

Quantum walks in higher dimensions

T. D. Mackay, S. D. Bartlett, L. T. Stephenson, and B. C. Sanders

Department of Physics, Macquarie University, Sydney, New South Wales 2109, Australia

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We analyze the quantum walk in higher spatial dimensions and compare classical and quantum spreading as a function of time. Tensor products of Hadamard transformations and the discrete Fourier transform arise as natural extensions of the “quantum coin toss” in the one-dimensional walk simulation, and other illustrative transformations are also investigated. We find that entanglement between the dimensions serves to reduce the rate of spread of the quantum walk. The classical limit is obtained by introducing a random phase variable.

I. INTRODUCTION

Classical random walks (also known as ‘drunken walks’) have found practical applications in mathematics, physics and computational science, for example in studies of diffusion, Wiener processes and search algorithms, respectively. Quantum physics introduces new perspectives, such as quantum diffusion [1], quantum stochastics [2], and quantum walks [3, 4, 5, 6]. The quantum walk is particularly appealing as an intuitively accessible model underpinning quantum diffusion and quantum stochastics. Remarkable properties of these quantum walks (QWs) have been discovered; of particular interest is that the spread (standard deviation) for the quantum walk is proportional to elapsed time t , as opposed to $\sqrt{t}$ for the classical random walk; thus, the QW offers a quadratic gain over its classical counterpart.

Physical implementations of the quantum walk have been proposed [3, 7], and possess the attractive property that they are inherently local in the sense that the spatial state shifts by one step along the lattice at each time step. One potential use of the QW is as a benchmark for assessing the non-classical performance of a quantum computer [7]. It is critically important in quantum information to develop algorithms and processes that behave in a distinct, observably different way than any classical one; the quantum walk is one such example.

We extend studies of QWs to a higher number of spatial dimensions and examine the time dependence of the standard deviation, which reveals the universal feature of a quadratic gain over the classical random walk. We analyze and discuss the effects of entanglement between the different spatial degrees of freedom. We also compare with the equivalent classical random walk, and obtain the classical limit from the quantum model via the introduction of a random phase variable at each time step and performing an ensemble average.

II. THE ONE-DIMENSIONAL QW

The classical random walk in one dimension describes a particle that moves in the positive or negative direction according to the random outcome of some unbiased binary variable (e.g., a fair coin). The one-dimensional

lattice on which the particle moves could be infinite or bounded (as in a circle). We may extend this to a QW by giving the particle an internal degree of freedom; for example, the particle may be a spin-1/2 system with internal Hilbert space $\mathcal{H}_2$ and basis states $|\pm\rangle$. The spatial state of the particle is given by a state in a Hilbert space $\mathcal{H}_{\text{spatial}}$ of a one-dimensional regular lattice. Let $|i\rangle$, with i an integer, denote the state of a particle located at position i ; the set $\{|i\rangle\}$ forms an orthonormal basis for $\mathcal{H}_{\text{spatial}}$. The total state of the particle is given by a state in the tensor product space

$$\mathcal{H}_T = \mathcal{H}_{\text{spatial}} \otimes \mathcal{H}_2. \quad (1)$$

Let the particle initially be in the spatial state $|0\rangle$ (i.e., localized at the origin) with internal state $|+\rangle$. To realize the 1-D QW [4], this particle is subjected to two alternating unitary transformations. The first step is the Hadamard transformation [8],

$$\mathbf{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad (2)$$

which acts only on the internal state of the particle (i.e., on $\mathcal{H}_2$), and transforms the initial state $|+\rangle$ into the superposition $\frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$. Following this transformation, we apply a unitary operator $\mathbf{F}$ that translates the position of the particle *conditionally* on the internal state: if the particle has internal state $|+\rangle$, it is moved one unit to the right, and if the internal state is $|-\rangle$, it is moved to the left, i.e.,

$$\begin{aligned} \mathbf{F}(|i\rangle \otimes |+\rangle) &= |i+1\rangle \otimes |+\rangle, \\ \mathbf{F}(|i\rangle \otimes |-\rangle) &= |i-1\rangle \otimes |-\rangle. \end{aligned} \quad (3)$$

The translation does not alter the internal state, i.e., the states $|\pm\rangle$ are internal translation eigenstates. Since the transformation is linear, it will transform the superposition state $\frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$ into a superposition state of the particle having moved left and right. Thus, the internal and spatial degrees of freedom become entangled. The Hadamard transformation is applied again, followed by $\mathbf{F}$, and these transformations are repeated alternately.

After n iterations, the particle is in an entangled state $|\Psi_n\rangle \in \mathcal{H}_T$. The probability P_i that the particle will be found at the i^{th} location is given by

$$P_i = |(\langle i| \otimes \langle +|) |\Psi_n\rangle|^2 + |(\langle i| \otimes \langle -|) |\Psi_n\rangle|^2. \quad (4)$$

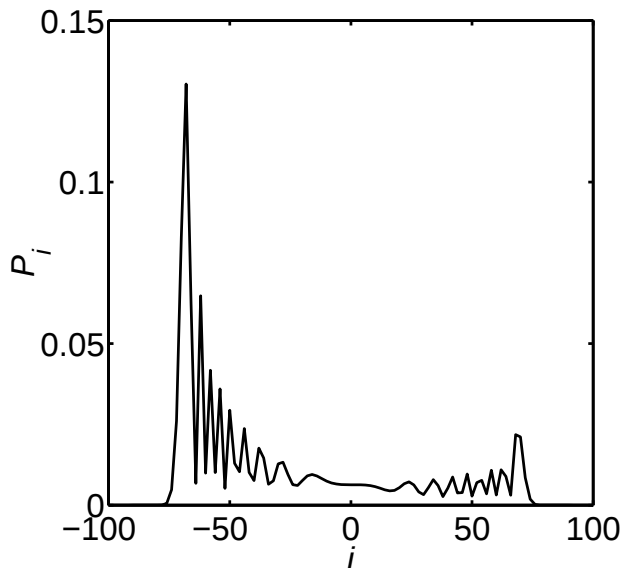


FIG. 1: The probability distribution of the 1-D quantum walk after 100 iterations. The internal state transformation used is the Hadamard transformation, and the initial internal state is $|-\rangle$.

In Fig. 1, we plot the probability distribution of this 1-D QW as a function of i [4, 5]. Analytical results are possible for the 1-D QW, and the $n \rightarrow \infty$ asymptotic behaviour has been investigated [4]. A key feature of the quantum walk is quantum interference, whereby two separate paths between two nodes can interfere according to the phase difference. In contrast, the classical model has additive probabilities for alternate paths. Perhaps most interesting is the relative uniformity of the central portion of the distribution ($-25 < i < 25$) and the standard deviation of the distribution increases linearly with the number of steps t ; this result is in contrast to the square root dependence of the classical random walk. Another peculiar feature is the asymmetry of the spatial probability distribution; this asymmetry is a consequence of the choice of initial state. The distribution resulting from the initial internal state $|\psi_s\rangle = \frac{1}{\sqrt{2}}(|+\rangle + i|-\rangle)$ is symmetric.

III. QW IN HIGHER DIMENSIONS

The analysis of the one-dimensional walk can be extended to higher dimensions. We define generalizations of the Hadamard gate, which place the internal state of the particle in superpositions of internal translation eigenstates, plus a generalization of $\mathbf{F}$, which moves the particle in the d -dimensional space conditional on the internal state of the particle.

For a QW in d -dimensions, we require the particle to have an internal state in a 2^d -dimensional Hilbert space. This internal state is simply described as the state of d coupled qubits [8]; thus, we can express the internal

Hilbert space $\mathcal{H}_{\text{int}}$ as

$$\mathcal{H}_{\text{int}} = \mathcal{H}_2 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_2 = \otimes^d \mathcal{H}_2, \quad (5)$$

and give a basis for internal states in binary notation as

$$|\epsilon_1 \epsilon_2 \dots \epsilon_d\rangle = |\epsilon_1\rangle \otimes |\epsilon_2\rangle \otimes \dots \otimes |\epsilon_d\rangle, \quad (6)$$

where $\epsilon_i = \pm$. The state of the i^{th} qubit (with basis $|\pm\rangle$) will determine the direction (positive or negative) that the particle moves in the i^{th} dimension. That is, we define a translation operator $\mathbf{F}$ which translates the state of the particle by one unit in every dimension: the direction in the i^{th} dimension is conditional on the state of the i^{th} qubit. The internal translation eigenstates are those given in Eq. (6).

For the 1-D QW, the quantum analogue of the classical “coin-flip” was the application of the Hadamard transformation of Eq. (2). This transformation maps an internal translation eigenstate of the translation operator $\mathbf{F}$ (either $|+\rangle$ or $|-\rangle$) into an equally weighted superposition of the two. The choice of phases in this transformation was to some extent arbitrary; the Hadamard transformation represents a choice with real entries.

For the d -dimensional QW, there exists a wide variety of unitary transformations on the internal state that could be used as a generalization of the Hadamard transformation for the 1-D case. One obvious generalization would be to apply a Hadamard transformation $\mathbf{H}$ to each qubit in the decomposition of Eq. (5); i.e., the transformation

$$\mathbf{H}_d = \mathbf{H} \otimes \mathbf{H} \otimes \dots \otimes \mathbf{H}. \quad (7)$$

This internal transformation is *separable*, in the sense that it does not produce entanglement between the spatial degrees of freedom. This choice could be viewed as the quantum analogue of using d independent coin tosses, one for each spatial dimension.

Another obvious generalization, which is not separable and does produce entanglement between spatial degrees of freedom, is the 2^d -dimensional discrete Fourier transform (DFT) $\mathbf{D}_d$, defined as follows. Expressing the basis of Eq. (6) as labelled by its numerical value $\{|\mu\rangle, \mu = 0, 1, \dots, 2^d - 1\}$, the DFT acts on this basis as

$$\mathbf{D}_d|\mu\rangle = \frac{1}{\sqrt{2^d}} \sum_{\nu=0}^{2^d-1} e^{2\pi i \mu \nu / 2^d} |\nu\rangle. \quad (8)$$

Note that the Hadamard transformation is the $d = 1$ discrete Fourier transform $\mathbf{D}_1$. As the Hadamard transformation does for the 1-D case, this DFT transforms any internal translation eigenstate into an equally weighted superposition of all the eigenstates. Unlike the tensor product of Hadamard transformations, it is non-separable and highly entangles the different internal qubits. Although this internal transformation can also be viewed as a quantum analogue of d independent coin tosses, this entanglement between the spatial degrees of freedom is a genuinely quantum effect.

The DFT transformation represents a natural choice for the phase relationship between the translation eigenstates of the superpositions. However, this choice of phases is arbitrary, and we may consider other choices, which will have a different effect on the QW. We also investigate another internal state transformation (the Grover operator [8]) that also produces an equally weighted superposition in the transformation (defined on the same basis as used above)

$$\mathbf{G}_d|\mu\rangle = \frac{1}{\sqrt{2^d}} \left(-2|\mu\rangle + \sum_{\nu=0}^{2^d-1} |\nu\rangle \right). \quad (9)$$

This choice, like the Hadamard transformation, possesses only real entries.

There are, of course, an infinite variety of other non-separable choices for the internal transformation by employing different phase relationships. Also, a bias could be introduced into the transformation, which would give an *unequally* weighted superposition of translation eigenstates; however, we consider only unbiased transformations here.

One of the remarkable properties of the 1-D QW is that, unlike its classical counterpart, it can produce an asymmetric distribution. Note, however, that with appropriate initial conditions (such as the state $|\psi_s\rangle = \frac{1}{\sqrt{2}}(|+\rangle + i|-\rangle)$) a symmetric distribution is obtained. It is of interest to question what effect the initial conditions will have on the higher-dimensional QWs. (Note that a symmetric distribution can always be obtained by averaging over initial conditions.)

IV. CALCULATIONS OF QWS

We begin our analysis with the straightforward generalization to higher dimensions of using the Hadamard transformation on each qubit. Fig. 1 and Fig. 2 show simulation results for the Hadamard walk both in one-dimension and a tensor product $\mathbf{H} \otimes \mathbf{H}$ for two-dimensions respectively. The initial condition for the internal state was chosen to be the separable state composed of all qubits in the $|-\rangle$ state, which leads to an asymmetric probability distribution.

For the case of separable transformations with separable initial conditions, the different spatial dimensions behave independently; thus, the variance can be expressed in terms of the one-dimensional case. For example, consider the family

$$\mathbf{H}, \mathbf{H} \otimes \mathbf{H}, \mathbf{H} \otimes \mathbf{H} \otimes \mathbf{H}, \dots; \quad (10)$$

the time dependence of the standard deviation for these walks is plotted in Fig. 3, and the corresponding slopes $\Delta\sigma/\Delta t$ are presented in Table I. We observe that

$$\left(\frac{\Delta\sigma_1}{\Delta t}, \frac{\Delta\sigma_2}{\Delta t}, \frac{\Delta\sigma_3}{\Delta t}, \dots \right) = \left(\frac{\Delta\sigma_1}{\Delta t}, \sqrt{2} \frac{\Delta\sigma_1}{\Delta t}, \sqrt{3} \frac{\Delta\sigma_1}{\Delta t}, \dots \right), \quad (11)$$

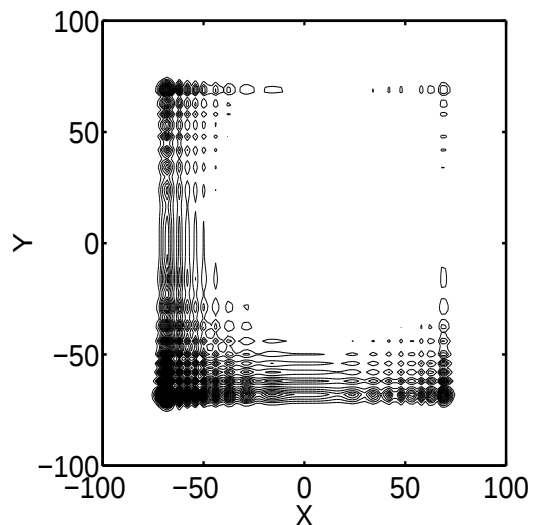


FIG. 2: Probability distribution of the 2-D quantum walk using the separable internal transformation $\mathbf{H} \otimes \mathbf{H}$ over 100 iterations, with initial condition given by $|-\rangle \otimes |-\rangle$.

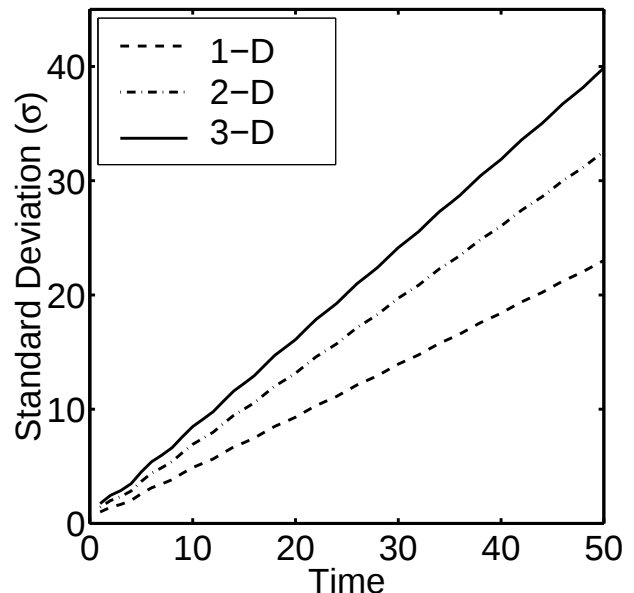


FIG. 3: Time dependence of standard deviation for the series $\mathbf{H}$, $\mathbf{H} \otimes \mathbf{H}$ and $\mathbf{H} \otimes \mathbf{H} \otimes \mathbf{H}$ with initial state given by $\otimes^d |-\rangle$.

where σ_d is the standard deviation for the d -dimensional QW, as expected for independent distributions. Also, by calculating a d -dimensional QW using this separable internal transformation and projecting the state onto the Hilbert space for any one dimension, the state of the 1-D QW is recovered. Again, this property illustrates that the different spatial dimensions are independent. Analytical results for these QWs follow from the 1-D case in a straightforward manner.

We now consider the behaviour of higher-dimensional QWs that possess entanglement between the spatial degrees of freedom, i.e., QWs that have non-separable in-

Transformation	$\Delta\sigma/\Delta t$	$(\sqrt{d})\Delta\sigma_1/\Delta t$
$\mathbf{H}$	0.4544 ± 0.0012	0.4544 ± 0.0012
$\mathbf{H} \otimes \mathbf{H}$	0.6427 ± 0.0017	0.6427 ± 0.0017
$\mathbf{H} \otimes \mathbf{H} \otimes \mathbf{H}$	0.7871 ± 0.0021	0.7871 ± 0.0021

TABLE I: The slope of the standard deviation as a function of time for the family $(\mathbf{H}, \mathbf{H} \otimes \mathbf{H}, \mathbf{H} \otimes \mathbf{H} \otimes \mathbf{H}, \dots)$. The slope $\Delta\sigma/\Delta t$ is found by linear regression of data points where $t \geq 10$ (such as to allow stabilization of irregularities caused by initial condition). σ_1 refers to the 1-D case.

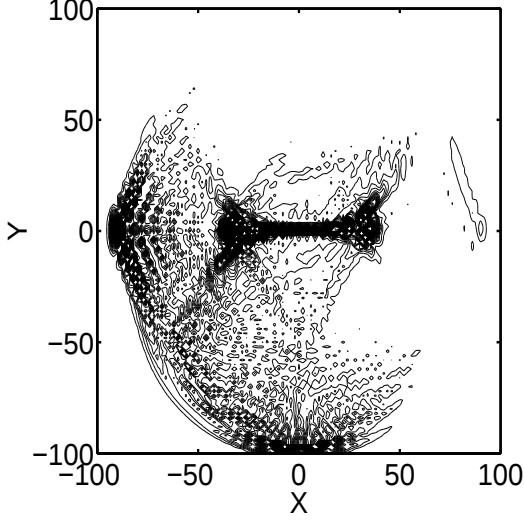


FIG. 4: Probability distribution for the quantum walk using the $d = 2$ DFT ($\mathbf{D}_2$) over 100 iterations, with initial condition given by $|-\rangle \otimes |-\rangle$.

ternal transformations, such as the DFT of Eq. (8). Fig. 4 shows the spatial probability distribution of the QW with internal transformation given by the $d = 2$ discrete Fourier transform $\mathbf{D}_2$; note that this distribution is distinct from that of the $\mathbf{H} \otimes \mathbf{H}$ QW. In particular, it has the feature that the density of the distribution is significant near the origin, in contrast to the separable $\mathbf{H} \otimes \mathbf{H}$ QW which possesses only average density at the origin. Note also that it is asymmetric for the initial condition $|-\rangle \otimes |-\rangle$; the asymmetry appears to be a general property of the higher-dimensional QWs as it is for the 1-D case.

The time dependence of the standard deviations for the $d = 1, 2, 3$ DFT walks are plotted in Fig. 5 and summarized in Table II. In contrast to the separable case, the trend observed in the DFT family is $\Delta\sigma_d/\Delta t = \sqrt{(d+1)/2}\Delta\sigma_1/\Delta t$. This trend is in agreement with the three calculations ($d = 1, 2, 3$). For the family of DFT walks, the standard deviation grows linearly with time, but the slope is less than that for the separable case (the tensor products of Hadamard transformations); see Table II. This suggests that the entanglement between the spatial degrees of freedom serves to reduce the rate of spread.

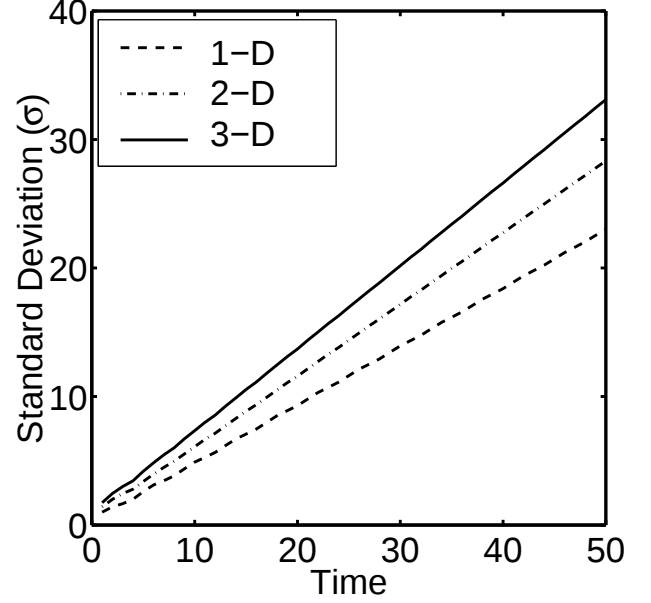


FIG. 5: Time dependence of the standard deviation for the $\mathbf{D}_d$ DFT series with initial state given by $\otimes^d |-\rangle$. Details are given in Table II.

Transformation	$\Delta\sigma/\Delta t$	$\sqrt{(d+1)/2}\Delta\sigma_1/\Delta t$
$\mathbf{D}_1$ ($\mathbf{H}$)	0.4544 ± 0.0012	0.4544 ± 0.0012
$\mathbf{D}_2$	0.5569 ± 0.0006	0.5565 ± 0.0015
$\mathbf{D}_3$	0.6449 ± 0.0007	0.6426 ± 0.0017

TABLE II: Slope of the standard deviation as a function of time, and comparison to the suggested pattern. $\Delta\sigma/\Delta t$ is the slope found by linear regression of data points where $t \geq 10$ (such as to allow stabilization of irregularities caused by initial condition).

Choosing different relative phases in the internal state transformation can lead to vastly different distributions. Fig. 6 shows the results of using the internal transformation $\mathbf{G}$ of Eq. (9). This distribution is characterized by its marked localization at the centre, as well as possessing peaks at the “maximum distance” attainable in the number of iterations (100 units from the origin).

Note that the time dependence of variance for the non-separable 2-D transformations ($\mathbf{D}_2$, $\mathbf{G}_2$) are quite similar, although the probability density functions are quite different in appearance. (See Table III.) The choice of initial condition does not appear to have a significant effect on the time dependence of the standard deviation.

V. OBTAINING THE CLASSICAL RANDOM WALK FROM THE QUANTUM MODEL

A classical distribution can be obtained from the quantum model by introducing a random element into the

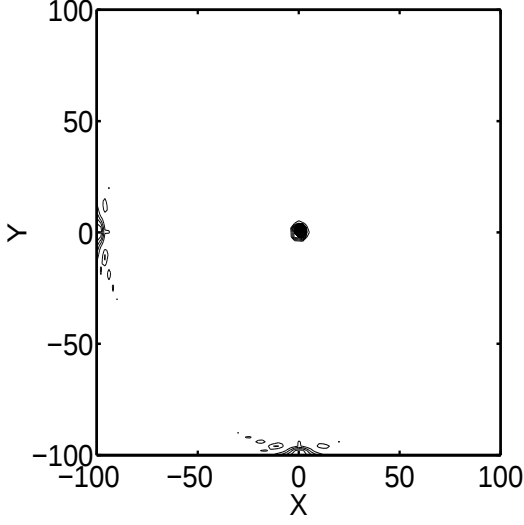


FIG. 6: Probability distribution of the 2-D quantum walk with internal transformation given by $\mathbf{G}$ (see Eq. 9) over 100 iterations with initial condition $|-\rangle \otimes |-\rangle$.

Transformation	Initial State	$\Delta\sigma/\Delta t$
$(\mathbf{H} \otimes \mathbf{H})$	$ -\rangle \otimes -\rangle$	0.6427 ± 0.0017
$\mathbf{D}_2$	$ -\rangle \otimes -\rangle$	0.5569 ± 0.0006
$\mathbf{D}_2$	$ +\rangle \otimes +\rangle$	0.5569 ± 0.0006
$\mathbf{D}_2$	$ \psi_s\rangle \otimes \psi_s\rangle$	0.6234 ± 0.0005
$\mathbf{D}_2$	$ \psi_-\rangle$	0.6009 ± 0.0006
$\mathbf{G}$ (see Eq. 9)	$ -\rangle \otimes -\rangle$	0.5418 ± 0.0020
$\mathbf{G}$	$ +\rangle \otimes +\rangle$	0.5418 ± 0.0020
$\mathbf{G}$	$ \psi_s\rangle \otimes \psi_s\rangle$	0.5988 ± 0.0006
$\mathbf{G}$	$ \psi_-\rangle$	0.5440 ± 0.0008

TABLE III: Slope of the standard deviation as a function of time for various 2-D transformations and initial conditions. $\Delta\sigma/\Delta t$ is the slope found by linear regression of data points where $t \geq 10$ (to allow stabilization of irregularities caused by initial condition). Here $|\psi_s\rangle = \frac{1}{\sqrt{2}}(|+\rangle + i|-\rangle)$ is the state that produces the 1-D symmetric distribution, and $|\psi_-\rangle = \frac{1}{\sqrt{2}}(|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle)$ is the entangled singlet state.

transformation at each time step. As shown previously, the “quantum” behaviour of the QW is due to the phase relationship (interference) between the separate paths of the walk. By adding a random element to the phase and averaging over many trials, we show that the quantum interference can be made to disappear and that the distribution of the classical random walk is regained. The introduction of this random phase is an example of decoherence.

Let us first investigate the one-dimensional case. In the internal translation eigenstate basis $|\pm\rangle$, the unitary operator that transforms the relative phase between these

states is

$$\mathbf{R}(\beta) = e^{\frac{i}{2}\beta\hat{\sigma}_z} = \begin{pmatrix} e^{i\beta/2} & 0 \\ 0 & e^{-i\beta/2} \end{pmatrix}, \quad (12)$$

where $\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ is the Pauli spin matrix, and $\beta \in [0, 2\pi)$. We then consider a QW where the phase between the $|+\rangle$ and $|-\rangle$ states is randomly selected at each interval from a uniform prior distribution over $[0, 2\pi)$. Rather than applying the Hadamard transformation as the internal transformation, we apply

$$\mathbf{H}(\beta) = \mathbf{R}(\beta) \mathbf{H} \mathbf{R}(\beta)^{-1} = \begin{pmatrix} 1 & e^{i\beta} \\ e^{-i\beta} & -1 \end{pmatrix}, \quad (13)$$

with a phase β chosen randomly from the set $[0, 2\pi)$ at each time step. The resulting distribution has a standard deviation comparable to that of the corresponding binomial distribution, but exhibits strong interference effects. By averaging over many trials, the distribution rapidly converges to the binomial distribution.

These results for the one-dimensional case can easily be generalized to higher dimensions. For the separable d -dimensional QW, the generalization is straightforward: one simply replaces each Hadamard transformation in the tensor product with a random $\mathbf{H}(\beta)$ at each step. The separability ensures that the resulting walk is equivalent to the 1-D walk in each dimension.

For non-separable internal transformations such as the DFT, a straightforward extension is to apply

$$(\mathbf{R}_1(\beta_1) \otimes \cdots \otimes \mathbf{R}_d(\beta_d)) \mathbf{D}_d (\mathbf{R}_d(\beta_d)^{-1} \otimes \cdots \otimes \mathbf{R}_1(\beta_1)^{-1}), \quad (14)$$

where $\beta_1, \dots, \beta_d$ are random phases, each from the set $[0, 2\pi)$. That is, an independent random phase is added for each dimension (qubit). Again, by averaging 400 walks of 50 iterations each, we obtained the 2-D binomial distribution to a high degree of confidence.

VI. CONCLUSIONS AND DISCUSSION

We present here a framework for calculating and analyzing quantum walks in higher dimensions. The generalization of these walks beyond one dimension gives a wide variety of choice for the phases involved in the “quantum coin toss”. We discuss the role of entanglement between the different spatial degrees of freedom as a possible non-classical property of the higher dimensional QWs. As different choices lead to different spatial probability distributions, it may be that specific unitary transformations of the internal Hilbert space are particularly well suited for certain computational tasks.

As with the one-dimensional QW, the increased rate of spread (given by the linear dependence of the standard deviation on time) is present in the higher dimensional walks. This property may be particularly valuable for

classical random walk based algorithms, such as quantum searches. We show that entanglement between the spatial degrees of freedom reduces the slope of this linear growth but not the linear dependence on t . These results are shown to be independent of the initial internal state in the cases investigated.

We show that the classical distribution can be obtained from the QW by introducing an internal transformation with a random phase and then averaging over many trials. This result is expected; the quantum behaviour of the QW is due to interference effects between the phases of different paths. For higher dimensional QW, more random parameters (one for each spatial dimension) are

needed.

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