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The ‘t/2 law’ for quantum random walks on the line starting in the classical state

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Abstract

Based on the theory of unitary matrices, our treatment of the theory of quantum random walks simplifies and clarifies certain prior derivations based on Fourier transform methods. Given a quantum random walk on the line determined by a 2×2 unitary matrix U, we show how the first two moments of the position probability distribution are determined by the eigenvalues of U. By varying the ‘coin operator’ A, we show that the leading term of the standard deviation of the position probability distribution is ct, where t denotes time and $0 \leqslant c \leqslant 1$. However, it turns out that the maximum value of c, namely $c = 1$, is achievable when and only when the coin operator A is diagonal, and the initial state is unbiased. Starting in the classical state $|0\rangle \otimes |1\rangle$, our approach confirms that the maximum value of the leading term of the standard deviation of the position probability distribution is $\frac{t}{2}$, which, by way of known examples, is verified to be achievable.

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1. Introduction

Some important algorithms in classical computation theory are based on the theory of classical random walks. Analogously, quantum random walks (henceforth abbreviated as QRW) on discrete lattices are of interest relative to the emerging field of quantum computation. The aim is to develop quantum analogues to the classical (non-quantum) theory. Recently, quantum random walks on the line have been investigated by a number of researchers in connection with the theory of quantum computing. We refer to Kempe [4] for an excellent overview.

A fundamental difference in behavior between classical and quantum random walks on the line is evidenced by the longrun-dependence on time t of the standard deviation $\sigma(X_t) = \sqrt{E\left(X_t^2\right) - [E(X_t)]^2}$ of the position probability distribution. Unlike classical random walks whose position probability distribution is essentially Gaussian, and therefore spread with velocity $\sqrt{t}$, the analogous distribution for a QRW can spread quadratically faster [1–3, 5–7].

In their analysis of quantum processes, the authors of [1, 2] employ the Schrödinger approach to obtain a description of the wave function in terms of Fourier-type integrals. They specify the leading terms of the first two moments of the position probability distribution in the longrun time limit for Hadamard walks, but stop short of presenting a clear derivation for the standard deviation of a general QRW on the line. In [3, 5] the authors present a closed expression, based on combinatorial arguments, for the rth moment of the position probability distribution, but the dependence on t of the standard deviation is not explicitly addressed. In [6], by way of Fourier transform methods, the authors obtain a closed formula for the rth moment of a QRW.

In this paper, we invoke some elementary analytic properties of 2×2 unitary matrices to derive improved versions of the closed formulae given in [6] for the first two moments of the position probability distribution. For a QRW, we demonstrate that the maximum value of the leading term of $\sigma(X_t)$ is t. However, this optimum value is attainable if and only if the coin operator A is *diagonal* and the initial state is *unbiased*. Also, we demonstrate the existence of an ample class of QRWs with non-trivial position probability distribution; the value of the leading term of whose standard deviation $\sigma(X_t)$ is arbitrarily close to t. For a QRW starting in classical state $|0\rangle \otimes |1\rangle$, we show that the leading terms of the first two moments of the position probability distribution are determined uniquely by the eigenvalues of the corresponding unitary matrix U. In particular, for a QRW on the line starting in classical state $|0\rangle \otimes |1\rangle$, we confirm that the maximum value of the leading term of the standard deviation $\sigma(X_t)$ of the position probability distribution is $\frac{t}{2}$. We offer some examples to illustrate the conditions under which this maximum value is achievable.

From this point forward, the remainder of this paper is organized as follows. In section 2, we offer a brief review of the relevant methods and results due to previous authors. In section 3, we investigate some basic analytic properties of unitary matrices as they pertain to the theory of QRWs on the line. In section 4, we derive clear and simple expressions for the first two moments of the position probability distribution of a QRW on the line. For clarity of exposition, proofs and details of some calculations are deferred to the appendix.

2. Related work

For a QRW on the line, the *position space* is the Hilbert space H_p spanned by an orthonormal basis $\{|x\rangle; x \in Z\}$. The *coin space* is the Hilbert space H_c spanned by an orthonormal basis $\{|j\rangle; j = 1, 2.\}$. The 'state space' is $H = H_c \otimes H_p$. Thus, a typical state ψ in H may be expressed as

$$\psi = \sum_{x \in Z} \sum_{j=1,2} \psi(x, j)|x\rangle \otimes |j\rangle.$$

To introduce the *evolution operator* of a QRW on a line, we begin with a *shift operator* and a *coin operator*. The shift operator $S : H \to H$ is defined by $S(|x\rangle \otimes |j\rangle) = |x+1\rangle \otimes |j\rangle$, if $j = 1$; $S(|x\rangle \otimes |j\rangle) = |x-1\rangle \otimes |j\rangle$, if $j = 2$. Meanwhile, the coin operator $A : H_c \to H_c$ can be any unitary operator. Accordingly, the evolution operator is defined by $U = S(I \otimes A)$, where I denotes the identity operator on H_p.

Given $\psi_0 \in H$ and $\psi_t = U^t \psi_0$, then the sequence $\{\psi_t\}_0^\infty$ models the temporal evolution of a QRW on the line with initial state ψ_0.

Let X denote the position operator on the position space H_p, so that $X|x\rangle = x|x\rangle$. Given a QRW with $\psi_t = \sum_{x\in Z}\sum_{j=1,2}\psi_t(x, j)|x\rangle \otimes |j\rangle$, where t denotes time, then the probability $p_t(x)$ of finding the particle at the position x at time t is given by the standard formula

$$p_t(x) = \sum_j |\psi_t(x, j)|^2.$$

Thus, at every instant t, the eigenvalues of the operator $X_t \doteq U^{\dagger t} X U^t$ equate to the possible values of the particle's position with corresponding probability $p_t(x)$.

Until further notice, let $H_c \otimes L^2([0, 2\pi))$ serve as the state space, sometimes also referred to as the k-space, and let $\psi = \sum_{x\in Z}\sum_{j=1,2}\psi(x, j)|x\rangle \otimes |j\rangle \in H$.

Let $\psi(x) = \binom{\psi(x,1)}{\psi(x,2)}$, and let $\psi(k) = \binom{\psi(k,1)}{\psi(k,2)} = \sum_{x\in Z}\psi(x)\,\mathrm{e}^{\mathrm{i}kx}$ denote the Fourier transform of $(\psi(x))$.

Then we have

$$\psi(x) = \int_0^{2\pi} \mathrm{e}^{-\mathrm{i}kx}\psi(k)\frac{\mathrm{d}k}{2\pi},$$

and

$$\langle\psi, \phi\rangle = \sum_{x\in Z}\sum_{j=1,2}\bar{\psi}(x, j)\phi(x, j) = \sum_{j=1,2}\int_0^{2\pi}\bar{\psi}(k, j)\phi(k, j)\frac{\mathrm{d}k}{2\pi}.$$

By definition,

$$S\begin{pmatrix}\psi(x,1)\\ \psi(x,2)\end{pmatrix} = \begin{pmatrix}\psi(x+1,1)\\ \psi(x-1,2)\end{pmatrix},$$

so that

$$S\begin{pmatrix}\psi(k,1)\\ \psi(k,2)\end{pmatrix} = \begin{pmatrix}\mathrm{e}^{\mathrm{i}k}\psi(k,1)\\ \mathrm{e}^{-\mathrm{i}k}\psi(k,2)\end{pmatrix}.$$

Therefore,

$$U\psi = \begin{pmatrix}\mathrm{e}^{\mathrm{i}k} & 0\\ 0 & \mathrm{e}^{-\mathrm{i}k}\end{pmatrix} A \begin{pmatrix}\psi(k,1)\\ \psi(k,2)\end{pmatrix} = U(k)\psi(k).$$

Thus, in k-space, the QRW may be modeled by the formula

$$\psi_t(k) = U(k)^t\psi_0(k).$$

In [6], using Fourier transform methods, Grimmett *et al* derived formulae for the rth moments of the position probability distribution. A brief statement of their main result is displayed below. For a more detailed account, the reader is advised to refer to [6].

Let $D = -\mathrm{i}/\mathrm{d}k$ denote the position operator in k-space. Assuming that all moments $E\big(X_0^r\big)$ of the initial state ψ_0 are finite, then, as $t \to \infty$, the rth moment of the position probability distribution is given by

$$E[(X_t/t)^r] = \int_0^{2\pi}\sum_j\left(\frac{D\lambda_j(k)}{\lambda_j(k)}\right)^r |\langle v_j(k), \psi_0(k)\rangle|^2\frac{\mathrm{d}k}{2\pi} + \mathrm{O}(t^{-1}),$$

where $\lambda_1(k)$ and $\lambda_2(k)$ denote the eigenvalues of $U(k)$, and $v_1(k)$ and $v_2(k)$ denote the corresponding orthonormal eigenvectors. Accordingly, the value of the leading term of the rth moment is $t^r\int_0^{2\pi}\sum_j\left(\frac{D\lambda_j(k)}{\lambda_j(k)}\right)^r|\langle v_j(k), \psi_0(k)\rangle|^2\frac{\mathrm{d}k}{2\pi}$.

3. Formulation of the evolution operator based on unitary matrices

In what follows, we denote by $\overline{\lambda}$ the complex conjugate of a complex number λ, by $|a|$ the modulus of a complex number a, and by $|A|$ the determinant of a matrix A. For x^T and y^T in C^2, the inner product is defined by $\langle x^T, y^T\rangle = \langle (x_1, x_2)^T, (y_1, y_2)^T\rangle = \overline{x_1}y_1 + \overline{x_2}y_2$.

For a unitary matrix

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad \text{with determinant} \quad |A| = \mathrm{e}^{\mathrm{i}\theta},$$

where a, b, c and d are complex constants, and θ is a real constant, set

$$U(k) = \begin{pmatrix} \mathrm{e}^{\mathrm{i}k} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}k} \end{pmatrix} A = \begin{pmatrix} a\,\mathrm{e}^{\mathrm{i}k} & b\,\mathrm{e}^{\mathrm{i}k} \\ c\,\mathrm{e}^{-\mathrm{i}k} & d\,\mathrm{e}^{-\mathrm{i}k} \end{pmatrix}.$$

Then, for each value of k, $U(k)$ has two eigenvalues $\lambda_1(k)$ and $\lambda_2(k)$, with $|\lambda_j(k)| = 1$, whose corresponding unit eigenvectors $v_1(k) = \left(v_1^1, v_1^2\right)^T$ and $v_2(k) = \left(v_2^1, v_2^2\right)^T \in C^2$ constitute an orthonormal basis for the k-space. To aid in the proof of the main result, we proceed to collect some basic facts about unitary matrices $U(k)$. The proofs are quite elementary, and are deferred to the appendix.

Proposition 1. *The eigenvalues* $\{\lambda_j(k)\}_{j=1}^2$ *of* $U(k)$ *are* C^∞ *functions of k, as are the corresponding eigenvectors* $\{v_j(k)\}_{j=1}^2$.

Henceforth, for simplicity of notation, the explicit dependence on the parameter k of the quantities U, $\{\lambda_j\}_{j=1}^2$, $\{v_j\}_{j=1}^2$ and the initial state ψ_0 will be suppressed.

Proposition 2. *As above, let* $D = -\mathrm{i}\,\mathrm{d}/\mathrm{d}k$ *denote the position operator. If u and w are two vectors in* C^2 *with differentiable components, then* $D(\langle u, w\rangle) = \langle u, Dw\rangle - \langle Du, w\rangle$.

Corollary 1. *If* v_1 *and* v_2 *are eigenvectors of U, then*

(i) $\langle v_j, Dv_j\rangle = \langle Dv_j, v_j\rangle$;
(ii) $\langle v_1, Dv_2\rangle = \langle Dv_1, v_2\rangle$.

As seen above, the expression $\overline{\lambda}D\lambda$ acts as an essential ingredient in the formulae for the moments of position probability distribution. The next two propositions capture some fundamental features of the expression $\overline{\lambda}D\lambda$.

Proposition 3. *If* λ_1 *and* λ_2 *are eigenvalues of U, then* $\overline{\lambda_1}D\lambda_1 = -\overline{\lambda_2}D\lambda_2$.

Proposition 4. *If* λ *is an eigenvalue and v is a corresponding unit eigenvector of U, then* $\overline{\lambda}D\lambda = 2|\langle v, \varepsilon_1\rangle|^2 - 1 = 1 - 2|\langle v, \varepsilon_2\rangle|^2$, *where* $\varepsilon_1 = (1, 0)^T$ *and* $\varepsilon_2 = (0, 1)^T$.

By proposition 4, $|\overline{\lambda}D\lambda| \leqslant 1$. In particular, when $|\overline{\lambda}D\lambda| \equiv 1$ or $\overline{\lambda}D\lambda \equiv 0$, then the shape of the coin operator matrix A is either diagonal or anti-diagonal, and we are faced with a 'trivial' scenario. The next two propositions pertain to the special cases where $\overline{\lambda}D\lambda \equiv 0$ or $\overline{\lambda}D\lambda \equiv \pm 1$.

Proposition 5. *For an eigenvalue* λ *of the matrix U, the following three statements are equivalent:*

(i) $\overline{\lambda}D\lambda \equiv 0$,
(ii) $A = \begin{pmatrix} 0 & b \\ c & 0 \end{pmatrix}$,
(iii) U possesses eigenvalues $\mathrm{e}^{\mathrm{i}\frac{\theta}{2}}$ *and* $-\mathrm{e}^{\mathrm{i}\frac{\theta}{2}}$ *which are independent of the parameter k.*

Proposition 6. *For an eigenvalue λ of the matrix U, the following three statements are equivalent:*

(i) $\overline{\lambda}D\lambda \equiv \pm 1$,
(ii) $A = \left(\begin{smallmatrix} a & 0 \\ 0 & d \end{smallmatrix}\right)$,
(iii) *U possesses eigenvalues $a\mathrm{e}^{\mathrm{i}k}$ and $d\mathrm{e}^{-\mathrm{i}k}$.*

Note that if A is a *Pauli matrix*, then either $\overline{\lambda}D\lambda \equiv 0$ or $|\overline{\lambda}D\lambda| \equiv 1$. When $\overline{\lambda}D\lambda \equiv 0$, the motion of the particle remains confined. When $|\overline{\lambda}D\lambda| \equiv 1$, the motion is completely decoupled into ballistic right drifting (spin-up) or left drifting (spin-down) states.

4. The SD and the first two moments of a QRW on the line

Based on the approach described in the previous section, we offer simplified versions of the formulae given in [6] for the first two moments of the position probability distribution of the QRW on the line. A rather simple expression emerges for the leading term of the standard deviation (SD), which permits us to specify explicitly its maximum value.

For simplicity, we may assume henceforth, without loss of generality, that the QRW is launched at the origin. Thus the initial state in k-space possesses the form $\psi_0 = \alpha_1\varepsilon_1 + \alpha_2\varepsilon_2$. We begin by presenting an explicit formula for the first moment of the position probability distribution. This formula refines the formula given in [6].

Proposition 7. *If the QRW starts in the initial state $\psi_0 = \alpha_1\varepsilon_1 + \alpha_2\varepsilon_2$, then the first moment of the position probability distribution is given by*

$$E(X_t) = \int_0^{2\pi} \langle \psi_t, D\psi_t\rangle \frac{\mathrm{d}k}{2\pi},$$

where $\langle \psi_t, D\psi_t\rangle = t\big[(2|\alpha_1|^2 - 1)\overline{\lambda_1}D\lambda_1 + 4\,\mathrm{Re}\big(\alpha_1\overline{\alpha_2}\overline{v_1^1}v_1^2\big)\big]\overline{\lambda_1}D\lambda_1 + 2\,\mathrm{Re}\big\{\big[\lambda_1^t(\overline{\lambda_2})^t - 1\big]\overline{\langle v_2, \psi_0\rangle}\langle v_1, \psi_0\rangle\langle v_2, Dv_1\rangle\big\}$.

If the QRW starts in the classical state $|0\rangle \otimes |1\rangle$, then $\psi_0 = \varepsilon_1$, in which case the formula for $E(X_t)$ simplifies as follows.

Corollary 2. *If the QRW starts in the classical state $|0\rangle \otimes |1\rangle$, then the first moment of position probability distribution is given by*

$$E(X_t) = t\int_0^{2\pi} (\overline{\lambda_1}D\lambda_1)^2 \frac{\mathrm{d}k}{2\pi} + \int_0^{2\pi} 2\,\mathrm{Re}\big\{\big[\lambda_1^t(\overline{\lambda_2})^t - 1\big]\overline{\langle v_2, \psi_0\rangle}\langle v_1, \psi_0\rangle\langle v_2, Dv_1\rangle\big\}\frac{\mathrm{d}k}{2\pi}.$$

Next, let us recall the formula for the second moment of the position probability distribution given in [6] by Grimmett *et al*:

$$E\big(X_t^2\big) = t^2\int_0^{2\pi} \sum_j \left(\frac{D\lambda_j}{\lambda_j}\right)^2 |\langle v_j, \psi_0\rangle|^2 \frac{\mathrm{d}k}{2\pi} + \mathrm{O}(t).$$

A simplified version of this formula is obtained by applying proposition 3. Interestingly, as noted by Konno in [3, 5] and Endrejat and Büttner in [8], the second moment of the position probability distribution turns out to be independent of the initial state of the QRW.

Proposition 8. *If the QRW starts in the initial state ψ_0, then the second moment of the position probability distribution is given by*

$$E\big(X_t^2\big) = t^2\int_0^{2\pi} (\overline{\lambda_1}D\lambda_1)^2 \frac{\mathrm{d}k}{2\pi} + \mathrm{O}(t).$$

Finally, we are ready to consider the standard deviation $\sigma(X_t)$ of the position probability distribution for a QRW on the line. The following theorem provides information about the upper and lower bounds of the leading term of the standard deviation $\sigma(X_t)$. In particular, it specifies conditions under which these bounds are sharp.

Theorem 1. *For a QRW on the line, with coin operator A and initial state ψ_0, an upper bound for the leading term of $\sigma(X_t)$ is t. The leading term of $\sigma(X_t)$ is identically equal to t if and only if the coin operator A is of diagonal format and the initial state is unbiased, i.e. $\psi_0 = \alpha_1\varepsilon_1 + \alpha_2\varepsilon_2$ with $|\alpha_1| = |\alpha_2| = \frac{\sqrt{2}}{2}$. At the other extreme, if the coin operator A is of anti-diagonal format, i.e. $\overline{\lambda_1}D\lambda_1 \equiv 0$, then, independent of the initial state ψ_0, the leading term of $\sigma(X_t)$ degenerates to* $\mathrm{O}(\sqrt{t})$.

According to theorem 1, the leading term of $\sigma(X_t)$ is identically equal to t when and only when the position probability distribution is 'trivial' in the sense that the particle is observed at time t to occupy positions t and $-t$ with equal probability $\frac{1}{2}$. However, by varying the coin operator A, we can find examples (see below) of *non-trivial* QRWs having coin operators A that are neither diagonal nor anti-diagonal, such that the leading term of $\sigma(X_t)$ is arbitrarily close to t. We cannot, at this time, completely rule out the existence of a non-trivial QRW whose leading term degenerates to $\mathrm{O}(\sqrt{t})$. However, if the QRW commences in the classical state $|0\rangle \otimes |1\rangle$, then, according to the following theorem and its corollaries, the leading term of $\sigma(X_t)$ of any non-trivial QRW *cannot* degenerate to $\mathrm{O}(\sqrt{t})$.

Theorem 2. *If the QRW starts in the classical state $|0\rangle \otimes |1\rangle$, then the variance of the position probability distribution is given by*

$$\sigma^2(X_t) = t^2 \left\{ \int_0^{2\pi} (\overline{\lambda_1}D\lambda_1)^2 \frac{\mathrm{d}k}{2\pi} - \left[\int_0^{2\pi} (\overline{\lambda_1}D\lambda_1)^2 \frac{\mathrm{d}k}{2\pi} \right]^2 \right\} + \mathrm{O}(t).$$

Corollary 3. *If the QRW starts in the classical state $|0\rangle \otimes |1\rangle$, then the variance $\sigma^2(X_t) = \mathrm{O}(t)$ if and only if $\overline{\lambda_1}D\lambda_1 \equiv 0$ or $\overline{\lambda_1}D\lambda_1 \equiv \pm 1$.*

In other words, the QRW spreads with the same level velocity $\mathrm{O}(\sqrt{t})$ as does a classical random walk if and only if the motion of the particle on the line either is confined to a finite interval or drifts monotonically to the right.

Corollary 4. *If the QRW starts in the classical state $|0\rangle \otimes |1\rangle$, then the maximum value of the leading term of $\sigma^2(X_t)$ is $\frac{1}{4}t^2$ if and only if $\int_0^{2\pi} (\overline{\lambda_1}D\lambda_1)^2 \frac{\mathrm{d}k}{2\pi} = \frac{1}{2}$.*

The following example shows that $\int_0^{2\pi} (\overline{\lambda_1}D\lambda_1)^2 \frac{\mathrm{d}k}{2\pi} = \frac{1}{2}$, as in corollary 4, is achievable, so that the corresponding QRW spreads at the highest possible velocity given by $\sigma(X_t) = \frac{1}{2}t + \mathrm{O}(1)$.

Consider a QRW with coin operator matrix

$$A(\beta) = \begin{pmatrix} \cos\beta & \sin\beta \\ \sin\beta & -\cos\beta \end{pmatrix},$$

where $\beta \in \left[0, \frac{\pi}{2}\right]$, and with corresponding evolution operator

$$U(k) = \begin{pmatrix} \mathrm{e}^{\mathrm{i}k}\cos\beta & \mathrm{e}^{\mathrm{i}k}\sin\beta \\ \mathrm{e}^{-\mathrm{i}k}\sin\beta & -\mathrm{e}^{-\mathrm{i}k}\cos\beta \end{pmatrix}.$$

By straightforward calculation, the eigenvalues are

$$\lambda_j(k) = \pm\sqrt{1 - \cos^2\beta\sin^2 k} + \mathrm{i}\cos\beta\sin k,$$

so that

$$\overline{\lambda_1}D\lambda_1 = (\cos\beta\cos k)/(\sqrt{1-\cos^2\beta\sin^2 k}), \qquad \text{and} \qquad \int_0^{2\pi}(\overline{\lambda}D\lambda)^2\frac{\mathrm{d}k}{2\pi} = 1-\sin\beta.$$

Depending on the initial state of the QRW, we have two cases:

Case 1. Suppose the initial state is the classical state $|0\rangle\otimes|1\rangle$. Then, by theorem 2, the variance $\sigma^2(X_t) = t^2(1-\sin\beta)\sin\beta + \mathrm{O}(t)$, so the standard deviation is $\sigma(X_t) = t\sqrt{\sin\beta(1-\sin\beta)} + \mathrm{O}(1)$. When $\beta = \frac{\pi}{6}$, the leading term of the standard deviation of the corresponding QRW attains the maximum value $\frac{1}{2}t$. When $\beta = \frac{\pi}{4}$, then the coin operator matrix is the Hadamard matrix, and the leading term of the standard deviation is $t\sqrt{(\sqrt{2}-1)/2}$. A similar result can be found in Nayak and Vishwanath [1], Ambainis *et al* [2], and Konno [3, 5].

Case 2. Suppose the initial state is $\psi_0 = \alpha_1\varepsilon_1 + \alpha_2\varepsilon_2$, where, for simplicity, both α_1 and α_1 are assumed to be real. After some laborious, though straightforward, calculations, the unit eigenvector of λ_1 becomes

$$\begin{pmatrix} v_1^1 \\ v_1^2 \end{pmatrix} = \frac{1}{\sqrt{N(k,\beta)}}\begin{pmatrix} \mathrm{e}^{\mathrm{i}k} \\ \frac{\lambda_1 - \mathrm{e}^{\mathrm{i}k}\cos\beta}{\sin\beta} \end{pmatrix},$$

where the normalization factor is given by

$$N(k,\beta) = (2 - 2\sqrt{1-\cos^2\beta\sin^2 k}\cos\beta\cos k - 2\cos^2\beta\sin^2 k)/\sin^2\beta,$$

so that

$$\left[\mathrm{Re}\left(\alpha_1\overline{\alpha_2}\overline{v_1^1}v_1^2\right)\right]\overline{\lambda_1}D\lambda_1 = (\alpha_1\overline{\alpha_2}\cos\beta\sin\beta\cos^2 k)/2(1-\cos^2\beta\sin^2 k).$$

Therefore

$$\int_0^{2\pi}\left[\mathrm{Re}\left(\alpha_1\overline{\alpha_2}\overline{v_1^1}v_1^2\right)\right]\overline{\lambda_1}D\lambda_1\frac{\mathrm{d}k}{2\pi} = (\alpha_1\overline{\alpha_2}\sin\beta(1-\sin\beta))/(2\cos\beta).$$

Finally, by proposition 7, we have

$$\sigma^2(X_t) = t^2(1-\sin\beta) - t^2[(2|\alpha_1|^2-1)(1-\sin\beta) + (2\alpha_1\sin\beta(1-\sin\beta)\sqrt{1-|\alpha_1|^2})/\cos\beta]^2 + \mathrm{O}(t).$$

Now, set $\alpha_1 = \frac{\sqrt{2}}{2}$. Then $\sigma^2(X_t) = t^2(1-\sin\beta) - t^2(1-\sin\beta)^2\tan^2\beta + \mathrm{O}(t)$. By taking values of β sufficiently close to 0, we see that the corresponding values of $\sigma^2(X_t)$ can come arbitrarily close to t^2. Since $\beta \neq 0$, the corresponding coin operator A is *not* diagonal and the QRW is *not* trivial. Under these conditions, it seems reasonable to believe that there are two regions at the extreme zones of the walk in which the particle is most likely to be found.

5. Conclusion

We have shown that the maximum value of the leading term of $\sigma(X_t)$ is t. This maximum value is reached if and only if the coin operator A is diagonal, and the initial state is unbiased. However, the position probability distribution of this QRW is not terribly interesting. It may be useless in designing quantum algorithms. Fortunately, as the above example assures us, QRWs exist with non-trivial position probability distributions and large enough standard deviations.

One rather evident fact is that if the coin operator A is of anti-diagonal type, then, regardless of the initial state ψ_0, the $\sigma(X_t) = O(\sqrt{t})$ which is the same order as the classical random walks. This evidence casts some doubt on the widespread notion that QRWs generally spread quadratically faster than their classical counterparts. The question might be worth investigating, whether a *non-trivial* QRW exists such that $\sigma(X_t) = O(\sqrt{t})$.

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Appendix

Proof of proposition 1. To justify the first one, we note that $\lambda_{1,2}(k) = (\mathrm{e}^{\mathrm{i}k}a + \mathrm{e}^{-\mathrm{i}k}d \pm \sqrt{(\mathrm{e}^{\mathrm{i}k}a+\mathrm{e}^{-\mathrm{i}k}d)^2 - 4\,\mathrm{e}^{\mathrm{i}\theta}})/2$. It is easy to see that $(\mathrm{e}^{\mathrm{i}k}a + \mathrm{e}^{-\mathrm{i}k}d)^2 - 4\,\mathrm{e}^{\mathrm{i}\theta} = 0$ for some k only if $|a| = |d| = 1$. In this case $\lambda_1(k) = \mathrm{e}^{\mathrm{i}k}a$, and $\lambda_2(k) = \mathrm{e}^{-\mathrm{i}k}d$, they are C^∞. Otherwise, if $(\mathrm{e}^{\mathrm{i}k}a + \mathrm{e}^{-\mathrm{i}k}d)^2 - 4\,\mathrm{e}^{\mathrm{i}\theta} \neq 0$ for every k, then the graph of the C^∞ function, $(\mathrm{e}^{\mathrm{i}k}a + \mathrm{e}^{-\mathrm{i}k}d)^2 - 4\,\mathrm{e}^{\mathrm{i}\theta}$, entirely lies inside of the circle centered at $4\,\mathrm{e}^{\mathrm{i}\theta}$ with radius 4. In this case $\sqrt{(\mathrm{e}^{\mathrm{i}k}a + \mathrm{e}^{-\mathrm{i}k}d)^2 - 4\,\mathrm{e}^{\mathrm{i}\theta}}$ is C^∞, therefore $\{\lambda_j(k)\}_{j=1}^2$ are also C^∞. The justification of the second claim is trivial.

Proof of proposition 2. $D[\langle u, w\rangle] = D(\overline{u}w) = -\mathrm{i}\big(\frac{\mathrm{d}(\overline{u}w)}{\mathrm{d}k}\big) = -\mathrm{i}\big(w\frac{\mathrm{d}\overline{u}}{\mathrm{d}k} + \overline{u}\frac{\mathrm{d}w}{\mathrm{d}k}\big) = wD\overline{u} + \overline{u}Dw = \overline{u}Dw - \overline{Du}w = \langle u, Dw\rangle - \langle Du, w\rangle$.

Proof of proposition 3. Since

$$\lambda_1\lambda_2 = |U| = \begin{vmatrix} \mathrm{e}^{\mathrm{i}k} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}k} \end{vmatrix} |A| = |A| = \mathrm{e}^{\mathrm{i}\theta}, \tag{A.1}$$

where θ is a constant, only depends on A, $\frac{\mathrm{d}(\lambda_1\lambda_2)}{\mathrm{d}k} = 0$. This implies that $\lambda_1\frac{\mathrm{d}\lambda_2}{\mathrm{d}k} + \frac{\mathrm{d}\lambda_1}{\mathrm{d}k}\lambda_2 = 0$. By (A.1), $\lambda_1 = \overline{\lambda_2}\,\mathrm{e}^{\mathrm{i}\theta}$ and $\lambda_2 = \overline{\lambda_1}\,\mathrm{e}^{\mathrm{i}\theta}$. So, we have

$$\overline{\lambda_2}\,\mathrm{e}^{\mathrm{i}\theta}\frac{\mathrm{d}\lambda_2}{\mathrm{d}k} = -\frac{\mathrm{d}\lambda_1}{\mathrm{d}k}\overline{\lambda_1}\,\mathrm{e}^{\mathrm{i}\theta}.$$

Therefore we obtain

$$\overline{\lambda_1}D\lambda_1 = -\overline{\lambda_2}D\lambda_2. \tag{A.2}$$

Proof of proposition 4. For simplicity, in this proof we temporarily assign the symbols v_1 and v_2 to the two components of the eigenvector v. Since λ is an eigenvalue of U, v is a corresponding unit eigenvector,

$$Uv = U\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \lambda\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} \lambda v_1 \\ \lambda v_2 \end{pmatrix}.$$

This implies the following equations:

$$\mathrm{e}^{\mathrm{i}k}av_1 + \mathrm{e}^{\mathrm{i}k}bv_2 = \lambda v_1 \tag{A.3}$$

and

$$\mathrm{e}^{-\mathrm{i}k}cv_1 + \mathrm{e}^{-\mathrm{i}k}\,\mathrm{d}v_2 = \lambda v_2. \tag{A.4}$$

Differentiating both sides of the above equations with respect to k, results in the two equations:

$$\mathrm{i}\mathrm{e}^{\mathrm{i}k}av_1 + \mathrm{e}^{\mathrm{i}k}a\frac{\mathrm{d}v_1}{\mathrm{d}k} + \mathrm{i}\mathrm{e}^{\mathrm{i}k}bv_2 + \mathrm{e}^{\mathrm{i}k}b\frac{\mathrm{d}v_2}{\mathrm{d}k} = \frac{\mathrm{d}\lambda}{\mathrm{d}k}v_1 + \lambda\frac{\mathrm{d}v_1}{\mathrm{d}k} \tag{A.5}$$

$$-\mathrm{i}\mathrm{e}^{-\mathrm{i}k}cv_1 + \mathrm{e}^{-\mathrm{i}k}c\frac{\mathrm{d}v_1}{\mathrm{d}k} - \mathrm{i}\mathrm{e}^{-\mathrm{i}k}dv_2 + \mathrm{e}^{-\mathrm{i}k}d\frac{\mathrm{d}v_2}{\mathrm{d}k} = \frac{\mathrm{d}\lambda}{\mathrm{d}k}v_2 + \lambda\frac{\mathrm{d}v_2}{\mathrm{d}k}. \tag{A.6}$$

Multiplying equation (A.5) by $\overline{\lambda v_1}$, we get

$$\overline{\lambda v_1}\left(\mathrm{i}\mathrm{e}^{\mathrm{i}k}av_1+\mathrm{e}^{\mathrm{i}k}a\frac{\mathrm{d}v_1}{\mathrm{d}k}+\mathrm{i}\mathrm{e}^{\mathrm{i}k}bv_2+\mathrm{e}^{\mathrm{i}k}b\frac{\mathrm{d}v_2}{\mathrm{d}k}\right)=\overline{\lambda}\frac{\mathrm{d}\lambda}{\mathrm{d}k}v_1\overline{v}_1+\frac{\mathrm{d}v_1}{\mathrm{d}k}\overline{v_1}. \tag{A.7}$$

Multiplying equation (A.6) by $\overline{\lambda v_2}$, we get

$$\overline{\lambda v_2}\left(-\mathrm{i}\mathrm{e}^{-\mathrm{i}k}cv_1+\mathrm{e}^{-\mathrm{i}k}c\frac{\mathrm{d}v_1}{\mathrm{d}k}-\mathrm{i}\mathrm{e}^{-\mathrm{i}k}\,\mathrm{d}v_2+\mathrm{e}^{-\mathrm{i}k}d\frac{\mathrm{d}v_2}{\mathrm{d}k}\right)=\overline{\lambda}\frac{\mathrm{d}\lambda}{\mathrm{d}k}v_2\overline{v}_2+\frac{\mathrm{d}v_2}{\mathrm{d}k}\overline{v_2}. \tag{A.8}$$

Adding (A.7) to (A.8) and solving for $\overline{\lambda}\frac{\mathrm{d}\lambda}{\mathrm{d}k}$ yields

$$\begin{aligned}\overline{\lambda}\frac{\mathrm{d}\lambda}{\mathrm{d}k}=\overline{\lambda v_1}&\left(\mathrm{i}\mathrm{e}^{\mathrm{i}k}av_1+\mathrm{e}^{\mathrm{i}k}a\frac{\mathrm{d}v_1}{\mathrm{d}k}+\mathrm{i}\mathrm{e}^{\mathrm{i}k}bv_2+\mathrm{e}^{\mathrm{i}k}b\frac{\mathrm{d}v_2}{\mathrm{d}k}\right)\\&+\overline{\lambda v_2}\left(-\mathrm{i}\mathrm{e}^{-\mathrm{i}k}cv_1+\mathrm{e}^{-\mathrm{i}k}c\frac{\mathrm{d}v_1}{\mathrm{d}k}-\mathrm{i}\mathrm{e}^{-\mathrm{i}k}dv_2+\mathrm{e}^{-\mathrm{i}k}d\frac{\mathrm{d}v_2}{\mathrm{d}k}\right)\\&-\left(\frac{\mathrm{d}v_1}{\mathrm{d}k}\overline{v_1}+\frac{\mathrm{d}v_2}{\mathrm{d}k}\overline{v_2}\right).\end{aligned} \tag{A.9}$$

Substituting the left-hand sides of (A.3) and (A.4) for λv_1 and λv_2, respectively, in the above equations, we obtain

$$\begin{aligned}\overline{\lambda}\frac{\mathrm{d}\lambda}{\mathrm{d}k}=\mathrm{i}|a|^2v_1\overline{v_1}&+|a|^2\overline{v_1}\frac{\mathrm{d}v_1}{\mathrm{d}k}+\mathrm{i}\overline{a}b\overline{v_1}v_2+\overline{a}b\overline{v_1}\frac{\mathrm{d}v_2}{\mathrm{d}k}+\mathrm{i}a\overline{b}v_1\overline{v_2}\\&+a\overline{b}\frac{\mathrm{d}v_1}{\mathrm{d}k}\overline{v_2}+\mathrm{i}|b|^2v_2\overline{v_2}+|b|^2\overline{v_2}\frac{\mathrm{d}v_2}{\mathrm{d}k}-\mathrm{i}|c|^2v_1\overline{v_1}+|c|^2\overline{v_1}\frac{\mathrm{d}v_1}{\mathrm{d}k}\\&-\mathrm{i}\overline{c}d\overline{v_1}v_2+\overline{c}d\overline{v_1}\frac{\mathrm{d}v_2}{\mathrm{d}k}-\mathrm{i}c\overline{d}v_1\overline{v_2}+c\overline{d}\frac{\mathrm{d}v_1}{\mathrm{d}k}\overline{v_2}\\&-\mathrm{i}|d|^2v_2\overline{v_2}+|d|^2\overline{v_2}\frac{\mathrm{d}v_2}{\mathrm{d}k}-\left(\overline{v_1}\frac{\mathrm{d}v_1}{\mathrm{d}k}+\overline{v_2}\frac{\mathrm{d}v_2}{\mathrm{d}k}\right).\end{aligned} \tag{A.10}$$

From the definition of a unitary matrix, the following identities are easily deduced:

$$\begin{array}{lll}|a|^2+|b|^2=1, & |a|^2+|c|^2=1, & |b|^2+|d|^2=1,\\ |c|^2+|d|^2=1, & \overline{a}b+\overline{c}d=0 \quad\text{and} & a\overline{c}+b\overline{d}=0.\end{array} \tag{A.11}$$

Applying the identities in (A.11) to the right-hand side of (A.10) and simplifying it, we conclude that

$$\overline{\lambda}\frac{\mathrm{d}\lambda}{\mathrm{d}k}=2\mathrm{i}(|a|^2v_1\overline{v_1}+|b|^2v_2\overline{v_2}+2\,\mathrm{Re}(\overline{a}b\overline{v_1}v_2))-\mathrm{i}. \tag{A.12}$$

By (A.3), we have

$$\lambda v_1\overline{\lambda v_1}=v_1\overline{v_1}=|a|^2v_1\overline{v_1}+|b|^2v_2\overline{v_2}+2\,\mathrm{Re}(\overline{a}b\overline{v_1}v_2). \tag{A.13}$$

Combining (A.12) and (A.13) together, leads to the desired result

$$\overline{\lambda}D\lambda=2|\langle v,\varepsilon_1\rangle|^2-1.$$

The proof is complete.

Proof of proposition 5. (1) (i) $\Rightarrow$ (ii). If $\overline{\lambda}D\lambda\equiv 0$, then λ_1 and λ_2 are independent of k. Since both λ_1 and λ_2 are solutions of the equation,

$$\lambda^2-[(a+d)\cos k+(a-d)\mathrm{i}\sin k]\lambda+ad-bc=0, \tag{A.14}$$

we derive that $a+d=0$ and $a-d=0$, so $a=d=0$. Thus we have

$$A=\begin{pmatrix}0 & b\\ c & 0\end{pmatrix}.$$

Both (ii) $\Rightarrow$ (iii) and (iii) $\Rightarrow$ (i) are obvious.

Proof of proposition 6. (i) $\Rightarrow$ (ii). The $\overline{\lambda}D\lambda \equiv 1$ is equivalent to $D\lambda \equiv \lambda$, which exactly is $\frac{\mathrm{d}\lambda}{\mathrm{d}k} = \mathrm{i}\lambda$. This gives that $\lambda(k) = \mathrm{e}^{\mathrm{i}(k+r)}$ for some $r \in [0, 2\pi)$. Since $\lambda_1 \cdot \lambda_2 = \mathrm{e}^{\mathrm{i}\theta}$, $\lambda_1 = \mathrm{e}^{\mathrm{i}k} \cdot \mathrm{e}^{\mathrm{i}r}$ and $\lambda_2 = \mathrm{e}^{-\mathrm{i}k} \cdot \mathrm{e}^{\mathrm{i}(\theta-r)}$.

Both λ_1 and λ_2 are the solutions of the equation

$$\lambda^2 - \lambda(\mathrm{e}^{\mathrm{i}k}a + \mathrm{e}^{-\mathrm{i}k}d) + ad - bc = 0, \tag{A.15}$$

hence $\lambda_1 + \lambda_2 = \mathrm{e}^{\mathrm{i}k}\mathrm{e}^{\mathrm{i}r} + \mathrm{e}^{-\mathrm{i}k}\mathrm{e}^{\mathrm{i}(\theta-r)} = \mathrm{e}^{\mathrm{i}k}a + \mathrm{e}^{-\mathrm{i}k}d$, which implies that $a = \mathrm{e}^{\mathrm{i}r}$ and $d = \mathrm{e}^{\mathrm{i}(\theta-r)}$. Due to that fact that A is unitary, we further deduce that $b = 0$ and $c = 0$. So we have

$$A = \begin{pmatrix} a & 0 \\ 0 & d \end{pmatrix}.$$

Similarly, we can prove it for the case of $\overline{\lambda}D\lambda \equiv -1$.

Both (ii) $\Rightarrow$ (iii) and (iii) $\Rightarrow$ (i) are evident. The proof is complete.

Proof of proposition 7. Recall that the tth time evolution is

$$\psi_t = U^t\psi_0 = \lambda_1^t\langle v_1, \psi_0\rangle v_1 + \lambda_2^t\langle v_2, \psi_0\rangle v_2.$$

Performing the position operator $D = -\mathrm{i}\,\mathrm{d}/\mathrm{d}k$ in k-space on both sides of the above equation, it becomes

$$D\psi_t = \sum_{j=1}^{2}\left(t\lambda_j^{t-1}D\lambda_j\langle v_j, \psi_0\rangle v_j + \lambda_j^t D\langle v_j, \psi_0\rangle v_j + \lambda_j^t\langle v_j, \psi_0\rangle Dv_j\right).$$

By appealing to corollary 1, propositions 3 and 4, we give a closed-form expression for the quantity

$$\begin{aligned}
\langle\psi_t, D\psi_t\rangle &= t\overline{\lambda_1}D\lambda_1|\langle v_1, \psi_0\rangle|^2 + D\langle v_1, \psi_0\rangle\overline{\langle v_1, \psi_0\rangle} + |\langle v_1, \psi_0\rangle|^2\langle v_1, Dv_1\rangle \\
&\quad + (\overline{\lambda_1})^t\lambda_2^t\overline{\langle v_1, \psi_0\rangle}\langle v_2, \psi_0\rangle\langle v_1, Dv_2\rangle + (\overline{\lambda_2})^t\overline{\langle v_2, \psi_0\rangle}\lambda_1^t\langle v_1, \psi_0\rangle\langle v_2, Dv_1\rangle \\
&\quad + t\overline{\lambda_2}D\lambda_2|\langle v_2, \psi_0\rangle|^2 + \overline{\langle v_2, \psi_0\rangle}D\langle v_2, \psi_0\rangle + |\langle v_2, \psi_0\rangle|^2\langle v_2, Dv_2\rangle \\
&= t\overline{\lambda_1}D\lambda_1(|\langle v_1, \psi_0\rangle|^2 - |\langle v_2, \psi_0\rangle|^2) \\
&\quad + (|\langle v_1, \psi_0\rangle|^2\langle v_1, Dv_1\rangle + |\langle v_2, \psi_0\rangle|^2\langle v_2, Dv_2\rangle) \\
&\quad + (\overline{\lambda_1})^t\lambda_2^t\overline{\langle v_1, \psi_0\rangle}\langle v_2, \psi_0\rangle\langle v_1, Dv_2\rangle + (\overline{\lambda_2})^t\lambda_1^t\overline{\langle v_2, \psi_0\rangle}\langle v_1, \psi_0\rangle\langle v_2, Dv_1\rangle \\
&\quad + (D\langle v_1, \psi_0\rangle\overline{\langle v_1, \psi_0\rangle} + D\langle v_2, \psi_0\rangle\overline{\langle v_2, \psi_0\rangle}) \\
&= t\overline{\lambda_1}D\lambda_1(|\langle v_1, \psi_0\rangle|^2 - |\langle v_2, \psi_0\rangle|^2) \\
&\quad + 2\,\mathrm{Re}\left\{\left[\lambda_1^t(\overline{\lambda_2})^t - 1\right]\overline{\langle v_2, \psi_0\rangle}\langle v_1, \psi_0\rangle\langle v_2, Dv_1\rangle\right\} \\
&= t\overline{\lambda_1}D\lambda_1(2|\langle v_1, \psi_0\rangle|^2 - 1) + 2\,\mathrm{Re}\left\{\left[\lambda_1^t(\overline{\lambda_2})^t - 1\right]\overline{\langle v_2, \psi_0\rangle}\langle v_1, \psi_0\rangle\langle v_2, Dv_1\rangle\right\} \\
&= t\overline{\lambda_1}D\lambda_1\left[(2|\alpha_1|^2 - 1)\overline{\lambda_1}D\lambda_1 + 4\,\mathrm{Re}\left(\alpha_1\overline{\alpha_2}\overline{v_1^1}v_1^2\right)\right] \\
&\quad + 2\,\mathrm{Re}\left\{\left[\lambda_1^t(\overline{\lambda_2})^t - 1\right]\overline{\langle v_2, \psi_0\rangle}\langle v_1, \psi_0\rangle\langle v_2, Dv_1\rangle\right\}.
\end{aligned} \tag{A.16}$$

This proof is done by noting that $E(X_t) = \langle\psi_t, X\psi_t\rangle = \int_0^{2\pi}\langle\psi_t(k), D\psi_t(k)\rangle\frac{\mathrm{d}k}{2\pi}$ from the last section.

Proof of theorem 1. Note that $\sigma^2(X_t) = E\left(X_t^2\right) - [E(X_t)]^2$. By propositions 4 and 8, the maximum leading term of $E\left(X_t^2\right)$ is t^2, and the leading term of $E\left(X_t^2\right)$ is t^2 if and only if $|\overline{\lambda_1}D\lambda_1| \equiv 1$. According to proposition 6, $|\overline{\lambda_1}D\lambda_1| \equiv 1$ if and only if A is diagonal, this implies that the second component of the eigenvector v_1 is zero, then by proposition 7,

$\sigma(X_t) = t(2|\alpha_1|^2 - 1) + O(1)$. Obviously, $\sigma(X_t) = O(1)$ if and only if $|\alpha_1| = \frac{\sqrt{2}}{2}$. A justification of the second statement in this theorem follows propositions 5, 7 and 8.

Proof of corollary 3. To justify them, it is easy to see $\sigma^2(X_t) = \mathrm{O}(t)$ if and only if $\int_0^{2\pi} (\overline{\lambda_1} D\lambda_1)^2 \frac{\mathrm{d}k}{2\pi} = 0$ or $\int_0^{2\pi} (\overline{\lambda_1} D\lambda_1)^2 \frac{\mathrm{d}k}{2\pi} = 1$. These are equivalent to $\overline{\lambda_1} D\lambda_1 \equiv 0$ or $\overline{\lambda_1} D\lambda_1 \equiv \pm 1$ since the quantity $\overline{\lambda_1} D\lambda_1$ is continuous and bounded by 1 according to proposition 4. Appealing to propositions 5 and 6, we know $\overline{\lambda_1} D\lambda_1 \equiv 0$ if and only if this quantum random walk remains confined, and $\overline{\lambda_1} D\lambda_1 \equiv 1$ if and only if this quantum random walk always moves to the right on the line.

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