# 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 integers: decoherence in the quantum "coin" which drives the walk, or the use of higher-dimensional (or multiple) 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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Considerable work has been done recently on quantum walks on lattices and graphs, which are unitary systems analogous to classical random walks, but with radically different behavior. Two approaches have been taken to the problem: *continuous-time* [1] and *discrete-time* [2–5] walks. This work is motivated by the hope it may lead to new algorithms for quantum computers, such as the recent demonstration of a problem solvable with a quantum walk exponentially faster than the best classical algorithm [6]. This raises questions: To what extent do the properties of quantum walks persist as we alter these models, allowing for experimental effects such as decoherence? At what point does the system "become classical?" We provide a partial answer in this Letter, while also using random walks as a new arena to study the quantum to classical transition in general.

We consider only the discrete-time walk on the integers. 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, $p(x, t)$ is a binomial distribution with a variance $\overline{x^2} - \bar{x}^2$ that grows linearly with time. The variance of the quantum walk, by contrast, grows *quadratically* with time [3]; and the distribution $p(x, t)$ has a complicated form [4]. Both of these are caused by interference between the possible paths of the particle. If the quantum coin is measured at every step, 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 a unique classical path; averaging over the outcomes would once again produce the classical result.

These two approaches, 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 more generally, use a coin with a higher-dimensional Hilbert space in order to dilute the effects of interference). 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 Letter 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 using even a large number of coins, the variance of the unitary walk grows quadratically.

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

$$\hat{E} \equiv (\hat{S} \otimes \hat{\mathcal{P}}_R + \hat{S}^\dagger \otimes \hat{\mathcal{P}}_L)(\hat{I} \otimes \hat{U}), \quad (1)$$

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 $\hat{S}, \hat{S}^\dagger$,

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

with eigenvalues

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

In the $k$ basis, the evolution operator becomes

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

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 $\chi$ for the coin degree of freedom is transformed as follows:

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

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

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

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

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

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

$$\langle \hat{x}^m\rangle_t = \frac{(-i)^m}{2\pi}\int dk \int dk' \delta^{(m)}(k-k'){\rm Tr}\{\mathcal{L}_{kk'}^t |\Phi_0\rangle\langle\Phi_0|\}, \tag{12}$$

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

In integrating (12) we need

$$\begin{aligned}\frac{d}{dk}{\rm Tr}\{\mathcal{L}_{kk'}\hat{O}\} &= -i{\rm Tr}\{\hat{Z}\mathcal{L}_{kk'}\hat{O}\}, \\ &= -i{\rm Tr}\{(\mathcal{L}_{kk'}\hat{O})\hat{Z}\}, \\ &= -\frac{d}{dk'}{\rm Tr}\{\mathcal{L}_{kk'}\hat{O}\},\end{aligned} \tag{13}$$

where $\hat{Z} \equiv \hat{\mathcal{P}}_{\rm R} - \hat{\mathcal{P}}_{\rm L}$. Making use of (13), when we carry out the integration by parts for the first moment we get

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

where we have 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:

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

Let us for the moment specialize on 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 $\hat{U}_k$:

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

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

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

Similarly, for the second moment

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

So in the long-time limit, the variance always grows *quadratically* in time for a unitary coin of finite dimension. If $\hat{U}_k$ is degenerate, Eqs. (17) and (18) have to be modified to include appropriate cross terms, but this does 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 $\hat{H}$:

$$\hat{H}|R\rangle = \frac{1}{\sqrt{2}}(|R\rangle + |L\rangle), \qquad \hat{H}|L\rangle = \frac{1}{\sqrt{2}}(|R\rangle - |L\rangle). \quad (19)$$

The projectors are $\hat{\mathcal{P}}_R = |R\rangle\langle R|$, $\hat{\mathcal{P}}_L = |L\rangle\langle L|$. 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 [7]; this is a particular case of a higher-dimensional coin with $D = 2^M$. In this case, (17) and (18) can be solved analytically; at long times, the variance goes as

$$\langle\Delta\hat{x}^2\rangle_t = t^2\frac{3-\sqrt{8}+1/M}{\sqrt{32}} + O(t) + \text{oscillatory terms.} \quad (20)$$

We compare this to the results of numerical simulations in Fig. 1, finding the agreement to be excellent. The variance grows quadratically in time, in contrast to the linear growth in the classical random walk. Note that the quadratic growth of the variance does not vanish even in the limit of large $M$. Only with a new coin for every step

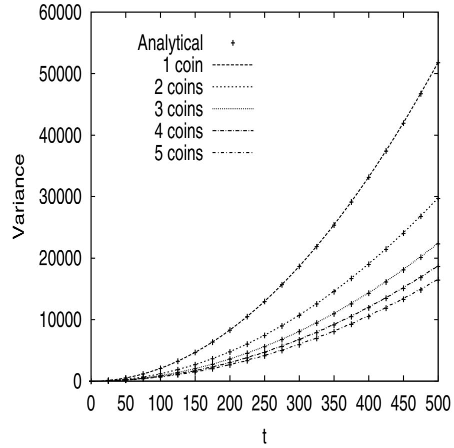


FIG. 1. The variance $\langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2$ for the unitary walk with multiple coins, $M = 1$–5. The coins all begin in state $|R\rangle$.

($M = t$) do we recover the classical behavior. (Note that this does not contradict the result (20), since that is only strictly valid for $t \gg M$.)

Let us 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 $|\lambda| < 1$ for all other eigenvalues of $\mathcal{L}_k$. It is handy then to separate out the traceless part $\chi_0$ of the coin's initial state

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

Inserting this into Eq. (14) we get

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

Note that $(1-\mathcal{L}_k)^{-1}$ acts only on the traceless operator $\chi_0$, 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 decays away. So in the long-time limit, the first moment of the walk with a decoherent coin tends to a constant.

The second moment is more complicated in detail, but similar in spirit. Again separating out $\chi_0$, we get

$$\langle\hat{x}^2\rangle_t = \int\frac{dk}{2\pi}\sum_{j=1}^{t}\Big[\mathrm{Tr}\{\hat{Z}^2\mathcal{L}_k^j(\hat{I}/D+\chi_0)\} + \sum_{j'=j+1}^{t}(\mathrm{Tr}\{\hat{Z}\mathcal{L}_k^{j'-j}(2\hat{Z}/D)\} + \mathrm{Tr}\{\hat{Z}\mathcal{L}_k^{j'-j}[\hat{Z}(\mathcal{L}_k^j\chi_0) + (\mathcal{L}_k^j\chi_0)\hat{Z}]\})\Big] \quad (23)$$

$$= \int\frac{dk}{2\pi}\sum_{j=1}^{t}[1 + (2/D)\mathrm{Tr}\{\hat{Z}(1-\mathcal{L}_k)^{-1}(\mathcal{L}_k - \mathcal{L}_k^{t-j+1})\hat{Z}\} + \mathrm{Tr}\{\hat{Z}(1-\mathcal{L}_k)^{-1}(\mathcal{L}_k - \mathcal{L}_k^{t-j+1})(\hat{Z}(\mathcal{L}_k^j\chi_0) + (\mathcal{L}_k^j\chi_0)\hat{Z})\}]. \quad (24)$$

The last term tends towards a constant for large $t$, while the first two grow linearly. So we get the approximate expression at long times,

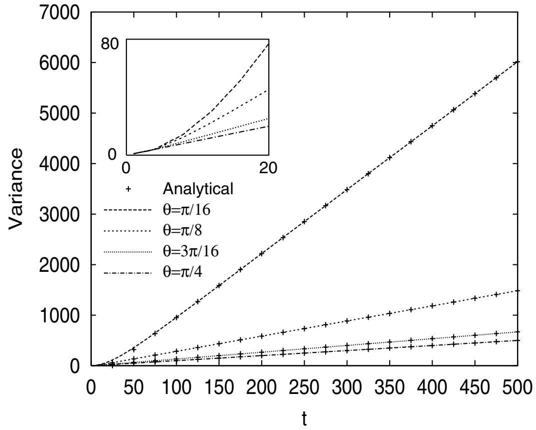


FIG. 2. $\langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2$ vs $t$ for the quantum random walk with decoherence, for $\theta = \pi/16, \pi/8, 3\pi/16, \pi/4$, coin initially in state $|R\rangle$. The inset shows the short-time quadratic behavior.

$$\langle\hat{x}^2\rangle_t \approx t\left(1 + \frac{1}{\pi D}\int dk \mathrm{Tr}\{\hat{Z}(1 - \mathcal{L}_k)^{-1}\mathcal{L}_k\hat{Z}\}\right) + \text{const}, \tag{25}$$

which is linear in $t$.

If we specialize on the case of a single two-level coin undergoing the Hadamard evolution, we can find exact solutions to (25). We first pick a model for the decoherence. The most convenient is *pure dephasing,*

$$\hat{A}_{0,1} = \frac{1}{\sqrt{2}}(e^{\pm i\theta}|R\rangle\langle R| + e^{\mp i\theta}|L\rangle\langle L|). \tag{26}$$

We then vary the parameter $\theta$. 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 [8]

$$\langle\Delta\hat{x}^2\rangle_t \approx t(\cot^2 2\theta + \csc^2 2\theta) + \text{const}. \tag{27}$$

The quantity multiplying $t$ goes to 1 as $\theta \rightarrow \pi/4$ and diverges as $\theta \rightarrow 0$, when the long-time approximation breaks down. In Fig. 2, we compare this result to the output of numerical simulations, once more finding excellent agreement. 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 $\theta = \pi/4$. Note also that while the variance grows linearly, as in the classical case, it grows *faster* than the classical case. This reflects the persistent effect of interference, which causes the particle to continue to drift in a particular direction based on the initial state of the coin. (In the unitary Hadamard walk, this drift is present except for the symmetric initial states $|R\rangle \pm i|L\rangle$.)

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. In fact, it can be shown [7] that even if each coin is flipped only twice, the variance still grows quadratically with time (letting both $t$ and $M$ increase). The decoherent system, by contrast, eventually becomes classical even in the limit of very weak noise. Moreover, from Eqs. (18) and (25) this behavior is generic for any high-dimensional unitary coin or model of decoherence.

We should emphasize that in this Letter we have altered only 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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