Quantum Walks driven by many coins

Todd A. Brun,[1,*] Hilary A. Carteret,[2,†] and Andris Ambainis[1,‡]

[1] *Institute for Advanced Study, Einstein Drive, Princeton, NJ 08540*

[2] *Department of Combinatorics and Optimization, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada*

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Abstract

Quantum random walks have been much studied recently, largely due to their highly nonclassical behavior. In this paper, we study one possible route to classical behavior for the discrete quantum random walk on the line: the use of multiple quantum "coins" in order to diminish the effects of interference between paths. We find solutions to this system in terms of the single coin random walk, and compare the asymptotic limit of these solutions to numerical simulations. We find exact analytical expressions for the time-dependence of the first two moments, and show that in the long time limit the "quantum mechanical" behavior of the one-coin walk persists. We further show that this is generic for a very broad class of possible walks, and that this behavior disappears only in the limit of a new coin for every step of the walk.

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*Electronic address: tbrun@ias.edu

†Electronic address: hcartere@cacr.math.uwaterloo.ca

‡Electronic address: ambainis@ias.edu

I. INTRODUCTION

In the classical discrete random walk, a particle is located at one of a set of positions. In response to a random event (such as the flipping of a coin), the particle moves in one direction or another. This sequence is repeated, and the motion of the particle is analyzed statistically. These systems provide good models for diffusion and other stochastic processes.

Considerable work has been done recently on quantum random walks. Quantum walks differ from classical walks in that their evolution is unitary and therefore reversible. Two classes of models have been studied: continuous [1, 2, 3] and discrete [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22], random walks. This paper is concerned solely with the discrete case.

A naïve generalization of the classical random walk behaves in a rather boring way: if its evolution is unitary, it can only move in one direction and keep on going that way [5]. To produce nontrivial behavior, we introduce an extra "coin" degree of freedom (usually a single quantum bit) into the system. Just as in the classical random walk, the outcome of a "coin flip" determines which way the particle moves; but in the quantum case, both the "flip" of the coin and the conditional motion of the particle are represented by unitary transformations; thus, there can be interference between different classical paths.

This paper is concerned with quantum walks on the infinite line. The particle is initially located at position $x = 0$ and is free to travel off to infinity in either direction. We will primarily consider the *position* of the particle after some number of flips t. At this point, we assume that the position is measured. We will look at both the probability distribution $p(x,t) = |\langle x|\psi(t)\rangle|^2$, and at the long-time behavior of the moments $\langle\hat{x}\rangle$ and $\langle\hat{x}^2\rangle$ as functions of t.

Unitary random walks behave quite differently from classical random walks. For a classical walk, $p(x,t)$ has approximately the form of a Gaussian distribution (actually, a binomial distribution), with a width which spreads like $\sqrt{t}$; the variance $\bar{x^2} - \bar{x}^2$ grows linearly with time. The variance in the quantum walk, by contrast, grows *quadratically* with time; and the distribution $p(x,t)$ has a complicated, oscillatory form. Both of these are effects of interference between the possible paths of the particle.

It should be possible to recover the classical behavior as some kind of limit of the quantum system. There are two obvious ways to regain the classical result. If the quantum coin is measured at every step, then the record of the measurement outcomes singles out a particular classical path. By averaging over all possible measurement records, one recovers the usual classical behavior [11].

Alternatively, rather than re-using the same coin every time, one could replace it with a *new* quantum coin for each flip. After a time t one would have accumulated t coins, all of them entangled with the position of the particle. By measuring them, one could reconstruct an unique classical path; averaging over the outcomes would once again produce the classical result. It is actually unnecessary, however, to measure the coins. Simply by tracing them out, one leaves the particle in the mixed state

$$\rho = \sum_x p(x,t)|x\rangle\langle x| \ , \tag{I.1}$$

where $p(x,t)$ is the probability distribution obtained after t steps of a classical random walk.

It is therefore certainly possible to recover the classical limit. But these two approaches give two different routes from quantum to classical. We might increase the number of coins used to generate the walk, cycling among M different coins, in the limit using a new coin at each step. Or we might *weakly* measure the coin after each step, reaching the classical limit with strong, projective measurements. This is equivalent to having the coin decohere with time.

In this paper we look at quantum random walks with multiple coins. (The case with a decoherent coin is considered elsewhere [23, 24]; systems with decoherence of the particle have also been considered [20, 22, 25].) We begin by reviewing the approaches to solving the single-coin walk. We extend these to walks with multiple coins, and derive expressions for the amplitudes of an M-coin walk which we can evaluate numerically. We look at the long-time behavior of the moments of position both numerically and analytically, and compare it to the usual classical random walk.

II. THE ONE-COIN QUANTUM WALK

Since our results will utilize the amplitudes for the *single-coin* quantum walk, we first go quickly over the single-coin derivation. We then make use of this in the following section to write down exact expressions for the multi-coin case.

There are two main approaches to analyzing quantum walks. One is to use Fourier analysis, which gives a good qualitative insight into the behavior of the system, but gives solutions for the wavefunction in terms of some rather unpleasant integrals. Indeed, no exact solution to them is known, and so they must be approximated in the limit as $t \to \infty$. The approximation methods become progressively more impractical as the number of coins increases; we examine these asymptotic expressions in Appendix B.

The other approach employs combinatorics. This gives expressions which are opaque, but are exact for all times. However, evaluating these expressions exactly is prohibitive for long times, and so approximation methods are again required for the long time limit.

A. Fourier Analysis of Quantum Walks

Following the analysis in [6] we consider the Hadamard walk, in which each coin performs the evolution

$$\begin{aligned} |\mathrm{R}\rangle \ &\mapsto \ \hat{H}|\mathrm{R}\rangle = \frac{1}{\sqrt{2}}\left(|\mathrm{R}\rangle + |\mathrm{L}\rangle\right) \\ |\mathrm{L}\rangle \ &\mapsto \ \hat{H}|\mathrm{L}\rangle = \frac{1}{\sqrt{2}}\left(|\mathrm{R}\rangle - |\mathrm{L}\rangle\right) \end{aligned} \tag{II.1}$$

at each time step for which that coin is active, where R and L can be respectively thought of as the "heads" and "tails" states of the coin, or equivalently as an internal chirality state of the particle. The value of the coin controls the direction in which the particle moves. When the coins shows "R" the particle moves right; when it shows "L" the particle moves left.

Let $\{|x\rangle\}$ be the position states of the particle, where the values x are integers. We define a unitary shift operator

$$\hat{S}|x\rangle = |x+1\rangle \ , \quad \hat{S}^{-1}|x\rangle = \hat{S}^{\dagger}|x\rangle = |x-1\rangle \ . \tag{II.2}$$

If $\hat{\mathcal{P}}_R = |R\rangle\langle R|$ and $\hat{\mathcal{P}}_L = |L\rangle\langle L|$ are projectors onto the two states of the coin, then one step of the quantum walks is given by the unitary operator

$$\hat{E} = (\hat{S} \otimes \hat{\mathcal{P}}_R + \hat{S}^{\dagger} \otimes \hat{\mathcal{P}}_L)(\hat{I} \otimes \hat{H}) \ . \tag{II.3}$$

If the initial state of the position and coin is $|\Psi_0\rangle$, then after t steps of the walk the state is

$$|\Psi(t)\rangle = \hat{E}^t|\Psi_0\rangle \ . \tag{II.4}$$

For the purposes of this paper, we will usually assume that the coin starts in the state $|R\rangle$.

Consider the wave function of the position of the particle. For a one coin walk, this wavefunction has just two amplitude components, which are labeled by their chiralities:

$$\Psi(x,t) = \begin{pmatrix} a_R(x,t) \\ a_L(x,t) \end{pmatrix} . \tag{II.5}$$

In Dirac notation this is

$$|\Psi(t)\rangle = \sum_x |x\rangle \otimes \left(a_R(x,t)|R\rangle + a_L(x,t)|L\rangle\right) . \tag{II.6}$$

We would like to solve for $a_{L,R}(x,t)$ explicitly. We can do this by diagonalizing the operator $\hat{E}$. Following the analysis in [6], we use the spatial discrete Fourier transformation, $\tilde{a}_{L,R}(k,t)$ for $k \in [-\pi,\pi]$

$$\begin{aligned} |\Psi(t)\rangle &= \int_{-\pi}^{\pi} |k\rangle \otimes \left(\tilde{a}_R(k,t)|R\rangle + \tilde{a}_L(k,t)|L\rangle\right) \frac{dk}{2\pi} , \\ \tilde{a}_{L,R}(k,t) &= \sum_{x=-\infty}^{\infty} a_{L,R}(x,t) e^{-ikx} , \\ |k\rangle &= \sum_{x=-\infty}^{\infty} |x\rangle e^{ikx} , \end{aligned} \tag{II.7}$$

where the usual integral is replaced by a sum, as the variable x is discrete. We note that these "momentum" states $|k\rangle$ are eigenstates of the shift operator $\hat{S}$ and its inverse:

$$\hat{S}|k\rangle = e^{-ik}|k\rangle , \quad \hat{S}^\dagger|k\rangle = e^{ik}|k\rangle . \tag{II.8}$$

These states are not normalizable; but we can think of them as the limit of the case where the number of position states is large but finite.

In this momentum basis, the effect of the evolution is given by the matrix

$$\hat{H}_k = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-ik} & e^{-ik} \\ e^{ik} & -e^{ik} \end{pmatrix} . \tag{II.9}$$

Since this is just a 2-by-2 matrix, it is easily diagonalized, and the final state found in terms of its eigenvectors and eigenvalues. The method of solution is now straightforward in principle, though complicated in detail. One first represents the initial state in the $\{|k\rangle\}$ basis; applies the diagonal form of the matrix H_k t times; and re-expresses the result in the original $\{|x\rangle\}$ and $|R\rangle, |L\rangle$ bases.

Nayak and Vishwanath [6] carried out this program and got exact results. For an initial state $|\Psi_0\rangle = |0\rangle|R\rangle$,

$$
\begin{aligned}
a_L(x,t) &= \frac{1+(-1)^{x+t}}{2}\int_{-\pi}^{\pi}\frac{dk}{2\pi}\left(1+\frac{\cos k}{\sqrt{1+\cos^2 k}}\right)e^{-i(\omega_k t+kx)} , \\
a_R(x,t) &= \frac{1+(-1)^{x+t}}{2}\int_{-\pi}^{\pi}\frac{dk}{2\pi}\frac{e^{ik}}{\sqrt{1+\cos^2 k}}e^{-i(\omega_k t+kx)} . \qquad \text{(II.10)}
\end{aligned}
$$

In the exponents, we define the frequencies ω_k by $\sin\omega_k = \sqrt{1/2}\sin k$, taking $\omega_k \in [-\pi/2,\pi/2]$.

These integrals, while exact, are difficult to evaluate. Nayak and Vishwanath found an approximation to these results, valid in the limit of large t, by making an asymptotic expansion of the integrals, to get the approximate expressions

$$
\begin{aligned}
a_L(x,t) &\approx \frac{1+(-1)^{x+t}}{\sqrt{8\pi t(1-x^2/t^2)\sqrt{1-2x^2/t^2}}} \\
&\quad \times(1-x/t)\left(\exp i(t\phi(x/t)+\pi/4)+\text{c.c.}\right) , \\
a_R(x,t) &\approx \frac{1+(-1)^{x+t}}{\sqrt{8\pi t(1-x^2/t^2)\sqrt{1-2x^2/t^2}}} \\
&\quad \times\left((x/t+i\sqrt{1-2x^2/t^2})\exp i(t\phi(x/t)+\pi/4)+\text{c.c.}\right) . \qquad \text{(II.11)}
\end{aligned}
$$

The results are conveniently represented in terms of a variable $\alpha = x/t$. This approximation is valid only within the range $-\sqrt{1/2} < \alpha < \sqrt{1/2}$; outside this range the amplitude becomes negligibly small. The phase $\phi(\alpha)$ is given by

$$
\phi(\alpha) = \arcsin\sqrt{\frac{1-2\alpha^2}{2-2\alpha^2}} + \alpha\arcsin\sqrt{\frac{1-2\alpha^2}{1-1\alpha^2}} . \qquad \text{(II.12)}
$$

B. Combinatorial Analysis

We can do a completely different analysis of the one-coin walk, using a combinatorial rather than a Fourier argument, similar to that done in [5] and [8]. Suppose we start with $x = 0$ and the coin in state $|R\rangle$. We see how the state evolves after the first few flips of the coin:

$$
\begin{aligned}
|\Psi_0\rangle &= |0\rangle|R\rangle , \\
|\Psi(1)\rangle &= \sqrt{1/2}\,(|1\rangle|R\rangle + |-1\rangle|L\rangle) , \\
|\Psi(2)\rangle &= \sqrt{1/2^2}\,(|2\rangle|R\rangle + |0\rangle|L\rangle + |0\rangle|R\rangle - |-2\rangle|L\rangle) . \qquad \text{(II.13)}
\end{aligned}
$$

At time t there will be 2^t terms, each with amplitude $\pm\sqrt{1/2^t}$. Each of these terms corresponds to a possible path for a *classical* random walk. To get the amplitude for a particular position x, conditioned on the coin showing R or L, one must sum up the amplitudes for all the paths which end at the position x with the appropriate coin face showing. This amounts to a nice problem in combinatorics.

For the coin to reach position x at time t, it must have moved to the left a total of $N_L = (t-x)/2$ times, and to the right a total of $N_R = (t+x)/2$ times. For a term corresponding to a given classical path, it turns out that the phase depends only on the values of N_L and N_R, and the number C of *clusters* of consecutive L flips. The details of the derivation are given in Appendix A, so we just quote the answer here:

$$\begin{aligned} a_L(x,t) &= \frac{1}{\sqrt{2^t}}\left[\sum_{C=1}^{\text{“}N\text{”}}(-1)^{N_L-C}\binom{N_L-1}{C-1}\binom{N_R}{C-1}\right], \\ a_R(x,t) &= \frac{1}{\sqrt{2^t}}\left[\sum_{C=1}^{\text{“}N\text{”}}(-1)^{N_L-C}\binom{N_L-1}{C-1}\binom{N_R}{C}\right], \end{aligned} \tag{II.14}$$

where the summation is to N_L for $x \geq 0$ and to N_R+1 for $x < 0$ (but only for $N_L \neq 0$; for $N_L = 0$ the amplitude is always $2^{-t/2}$). We can, of course, re-express N_R and N_L as functions of x and t.

If we had started instead with the coin in the state $|L\rangle$, the amplitudes would then become

$$\begin{aligned} b_L(x,t) &= \frac{1}{\sqrt{2^t}}\left[\sum_{C=1}^{\text{“}N\text{”}}(-1)^{N_L-C}\binom{N_L-1}{C-1}\binom{N_R}{C-1}\frac{N_R-2C+2}{N_R}\right], \\ b_R(x,t) &= \frac{1}{\sqrt{2^t}}\left[\sum_{C=1}^{\text{“}N\text{”}}(-1)^{N_L-C}\binom{N_L-1}{C-1}\binom{N_R}{C}\frac{N_R-2C}{N_R}\right], \end{aligned} \tag{II.15}$$

where the summation is to N_L for $x \geq 0$ and to N_R+1 for $x < 0$, and $N_L = 0$ is done separately, as before.

The solution given by Eq. (II.14) looks very different from that given by Eq. (II.10); it is rather extraordinary that they should describe exactly the same outcome. Moreover, a long-time approximation similar to Eq. (II.11) can be derived from Eq. (II.14), by using the asymptotics of Jacobi polynomials. See [8] for details.

If the coin starts in an arbitrary state

$$\psi_{\text{init}} = \alpha|R\rangle + \beta|L\rangle \tag{II.16}$$

the amplitudes will be

$$g_L(x,t) = \alpha a_L(x,t) + \beta b_L(x,t) \tag{II.17}$$

$$g_R(x,t) = \alpha a_L(x,t) + \beta b_L(x,t), \tag{II.18}$$

respectively.

III. WALKS WITH MULTIPLE COINS

For a walk driven by M coins, the wavefunction has 2^M components; for example, a two coin walk will be described by the wavefunction

$$|\Psi(x,t)\rangle = \begin{pmatrix} a_{RR}(x,t) \\ a_{RL}(x,t) \\ a_{LR}(x,t) \\ a_{LL}(x,t) \end{pmatrix} . \tag{III.1}$$

At each step, the particle moves in the direction dictated by the coin that is active at that step, with the other coins remaining inert until it is their turn once again. We will initially assume that we cycle through the coins in a deterministic, regular way, although we will discover later that we can relax that condition in certain specific ways.

The unitary transformation which results from flipping the mth coin is

$$\hat{E}_m = (\hat{S} \otimes \hat{\mathcal{P}}_{Rm} + \hat{S}^\dagger \otimes \hat{\mathcal{P}}_{Lm})(\hat{I} \otimes \hat{H}_m) , \tag{III.2}$$

where $\hat{H}_m$ is the Hadamard transformation on the mth coin, and $\hat{\mathcal{P}}_{L,Rm}$ is the projector onto the mth coin being in state L or R, respectively. If we cycle among the coins, doing a total of t flips (t/M flips with each coin), then the state will be

$$|\Psi(Mt)\rangle = (\hat{E}_M \cdots \hat{E}_1)^{t/M} |\Psi_0\rangle . \tag{III.3}$$

We have simulated this system numerically for different numbers M of coins. The probability distributions $p(x,t)$ agree with the classical results only up to $t = M$; beyond that, they diverge sharply, with the multicoin distributions exhibiting highly oscillatory behavior and rapid spreading (linear with t), similar to the behavior of the single-coin case. (See figure 1.)

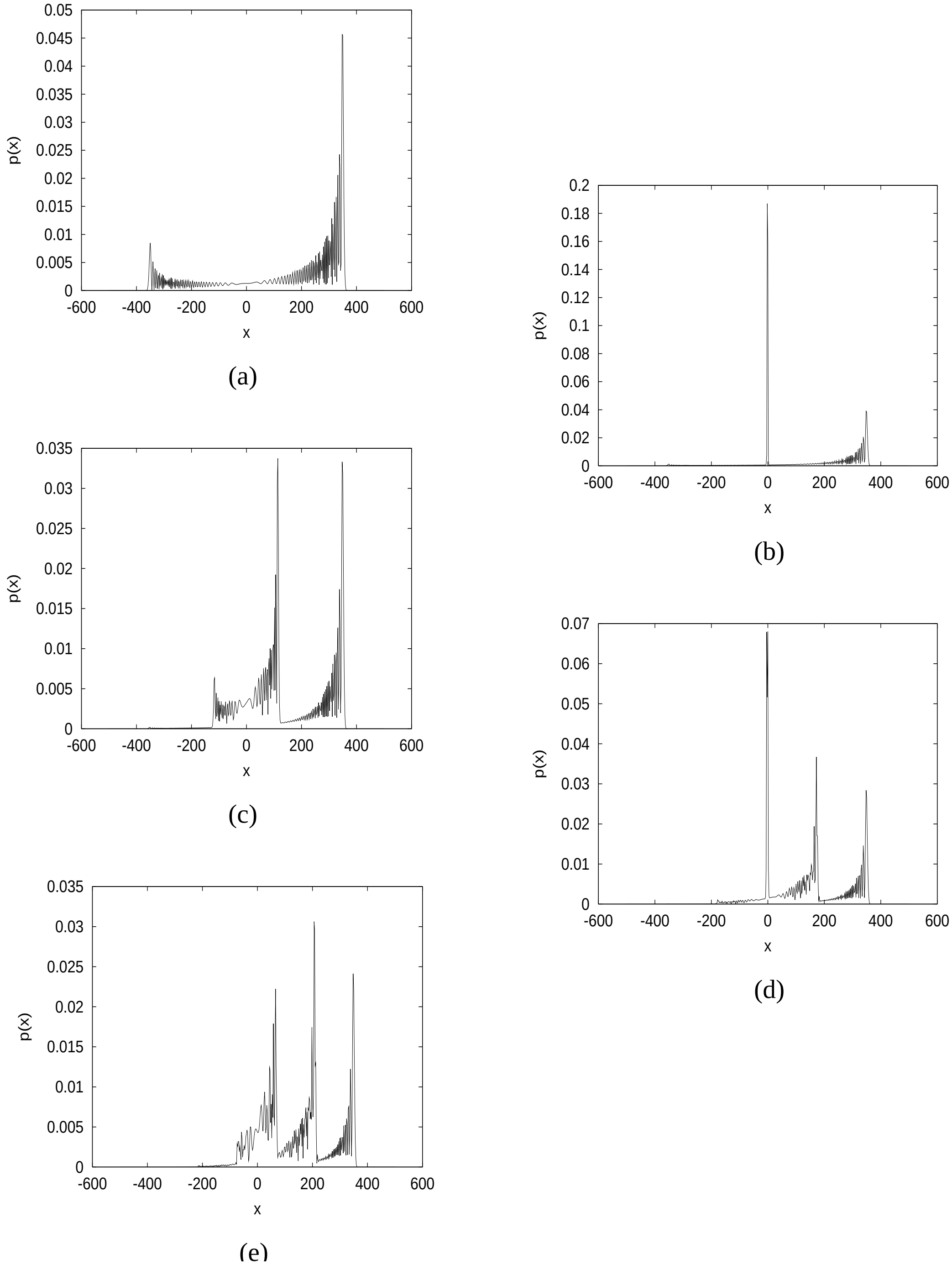

FIG. 1: These figures plot the particle position distribution $p(x)$ vs. x at time $t = 500$ for multicoin quantum random walks with 1–5 coins. In each of these plots, all the coins begin in state $|R\rangle$, which is the reason for the asymmetry of the distributions. Note that only even points x are plotted, since $p(x) = 0$ for odd values of $t - x$.

How can we understand these M-coin results? An important thing to notice is that these M unitary transformations $\{\hat{E}_m\}$ all commute:

$$[\hat{E}_m, \hat{E}_n] = 0 \ . \qquad \text{(III.4)}$$

Because of that, the order in which they are listed is irrelevant. We can equally well write

$$|\Psi(Mt)\rangle = (\hat{E}_M)^{t/M} \cdots (\hat{E}_1)^{t/M} |\Psi_0\rangle \ . \qquad \text{(III.5)}$$

We can either let the walk evolve for t steps using M coins, or we could use one coin for t/M steps, and then replace the coin with another one, and use that for another t/M steps, and so on, until we've used all M coins. The final probability distribution will be the same.

Suppose we decide to use our coins cyclically. Then it can be seen that at the end of the walk, the M coins act as a quantum memory of the last M moves that the particle made. The "which path" information from before then is lost, so we will see interference between paths arising from moves dating from before that time.

Now consider M walks controlled by one coin each, concatenated in the following recipe: Do the first one-coin walk. Measure the final state of the coin only, doing nothing that would give any further information about the position of the particle. Reset the coin state to the appropriate starting state for the next walk, and use the conditioned state produced by the measurement as the starting state for the next one-coin walk. Repeat this procedure until you've concatenated M walks in this way. The *final* probability distribution obtained after the last coin has been measured will be exactly the same as the on obtained after measuring the M coins from the single cyclic M coin walk.

How can we use this to solve the multicoin walk? Assume (for the moment) that the coins all start in the state $|R\rangle$, and the particle starts in the state $|0\rangle$. We flip the coins t/M times each (with t/M even for convenience). After each coin has been flipped t/M times, we measure it, and find it in state L or R. We then define *conditional evolution operators* for the particle position:

$$\begin{aligned} \hat{A}_L(t) &= \sum_{j=-t/2M}^{t/2M-1} a_L(2j, t/M)\hat{S}^{2j} \\ \hat{A}_R(t) &= \sum_{j=-t/2M+1}^{t/2M} a_R(2j, t/M)\hat{S}^{2j}, \end{aligned} \qquad \text{(III.6)}$$

where $x = 2j$. If we flipped M coins t/M times each and then measured them, getting N results R and $M - N$ results L, then the particle must have ended up in the (unnormalized) state

$$\left[\hat{A}_R(t)\right]^N \left[\hat{A}_L(t)\right]^{M-N} |0\rangle \ . \qquad \text{(III.7)}$$

The probability of the particle arriving at the final position x at time Mt is then $p(x, Mt) = |\Psi(x, Mt)|^2$, which is

$$p(x, Mt) = \sum_{N=0}^{M} \binom{M}{N} |\langle x| \left[\hat{A}_R(t)\right]^N \left[\hat{A}_L(t)\right]^{M-N} |0\rangle|^2. \qquad \text{(III.8)}$$

Note that this distribution doesn't depend on the order in which the coins were flipped, nor the order in which the measurement results occurred, provided that the measurement on coin m was made after it had been flipped exactly t/M times.

For the amplitudes $a_{L,R}(x, t)$ in (III.6), we can use any of the expressions (II.10), (II.11), or (II.14), whichever is convenient. We can also calculate them numerically; Eq. (III.8) provides a much more practical method of numerical calculation for multicoin systems than direct simulation, which requires a Hilbert space that grows exponentially in dimension with the number of coins. By contrast, the difficulty of evaluating (III.8) grows only linearly with the number of coins. We have used this to simulate systems with large numbers of coins, which would otherwise be impractical; see, e.g., figure 2.

One can find asymptotic expressions for $p(x, t)$ at long times which are analogous to the single-coin expressions (II.11), though the difficulties mount rapidly with the number of coins. We plot the approximate solution for two coins in figure 3, which matches the numerical results of figure 1b quite well. For details of the calculation, see Appendix B.

While having points of similarity, these multicoin walks differ from the tensor product walks studied in [11], in which each component in the tensor product corresponds to a different spatial dimension. There are also points of similarity to quantum Parrondo games, as studied in [9].

IV. MOMENTS OF THE DISTRIBUTIONS

While the probability distributions $p(x, t)$ for the quantum random walk clearly differ markedly from their classical counterparts, it is difficult to use this to give a quantitative criterion for quantum vs. classical behavior. In particular, we would like to know if the

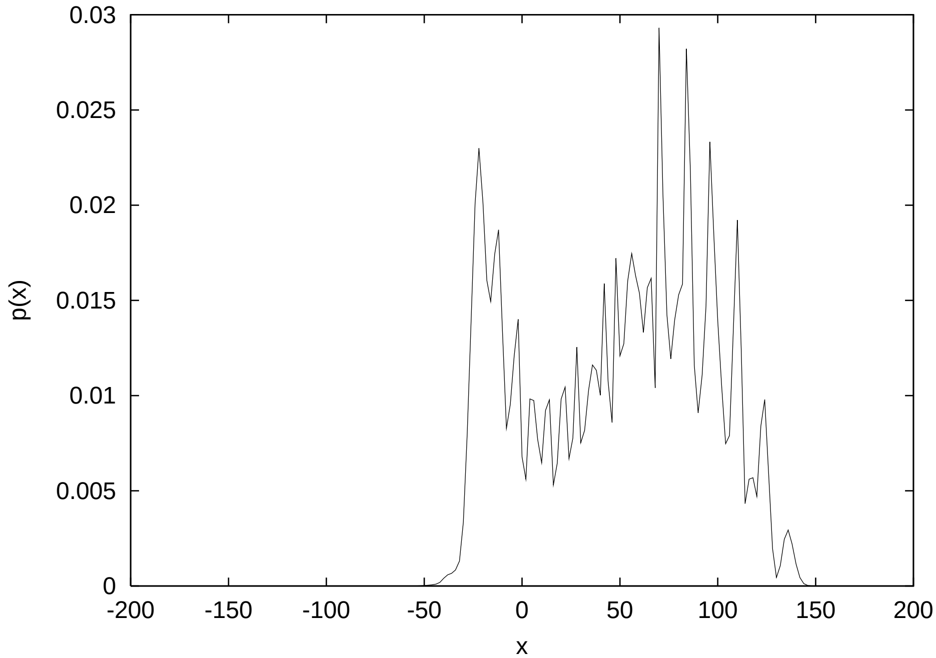

FIG. 2: This figure plots the numerical results for $p(x,t)$ at $t = 200$ for 20 coins, each initially in the state $|R\rangle$, using the formula (III.8). As we see, the highly oscillatory form of the probability distribution persists even for large numbers of coins. (Only even points are plotted.)

quantum walks become "more classical" in any meaningful sense as we let $M \to t$. It would be useful to look at one or two numbers instead of the entire probability distribution in answering this question.

One obvious criterion suggested by the single-coin case is to look at the long-time behavior of the moments of $p(x,t)$, and see if (for instance) the variance increases linearly or quadratically with time. Since it becomes more and more difficult to calculate $p(x,t)$ as we increase M, this might seem like an unhelpful approach; but as it happens, we can extract expressions for the long time behavior of the moments without having to evaluate $p(x,t)$ itself [24].

Note that in the following two subsections, we fix the number of coins M (or more generally the dimension D of the "coin") and then go to the long-time limit. What constitutes a long time will depend on the choice of M or D. In the final subsection, we let the number of coins used (or the dimension of the "coin") increase with time, and look at the long-time limit in that case.

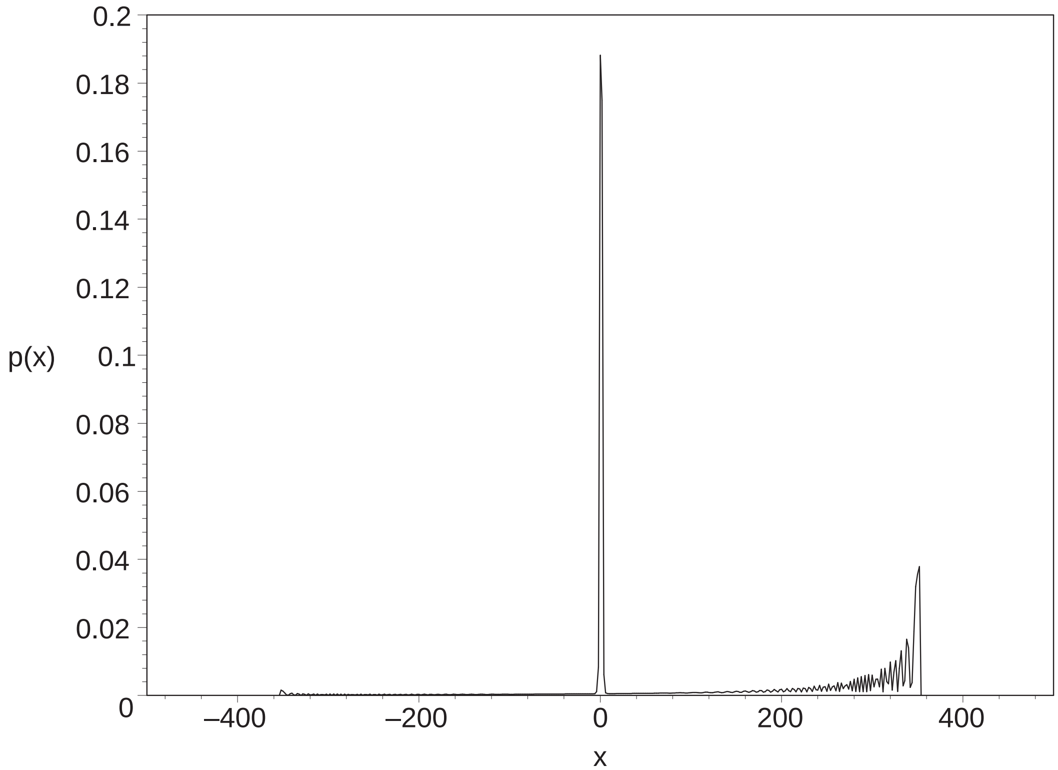

FIG. 3: This figure plots $p(x,t)$ at $t = 500$ for the two-coin quantum walk, using the long-time approximation derived in Appendix B. Comparison to figure 1b shows that this result matches direct numerical simulation very closely.

A. The general case

Let's consider a very general linear random walk, which includes the multicoin case as a subcase. Let the "coin" be a D-dimensional system with an initial state $|\Phi_0\rangle$; let $\hat{\mathcal{P}}_{R,L}$ be two orthogonal projectors on the Hilbert space of the coin, such that $\hat{\mathcal{P}}_R + \hat{\mathcal{P}}_L = \hat{I}$, and $\mathrm{Tr}\hat{\mathcal{P}}_R = \mathrm{Tr}\hat{\mathcal{P}}_L = D/2$. We also define a unitary transformation $\hat{U}$ which "flips" the coin. Then one step of the quantum random walk is given by the unitary operator

$$\hat{E} \equiv \left(\hat{S} \otimes \hat{\mathcal{P}}_R + \hat{S}^\dagger \otimes \hat{\mathcal{P}}_L\right)\left(\hat{I} \otimes \hat{U}\right) , \tag{IV.1}$$

where $\hat{S}, \hat{S}^\dagger$ are the usual shift operators (II.2) on the particle position. The full initial state of the system (particle and coin) is

$$|\Psi_0\rangle = |0\rangle \otimes |\Phi_0\rangle . \tag{IV.2}$$

We can identify the eigenvectors $|k\rangle$ of $\hat{S}, \hat{S}^\dagger$, with eigenvalues $\exp(\mp ik)$, as defined in

(II.7). In particular,

$$|0\rangle = \int_{-\pi}^{\pi} \frac{dk}{2\pi} |k\rangle \ . \tag{IV.3}$$

In the k basis, the evolution operator becomes

$$\begin{aligned} \hat{E}\left(|k\rangle \otimes |\Phi\rangle\right) &= |k\rangle \otimes \left(\mathrm{e}^{-ik} \hat{\mathcal{P}}_R + \mathrm{e}^{ik} \hat{\mathcal{P}}_L \right) \hat{U} |\Phi\rangle \ , \\ &\equiv |k\rangle \otimes \hat{U}_k |\Phi\rangle \ , \end{aligned} \tag{IV.4}$$

where $\hat{U}_k$ is a unitary operator on the coin degree of freedom.

Let the quantum random walk proceed for t steps. Then the state evolves to

$$\begin{aligned} |\Psi_0\rangle = |0\rangle \otimes |\Phi_0\rangle \ \rightarrow \ & \hat{E}^t |\Psi_0\rangle \\ &= \int_{-\pi}^{\pi} \frac{dk}{2\pi} |k\rangle \otimes \left(\hat{U}_k \right)^t |\Phi_0\rangle \equiv |\Psi(t)\rangle \ . \end{aligned} \tag{IV.5}$$

The probability to reach a point x at time t is

$$\begin{aligned} p(x,t) &= \langle \Psi(t)| \left(|x\rangle\langle x| \otimes \hat{I} \right) |\Psi(t)\rangle \\ &= \frac{1}{(2\pi)^2} \int dk \int dk' \langle k|x\rangle \langle x|k'\rangle \langle \Phi_0| \left(\hat{U}_k^\dagger \right)^t \left(\hat{U}_{k'} \right)^t |\Phi_0\rangle \\ &= \frac{1}{(2\pi)^2} \int dk \int dk' \mathrm{e}^{-ix(k-k')} \langle \Phi_0| \left(\hat{U}_k^\dagger \right)^t \left(\hat{U}_{k'} \right)^t |\Phi_0\rangle \ . \end{aligned} \tag{IV.6}$$

This will, in general, be difficult to calculate. However, all we are interested in are the *moments* of this distribution:

$$\begin{aligned} \langle \hat{x}^m \rangle_t &= \frac{1}{(2\pi)^2} \sum_x x^m p(x,t) \\ &= \frac{1}{(2\pi)^2} \sum_x x^m \int dk \int dk' \mathrm{e}^{-ix(k-k')} \langle \Phi_0| \left(\hat{U}_k^\dagger \right)^t \left(\hat{U}_{k'} \right)^t |\Phi_0\rangle \ . \end{aligned} \tag{IV.7}$$

We can then invert the order of operations and do the x sum first. This sum can be exactly carried out in terms of derivatives of the delta function:

$$\frac{1}{2\pi} \sum_x x^m \mathrm{e}^{-ix(k-k')} = (-i)^m \delta^{(m)}(k-k') \ . \tag{IV.8}$$

Inserting this result back into our expression for $\langle x^m \rangle_t$ yields

$$\langle \hat{x}^m \rangle_t = \frac{(-i)^m}{2\pi} \int dk \int dk' \delta^{(m)}(k-k') \langle \Phi_0| \left(\hat{U}_k^\dagger \right)^t \left(\hat{U}_{k'} \right)^t |\Phi_0\rangle \ . \tag{IV.9}$$

We can then integrate this by parts to obtain expressions such as

$$\begin{aligned}
\langle \hat{x}^m \rangle_t &= \frac{(-i)^m}{2\pi} \int dk \int dk' \delta^{(m)}(k-k') \langle \Phi_0 | \left(\hat{U}_k^\dagger\right)^t \left(\hat{U}_{k'}\right)^t |\Phi_0\rangle \\
&= \frac{(-i)^m}{2\pi} \int dk \int dk' \delta(k-k') \langle \Phi_0 | \left(\hat{U}_k^\dagger\right)^t \left[\frac{d^m}{dk'^m}\left(\hat{U}_{k'}\right)^t\right] |\Phi_0\rangle \\
&= \frac{(-i)^m}{2\pi} \int dk \langle \Phi_0 | \left(\hat{U}_k^\dagger\right)^t \left[\frac{d^m}{dk^m}\left(\hat{U}_{k}\right)^t\right] |\Phi_0\rangle
\end{aligned} \tag{IV.10}$$

For the first moment we get

$$\langle \hat{x} \rangle_t = -\frac{i}{2\pi} \int dk \langle \Phi_0 | \left(\hat{U}_k^\dagger\right)^t \left[\frac{d}{dk}\left(\hat{U}_{k}\right)^t\right] |\Phi_0\rangle \ , \tag{IV.11}$$

where

$$\begin{aligned}
\frac{d\hat{U}_k}{dk} &= \left(-i\mathrm{e}^{-ik}\hat{\mathcal{P}}_R + i\mathrm{e}^{ik}\hat{\mathcal{P}}_L\right)\hat{U} = -i(\hat{\mathcal{P}}_R - \hat{\mathcal{P}}_L)\hat{U}_k \equiv -i\hat{Z}\hat{U}_k \\
\frac{d\hat{U}_k^\dagger}{dk} &= i\hat{U}_k^\dagger(\hat{\mathcal{P}}_R - \hat{\mathcal{P}}_L) \equiv i\hat{U}_k^\dagger \hat{Z} \\
\hat{Z} &\equiv \hat{\mathcal{P}}_R - \hat{\mathcal{P}}_L = \hat{I} - 2\hat{\mathcal{P}}_L \ .
\end{aligned} \tag{IV.12}$$

Substituting this into (IV.11) gives us

$$\langle \hat{x} \rangle_t = -\frac{1}{2\pi} \sum_{j=1}^{t} \int dk \langle \Phi_0 | \left(\hat{U}_k^\dagger\right)^j \hat{Z} \left(\hat{U}_k\right)^j |\Phi_0\rangle \ . \tag{IV.13}$$

We can carry out a similar integration by parts to get the second moment:

$$\begin{aligned}
\langle \hat{x}^2 \rangle_t &= \frac{1}{2\pi} \int dk \langle \Phi_0 | \left[\frac{d}{dk}\left(\hat{U}_k^\dagger\right)^t\right] \left[\frac{d}{dk}\left(\hat{U}_k\right)^t\right] |\Phi_0\rangle \\
&= \frac{1}{2\pi} \sum_{j=1}^{t} \sum_{j'=1}^{t} \int dk \langle \Phi_0 | \left(\hat{U}_k^\dagger\right)^j \hat{Z} \left(\hat{U}_k\right)^{j-j'} \hat{Z} \left(\hat{U}_k\right)^{j'} |\Phi_0\rangle \ .
\end{aligned} \tag{IV.14}$$

Can we now evaluate these expressions? Let us suppose that we can find the eigenvectors $|\phi_{kl}\rangle$ and corresponding eigenvalues $\exp(i\theta_{kl})$ of $\hat{U}_k$. We expand the initial state

$$|\Phi_0\rangle = \sum_l c_{kl} |\phi_{kl}\rangle \ . \tag{IV.15}$$

After t steps

$$\left(\hat{U}_k\right)^t |\Phi_0\rangle = \sum_l c_{kl} |\phi_{kl}\rangle \mathrm{e}^{i\theta_{kl}t} \ . \tag{IV.16}$$

Substituting this into the equation for the first moment (IV.13) we get

$$\langle x \rangle_t = -t + \frac{1}{\pi} \int dk \sum_{l,l'} c_{kl}^* c_{kl'} \langle \phi_{kl} | \hat{\mathcal{P}}_L | \phi_{kl'} \rangle \sum_{j=1}^{t} \mathrm{e}^{i(\theta_{kl'} - \theta_{kl})j} \ . \tag{IV.17}$$

If the unitary matrix is nondegenerate, then most of the terms in (IV.17) will be *oscillatory*; hence, over time, they will average to zero. Only the diagonal terms in the above sum are nonoscillatory. We can therefore write

$$\begin{aligned} \langle x \rangle_t &= C_1 t + \text{oscillatory terms} , \\ C_1 &= -1 + \frac{1}{\pi} \int dk \sum_l |c_{kl}|^2 \langle \phi_{kl} | \hat{\mathcal{P}}_L | \phi_{kl} \rangle . \end{aligned} \quad \text{(IV.18)}$$

Making the same substitutions in the equation for the second moment (IV.14), we get

$$\langle x^2 \rangle_t = \frac{1}{2\pi} \int dk \sum_{l,l',l''} c_{kl}^* c_{kl'} \langle \phi_{kl} | \hat{Z} | \phi_{kl''} \rangle \langle \phi_{kl''} | \hat{Z} | \phi_{kl'} \rangle \sum_{j,j'=1}^{t} \mathrm{e}^{i(\theta_{kl''} - \theta_{kl})j} \mathrm{e}^{i(\theta_{kl'} - \theta_{kl''})j'} . \quad \text{(IV.19)}$$

Once again, most of these terms are oscillatory. There are two sets of nonoscillatory terms: terms with $l = l' = l''$ (which give a quadratic dependence on t) and terms with $j = j'$ and $l = l'$ (which give a linear dependence). Therefore we can write the second moment as

$$\begin{aligned} \langle x^2 \rangle_t &= C_2 t^2 + \text{oscillatory terms} + O(t) , \\ C_2 &= 1 - \frac{2}{\pi} \int dk \sum_l |c_{kl}|^2 \langle \phi_{kl} | \hat{\mathcal{P}}_L | \phi_{kl} \rangle \langle \phi_{kl} | \hat{\mathcal{P}}_R | \phi_{kl} \rangle . \end{aligned} \quad \text{(IV.20)}$$

Of course, if the spectrum of $\hat{U}_k$ is degenerate, we will have to modify (IV.20) and (IV.18) to include appropriate cross terms. This does not, however, alter the qualitative behavior. We see that generically in the long time limit, the first moment of the quantum random walk on the line will undergo a linear drift, and the variance will grow quadratically with time, so long as the coin is a finite-dimensional system.

B. The multicoin model

Now let us specialize to the case of our multicoin model. In this case our coin is a tensor-product of M 2-level coins, with a Hilbert space of 2^M dimensions. The "flip operator" is

$$\hat{U} = \left[\hat{H} \otimes \hat{I}^{\otimes M-1} \right] \hat{P} , \quad \text{(IV.21)}$$

where $\hat{H}$ is the usual Hadamard operator (II.1) and $\hat{P}$ is a cyclic permutation of the M coins:

$$\hat{P}(|\psi_0\rangle \otimes |\psi_1\rangle \otimes \cdots \otimes |\psi_{M-1}\rangle) = |\psi_1\rangle \otimes \cdots \otimes |\psi_{M-1}\rangle \otimes |\psi_0\rangle) . \quad \text{(IV.22)}$$

The two projectors onto the flip results are

$$\hat{\mathcal{P}}_R = |R\rangle\langle R| \otimes \hat{I}^{\otimes M-1} ,$$
$$\hat{\mathcal{P}}_L = |L\rangle\langle L| \otimes \hat{I}^{\otimes M-1} . \qquad \text{(IV.23)}$$

When we switch to the k representation, these give us the effective unitary evolution

$$\hat{U}_k = \left[\hat{H}_k \otimes \hat{I}^{\otimes M-1}\right] \hat{P} , \qquad \text{(IV.24)}$$

where $\hat{H}_k$ is given by (II.9). In the case $M = 1$, $\hat{U}_k = \hat{H}_k$.

The eigenvectors of $\hat{H}_k$ are

$$|\pm\rangle = \frac{1}{\sqrt{2}} \left(1 + \cos^2 k \pm \cos k \sqrt{1 + \cos^2 k}\right)^{-1/2} \begin{pmatrix} \mathrm{e}^{-ik} \\ \mp\sqrt{2}\mathrm{e}^{\pm i\omega_k} - \mathrm{e}^{-ik} \end{pmatrix} , \qquad \text{(IV.25)}$$

with eigenvalues $\mathrm{e}^{i(\pi+\omega_k)}$, $\mathrm{e}^{-i\omega_k}$, respectively, where we define ω_k to satisfy

$$\sin \omega_k \equiv \frac{1}{\sqrt{2}} \sin k , \quad -\pi/2 < \omega_k < \pi/2 . \qquad \text{(IV.26)}$$

A basis for the full M-coin space is given by product vectors of $|+\rangle$ and $|-\rangle$. (E.g., for $M = 2$ the basis vectors would be $|--\rangle, |-+\rangle, |+-\rangle, |++\rangle$.) Can we find the eigenvectors and eigenvalues of $\hat{U}_k$ in terms of this basis?

Note first that if we apply $\hat{U}_k$ to such a basis vector, we get another basis vector multiplied by a phase. Second, if we apply $\hat{U}_k$ to a basis vector M times, we get the *same* basis vector back, multiplied by a phase.

Two obvious eigenvectors appear at once: the vectors

$$|++\cdots+\rangle \equiv |+\rangle^{\otimes M} ,$$
$$|--\cdots-\rangle \equiv |-\rangle^{\otimes M} , \qquad \text{(IV.27)}$$

are both eigenvectors of $\hat{U}_k$ with eigenvalues $\mathrm{e}^{i(\pi+\omega_k)}$, $\mathrm{e}^{-i\omega_k}$, respectively. Let us suppose for the moment that M is a prime number. Then for all basis vectors $|\phi\rangle$ other than those two, the vectors

$$\left(\hat{U}_k\right)^j |\phi\rangle , \quad 0 \leq j \leq M - 1 \qquad \text{(IV.28)}$$

are all distinct. Together they span an M-dimensional subspace which is preserved under the action of $\hat{U}_k$. If $|\phi\rangle$ contains exactly m $|-\rangle$s and $(M - m)$ $|+\rangle$s, then every vector in this subspace is an eigenvector of $(\hat{U}_k)^M$ with eigenvalue $\exp i((M-m)(\pi+\omega_k)-m\omega_k)$. This implies that the subspace is spanned by M eigenvectors of $\hat{U}_k$ with eigenvalues

$$\lambda_n = \mathrm{e}^{i(-m\omega_k+(M-m)(\pi+\omega_k)+2\pi n)/M} \ , \quad 0 \le n < M \ . \tag{IV.29}$$

Let's restrict ourselves to this M-dimensional subspace for the moment. Starting with our original basis state $|\phi\rangle$, we label the basis states which span this space

$$|\phi_j\rangle = \hat{P}^j|\phi\rangle \ . \tag{IV.30}$$

The eigenvectors of $\hat{U}_k$ must have the form

$$|\chi_n\rangle = \frac{1}{\sqrt{M}} \sum_{j=0}^{M-1} e^{i\nu_{nj}}|\phi_j\rangle \ . \tag{IV.31}$$

Plugging the above expression and equation (IV.29) into the equation

$$\hat{U}_k|\chi_n\rangle = \lambda_n|\chi_n\rangle \tag{IV.32}$$

gives the result

$$\nu_{nj+1} = \nu_{nj} - \left(m\omega_k - (M-m)(\pi+\omega_k) - 2\pi n\right)/M + \theta_{j+1} \ , \tag{IV.33}$$

where we define θ_j to be $\mathrm{e}^{-i\omega_k}$ if the first factor of $|\phi_j\rangle$ is $|-\rangle$ and to be $\mathrm{e}^{i(\pi+\omega_k)}$ if the first factor is $|+\rangle$. Since the overall phase is arbitrary, we take $\nu_0 = 0$, which gives us

$$\nu_{nj} = -\frac{j}{M}\left(m\omega_k - (M-m)(\pi+\omega_k) + 2\pi n\right) + \sum_{j'=1}^{j} \theta_{j'} \ . \tag{IV.34}$$

For each value of m, $1 \le m \le M-1$, there are $\frac{1}{M}\binom{M}{m}$ such M-dimensional subspaces which are preserved by the action of $\hat{U}_k$; each eigenvalue is thus $\frac{1}{M}\binom{M}{m}$-fold degenerate. However, this doesn't complicate the expressions (IV.18) and (IV.20), because the cross-terms vanish:

$$\langle\phi_{kl}|\hat{\mathcal{P}}_R|\phi_{kl'}\rangle = \langle\phi_{kl}|\hat{\mathcal{P}}_L|\phi_{kl'}\rangle = 0 \tag{IV.35}$$

for all such degenerate eigenvectors $|\phi_{kl}\rangle, |\phi_{kl'}\rangle$. Thus, we can use the expressions we've already derived.

Using the results in Eq. (IV.34) we can calculate the necessary matrix elements:

$$\begin{aligned}
\langle\chi_n|\hat{\mathcal{P}}_L|\chi_n\rangle &= \frac{1}{M}\left[m\langle-|L\rangle\langle L|-\rangle + (M-m)\langle+|L\rangle\langle L|+\rangle\right] \\
&= \frac{1}{M}\left[\frac{m(\sqrt{1+\cos^2 k}-\cos k)^2}{2(1+\cos^2 k-\cos k\sqrt{1+\cos^2 k})}\right. \\
&\qquad \left.+\frac{(M-m)(\sqrt{1+\cos^2 k}+\cos k)^2}{2(1+\cos^2 k+\cos k\sqrt{1+\cos^2 k})}\right], \\
\langle\chi_n|\hat{\mathcal{P}}_R|\chi_n\rangle &= \frac{1}{M}\left[m\langle-|R\rangle\langle R|-\rangle + (M-m)\langle+|R\rangle\langle R|+\rangle\right] \\
&= \frac{1}{M}\left[\frac{m}{2(1+\cos^2 k-\cos k\sqrt{1+\cos^2 k})}\right. \\
&\qquad \left.+\frac{M-m}{2(1+\cos^2 k+\cos k\sqrt{1+\cos^2 k})}\right].
\end{aligned} \tag{IV.36}$$

We also need the amplitudes of the coin's initial state. If

$$|\Phi_0\rangle = |\psi_0\rangle\otimes\cdots\otimes|\psi_0\rangle = |\psi_0\rangle^{\otimes M}, \tag{IV.37}$$

then

$$|\langle\Phi_0|\chi_n\rangle|^2 = |\langle\psi_0|-\rangle|^{2m}|\langle\psi_0|+\rangle|^{2(M-m)}\sum_{j,j'}\frac{1}{M}\mathrm{e}^{i(\nu_{nj}-\nu_{nj'})}. \tag{IV.38}$$

Note that

$$\sum_{n=0}^{M-1}\mathrm{e}^{i(\nu_{nj}-\nu_{nj'})} = M\delta_{jj'}. \tag{IV.39}$$

We now have everything we need to get the moments!

To evaluate the expression (IV.18) to get C_1 we calculate

$$\begin{aligned}
\sum_l |c_{kl}|^2\langle\phi_{kl}|\hat{\mathcal{P}}_L|\phi_{kl}\rangle &= \sum_{m=1}^{M-1}\frac{1}{M}\binom{M}{m}\sum_{n=0}^{M-1}|\langle\Phi_0|\phi_n\rangle|^2\langle\phi_n|\hat{\mathcal{P}}_L|\phi_n\rangle \\
&\quad +|\langle\psi_0|-\rangle|^2\langle-|L\rangle\langle L|-\rangle + |\langle\psi_0|+\rangle|^2\langle+|L\rangle\langle L|+\rangle \\
&= \sum_{m=0}^{M}\binom{M}{m}|\langle\psi_0|-\rangle|^{2m}|\langle\psi_0|+\rangle|^{2(M-m)} \\
&\qquad \times\frac{1}{M}\left[\frac{m(\sqrt{1+\cos^2 k}-\cos k)^2}{2(1+\cos^2 k-\cos k\sqrt{1+\cos^2 k})}\right. \\
&\qquad \left.+\frac{(M-m)(\sqrt{1+\cos^2 k}+\cos k)^2}{2(1+\cos^2 k+\cos k\sqrt{1+\cos^2 k})}\right].
\end{aligned} \tag{IV.40}$$

We can simplify this considerably by noting that this equation (IV.40) has the form

$$\sum_{m=0}^{M} \binom{M}{m} p^m (1-p)^{M-m} [(m/M)(A-B)+B] = pA + (1-p)B \;, \tag{IV.41}$$

where

$$\begin{aligned} p &= |\langle \psi_0 | - \rangle|^2 \;, \\ A &= \frac{(\sqrt{1+\cos^2 k} - \cos k)^2}{2(1+\cos^2 k - \cos k \sqrt{1+\cos^2 k})} \;, \\ B &= \frac{(\sqrt{1+\cos^2 k} + \cos k)^2}{2(1+\cos^2 k + \cos k \sqrt{1+\cos^2 k})} \;, \end{aligned} \tag{IV.42}$$

and we've invoked some combinatorial identities

$$\begin{aligned} \sum_{m=0}^{M} \binom{M}{m} p^m (1-p)^{M-m} &= (p + (1-p))^M = 1 \;, \\ \sum_{m=0}^{M} \binom{M}{m} p^m (1-p)^{M-m} (m/M) &= p \sum_{m=0}^{M-1} \binom{M-1}{m} p^m (1-p)^{M-m-1} = p \;. \end{aligned} \tag{IV.43}$$

This leaves us with the simple expression

$$\begin{aligned} \sum_l |c_{kl}|^2 \langle \phi_{kl} | \hat{\mathcal{P}}_L | \phi_{kl} \rangle = \Bigg[& \frac{|\langle \psi_0 | - \rangle|^2 (\sqrt{1+\cos^2 k} - \cos k)^2}{2(1+\cos^2 k - \cos k \sqrt{1+\cos^2 k})} \\ & + \frac{|\langle \psi_0 | + \rangle|^2 (\sqrt{1+\cos^2 k} + \cos k)^2}{2(1+\cos^2 k + \cos k \sqrt{1+\cos^2 k})} \Bigg] \;, \end{aligned} \tag{IV.44}$$

in which all M dependence is gone!

Let us choose the initial condition $|\psi_0\rangle = |R\rangle$. Then

$$\begin{aligned} |\langle \psi_0 | - \rangle|^2 &= \frac{1}{2(1+\cos^2 k - \cos k \sqrt{1+\cos^2 k})} \\ |\langle \psi_0 | + \rangle|^2 &= \frac{1}{2(1+\cos^2 k + \cos k \sqrt{1+\cos^2 k})} \;. \end{aligned} \tag{IV.45}$$

We can plug this into the above equation (IV.44); after a bit of algebra, this boils down to the result

$$\sum_l |c_{kl}|^2 \langle \phi_{kl} | \hat{\mathcal{P}}_L | \phi_{kl} \rangle = \frac{1}{2(1+\cos^2 k)} \;, \tag{IV.46}$$

This gives us the final equation for C_1,

$$C_1 = -1 + \frac{1}{2\pi} \int \frac{dk}{1+\cos^2 k} = -1 + 1/\sqrt{2} \;, \tag{IV.47}$$

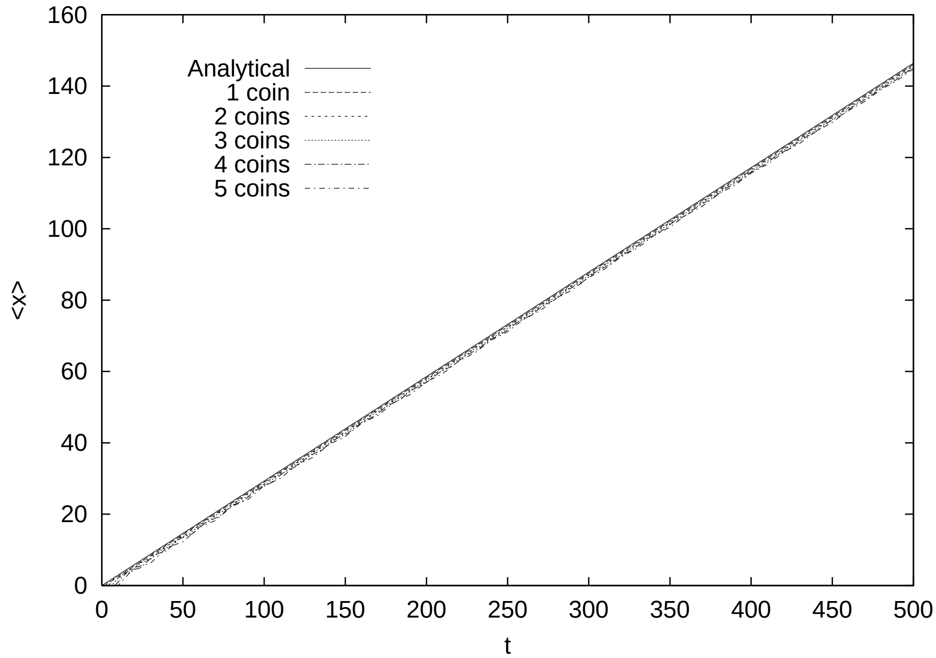

FIG. 4: This plots the first moment of position vs. time for multicoin quantum random walks with M =1–5 coins, using both direct numerical simulation and the analytical result (IV.47). As calculated, the long time behavior is essentially independent of the number of coins, and grows linearly with time. All coins begin in the initial state $|R\rangle$.

which exactly matches the observed numerical results. (See figure 4.)

We can do a similar derivation for the second moment, in order to get C_2. For this we use

$$\begin{aligned}
&\sum_l |c_{kl}|^2 \langle\phi_{kl}|\hat{\mathcal{P}}_L|\phi_{kl}\rangle\langle\phi_{kl}|\hat{\mathcal{P}}_R|\phi_{kl}\rangle \\
&= \sum_{m=0}^{M} \binom{M}{m} |\langle\psi_0|-\rangle|^{2m} |\langle\psi_0|+\rangle|^{2(M-m)} \\
&\quad \times \frac{1}{M}\left[\frac{m(\sqrt{1+\cos^2 k}-\cos k)^2}{2(1+\cos^2 k - \cos k\sqrt{1+\cos^2 k})}\right. \\
&\quad \left. + \frac{(M-m)(\sqrt{1+\cos^2 k}+\cos k)^2}{2(1+\cos^2 k + \cos k\sqrt{1+\cos^2 k})}\right] \\
&\quad \times \frac{1}{M}\left[\frac{m}{2(1+\cos^2 k - \cos k\sqrt{1+\cos^2 k})}\right. \\
&\quad \left. + \frac{(M-m)}{2(1+\cos^2 k + \cos k\sqrt{1+\cos^2 k})}\right] . \qquad \text{(IV.48)}
\end{aligned}$$

We can again simplify by observing that (IV.48) has the form

$$\sum_{m=0}^{M} \binom{M}{m} p^m (1-p)^{M-m} [(m/M)(A-B)+B][A+(m/M)(B-A)] = AB + p(1-p)\frac{M-1}{M}(A-B)^2 \; . \qquad \text{(IV.49)}$$

If we specialize once more to $|\psi_0\rangle = |0\rangle$, we can make similar algebraic simplifications to get

$$\begin{aligned} C_2 &= 1 - \frac{1}{2\pi}\int dk \left[\frac{1+2\cos^2 k}{(1+\cos^2 k)^2} - \frac{1}{M}\frac{\cos^2 k}{(1+\cos^2 k)^2} \right] \\ &= 1 - \frac{5}{4\sqrt{2}} + \frac{1}{M}\frac{1}{4\sqrt{2}} \; . \end{aligned} \qquad \text{(IV.50)}$$

Of course, numerically we calculated not the second moment but the *variance* of x. Given our results,

$$\langle \hat{x}^2 \rangle_t - \langle \hat{x} \rangle_t^2 = (C_2 - C_1^2)t^2 + O(t) + \text{osc. terms} \; , \qquad \text{(IV.51)}$$

we get the result

$$C_2 - C_1^2 = \frac{3 - 2\sqrt{2} + 1/M}{4\sqrt{2}} \; . \qquad \text{(IV.52)}$$

Note that this doesn't vanish as M becomes large!

The derivation used above was only strictly valid for prime M. However, it turns out that the additional complications arising from composite M all cancel out, yielding the same expressions for C_1 and C_2. Upon comparison to the numerical results, we see that these analytical expressions for the first moment and the variance match the simulations extremely well. (See figure 5.)

C. Constant flips per coin

We see that in the long time limit, an M-coin quantum random walk with fixed M has qualitative behavior similar to that one of the one-coin walk, and is markedly nonclassical. A reasonable question to ask is, how long is a long time? Suppose we flip each coin at most d times, and add more coins as we go to long times, so that M and t are both growing in a fixed ratio $t/M \rightarrow d$. Does this still behave nonclassically? The fact that $C_2 - C_1^2$ does not vanish as $M \rightarrow \infty$ makes this conjecture plausible. If so, how big must d be for this nonclassical behavior to manifest itself?

Let us now consider a quantum random walk on a line driven by a sequence of two-level coins, each flipped d times. By the reordering principle described in section III, this is the

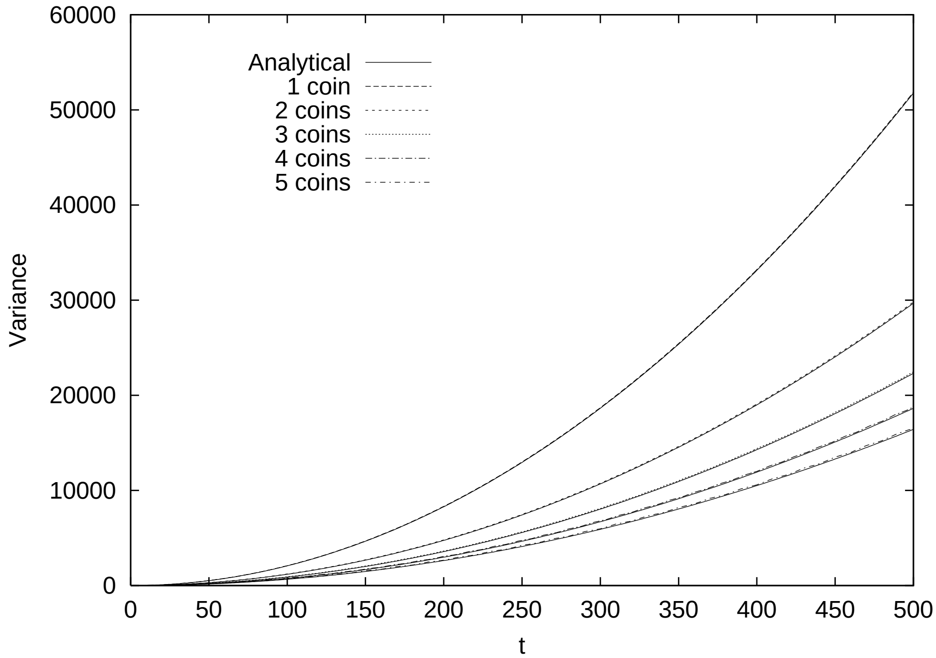

FIG. 5: This plots the variance of position vs. time for multicoin quantum random walks with M =1–5 coins, using both direct numerical simulation and the analytical result (IV.52). All coins begin in the initial state $|R\rangle$.

same as having a single coin which is measured and reset to the initial state $|\Phi_0\rangle$ after every d steps. We describe this evolution by a *superoperator* $\mathcal{L}$ which acts on the density matrix of the particle and coin:

$$\begin{aligned} \rho \rightarrow \rho' &= \mathcal{L}\rho \\ &= \sum_n \hat{A}_n \left(\hat{E}\right)^d \rho \left(\hat{E}^\dagger\right)^d \hat{A}_n^\dagger \ , \end{aligned} \qquad \text{(IV.53)}$$

where $\hat{E}$ is the usual unitary evolution (II.3), and

$$\begin{aligned} \hat{A}_0 &= \hat{I} \otimes |\Phi_0\rangle\langle R| \ , \\ \hat{A}_1 &= \hat{I} \otimes |\Phi_0\rangle\langle L| \ . \end{aligned} \qquad \text{(IV.54)}$$

The superoperator $\mathcal{L}$ represents d steps of the walk. Note that

$$\mathcal{L}\rho = \mathrm{Tr}_{\mathrm{coin}} \left\{ \left(\hat{E}\right)^d \rho \left(\hat{E}^\dagger\right)^d \right\} \otimes |\Phi_0\rangle\langle\Phi_0| \ . \qquad \text{(IV.55)}$$

We rewrite this in terms of the eigenvectors $|k\rangle$ of $\hat{S}, \hat{S}^\dagger$. In the k basis, a general density operator for the joint particle/coin system is written

$$\rho = \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} |k\rangle\langle k'| \otimes \chi_{kk'} \ , \tag{IV.56}$$

and the evolution superoperator becomes

$$\begin{aligned}\mathcal{L}\rho &= \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} |k\rangle\langle k'| \otimes \sum_{n=R,L} |\Phi_0\rangle\langle n| \left(\hat{H}_k \chi_{kk'} \hat{H}^\dagger_{k'}\right) |n\rangle\langle\Phi_0| \\ &\equiv \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} |k\rangle\langle k'| \otimes \mathcal{L}_{kk'}\chi_{kk'} \ ,\end{aligned} \tag{IV.57}$$

where $\mathcal{L}_{kk'}$ is now a superoperator on the coin degree of freedom alone.

The initial state of the system (particle and coin) is

$$\begin{aligned}\rho_0 &= |\Psi_0\rangle\langle\Psi_0| = |0\rangle\langle 0| \otimes |\Phi_0\rangle\langle\Phi_0| \\ &= \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} |k\rangle\langle k'| \otimes |\Phi_0\rangle\langle\Phi_0| \ .\end{aligned} \tag{IV.58}$$

Let the quantum random walk proceed for t steps. Then the state evolves to

$$\rho_t = \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} |k\rangle\langle k'| \otimes \mathcal{L}^{t/d}_{kk'} |\Phi_0\rangle\langle\Phi_0| \ . \tag{IV.59}$$

The probability to reach a point x at time t is

$$\begin{aligned}p(x,t) &= \mathrm{Tr}\left\{(|x\rangle\langle x| \otimes \hat{I})\rho_t\right\} \\ &= \frac{1}{(2\pi)^2} \int dk \int dk' \langle k|x\rangle\langle x|k'\rangle \mathrm{Tr}\left\{\mathcal{L}^{t/d}_{kk'}|\Phi_0\rangle\langle\Phi_0|\right\} \\ &= \frac{1}{(2\pi)^2} \int dk \int dk' \mathrm{e}^{-ix(k-k')} \mathrm{Tr}\left\{\mathcal{L}^{t/d}_{kk'}|\Phi_0\rangle\langle\Phi_0|\right\} \ .\end{aligned} \tag{IV.60}$$

We are interested in the moments of this distribution.

$$\begin{aligned}\langle\hat{x}^m\rangle_t &= \sum_x x^m p(x,t) \\ &= \frac{1}{(2\pi)^2} \sum_x x^m \int dk \int dk' \mathrm{e}^{-ix(k-k')} \mathrm{Tr}\left\{\mathcal{L}^{t/d}_{kk'}|\Phi_0\rangle\langle\Phi_0|\right\} \ .\end{aligned} \tag{IV.61}$$

Just as before, we invert the order of operations and do the x sum first, which yields

$$\langle\hat{x}^m\rangle_t = \frac{(-i)^m}{2\pi} \int dk \int dk' \delta^{(m)}(k-k') \mathrm{Tr}\left\{\mathcal{L}^{t/d}_{kk'}|\Phi_0\rangle\langle\Phi_0|\right\} \ . \tag{IV.62}$$

We can then integrate this by parts. In carrying out this integration by parts, we will need

$$\begin{aligned}\frac{d}{dk}\mathcal{L}_{kk'}\rho &= -i \sum_n \hat{A}_n \left(\sum_{j=0}^{d-1} (\hat{H}_k)^j \hat{Z} (\hat{H}^\dagger_k)^j\right) (\hat{H}_k)^d \rho (\hat{H}^\dagger_k)^d \hat{A}^\dagger_n \\ &= -i|\Phi_0\rangle\langle\Phi_0| \mathrm{Tr}\left\{\left(\sum_{j=0}^{d-1} (\hat{H}_k)^j \hat{Z} (\hat{H}^\dagger_k)^j\right) (\hat{H}_k)^d \rho (\hat{H}^\dagger_k)^d\right\} \ ,\end{aligned} \tag{IV.63}$$

where $\hat{H}_k$ is given by (II.9) and $\hat{Z}$ by (IV.12).

Using this, we can carry out the integration by parts for the first moment to get

$$\begin{aligned}\langle \hat{x} \rangle_t &= -\frac{1}{2\pi} \sum_{j=0}^{t/d-1} \int dk \mathrm{Tr} \left\{ \hat{Z}_{kd} \mathcal{L}_{kk}^j |\Phi_0\rangle\langle\Phi_0| \right\} \\ &= -\frac{1}{2\pi} \sum_{j=0}^{t/d-1} \int dk \mathrm{Tr} \left\{ \hat{Z}_{kd} |\Phi_0\rangle\langle\Phi_0| \right\} \\ &= -\frac{t}{d} \int \frac{dk}{2\pi} \langle\Phi_0|\hat{Z}_{kd}|\Phi_0\rangle \ , \end{aligned} \tag{IV.64}$$

where we define

$$\hat{Z}_{kd} = \sum_{l=1}^{d} (\hat{H}_k^\dagger)^l \hat{Z} (\hat{H}_k)^l \ . \tag{IV.65}$$

Generically, then, we see from (IV.64) that the first moment of position grows linearly with time provided $\langle\Phi_0|\hat{Z}_{kd}|\Phi_0\rangle$ is nonzero.

We can carry out a similar integration by parts to get the second moment:

$$\begin{aligned}\langle \hat{x}^2 \rangle_t &= \frac{1}{2\pi} \int dk \Bigg[\sum_{j=0}^{t/d-1} \mathrm{Tr} \left\{ \left(\hat{Z}_{kd} \right)^2 \mathcal{L}_{kk}^j |\Phi_0\rangle\langle\Phi_0|) \right\} \\ &\quad + \sum_{j=0}^{t/d-1} \sum_{j'=0}^{j-1} \mathrm{Tr} \left\{ \hat{Z}_{kd} \mathcal{L}_{kk}^{j-j'} ((\mathcal{L}_k^{j'} |\Phi_0\rangle\langle\Phi_0|) \hat{Z}_{kd} + \hat{Z}_{kd} \mathcal{L}_{kk}^{j'} |\Phi_0\rangle\langle\Phi_0|) \right\} \Bigg] \\ &= \frac{1}{2\pi} \int dk \Bigg[(t/d) \langle\Phi_0| \left(\hat{Z}_{kd} \right)^2 |\Phi_0\rangle + (t^2/d^2 - t/d) \langle\Phi_0|\hat{Z}_{kd}|\Phi_0\rangle^2 \ . \end{aligned} \tag{IV.66}$$

So here we expect the second moment to grow quadratically with time, qualitatively like the single-coin walk.

Let's choose the initial condition $|\Phi_0\rangle = |R\rangle$, and look at a few values of d. We are interested in the coefficients C_1 and C_2, where

$$\begin{aligned}\langle \hat{x} \rangle_t &= C_1 t \ , \\ \langle \hat{x}^2 \rangle_t &= C_2 t^2 + O(t) \ . \end{aligned} \tag{IV.67}$$

From the equations (IV.64), (IV.66), we get

$$\begin{aligned} C_1 &= -\frac{1}{d} \int \frac{dk}{2\pi} \langle R|\hat{Z}_{kd}|R\rangle \ , \\ C_2 &= \frac{1}{d^2} \int \frac{dk}{2\pi} \langle R|\hat{Z}_{kd}|R\rangle^2 \ . \end{aligned} \tag{IV.68}$$

From the definitions of $\hat{Z}_{kd}$ and $\hat{H}_k$ we can work out the values of $C_{1,2}$ in specific cases.

For $d = 1$, the matrix element $\langle R|\hat{Z}_{k1}|R\rangle = 0$, so both C_1 and C_2 vanish. We recover the classical case.

For $d = 2$, the matrix element $\langle R|\hat{Z}_{k2}|R\rangle = \cos 2k$, so C_1 vanishes in this case as well. However, $C_2 = 1/8 \neq 0$. So even with only two flips per coin, the variance already grows quadratically with time.

For $d = 3$, the matrix element $\langle R|\hat{Z}_{k3}|R\rangle = \cos 2k + \sin^2 2k$, so both C_1 and C_2 are nonzero. In this case, $C_1 = -1/6$ and $C_2 = 7/72$.

If we let both d and t/d become large, then we can evaluate (IV.64) and (IV.66) to get $C_1 \to -1 + \sqrt{1/2}$ and $C_2 \to 1 - 5/\sqrt{32}$, which are in agreement with our earlier results for large M in the multicoin case.

V. CONCLUSIONS

We have examined one possible path from quantum to classical behavior: the use of multiple coins (or, more generally, higher-dimensional systems) to drive the walk and reduce the effects of interference. We have seen that quantum behavior, as typified by quadratic growth of the variance with time, persists except in the extreme limit of a new coin for every step. Furthermore, quadratic growth of the variance seems to be a generic feature of such unitary walks.

From the multicoin example we might speculate that classical behavior is only recovered in the limit where the coin system retains enough information about the walk to reconstruct a unique classical path for the particle. Since there are 2^t such paths up to time t, the coin must have a Hilbert space dimension which grows exponentially in time in order to exhibit classical behavior.

Another plausible route to classical behavior adds decoherence to the coin, which also effectively suppresses interference effects. The results of this study are presented elsewhere [23].

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APPENDIX A: COMBINATORIAL DERIVATION OF ONE-COIN WALK

Assume that the coin starts at $x = 0$. After t coin flips, the particle might have reached locations anywhere between $x = -t, -t+2, \ldots, t-2, t$. The number of paths that finish at a point x after t steps is

$$\#\ \text{paths} = \binom{t}{(t-x)/2}. \tag{A.1}$$

Paths ending with the coin in state $|L\rangle$ cannot interfere with paths ending with the coin in state $|R\rangle$.

A given path can be written as a sequence S of t symbols, L or R like this one:

$$L\ R\ R\ L\ R \underbrace{L\ L\ L}_{\substack{\text{a cluster}\\ \text{of 3 } Ls}} R\ R \ldots \tag{A.2}$$

We let $N_L(S)$ be the number of L's in S and $N_R(S)$ the number of R's. Then

$$N_L(S) + N_R(S) = t, \qquad N_R(S) - N_L(S) = x\ , \tag{A.3}$$

so we can write

$$N_R(S) = (t+x)/2, \qquad N_L(S) = (t-x)/2\ . \tag{A.4}$$

Each path has an associated phase factor, which can take the values ± 1. A factor of -1 is acquired whenever the coin flips two successive lefts, so a pair LL contributes a phase factor of -1, the sequence LLL produces a factor of $+1$, and $LLLL$ results in a -1, and so on. Each cluster of m Ls contributes a factor of $(-1)^{m-1}$ to the phase for that path.

Let $C(S)$ be the number of L-clusters in S. (An L-cluster must contain at least one L.) Swapping an L from one cluster to another changes the phase contributed by each cluster by -1, thus having no overall effect on the phase of the path as a whole. Therefore, only the number of L-clusters and the total number of Ls matters.

If the number of L-clusters is C and the total number of Ls is N_L, then these could be arranged thus

$$\underbrace{L \quad L \quad L \quad \ldots \quad L}_{C-1 \quad \text{singletons}} \quad \underbrace{L\,L\,\ldots\,L}_{\substack{N_L-(C-1)\\ \text{consecutively}}}. \tag{A.5}$$

This path will have a phase of

$$\varphi(S) = (-1)^{N_L-(C-1)-1} = (-1)^{N_L-C}. \tag{A.6}$$

So when $N_L - C$ is odd the overall phase is -1.

Each cluster must have at least one R between itself and the next cluster. Call these groups of Rs "partitions." Every sequence S is then a succession of alternating clusters and partitions. Let

$$P(S) = \#\text{ of partitions in} \quad S. \tag{A.7}$$

Clearly $C(S)$ cannot be higher than $N_L(S)$, and $P(S)$ cannot be higher than $N_R(S)$. Also, it must be the case that

$$P(S) = C(S) \quad \text{or} \quad C(S) \pm 1. \tag{A.8}$$

Allocating N_L Ls among C clusters can be done in $\binom{N_L-1}{C-1}$ ways; similarly, N_R Rs can be allocated among P partitions in $\binom{N_R-1}{P-1}$ ways. For a given C and P, then, the total number of paths must be

$$\#\text{ paths } = \binom{N_L-1}{C-1}\binom{N_R-1}{P-1}. \tag{A.9}$$

Let us now fix t and x, and hence also N_L and N_R. What values of C and P are possible, and how many paths have each value?

Case I: $x > 0 \implies N_R > N_L$. The number of clusters, C, can range from 0 (only when $x = t$) to N_L. The number of partitions P can be $C, C+1$ or $C-1$, except when $C = 0, 1$.

Case II: $x < 0 \implies N_L > N_R$. This time C can range from 1 to $N_R + 1$. Likewise, P can take values of $C, C+1, C-1$ except at the extremes.

Case III: $x = 0 \implies N_L = N_R$ and C and P can be anything from 1 to $N_L = N_R$.

Consider now the arrangements of clusters and partitions. There are four distinct possible arrangements.

Arrangement 1: $P = C - 1$.

$$\text{[cluster] partition [cluster] partition} \ldots \text{[cluster]}\,. \tag{A.10}$$

Arrangement 2: $P = C$, starting with a partition. This looks like

$$\text{partition [cluster] partition} \ \ldots \ \text{[cluster]}\,. \tag{A.11}$$

Arrangement 3: $P = C$, starting with a cluster.

$$\text{[cluster] partition [cluster]} \ \ldots \ \text{partition.} \tag{A.12}$$

Arrangement 4: $P = C + 1$.

$$\text{partition [cluster] partition [cluster]} \ \ldots \ \text{partition.} \tag{A.13}$$

We adopt the convention

$$\binom{a}{b} = 0, \quad \text{if} \quad b > a,\ b < 0, \quad \text{or} \quad a < 0. \tag{A.14}$$

Then we can write that the amplitude to reach x after t coin flips, ending in an L is:

$$a_L(x,t) = \frac{1}{\sqrt{2^t}} \left[\sum_{C=1}^{\text{“}N\text{”}} (-1)^{N_L - C} \binom{N_L - 1}{C - 1} \left\{ \binom{N_R - 1}{C - 2} + \binom{N_R - 1}{C - 1} \right\} \right], \tag{A.15}$$

where the summation is to N_L for $x \geq 0$ and to $N_R + 1$ for $x < 0$.

Likewise, the amplitude to reach x in t flips, ending in an R is

$$a_R(x,t) = \frac{1}{\sqrt{2^t}} \left[\sum_{C=1}^{\text{“}N\text{”}} (-1)^{N_L - C} \binom{N_L - 1}{C - 1} \left\{ \binom{N_R - 1}{C - 1} + \binom{N_R - 1}{C} \right\} \right], \tag{A.16}$$

but only if $N_L \neq 0$; that case (which corresponds to $t = x$) always has amplitude $2^{-t/2}$.

We can use the binomial relations

$$\begin{aligned} \binom{N_R - 1}{C - 2} + \binom{N_R - 1}{C - 1} &= \binom{N_R}{C - 1} \\ \binom{N_R - 1}{C - 1} + \binom{N_R - 1}{C} &= \binom{N_R}{C}, \end{aligned} \tag{A.17}$$

to simplify these somewhat to give the final equations (II.14).

If we had started instead with the coin in the state $|L\rangle$, all sequences which begin with an L (i.e., arrangements 1 and 3) would pick up an extra minus sign. The amplitudes then become those given by the equations (II.15).

APPENDIX B: ASYMPTOTIC APPROXIMATION TO THE FOURIER INTEGRALS

Following the analysis in [6], the Fourier analysis of the many coin quantum walk can be completed in the same way. We represent the state of the particle in the $\{|k\rangle\}$ basis, and make use of the eigenvectors and eigenvalues of $\hat{H}_k$, as given by (IV.25) and (IV.26). We will also use the identity

$$\pm\sqrt{2}e^{\mp i\omega_k} - e^{-ik} = \pm\sqrt{1+\cos^2(k)} - \cos(k) \tag{B.1}$$

We can now use the tensor-product structure of the evolution matrix and the integral simplifications in [6] to simplify the integrals for a_R and a_L. The expression for a_R becomes

$$\int_{-\pi}^{\pi}\left(1-\frac{\cos(k)}{\sqrt{1+\cos^2(k)}}\right)e^{i((\omega_k+\pi)t-kx)}dk = (-1)^{x+t}\int_{-\pi}^{\pi}\left(1+\frac{\cos(k')}{\sqrt{1+\cos^2(k')}}\right)e^{-i(\omega_{k'}t+k'x)}dk' \tag{B.2}$$

where $k' = k-\pi, \quad \omega_{k'} = -\omega_k$ and we are free to move the limits of integration because the integral is over a whole period of the function. The two terms in the integral for a_L can be simplified in a similar way:

$$\int_{-\pi}^{\pi}\frac{-e^{ik}(\sqrt{1+\cos^2(k)}+\cos(k))}{((1+\cos^2(k))+\cos(k)\sqrt{1+\cos^2(k)})}e^{i(\omega_k+\pi)t-kx}dk$$
$$= -(-1)^{x+t}\int_{-\pi}^{\pi}\frac{e^{ik'}}{2\sqrt{1+\cos^2(k')}}e^{-i(\omega_{k'}t+k'x)}dk'\,. \tag{B.3}$$

Before we can write down a closed form for the M-coin momentum wave-function, we need one more construction. This is a timelike parameter that we'll call $|\tau|$. Let t_i be the total number of turns that coin i has. The tensor product structure of the evolution matrix for the multicoin system means that the eigenvalues for the combined system are just products of the eigenvalues for the one coin system. So we'll see things like

$$\lambda_{\mathbf{k}}^t = e^{-i\omega_k t_1}e^{i(\omega_k+\pi)t_2}e^{-i\omega_k t_3}e^{i(\omega_k+\pi)t_4}e^{i(\omega_k+\pi)t_5}\dots \tag{B.4}$$
$$= (-1)^{t_2+t_4+t_5}e^{-i\omega_k(t_1-t_2+t_3-t_4-t_5\dots)}. \tag{B.5}$$

If we now write

$$(t_1-t_2+t_3-t_4-t_5\dots) = \text{“}\tau\text{”} \tag{B.6}$$

we can see that, up to a minus sign, we will obtain expressions of much the same form as in the one coin case, but parametrized by τ instead of t, where τ is defined

$$\tau \in \{\pm t_1 \pm t_2 \pm \ldots \pm t_M\}, \tag{B.7}$$

with each $\pm$ independent. The modulus sign arises naturally when the integral expressions for the wavefunction are simplified in a way analogous to the one coin case, as τ can be chosen to be positive without loss of generality. When performing the simplification, it is also convenient to introduce the integer j_τ, which is useful because for each τ we get terms like

$$\left(1 + \frac{\cos^2(k)}{\sqrt{1+\cos^2(k)}}\right)^{\#(t_i s \text{ ending in } L)} \left(1 - \frac{\cos^2(k)}{\sqrt{1+\cos^2(k)}}\right)^{\#(-t_i s \text{ ending in } L)} \tag{B.8}$$

These are of the form $(a+b)^r(a-b)^s$, and j_τ counts the $(a^2-b^2)^{|r-s|}$ terms in the expansion of that product. These are of the form $(\frac{1}{1+\cos^2(k)})^{|r-s|}$ and so they only appear in the denominator. The term raised to the power of $n-2j_\tau$ is just the two sets of left-overs from that (one multiplied by $e^{-i(\omega_k|\tau|+kx)}$ and the other by $e^{i((\omega_k+\pi)|\tau|-kx)}$) which have then been combined using the integral simplification identities as before.

We can now write down the wavefunction for a particle that started out with all the coins in the state $|R\rangle$ and ended in them in (any) one of the $\binom{M}{n}$ components with n coins in the state R :

$$|\psi_{n,(M-n)}(x,t)\rangle = \sum_\tau \frac{1+(-1)^{x+|\tau|}}{2^M} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left(\frac{e^{ik(M-n)}\left(\cos(k)+\sqrt{1+\cos^2(k)}\right)^{n-2j_\tau}}{(1+\cos^2(k))^{M/2}} \right) e^{-i(\omega_k|\tau|+kx)}\ , \tag{B.9}$$

where the sum over τ indicates a sum over all 2^M possible signs in (B.7).

To write down the wavefunction for a particle that started with its coins in any state in the computational basis for the coins, we need yet another definition. We will introduce the notation σ to be the L-sign weight of τ, which will be the number of minuses in that particular τ. So for

$$\begin{aligned} \tau &= t_1 + t_2 - t_3 + t_4 - t_5 - t_6 + t_7, \\ \text{initial coin state} &= R \quad L \quad R \quad L \quad L \quad L \quad R, \end{aligned} \tag{B.10}$$

we define $\sigma = 2$. In other words, for all the coins that started out in the state L, count the number of minuses in front of the number of turns taken by those coins for that τ. Ignore any minuses for coins that start in the state R. Without loss of generality, σ can be taken to be in $[0, \lfloor M/2 \rfloor]$, as only $|\tau|$ actually matters in the wavefunction.

Then the wavefunction for a walk starting with its M coins in a state in the computational basis of the coins, where there are initially q coins in the state L and $M-q$ in the state R will be

$$
\begin{aligned}
|\psi_{n,(M-n):\text{coins}}(x,t)\rangle &= \sum_{\tau} \frac{1+(-1)^{x+|\tau|}}{2^M} \\
&\times \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{i\sigma\pi} \left(\sqrt{1+\cos^2(k)} - \cos(k)\right)^{M-q-\sigma} \left(\sqrt{1+\cos^2(k)} + \cos(k)\right)^{\sigma} \\
&\times \left(\frac{e^{-ikn} \left(\cos(k) + \sqrt{1+\cos^2(k)}\right)^{n-2j_\tau} e^{ikq}}{(1+\cos^2(k))^{M/2}} \right) e^{-i(\omega_k|\tau|+kx)}. \qquad \text{(B.11)}
\end{aligned}
$$

The wavefunction for a general starting state can be obtained from those for the computational basis states by forming the corresponding linear combination.

If τ is an asymptotic parameter: i.e., $\tau \to \infty$ as $t \to \infty$ then these integrals may be approximated using the method of stationary phase. If $\tau = 0$ or $\tau =$ constant (which can happen if the coins are used cyclically: for example if we have two coins, then we will get terms where $t_1 - t_2 = 0$ or 1 for all time) then the integrals must be performed by some other method. It is these constant-τ cases that produce the "stationary" central spikes seen in the simulations for an even number of coins (more on these below).

If we restrict to the special case where $t_1 = t_2 = \ldots = t_m = t/M$ is an integer, then equation (B.9) simplifies somewhat to

$$
\begin{aligned}
|\psi_{n,(M-n)}(x,t)\rangle &= \sum_{r=0}^{\lfloor M/2 \rfloor} \sum_{j=0}^{\lfloor n/2 \rfloor} \binom{M}{r} \frac{1+(-1)^{x+(M-2r)t/M}}{2^M} \times \\
&\int_{\pi}^{\pi} \frac{dk}{2\pi} \left(\frac{\left(\cos(k) + \sqrt{1+\cos^2(k)}\right)^{n-2j} e^{ik(M-n)}}{(1+\cos^2(k))^{M/2}} \right) e^{-i(\omega_k(M-2r)t/M+kx)} . \qquad \text{(B.12)}
\end{aligned}
$$

All of the time-dependent integrals are of the form

$$
I(\alpha,\tau) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} g(k) e^{i\varphi(k,\alpha_\tau)|\tau|}, \qquad \text{(B.13)}
$$

i.e., these are one-parameter families of generalized Fourier integrals, with parameter $\alpha_\tau = x/\tau$. They can therefore be approximated in the limit as $\tau \to \infty$ by the method of stationary phase, as used in [6], and references therein, principally [26] and [27]. When each coin is used the same number of times, it can be seen that the spikes are equally spaced between $-t/\sqrt{2}$ and $t/\sqrt{2}$. It can also be shown that the height of the peaks scales like $1/\sqrt[3]{t}$.

The asymptotic behavior of the time-dependent terms in the above components is as follows. Just as in the one coin case, the integral displays three different types of behavior, depending on α_τ, and we refer readers interested in the details of the analysis to [6]. For the purposes of calculating the moments of the distribution, we can treat the support of the integral as confined to the region $\alpha_\tau \in (-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ to a good approximation, and so we will only do the calculations for α_τ in this range. All the integrals have the same form, and differ only by a linear rescaling.

The values of k corresponding to the two stationary points of $\varphi(\alpha_\tau)$ are $\pm k_{\alpha\tau}$, where k is a function of α_τ, and

$$\cos(k_{\alpha\tau}) = \frac{-\alpha_\tau}{\sqrt{1-\alpha_\tau^2}}. \tag{B.14}$$

We also write

$$\varphi(\alpha_\tau) = (\omega_{k_{\alpha\tau}} + \alpha_\tau k_{\alpha\tau}) \qquad\qquad \omega_{k_{\alpha\tau}} = \arcsin\left(\sqrt{\frac{1-2\alpha_\tau^2}{2(1-\alpha_\tau^2)}}\right), \tag{B.15}$$

and note that

$$|\omega''_{k_{\alpha\tau}}| = (1-\alpha_\tau^2)\sqrt{1-2\alpha_\tau^2} \tag{B.16}$$

$$1 + \frac{\cos(k)}{\sqrt{1+\cos^2(k)}} = 1 - \alpha_\tau \tag{B.17}$$

$$\frac{e^{ik}}{\sqrt{1+\cos^2(k)}} = -\alpha_\tau + i\sqrt{1-2\alpha_\tau^2}. \tag{B.18}$$

Using these, we can now write down our asymptotic approximations for the time-dependent components. Let us consider the two-coin walk as an example. The time-dependent components $\tilde{\psi}(x,t)$ for the two-coin wavefunction are then

$$|\tilde{\psi}_{RR}(x,t)\rangle = \frac{1+(-1)^{(\alpha+1)t}}{\sqrt{2\pi t(1-\alpha^2)\sqrt{1-2\alpha^2}}}(1-\alpha)^2\cos(\varphi(\alpha)t + \pi/4)\ , \tag{B.19}$$

$$|\tilde{\psi}_{LR}\rangle = |\tilde{\psi}_{RL}\rangle = \frac{1+(-1)^{(\alpha+1)t}}{\sqrt{2\pi t(1-\alpha^2)\sqrt{1-2\alpha^2}}}$$

$$\times \Big((\alpha(\alpha-1)\cos(\varphi(\alpha)t+\pi/4) + (\alpha-1)\sqrt{1-2\alpha^2}\sin(\varphi(\alpha)t+\pi/4) \Big) \ , \quad \text{(B.20)}$$

and

$$|\tilde{\psi}_{LL}\rangle = \frac{1+(-1)^{(\alpha+1)t}}{\sqrt{2\pi t(1-\alpha^2)\sqrt{1-2\alpha^2}}}$$

$$\times \Big((3\alpha^2-1)\cos(\varphi(\alpha)t+\pi/4) + 2\alpha\sqrt{1-2\alpha^2}\sin(\varphi(\alpha)t+\pi/4) \Big) \ , \quad \text{(B.21)}$$

where we have dropped the τ subscript on α because there is only one set of asymptotic integrals for this system. These expressions can be used to calculate $p(x,t)$ in the long time limit; we plot this result in figure 3.

More generally, for those components which can be obtained using the method of stationary phase, we can write

$$|\psi_{n,(M-n)}(x,t_1,\ldots,t_M)\rangle = \sum_{\tau} \frac{(1+(-1)^{x+|\tau|})(1-\alpha_\tau)^{(n-2j_\tau)}(1-\alpha_\tau^2)^{(M+j_\tau-n/2)}}{2^{M-1}\sqrt{2\pi|\tau|(1-\alpha_\tau^2)\sqrt{1-2\alpha_\tau^2}}}$$

$$\times \cos(\varphi(\alpha_\tau)|\tau| + (M-n)k_{\alpha_\tau} + \pi/4), \quad \text{(B.22)}$$

where $|\psi_{n,(M-n)}(x,t_1,\ldots,t_M)\rangle$ denotes any of the $\binom{M}{n}$ components of the wavefunction which end up with n coins in the state R and $(M-n)$ coins in the state L.

If M is an even number, the wavefunction will have components $\hat{\psi}(x)$ that are central spikes which perform periodic motion for a cyclic walk as the walk cycles through the coins. If the coins are used in some other order, these spikes are the final positions of part of the wavefunction. In any event, these central spikes make no contribution to the moments of the distribution.

Let us write the total wavefunction $\psi(x,t) = \hat{\psi}(x) + \tilde{\psi}(x,t)$, where $\tilde{\psi}(x,t)$ denotes the rest of the components. For the two-coin case, the central spike components are as follows:

$$|\hat{\psi}_{RR}(x)\rangle = \frac{(-1)^{t_1}+(-1)^{t_2}}{8\pi}\int_{-\pi}^{\pi}\frac{e^{-ikx}}{1+\cos^2(k)}dk \quad \text{(B.23)}$$

$$|\hat{\psi}_{LR}(x)\rangle = \frac{(-1)^{t_1}+(-1)^{t_2}}{8\pi}\int_{-\pi}^{\pi}\frac{e^{-ik(x-1)}\cos(k)}{1+\cos^2(k)}dk \quad +$$

$$\frac{(-1)^{t_1}-(-1)^{t_2}}{8\pi}\int_{-\pi}^{\pi}\frac{e^{-ik(x-1)}}{\sqrt{1+\cos^2(k)}}dk \quad \text{(B.24)}$$

$$|\hat{\psi}_{LL}(x)\rangle = \frac{(-1)^{t_1} + (-1)^{t_2}}{8\pi} \int_{-\pi}^{\pi} \frac{e^{-ik(x-2)}}{1+\cos^2(k)} dk. \tag{B.25}$$

These integrals shrink to zero very rapidly away from $x = 0$, but they are still visibly non-zero out as far as $x = \pm 6$ or so.

These time-independent stationary spike integrals are similar in form to the time-dependent ones, but this time the method of stationary phase isn't helpful. That asymptotic approximation method can only tell us about their behavior as $x \to \infty$. Since we already know that they're independent of time, we can say that these represent something that stays in the vicinity of the origin and doesn't go anywhere: so we already know they'll tend to zero very rapidly for large x. This means that we're only interested in their behavior for a few points in the vicinity of the origin. Since the kernel of the integrand oscillates fairly slowly for small values of x, it is practical to evaluate these terms numerically.

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