The quantum to classical transition for random walks

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We look at two possible routes to classical behavior for the discrete quantum random walk on the line: decoherence in the quantum "coin" which drives the walk, or the use of higher-dimensional coins to dilute the effects of interference. We use the position variance as an indicator of classical behavior, and find analytical expressions for this in the long-time limit; we see that the multicoin walk retains the "quantum" quadratic growth of the variance except in the limit of a new coin for every step, while the walk with decoherence exhibits "classical" linear growth of the variance even for weak decoherence.

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INTRODUCTION

Considerable work has been done recently on quantum random walks, which are unitary (and hence reversible) systems designed as analogues to the usual classical case. Two approaches have been taken to the problem: *continuous* [1] and *discrete* [2, 3, 4, 5] walks. This paper is exclusively concerned with the discrete walk on the infinite line. In this case, we introduce an extra "coin" degree of freedom into the system. As in the classical random walk, the outcome of a "coin flip" determines the direction that the particle moves. In the quantum case, however, both the flip of the coin and the conditional motion of the particle are unitary transformations. Different possible classical paths can therefore interfere.

For the classical walk, $p(x,t)$ has the form of a binomial distribution, with a variance $\bar{x^2} - \bar{x}^2$ which grows linearly with time. The variance in the quantum walk, by contrast, grows *quadratically* with time [3]; and the distribution $p(x,t)$ has a complicated, oscillatory form [4]. Both of these are effects of interference between the possible paths of the particle. There are two obvious ways to regain the classical behavior. 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.

Alternatively, rather than measuring the 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.

These two approaches, which are equivalent in the classical limit, 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 a coin which is subject to *decoherence*.

In this paper we contrast these two approaches, using the functional dependence of the variance on time as an indicator of "classical" vs. "quantum" behavior. In the presence even of very weak decoherence, the variance of the quantum walk grows linearly with t at long times; while even using a large number of coins, the the variance of the unitary walk grows quadratically.

Let us consider a fairly general quantum walk on the line. The particle degree of freedom has a basis of position eigenstates $\{|x\rangle\}$, $\hat{x}|x\rangle = x|x\rangle$, where x can be any integer. We will assume that the particle begins the walk at the origin, in state $|0\rangle$. The walk is driven by a separate "coin" degree of freedom: a D-dimensional system with an initial state $|\Phi_0\rangle$. Let $\hat{\mathcal{P}}_{\rm R}, \hat{\mathcal{P}}_{\rm L}$ be two orthogonal projectors on the Hilbert space of the "coin," such that $\hat{\mathcal{P}}_{\rm R} + \hat{\mathcal{P}}_{\rm L} = \hat{I}$. These represent the two possible outcomes of the coin flip, Right or Left. We assume that the coin is unbiased, meaning ${\rm Tr}\hat{\mathcal{P}}_{\rm R} = {\rm Tr}\hat{\mathcal{P}}_{\rm L} = D/2$. We also define a unitary transformation $\hat{U}$ which "flips" the coin. One step of the quantum walk is given by the unitary operator

$$\hat{E} \equiv \left(\hat{S}\otimes\hat{\mathcal{P}}_{\rm R} + \hat{S}^\dagger\otimes\hat{\mathcal{P}}_{\rm L}\right)\left(\hat{I}\otimes\hat{U}\right) , \tag{1}$$

where $\hat{S}, \hat{S}^\dagger$ are shift operators on the particle position, $\hat{S}|x\rangle = |x+1\rangle$, $\hat{S}^\dagger|x\rangle = |x-1\rangle$. The full initial state of the system (particle and coin) is $|\Psi_0\rangle = |0\rangle\otimes|\Phi_0\rangle$.

We can identify the eigenvectors $|k\rangle$ of $\hat{S}, \hat{S}^\dagger$,

$$|x\rangle = \int_{-\pi}^{\pi} \frac{dk}{2\pi} {\rm e}^{-ikx}|k\rangle , \tag{2}$$

with eigenvalues

$$\hat{S}|k\rangle = {\rm e}^{-ik}|k\rangle , \quad \hat{S}^\dagger|k\rangle = {\rm e}^{+ik}|k\rangle . \tag{3}$$

In the k basis, the evolution operator becomes

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

where $\hat{U}_k$ is also a unitary operator.

We now generalize to allow for decoherence. Suppose that before each unitary "flip" of the coin, a *completely positive* and *unital* map is performed on the coin. This map is given by a set of operators $\{\hat{A}_n\}$ on the coin degree of freedom which satisfy

$$\sum_n \hat{A}_n^\dagger \hat{A}_n = \sum_n \hat{A}_n \hat{A}_n^\dagger = \hat{I} . \tag{5}$$

A density operator χ for the coin degree of freedom is transformed

$$\chi \rightarrow \chi' = \sum_n \hat{A}_n \chi \hat{A}_n^\dagger . \tag{6}$$

We combine this with the unitary evolution to define an evolution *superoperator*

$$\mathcal{L}_{kk'}\chi \equiv \sum_n \hat{U}_k \hat{A}_n \chi \hat{A}_n^\dagger \hat{U}_{k'}^\dagger . \tag{7}$$

Note that for the diagonal case $k = k'$, this superoperator is also unital, and hence preserves the identity.

The initial state is

$$\rho_0 = |\Psi_0\rangle\langle\Psi_0| = \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} |k\rangle\langle k'| \otimes |\Phi_0\rangle\langle\Phi_0| . \tag{8}$$

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

$$\rho_t = \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} |k\rangle\langle k'| \otimes \mathcal{L}_{kk'}^t |\Phi_0\rangle\langle\Phi_0| . \tag{9}$$

From this, the probability to reach a point x at time t is

$$\begin{aligned} p(x,t) &= \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} \langle x|k\rangle\langle k'|x\rangle \mathrm{Tr}\left\{\mathcal{L}_{kk'}^t |\Phi_0\rangle\langle\Phi_0|\right\} \\ &= \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} \mathrm{e}^{-ix(k-k')} \mathrm{Tr}\left\{\mathcal{L}_{kk'}^t |\Phi_0\rangle\langle\Phi_0|\right\} \end{aligned} \tag{10}$$

Eq. (10) for $p(x,t)$ will be difficult to evaluate analytically; hence, we restrict our interest to the *moments* of this distribution.

$$\begin{aligned} \langle\hat{x}^m\rangle_t &= \sum_x x^m p(x,t) \\ &= \sum_x x^m \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} \mathrm{e}^{-ix(k-k')} \\ &\quad \times \mathrm{Tr}\left\{\mathcal{L}_{kk'}^t |\Phi_0\rangle\langle\Phi_0|\right\} . \end{aligned} \tag{11}$$

We invert the order of operations and do the x sum first, yielding

$$\begin{aligned} \langle\hat{x}^m\rangle_t &= \frac{(-i)^m}{2\pi} \int dk \int dk' \delta^{(m)}(k-k') \\ &\quad \times \mathrm{Tr}\left\{\mathcal{L}_{kk'}^t |\Phi_0\rangle\langle\Phi_0|\right\} , \end{aligned} \tag{12}$$

where $\delta^{(m)}(k-k')$ is the mth derivative of the delta function. We can then integrate this by parts.

In integrating (12) we will need

$$\begin{aligned} \frac{d}{dk}\mathrm{Tr}\left\{\mathcal{L}_{kk'}\hat{O}\right\} &= -i\mathrm{Tr}\left\{\hat{Z}\mathcal{L}_{kk'}\hat{O}\right\} , \\ &= -i\mathrm{Tr}\left\{(\mathcal{L}_{kk'}\hat{O})\hat{Z}\right\} , \\ &= -\frac{d}{dk'}\mathrm{Tr}\left\{\mathcal{L}_{kk'}\hat{O}\right\} , \\ \hat{Z} &\equiv \hat{\mathcal{P}}_{\mathrm{R}} - \hat{\mathcal{P}}_{\mathrm{L}} . \end{aligned} \tag{13}$$

Making use of (13), when we carry out the integration by parts for the first moment we get

$$\langle\hat{x}\rangle_t = -\int \frac{dk}{2\pi} \sum_{j=1}^t \mathrm{Tr}\left\{\hat{Z}\mathcal{L}_k^j |\Phi_0\rangle\langle\Phi_0|\right\} , \tag{14}$$

where we've introduced the simplified notation $\mathcal{L}_k \equiv \mathcal{L}_{kk}$.

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

$$\begin{aligned} \langle\hat{x}^2\rangle_t &= \int \frac{dk}{2\pi} \left[\sum_{j=1}^t \sum_{j'=1}^j \mathrm{Tr}\left\{\hat{Z}\mathcal{L}_k^{j-j'}(\hat{Z}\mathcal{L}_k^{j'}|\Phi_0\rangle\langle\Phi_0|)\right\} \right. \\ &\quad \left. + \sum_{j=1}^t \sum_{j'=1}^{j-1} \mathrm{Tr}\left\{\hat{Z}\mathcal{L}_k^{j-j'}((\mathcal{L}_k^{j'}|\Phi_0\rangle\langle\Phi_0|)\hat{Z})\right\} \right] \end{aligned} \tag{15}$$

Let us for the moment specialize to the unitary case, so $\mathcal{L}_k\rho = \hat{U}_k \rho \hat{U}_k^\dagger$. In this case, we can expand $|\Phi_0\rangle$ in terms of the eigenvectors of $\hat{U}_k$:

$$|\Phi_0\rangle = \sum_l c_{kl}|\phi_{kl}\rangle , \quad \hat{U}_k|\phi_{kl}\rangle = \mathrm{e}^{i\theta_{kl}}|\phi_{kl}\rangle . \tag{16}$$

Assume, for the moment, that $\hat{U}_k$ is nondegenerate, so the θ_{kl} are all distinct. If we plug these expressions into (14) and (15), we notice that most of the terms will be *oscillatory*; at long times t, they will average to zero. The only terms that survive will be diagonal in l:

$$\begin{aligned} \langle\hat{x}\rangle_t &= -\sum_{j=1}^t \int \frac{dk}{2\pi} \langle\Phi_0|(\hat{U}_k)^j \hat{Z} (\hat{U}_k^\dagger)^j|\Phi_0\rangle \\ &= -t \int \frac{dk}{2\pi} \sum_{l=1}^D |c_{kl}|^2 \langle\phi_{kl}|\hat{Z}|\phi_{kl}\rangle \\ &\quad + \text{oscillatory terms} . \end{aligned} \tag{17}$$

Similarly, for the second moment

$$\begin{aligned} \langle\hat{x}^2\rangle_t &= t^2 \int \frac{dk}{2\pi} \sum_{l=1}^D |c_{kl}|^2 \langle\phi_{kl}|\hat{Z}|\phi_{kl}\rangle^2 \\ &\quad + O(t) + \text{oscillatory terms} . \end{aligned} \tag{18}$$

So in the long-time limit, the variance will always grow *quadratically* in time for a unitary coin of finite dimension. If $\hat{U}_k$ is degenerate, the expressions (17) and (18)

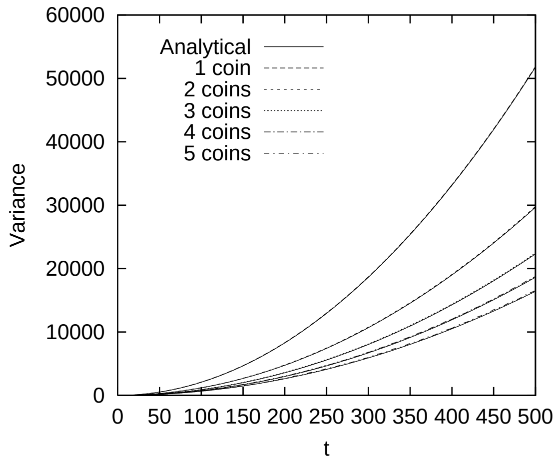

FIG. 1: The variance $\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2$ for the unitary walk with multiple coins, M=1–5. The coins all begin in state $|R\rangle$. The variance grows quadratically in time, in contrast to the linear growth in the classical random walk.

will have to be modified to include appropriate cross-terms; but this will not change the functional dependence on t.

The usual case considered in the literature has taken the coin to be a simple two-level system, and the "flip" operator $\hat{U}$ to be the usual Hadamard transformation $\hat{H}$:

$$\begin{aligned} \hat{H}|R\rangle &= \frac{1}{\sqrt{2}}\left(|R\rangle + |L\rangle\right) , \\ \hat{H}|L\rangle &= \frac{1}{\sqrt{2}}\left(|R\rangle - |L\rangle\right) . \end{aligned} \tag{19}$$

The projectors are $\hat{\mathcal{P}}_{\rm R} = |R\rangle\langle R|$, $\hat{\mathcal{P}}_{\rm L} = |L\rangle\langle L|$. The walk on the line in this case has been exactly solved by Nayak and Vishwanath [4], and agrees with the expression (18) given above. We have also considered the case of a walk driven by M coins, flipped cyclically [6]. In this case, (17) and (18) can be solved analytically; at long times, the variance goes like

$$\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2 = t^2 \left(\frac{3 - \sqrt{8} + 1/M}{\sqrt{32}} \right) + O(t) + \text{osc. terms} . \tag{20}$$

We compare this to the results of numerical simulations in figure 1, finding the agreement to be excellent. Note that the quadratic growth of the variance doesn't vanish even in the limit of large M. Only with a new coin for every step ($M = t$) do we recover the classical behavior. (Note that this doesn't contradict the result (20), since that is only strictly valid for $t \gg M$.)

Let's now allow for decoherence. Because the superoperator $\mathcal{L}_k$ is unital it preserves the identity $\mathcal{L}_k \hat{I} = \hat{I}$; its largest eigenvalue is 1. We explicitly assume that all the other eigenvalues of $\mathcal{L}_k$ obey $|\lambda| < 1$. It is handy then to separate out the traceless part of the initial state

$$\rho_0 = \hat{I}/D + (|\Phi_0\rangle\langle\Phi_0| - \hat{I}/D) \equiv \hat{I}/D + \chi_0 . \tag{21}$$

Plugging this into the equation (14) we get

$$\begin{aligned} \langle \hat{x} \rangle_t &= -\sum_{j=1}^{t} \int \frac{dk}{2\pi} \mathrm{Tr}\left\{ \hat{Z}/D \right\} + \mathrm{Tr}\left\{ \hat{Z}\mathcal{L}_k^j \chi_0 \right\} \\ &= -t\mathrm{Tr}\left\{ \hat{Z}/D \right\} \\ &\quad - \int \frac{dk}{2\pi} \mathrm{Tr}\left\{ \hat{Z}(1-\mathcal{L}_k)^{-1}(\mathcal{L}_k - \mathcal{L}_k^{t+1})\chi_0 \right\} \end{aligned} \tag{22}$$

Note that $(1-\mathcal{L}_k)^{-1}$ acts only on the traceless operator χ_0, so it is well-defined. If the coin is unbiased (as we assumed), then $\mathrm{Tr}\hat{Z} = 0$ and the first term vanishes. At long times the $\mathcal{L}_k^{t+1}$ term will decay away. So in the long time limit, the first moment of the walk with a decoherent coin will tend to a constant.

The second moment is more complicated in detail, but similar in spirit. Again separating out the traceless part χ_0, we get

$$\begin{aligned} \langle \hat{x}^2 \rangle_t &= \int \frac{dk}{2\pi} \sum_{j=1}^{t} \Bigg[\mathrm{Tr}\left\{ \hat{Z}^2 \mathcal{L}_k^j \rho_0 \right\} \\ &\quad + \sum_{j'=j+1}^{t} \Bigg(\mathrm{Tr}\left\{ \hat{Z}\mathcal{L}_k^{j'-j}(2\hat{Z}/D) \right\} \\ &\quad + \mathrm{Tr}\left\{ \hat{Z}\mathcal{L}_k^{j'-j}(\hat{Z}(\mathcal{L}_k^j\chi_0) + (\mathcal{L}_k^j\chi_0)\hat{Z}) \right\} \Bigg) \Bigg] \\ &= \int \frac{dk}{2\pi} \sum_{j=1}^{t} \Bigg[1 + (2/D)\mathrm{Tr}\Big\{ \hat{Z}(1-\mathcal{L}_k)^{-1} \\ &\quad \times (\mathcal{L}_k - \mathcal{L}_k^{t-j+1})\hat{Z} \Big\} \\ &\quad + \mathrm{Tr}\Big\{ \hat{Z}(1-\mathcal{L}_k)^{-1}(\mathcal{L}_k - \mathcal{L}_k^{t-j+1}) \\ &\quad \times (\hat{Z}(\mathcal{L}_k^j\chi_0) + (\mathcal{L}_k^j\chi_0)\hat{Z}) \Big\} \Bigg] . \end{aligned} \tag{23}$$

It is not difficult to see that the last term will tend towards a constant for large t, while the first two will grow linearly. So we get the approximate expression at long times

$$\begin{aligned} \langle \hat{x}^2 \rangle_t &\approx t \left(1 + \frac{1}{\pi D} \int dk \mathrm{Tr}\left\{ \hat{Z}(1-\mathcal{L}_k)^{-1}\mathcal{L}_k\hat{Z} \right\} \right) \\ &\quad + \text{const.} , \end{aligned} \tag{24}$$

which is linear in t.

If we specialize to the case of a single two-level coin undergoing the Hadamard evolution, we can find exact solutions to (24). We first pick a particular form for the

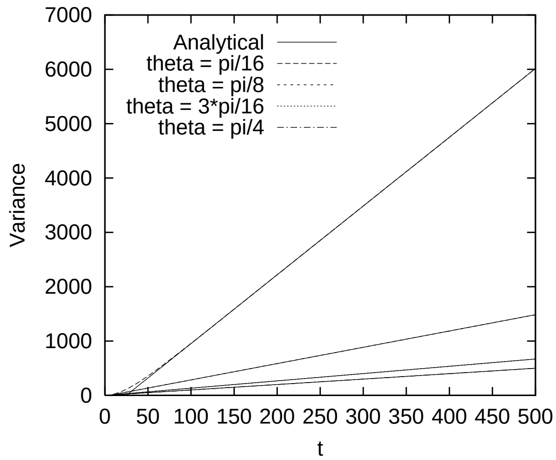

FIG. 2: $\langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2$ vs. t for the quantum random walk with decoherence, for $\theta = \pi/16, \pi/8, 3\pi/16, \pi/4$. For all cases the coin began in the initial state $|R\rangle$. Note that the variance goes asymptotically to a linear growth at long times which matches our analytical estimate; the rate of growth goes to one with increasing decoherence, matching the classical case at $\theta = \pi/4$.

decoherence. The most convenient numerically is *pure dephasing*

$$\hat{A}_{0,1} = \frac{1}{\sqrt{2}} \left(\mathrm{e}^{\pm i\theta} |R\rangle\langle R| + \mathrm{e}^{\mp i\theta} |L\rangle\langle L| \right) \ . \tag{25}$$

For $\theta = 0$ this reverts to the unitary case, while for $\theta = \pi/4$ there is complete decoherence at each step. At long times we have [7]

$$\langle\hat{x}^2\rangle_t - \langle\hat{x}\rangle_t^2 \approx t \left(\cot^2 2\theta + \csc^2 2\theta \right) + \text{const.} \ , \tag{26}$$

which goes to 1 as $\theta \to \pi/4$, and diverges as $\theta \to 0$, when the long-time approximation breaks down. In figure 2, we compare this result to the output of numerical simulations, once more finding excellent agreement. Note that while the variance grows linearly, as in the classical case, it grows *faster* than the classical case. The reflects the persistent effect of interference, which causes the particle to continue to drift in a particular direction.

From the time-dependence of the moments, one might reasonably claim that the multicoin system remains "quantum" even in the limit of very large numbers of coins, while the decoherent system remains "classical" even in the limit of very weak noise. Moreover, from equations (18) and (24) this behavior seems to be generic, independent of the particular model chosen.

We should emphasize that in this paper we have only altered the coin degree of freedom. One might naturally consider modifications of the evolution of the particle as well, such as allowing decoherence of the position as well as the coin. There have been numerical studies of this, and of the transition to classical behavior that results [5].

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