Quantum and random walks as universal generators of probability distributions

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Quantum walks and random walks bear similarities and divergences. One of the most remarkable disparities affects the probability of finding the particle at a given location: typically, almost a flat function in the first case and a bell-shaped one in the second case. Here I show how one can impose in practice any desired probabilistic behavior on both systems by the appropriate choice of time- and site-dependent coins. This implies, in particular, that one can devise quantum walks that show diffusive spreading without loosing coherence, as well as random walks that exhibit the characteristic fast propagation of a quantum particle driven by a Hadamard coin.

Quantum walks and random walks have a long list of affinities and disparities. One can find the (now mostly deprecated) mixed expression “quantum random walks” in the first references exploring these new processes [3–6], because they were developed as the quantum variants of the discrete random walk in one dimension: the Markov process in which, at every time step, a particle moves (either leftward or rightward) to one of the two neighboring sites as a result of the random outcome of a coin toss. The quantum particle however, like in the renowned case of the double-slit experiment, moves to both directions simultaneously, and this propagation takes place in a deterministic way: the wave function describing the system evolves unambiguously according to the value of some inner binary property —as, e.g., the spin or the chirality— whose state is locally updated by the action a unitary operator, known as the coin operator. Therefore, in this case, the location of the particle at a given instant of time is a probabilistic magnitude due to the intrinsic uncertainty inherent in every quantum phenomenon.

One of the first coin operators considered in the quantum-walk literature is the Hadamard coin $|\rangle$, a real-valued unitary operator that performs a Hadamard transformation on the chirality of the particle. Since all the probabilities associated with this transformation are identical, the Hadamard walk can be considered as the quantum counterpart of a random walk with a fair coin. In both cases, the occupation probabilities of the more distant (although accessible) locations are exponentially small. But, while the central part of the distribution of the unbiased random walk quickly converges to a Gaussian, the location of a particle doing a Hadamard walk after $t$ steps is almost uniformly distributed in the range $[-t/\sqrt{2}, t/\sqrt{2}]$, centered around the initial position of the particle, and therefore the quantum walker connects this point with any site within this interval after a lapse of time that is thus proportional to their relative distance. To perform the same operation, the unbiased random walker needs an amount of time that grows quadratically with the separation between the sites.

These two diverging statistical traits are sometimes seen as paradigms of the two processes. The truth, however, is that these properties depend strongly on how the coin (operator) is chosen, and correspond to the homogeneous, time-independent (Markovian) case. Researchers have relaxed these conditions in the past and detected the emergence of new features in the system as, e.g., Anderson localization. Thus, among the publications on quantum walks, one can find examples of processes whose evolution is driven by site-dependent coins [8–12], time-dependent coins [13–17], history-dependent coins [18, 19], and even random coins, unitary operators which are randomly chosen [20–24]. The lack of homogeneity is also a recurrent topic in the random-walk literature [25–28].

My goal in this letter is, in a sense, just the opposite: starting from a given probability function, I want to deduce what is the proper coin selection to retrieve this distribution. With this aim, I consider here the discrete-time evolution of a particle moving on the integers as a result of the interaction with a set of site- and time-dependent (either quantum or random) coins. In a previous work [29], I examined a particular instance of this problem, the design of a quantum walk that shown a binomial probability function, the distribution of a random walk with a fair coin. Here, I am going to generalize these results in both directions: I will find quantum walks with classical distributions, as well as random walks with quantum-like properties, provided that the comparison is limited to their common probabilistic aspects.

Let us begin with the fundamentals of the quantum-mechanical side of the problem. As I announced previously, along this letter we will identify particle positions through integer numbers, so let us call $\mathcal{H}^p$ the associated Hilbert space, with the usual span $\{|n\rangle : n \in \mathbb{Z}\}$. $\mathcal{H}^c$ will represent the Hilbert space of coin states and its orthogonal basis. The mathematical representation of the state of our discrete-time, discrete-space quantum walk resides in the tensor-product space $\mathcal{H} \equiv \mathcal{H}^c \otimes \mathcal{H}^p$ and changes as a result of the action of the evolution operator $\hat{T}_t$ on it: $\hat{T}_t \equiv \hat{S}\hat{U}_t$, where the coin $\hat{U}_t$ is a time- and site-dependent, real-valued unitary operator of the
The free parameters that determine the features of the particular position \( n \) long as the null sets are kept unchanged. So, let us in-operators and wave functions are not discarded, however.

Approaches to this same issue based on complex-valued real-valued magnitudes is to clearly ensure that quan-

The reason behind considering the origin, \( \psi(0, t) = 0 \) if \( n \neq 0 \), implying this that \( \psi_{\pm}(n, 0) = 0 \) for \( |n| > 0 \), in general. We also assume that the wave function is real. The reason behind considering real-valued magnitudes is to clearly ensure that quantum walks and random walks to be introduced here share the same number of degrees of freedom. The viability of approaches to this same issue based on complex-valued operators and wave functions are not discarded, however.

My first aim is to show how a quantum experiment can be designed with custom probabilistic properties—as long as the null sets are kept unchanged. So, let us introduce \( \rho(n, t) \), the likelihood of finding the particle in a particular position \( n \) at a given time \( t \), the probability function. In the case of a quantum walker, this probability is recovered through the wave-function components:

\[
\rho(n, t) \equiv \psi_+^2(n, t) + \psi_-^2(n, t).
\]

The free parameters that determine the features of the coin operators are in this case the angular variables \( \theta_{n,t} \).

Therefore, one has as many unknown quantities as independent equations, \( 8 \) so, it is not surprising that our objective can be readily attained. To this end, let us begin by focusing our attention on the conditions that the wave-function components must satisfy for ensuring the self-consistency of the problem. From Eqs. (4) and (5) one gets

\[
\psi_+^2(n + 1, t + 1) + \psi_-^2(n - 1, t + 1) = \rho(n, t),
\]

but, at the same time, cf. Eq. (8),

\[
\psi_+^2(n + 1, t + 1) + \psi_-^2(n + 1, t + 1) = \rho(n + 1, t + 1).
\]

In particular, for \( n = t, t \geq 1 \), one has \( \psi_-(t, t) = 0 \), see Eq. (8), and therefore

\[
\psi_+(t + 1, t + 1) = \rho(t + 1, t + 1).
\]

This means that

\[
\psi_-(t - 1, t + 1) = \rho(t, t) - \rho(t + 1, t + 1).
\]

One can use this result to compute \( \psi_+(t - 1, t + 1) \) through Eq. (8), and continue with this reasoning until obtaining the general rule, valid for \( t \geq 1 \),

\[
\psi_+^2(n, t) = \sum_{m=n}^{t} \rho(m, t) - \sum_{m=n+1}^{t-1} \rho(m, t - 1),
\]

\[
\psi_-^2(n, t) = \sum_{m=n+1}^{t-1} \rho(m, t - 1) - \sum_{m=n+2}^{t} \rho(m, t).
\]

On can check how constraints (8) and (9) are satisfied, as well as the boundary conditions: \( \psi_+(t, t) = 0 \), and \( \psi_2(-t, t) = \rho(-t, t) \). Alternatively, one can show the soundness of the solution by induction. Now we can use either Eq. (9) or Eq. (10) to finally find

\[
\cos \theta_{n,t} = \frac{\psi_+(n, t)\psi_+(n + 1, t + 1) - \psi_-(n, t)\psi_-(n - 1, t + 1)}{\rho(n, t)},
\]

\[
\sin \theta_{n,t} = \frac{\psi_+(n, t)\psi_-(n + 1, t + 1) + \psi_-(n, t)\psi_+(n - 1, t + 1)}{\rho(n, t)}.
\]

1 After a raw inspection, it could be concluded that in this problem the number of unknown quantities exceeds the number of constraints and that the system of equations is underdetermined: after all, different choices for \( \psi_+(n, t) \) and \( \psi_-(n, t) \) may be (in principle) congruent with the same value of \( \rho(n, t) \). This is not true here, with only one marginal exception: \( \psi_+(0, 0) \) and \( \psi_-(0, 0) \) are arbitrary, provided that \( \rho(0, 0) = 1 \). The adequate choice for \( \theta_{0,0} \) is recovered from Eqs. (14) and (15) below.
Equation (15) reflects the law of probability conservation. Rearranging this expression, one can see how the same statement can be also expressed as follows

\[
\rho(n,t) = \frac{1}{2} [\rho(n-1,t-1) + J(n-1,t-1) + \rho(n+1,t-1) - J(n+1,t-1)],
\]

(16)

where \(J(n,t)\) is the net flux of probability leaving site \(n\)

\[
J(n,t) \equiv \psi_+^2(n+1,t+1) - \psi_-^2(n-1,t+1) = \cos 2\theta_{n,t} [\psi_+^2(n,t) - \psi_-^2(n,t)] + 2\sin 2\theta_{n,t} \psi_+(n,t) \psi_-(n,t),
\]

(17)

a vectorial quantity: it is positive if there is a net flux of probability to larger values of \(n\), and negative otherwise. This magnitude is very useful in subsequent derivations, as we will see below.

The inhomogeneous, time-dependent random walk, \(X_t\), is a non-Markovian process whose one-step evolution can be expressed as follows: If at time \(t\) the walker is at a given location, \(X_t = n\), then at time \(t+1\) one has

\[
X_{t+1} = \begin{cases} 
   n + 1, & \text{with probability } p_{n,t}, \\
   n - 1, & \text{with probability } (1 - p_{n,t}).
\end{cases}
\]

(18)

The corresponding recursive equation for the probability function reads:

\[
\rho(n,t) = \cos^2 \theta_{n-1,t-1} \rho(n-1,t-1) + \sin^2 \theta_{n+1,t-1} \rho(n+1,t-1),
\]

(19)

where we have expressed \(p_{n,t}\) as \(p_{n,t} = \cos^2 \theta_{n,t}\) for comparison purposes. From Eq. (19) one can easily conclude the validity of expression (16) also in this case, since now

\[
J(n,t) \equiv (2p_{n,t} - 1) \rho(n,t) = \cos 2\theta_{n,t} \rho(n,t).
\]

(20)

The general solution of the classical problem for arbitrary \(\rho(n,t)\) can be attained, in this case, with the help of the \(z\) transform,

\[
\hat{\rho}(z,t) \equiv \mathcal{Z} [\rho(n,t), n, z] = \sum_{n=-\infty}^{\infty} \rho(n,t) z^{-n},
\]

\[
\hat{J}(z,t) \equiv \mathcal{Z} [J(n,t), n, z] = \sum_{n=-\infty}^{\infty} J(n,t) z^{-n}.
\]

Equation (16) leads to

\[
\hat{J}(z,t) = \frac{2z\hat{\rho}(z,t+1) - (1+z^2)\hat{\rho}(z,t)}{1-z^2},
\]

(21)

and therefore

\[
\cos 2\theta_{n,t} = \frac{1}{\rho(n,t)} \mathcal{Z}^{-1} [\hat{J}(z,t), n, z].
\]

(22)

I will illustrate these ideas through a simple but paradigmatic example where closed expressions can be found. Consider, for instance, the uniform distribution:

\[
\rho(n,t) = \frac{1}{t+1},
\]

(23)

for \(n \in \{-t, -t+2, \cdots, t-2, t\}\). Equations (12) and (13) lead to

\[
\psi_+(n,t) = \sqrt{\frac{t+n}{2(t+1)}},
\]

(24)

\[
\psi_-(n,t) = \sqrt{\frac{t-n}{2(t+1)}},
\]

(25)

and correspondingly

\[
\cos \theta_{n,t} = \frac{1}{2} \begin{pmatrix} (t+n)(t+n+2) & t(t+2) \\ -t(t+n+2) & t(t+2) \end{pmatrix},
\]

(26)

\[
\sin \theta_{n,t} = \frac{1}{2} \begin{pmatrix} (t-n)(t+n+2) & t(t+2) \\ t(t+n+2) & t(t+2) \end{pmatrix},
\]

(27)

We can use the results above to assess the value of \(J(n,t)\),

\[
J(n,t) = \frac{n}{(t+1)(t+2)}.
\]

(28)

Provided with this information, we can solve the classical problem without passing through Eq. (21) in this case: I recall that \(J(n,t)\) is the same in both flavors of the walk, so we can substitute (23) and (28) in Eq. (22) to find

\[
\cos 2\theta_{n,t} = \frac{J(n,t)}{\rho(n,t)} = \frac{n}{t+2},
\]

(29)

3 The explicit functional forms of \(\hat{\rho}(z,t)\) and \(\hat{J}(z,t)\) for this case are:

\[
\hat{\rho}(z,t) = \frac{z^{-t}}{t+1} - \frac{z^{2(t+1)}}{1-z^2},
\]

\[
\hat{J}(z,t) = \frac{z^{-t}}{(t+1)(t+2)} \left[(1+z^2)(1+z^{2(t+1)}) - 2z^2(1-z^{2t})\right].
\]

The surprisingly disparity in the complexity of these formulas when compared to Eqs. (23) and (28) is in great measure due to the fact that the last expressions only apply for alternating sites, i.e., \(n \in \{-t, -t+2, \cdots, t-2, t\}\), being zero otherwise.
and, on the one side, see Eq. (17), means that, on the other side, see Eq. (20),

\[ \rho(n, t) = \frac{t!}{(\frac{t}{2})!(\frac{t}{2})!} p^{\frac{t}{2}} (1 - p)^{\frac{t}{2}}, \tag{31} \]

for \( n \in \{ -t, -t + 2, \ldots, t - 2, t \} \). There it was shown that the solution for this problem reads

\[
\psi_+(n, t) = \sqrt{p} \rho(n - 1, t - 1), \tag{32}
\]

\[
\psi_-(n, t) = \sqrt{1 - p} \rho(n + 1, t - 1), \tag{33}
\]

two expressions whose suitability can be checked by direct insertion in Eqs. (3) and (4). Alternatively, it is very elucidative the computation of \( J(n, t) \), since in this case

\[ J(n, t) = (2p - 1)\rho(n, t), \tag{34} \]

what corresponds to the flux of probability of a random walk with a constant jump likelihood, cf. Eq. (24).

Here, I will examine the opposite situation: how a time- and site-dependent random walk can mimic the characteristic properties of a standard quantum walk. In particular, we are going to focus our attention on the celebrated Hadamard walk, for which \( \theta_{n,t} = \pi/4 \). This means that, on the one side, see Eq. (17),

\[ J(n, t) = 2\psi_+(n, t)\psi_-(n, t), \tag{35} \]

and, on the other side, see Eq. (20),

\[ p_{n,t} = \frac{\rho(n, t) + J(n, t)}{2\rho(n, t)}, \tag{36} \]

that is

\[ p_{n,t} = \frac{[\psi_+(n, t) + \psi_-(n, t)]^2}{2\rho(n, t)}. \tag{37} \]

Closed expressions for the wave-function components of plain quantum walks (including Hadamard walks) are unwieldy but available [24]. In Fig. 1 we can observe the almost perfect correspondence between the probability function of the random walk with inhomogeneous probabilities, and the one of the Hadamard walk with initial state:

\[ |\psi\rangle_0 = \left( \frac{\sqrt{2} - \sqrt{2}}{2} |+\rangle + \frac{\sqrt{2} + \sqrt{2}}{2} |\rangle \right) \otimes |0\rangle. \tag{38} \]

This apparently capricious choice was made to get a quasi-symmetrical \( \rho(n, t) \). Full symmetry in Hadamard walks necessarily involves the use of complex coefficients for describing the initial coin state.

In this letter, I have shown how a time- and site-dependent coin is an extremely useful and versatile tool for the design of both quantum and random walks on the line. Such approach entails enough generality to give rise to any desired probabilistic fingerprint either through quantum or classical randomness: I have deduced the rules that must be employed for unambiguously assessing the values of the parameters that fully determine the evolution of the two kind of systems.

This means, in particular, that the extra degree of freedom of the quantum walker associated with its chirality does not introduce further arbitrariness into the problem. This fact is not the consequence of the restriction that I have considered along the text by demanding that the Hilbert space of the quantum particle is defined on the reals rather than on the complex plane: Since a quantum walk with a time- and site-dependent coin operator taking values on the reals can mimic any desired probability function, it is also capable of reproducing the probabilistic behavior of general, complex-valued quantum walks.

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[1] S. E. Venegas-Andraca, Quantum walks: a comprehensive review, Quantum Inf. Process. 11, 1015 (2012).
[2] G. H. Weiss, Aspects and Applications of the Random Walk (North Holland, New York, 1994).
[3] Y. Aharonov, L. Davidovich, and N. Zagury, Quantum random walks, Phys. Rev. A 48, 1687 (1993).
[4] B. C. Travaglione and G. J. Milburn, Implementing the quantum random walk, Phys. Rev. A 65, 032310 (2002).
[5] N. Konno, Quantum random walks in one dimension, Quantum Inf. Process. 1, 345 (2003).
[6] J. Kempe, Quantum random walks: An introductory overview, Contemp. Phys. 44, 307 (2003).
[7] A. Ambainis, E. Bach, A. Nayak, A. Vishwanath, and J. Watrous in *One Dimensional Quantum Walks*, Proceedings of the thirty-third annual ACM symposium on Theory of Computing (ACM New York, New York, 2001), p. 37.
[8] D. Bulger, J. Freckleton, and J. Twamley, Position-dependent and cooperative quantum Parrondo walks, New J. Phys. 10, 093014 (2008).
[9] Y. Shikano and H. Katsura, Localization and fractality in inhomogeneous quantum walks with self-duality, Phys. Rev. E 82, 031122 (2010).
[10] N. Konno, T. Luczak, and E. Segawa, Limit measures of inhomogeneous discrete-time quantum walks in one dimension, Quantum Inf. Process. 12, 33 (2013).
[11] R. Zhang, P. Xue, and J. Twamley, One-dimensional quantum walks with single-point phase defects, Phys. Rev. A 89, 042317 (2014).
[12] P. Xue, H. Qin, B. Tang, and B. C. Sanders, Observation of quasiperiodic dynamics in a one-dimensional quantum walk of single photons in space, New J. Phys. 16, 053009 (2014).
[13] P. Ribeiro, P. Milman, and R. Mosseri, Aperiodic Quantum Random Walks, Phys. Rev. Lett. 93, 190503 (2004).
[14] M. C. Bañuls, C. Navarrete, A. Pérez, E. Roldán, and J. C. Soriano, Quantum walk with a time-dependent coin, Phys. Rev. A 73, 062304 (2006).
[15] A. Romanelli, The Fibonacci quantum walk and its classical trace map, Physica A 388, 3985 (2009).
[16] A. Romanelli, Driving quantum-walk spreading with the coin operator, Phys. Rev. A 80, 042332 (2009).
[17] M. Montero, Invariance in quantum walks with time-dependent coin operators, Phys. Rev. A 90, 062312 (2014).
[18] A. P. Flitney, D. Abbott, and N. F. Johnson, Quantum walks with history dependence, J. Phys. A 37, 7581 (2004).
[19] Y. Shikano, T. Wada, and J. Horikawa, Discrete-time quantum walk with feed-forward quantum coin, Sci. Rep. 4, 4427 (2014).
[20] A. Joye and M. Merkli, Dynamical Localization of Quantum Walks in Random Environments, J. Stat. Phys. 140, 1025 (2010).
[21] A. Joye, Random Time-Dependent Quantum Walks, Commun. Math. Phys. 307, 65 (2011).
[22] A. Ahlbrecht, H. Vogts, A. H. Werner, and R. F. Werner, Asymptotic evolution of quantum walks with random coin, J. Math. Phys. 52, 042201 (2011).
[23] A. Ahlbrecht, C. Cedzich, V. B. Scholz, A. H. Werner, and R. F. Werner, Asymptotic behavior of quantum walks with spatio-temporal coin fluctuations, Quantum Inf. Process. 11, 1219 (2012).
[24] A. Joye, Dynamical localization for d-dimensional random quantum walks, Quantum Inf. Process. 11, 1251 (2012).
[25] R. Metzler, Non-homogeneous random walks, generalised master equations, fractional Fokker-Planck equations, and the generalised Kramers-Moyal expansion, Eur. Phys. J. B 19, 249 (2001).
[26] O. Flomenbom and R. J. Silbey, Path-probability density functions for semi-Markovian random walks, Phys. Rev. E 76, 041101 (2007).
[27] P. Lafitte-Godillon, K. Raschel, and V. C. Tran, Extinction probabilities for a distylous plant population modeled by an inhomogeneous random walk on the positive quadrant, SIAM J. Appl. Math. 73, 700 (2013).
[28] M. Menshikov, S. Popov, and A. Wade, *Non-homogeneous Random Walks: Lyapunov Function Methods for Near-Critical Stochastic Systems* (Cambridge University Press, New York, 2017).
[29] M. Montero, Classical-like behavior in quantum walks with inhomogeneous, time-dependent coin operators, Phys. Rev. A 93, 062316 (2016).
[30] M. Montero, Quantum walk with a general coin: exact solution and asymptotic properties, Quantum Inf. Process. 14, 839 (2015).