Quantum random walks on the integer lattice

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1 Introduction

Random walks have proven to be a useful tool in creating optimized algorithms for many situations. For example, random walks can contribute to algorithms for counting and sampling, and also algorithms which test properties such as the satisfiability of Boolean formulae or graph connectivity [BP07].

Quantum random walks provide the opportunity to expand upon and better these algorithms. The process was first constructed in the 1990’s by [ADZ93], with the idea of using such a process for quantum computing. In their 2001 paper, Ambainis et al pointed out that “quantum random walks have the potential to offer new tools for quantum algorithms,” including that they “may yield techniques for analyzing discrete quantum processes [...] more generally.”

Quantum random walks differ from their classical counterparts because they allow for destructive interference between different paths between the same two locations. In particular, quantum walks frequently encounter this interference near the origin. As a result, particles tend to spread much faster in quantum random walks than in classical random walks. Explicitly, at time $n$, the location of a quantum random walk’s particle is typically found at distance $\theta(n)$ from the origin, while in a classical random walk, the particle is found at distance $\theta(\sqrt{n})$ from the origin.
1.1 Preliminaries

For our discrete quantum random walks, we first choose a dimension $d$ for the integer lattice $\mathbb{Z}^d$ around which the particle moves. Next, we need to add a degree of freedom to allow for quantum interference. This extra degree of freedom, called a chirality, is somewhat like the spin of a particle. Each chirality $j$ corresponds to one way a particle can move throughout the walk, defined by a vector $\mathbf{v}^{(j)} \in \mathbb{Z}^d$. For example, in a simple 1-dimensional case, there may be 2 chiralities: one which corresponds to moving one step to the left, and one which corresponds to moving one step to the right. Throughout our models of a walk, the chirality of a particle will describe the last step the particle took. Overall, this gives the state space for the quantum random walk,

$$\Omega := L^2(\mathbb{Z}^d \times \{1, \ldots, k\})$$

A Hilbert Basis for $\Omega$ is the set of elementary states $\delta_{r,j}$, as $r$ ranges over $\mathbb{Z}^d$ and $1 \leq j \leq k$; we will also denote $\delta_{r,j}$ simply by $(r,j)$.

Next, the walk needs a unitary matrix $U$ to describe how any chirality transforms into the other chiralities during a step of the walk. Although in general $U$ can take complex values, we restrict to the case where $U$ is real for ease of computations. For a $k$-chirality walk, $U$ will be a $k \times k$ unitary matrix. Let $I \otimes U$ denote the unitary operator on $\Omega$ whose value on the elementary state $(r,j)$ is equal to $\sum_{i=1}^{k} U_{ij}(r,i)$. Let $T$ denote the operator whose action on the elementary states is given by $T(r,j) = (r + \mathbf{v}^{(j)}, j)$. The QRW operator $S = S_{d,k;\mathbf{U};\{\mathbf{v}^{(j)}\}}$ is defined by
More informally, a step of a QRW may be broken down into two parts: first, change the chiralities of the particle by acting on it by $U$. The $nj$th entry of $U$ gives a square root of the probability that a particle starting in chirality $n$ changes to chirality $j$ in any given step - so, the $n$th column of the matrix describes the distribution of a particle of chirality $n$ after it has taken its next step. For the second part of the step, move the particles according to their new chiralities. It is important to notice that even when we restrict to real values, $U$ matrix will have both positive and negative entries. This is because these values represent amplitudes, which are squared to give probabilities. By allowing negative amplitudes, the particles may interfere with each other throughout the walk. The fact that the matrix is unitary guarantees that the total probability of a particle being anywhere always adds up to 1 after every step.

Therefore, to fully set up any quantum random walk, we need a collection of chiralities, a corresponding unitary matrix, and an initial distribution. The initial distribution simply tells the probability of our particle starting at any location, with any given amplitudes.

Notice that the QRW is translation invariant, meaning that if $\sigma$ is any translation operator $(r, j) \mapsto (r + u, j)$ then $S \circ \sigma = \sigma \circ S$. The $n$-step operator is $S^n$. Using bracket notation, we denote the amplitude for finding the particle in chirality $j$ and
location $\mathbf{x} + \mathbf{r}$ after $n$ steps, starting in chirality $i$ and location $\mathbf{x}$, by

$$a(i, j, n, r) := \langle (\mathbf{x}, i) \left| S^n \right| (\mathbf{x} + \mathbf{r}, j) \rangle .$$

(1.2)

By translation invariance, this quantity is independent of $\mathbf{x}$. The squared modulus $|a(i, j, n, r)|^2$ is interpreted as the probability of finding the particle in chirality $j$ and location $\mathbf{x} + \mathbf{r}$ after $n$ steps, starting in chirality $i$ and location $\mathbf{x}$, if a measurement is made. Unlike the classical random walk, the quantum random walk can be measured only at one time without disturbing the process. We may therefore study limit laws for the quantities $a(i, j, n, r)$ but not joint distributions of these.

## 2 Examples

### 2.1 Hadamard QRW

As an example, we look at the classic Hadamard walk, which was defined in [ADZ93] and analyzed in [ABN+01] and [CIR03]. The walk has two chiralities, which correspond to staying still and moving one step to the right - and in this special case, we name them accordingly: $\{0, 1\}$. The unitary matrix for the walk is as follows:

$$U = \begin{pmatrix}
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}
\end{pmatrix}$$

In general, we assume that all of our particles start at the origin, because a simple translation could make the starting location a new origin. Therefore, we can choose our starting state to be a particle with amplitude 1 in chirality 1. Then, after one
step, the distribution of the particle will be as follows: there is a particle at location 0 with an amplitude of $\frac{1}{\sqrt{2}}$ and a chirality of 0, and there is another particle at location 1 with an amplitude of $-\frac{1}{\sqrt{2}}$ and a chirality of 1.

For the second step, the unitary matrix acts upon each theoretical location of the particle. We will get the following four particles, labelled as [location, amplitude, chirality]:

\[
\begin{align*}
[0, \frac{1}{2}, 0] & \quad \text{coming from the particle at location 0} \\
[1, \frac{1}{2}, 1] & \\
[1, -\frac{1}{2}, 0] & \quad \text{coming from the particle at location 1} \\
[2, \frac{1}{2}, 1] & 
\end{align*}
\]

Notice that the particles at 1 do not yet interfere because they have different chiralities. It is not until the next step of the walk that the particles first interfere: this happens only with the particles at 1, who will necessarily move to the same locations with the same chiralities. The distribution of the particles $[1, \frac{1}{2}, 1]$ and $[1, -\frac{1}{2}, 0]$ are as follows:

\[
\begin{align*}
[1, \frac{1}{2}, 0] & \quad \text{coming from the particle with chirality 1} \\
[2, -\frac{1}{2}, 1] & \\
[1, -\frac{1}{2}, 0] & \quad \text{coming from the particle with chirality 0} \\
[2, -\frac{1}{2}, 1] & 
\end{align*}
\]
So here, the two paths which led to a particle at position 1 will cancel with each other completely, leaving no particle at this location with chirality 0. On the other hand, the particles at location 2 will constructively interfere, giving a particle with amplitude $-\frac{1}{\sqrt{2}}$ and chirality 1 at this location.

As previous works have shown, up to a rapidly oscillating factor due to a phase difference in two summands in the amplitude, the rescaled amplitudes $n^{1/2}a(i, j, n, n\theta)$ converge to a profile $f(\theta)$ supported on the interval $J := \left[\frac{1}{2} - \frac{\sqrt{2}}{4}, \frac{1}{2} + \frac{\sqrt{2}}{4}\right]$. The function $f$ is continuous on the interior of $J$ and blows up like $|\theta - \theta_0|^{-1/2}$ when $\theta_0$ is an endpoint of $J$. These results are extended in [BP07] to arbitrary unitary matrices. The limiting profiles are all qualitatively similar; a plot for the Hadamard QRW is shown in figure 1, with the upper envelope showing what happens when the phases of the summands line up.
2.2 Walks with Three or More Chiralities

When the number of chiralities is allowed to exceed two, new phenomena emerge. The possibility of a bound state arises. This means that for some fixed location \( x \), the amplitude \( a(i, j, n, x) \) does not go to zero as \( n \to \infty \). This was first shown to occur in [BCA03, IKS05]. From a generating function viewpoint, bound states occur when the denominator \( Q \) of the generating function factors. The occurrence of bound states appears to be a non-generic phenomenon.

To investigate these phenomena further, my coworker Rajarshi Das and I wrote
codes that would model 1-dimensional quantum random walks with 3 or 4 chiralities, and generalized matrices $U$ and step sizes $\{v^{(j)}\}$. Many of the walks we modelled are catalogued here:


The probability profile shown in figure 2 is typical of what we found and is the basis for an example running throughout this section. In this example,

$$U = \frac{1}{27} \begin{bmatrix}
17 & 6 & 20 & -2 \\
-20 & 12 & 13 & -12 \\
-2 & -15 & 4 & -22 \\
-6 & -18 & 12 & 15
\end{bmatrix} \quad (2.1)$$

and $v^{(j)} = -1, 0, 1, 2$ for $j = 1, 2, 3, 4$ respectively. The profile shown in the figure is a plot of $|a(1, 1, 1000, x)|^2$ against $x$ for integers $x$ in the interval $[-1000, 2000]$. 
Figure 2: probability profile for a four-chirality QRW in one dimension

The values were computed exactly by recursion and then plotted. The most obvious new feature is the existence of a number of peaks in the interior of the feasible region. The phase factor is somewhat more chaotic as well, which turns out to be due to a greater number of summands in the amplitude function. Our aim is to use the theory described in Section 2 to establish the locations of these peaks, that is to say, the values of $\theta$ for which $n^{1/2}a(i, j, n, x)$ become unbounded for $x$ sufficiently near $n\theta$. 
2.3 2-dimensional example

We can extend the quantum random walks to two dimensions, adding a component to each chirality to describe the step sizes in the new dimension. For example, we can take a walk with chiralities \( \{(1, 0), (-1, 0), (0, 1), (0, -1)\} \), the unitary matrix

\[
U := \begin{pmatrix}
  51 & -188 & -18 & -234 \\
  116 & -3 & 282 & 6 \\
  -258 & 54 & 109 & -108 \\
  -102 & -234 & 36 & 163
\end{pmatrix},
\]

and a starting distribution of the particle with amplitude \( \frac{1}{\sqrt{2}} \) in each of the first two chiralities. We plot the graph for 200 steps and get the distribution in Figure 2.3, where the darker lines represent higher probabilities of being at that location:

![Figure 3: The probability distribution of a 2-dimensional QRW after 200 steps.](image)
3 Asymptotics

In the following sections, the notation and results mimic those of [BGPP09].

3.1 Generating Functions

Quantum random walks show pronounced asymptotes. In particular, for each walk, there are set ratios $r/s$ of location to time where the amplitude of the particle explodes, relative to the amplitudes of nearby locations. Precisely, the peaks are values $\theta$ such that $\sqrt{n}a(i, j, n, x)$ becomes unbounded for $x$ sufficiently close to $n\theta$.

We wish to determine exactly where these values of $\theta$ are, without approximating them through merely iterating a QRW. The key to analyzing a QRW’s graphs is through generating functions. In his book [Wil06], Herbert Wilf describes a generating function as “a clothesline on which we hang up a sequence of numbers for display.” Generating functions encode a sequence of numbers $\{a_n\}_{n=0}^\infty$ by encapsulating the information an expression whose power series has the same coefficients $\{a_n\}$.

In what follows, we let $x$ denote the vector $(x_1, \ldots, x_d)$. Given a lattice QRW, for $1 \leq i, j \leq k$ we may define a power series in $d + 1$ variables via

$$F_{ij}(x, y) := \sum_{n \geq 0} \sum_{r \in \mathbb{Z}^d} a(i, j, n, r)x^r y^n. \quad (3.1)$$

Here and throughout, $x^r$ denotes the monomial power $x_1^{r_1} \cdots x_d^{r_d}$. We let $F$ denote the generating matrix $(F_{ij})_{1 \leq i, j \leq k}$, which is a $k \times k$ matrix with entries in the formal power series ring in $d + 1$ variables. The following result from [BP07] is obtained via
a straightforward use of the transfer matrix method.

**Lemma 3.1** ([BP07, Proposition 3.1]). Let $M(x)$ denote the $k \times k$ diagonal matrix whose diagonal entries are $x^{v(1)}, \ldots, x^{v(k)}$. Then

$$F(x, y) = (I - yM(x)U)^{-1}. \tag{3.2}$$

Consequently, there are polynomials $P_{ij}(x, y)$ such that

$$F_{ij} = \frac{P_{ij}}{Q} \tag{3.3}$$

where $Q(x, y) := \det(I - yM(x)U)$.

Within these generating functions, $x$ is a placeholder whose power represents the location of a particle, and $y$ is a placeholder whose power represents the number of steps taken by the particle.

Let $z$ denote the vector $(x, y)$ and let

$$\mathcal{V} := \{z \in \mathbb{C}^{d+1} : Q(z) = 0\}$$

denote the algebraic variety which is the common pole of the generating functions $F_{ij}$. Let $\mathcal{V}_1 := \mathcal{V} \cap T^{d+1}$ denote the intersection of the singular variety $\mathcal{V}$ with the unit torus $T^{d+1} := \{|x_1| = \cdots = |x_d| = |y| = 1\}$. An important map on $\mathcal{V}$ is the logarithmic Gauss map $\mu : \mathcal{V} \to \mathbb{CP}^d$ defined by

$$\mu(z) := \left( z_1 \frac{\partial Q}{\partial z_1} : \cdots : z_{d+1} \frac{\partial Q}{\partial z_{d+1}} \right). \tag{3.4}$$
The map $\mu$ is defined only at points of $\mathcal{V}$ where the gradient $\nabla Q$ does not vanish. Here, we will be concerned only with instances of QRW satisfying

$$\nabla Q \text{ vanishes nowhere on } \mathcal{V}_1.$$ \hspace{1cm} (3.5)

This condition holds generically.

### 3.2 Previous Results

It is shown in [BBBP08, Proposition 2.1] that the image $\mu[\mathcal{V}_1]$ is contained in the real subspace $\mathbb{RP}^d \subseteq \mathbb{CP}^d$. Also, under the hypothesis (3.5), $\partial Q/\partial y$ cannot vanish on $\mathcal{V}_1$, hence we may interpret the range of $\mu$ as $\mathbb{R}^d \subseteq \mathbb{RP}^d$ via the identification $$(x_1 : \cdots : x_d : y) \leftrightarrow ((x_1/y), \ldots, (x_d/y)).$$ In what follows, we draw heavily on two results from [BBBP08].

**Theorem 3.2** (shape theorem [BBBP08, Theorem 4.2]). Assume (3.5) and let $G \subseteq \mathbb{R}^d$ be the closure of the image of $\mu$ on $\mathcal{V}_1$. If $K$ is any compact subset of $G^c$, then

$$a(i, j, n, r) = O(e^{-cn})$$

for some $c = c(K) > 0$, uniformly as $r/n$ varies over $K$.

In other words, under ballistic rescaling, the region of non-exponential decay or feasible region is contained in $G$. The converse, and much more, is provided by the second result, also from the same theorem. For $z \in \mathcal{V}_1$, let $\kappa(z)$ denote the curvature
of the real hypersurface $-i \log V_1 \subseteq \mathbb{R}^{d+1}$ at the point $\log z$, where $\log$ is applied to vectors coordinatewise and manifolds pointwise.

**Theorem 3.3** (asymptotics in the feasible region). Suppose $Q$ satisfies (3.5). For $r \in \mathbf{G}$, let $Z(r)$ denote the set $\mu^{-1}(r)$ of pre-images in $V_1$ of the projective point $r$ under $\mu$. If $\kappa(z) \neq 0$ for all $z \in Z(r)$, then

$$a(i,j,n,r) = n^{-d/2} \left[ \sum_{z \in Z(r)} \frac{P_{ij}(z)}{|\nabla \log Q(z)|} |\kappa(z)|^{-1/2} e^{i\omega(r,n)} \right] + O\left(n^{-(d+1)/2}\right)$$

(3.6)

where the argument $\omega(r,n)$ is given by $-r \cdot \text{Arg}(z) + i\pi \tau(z)/4$ and $\tau(z)$ is the index of the quadratic form defining the curvature at the point $(1/i) \log z \in (1/i) \log V_1$.

4 Results and Conjectures

The results of Section 2.2 may be summarized informally in the case of one-dimensional QRW as follows. Provided the quantities $\nabla Q$ and $\kappa$ do not vanish for the points $z$ associated with a direction $r$, then the amplitude profile will be a the sum of terms whose phase factors may be somewhat chaotic, but whose magnitudes are proportional to $\kappa^{-1/2}/|\nabla \log Q|$. In practice the magnitude of the amplitude will vary between zero and the sum of the magnitudes of the pieces, depending on the behavior of the phase terms. In the two-chirality case, with only two summands, it is easy to identify the picture with the theoretical result. However, in the multi-chirality case, the empirical results in figure 2 are not easily rectified with the theoretical result, firstly because
the theoretical result is not trivial to compute, and secondly because the computation appears at first to be at odds with the data. In the remainder of Section 2.2, we show how the theoretical computations may be executed in a computer algebra system, and then recify these with the data in figure 2. The first step is to verify some of the hypotheses of Theorems 3.2–3.3. The second step, reconciling the theory and the data, will be done in Section 4.1.

**Proposition 4.1.** Let $Q(x, y)$ be the denominator of the generating function for any QRW in any dimension that satisfies the smoothness hypothesis (3.5). Let $\pi$ be the projection from $V_1$ to the $d$-torus $T^d$ that forgets the last coordinate. Then the following properties hold.

(i) $\partial Q/\partial y$ does not vanish on $V_1$;

(ii) $V_1$ is a compact $d$-manifold;

(iii) $\pi : V_1 \to T^d$ is smooth and nonsingular;

(iv) In fact, $V_1$ is homeomorphic to a union of some number $s$ of $d$-tori, each mapping smoothly to $T^d$ under $\pi$ and covering $T^d$ some number $n_j$ times for $1 \leq j \leq s$.

(v) $\kappa : V_1 \to \mathbb{R}$ vanishes exactly when the determinant of the Jacobian of the map $\mu$ vanishes.

(vi) $\kappa$ vanishes on the boundary $\partial \mu[V_1]$ of the range of $\mu$. 

Proof. The first two conclusions are shown as [BBBP08, Proposition 2.2]. The map \( \pi \) is smooth on \( T^{d+1} \), hence on \( \mathcal{V}_1 \), and nonsingularity follows from the nonvanishing of the partial derivative with respect to \( y \). The fourth conclusion follows from the classification of compact \( d \)-manifolds covering the \( d \)-torus. For the fifth conclusion, recall that the Gauss-Kronecker curvature of a real hypersurface is defined as the determinant of the Jacobian of the map taking \( p \) to the unit normal at \( p \). We have identified projective space with the slice \( z_{d+1} = 1 \) rather than with the slice \( |z| = 1 \), but these are locally diffeomorphic, so the Jacobian of \( \mu \) still vanishes exactly when \( \kappa \) vanishes. Finally, if an interior point of a manifold maps to a boundary point of the image of the manifold under a smooth map, then the Jacobian vanishes there, hence the last conclusion follows from the fifth.

An empirical fact is that in all of the several dozen quantum random walks we have investigated, the number of components of \( \mathcal{V}_1 \) and the degrees of the map \( \pi \) on each component depend on the dimension \( d \) and the vector of chiralities, but not on the unitary matrix \( U \).

**Conjecture 4.2.** If \( d, k, v^{(1)}, \ldots, v^{(k)} \) are fixed and \( U \) varies over unitary matrices, then the number of components of \( \mathcal{V} \) and the degrees of the map \( \pi \) on each component are constant, except for a set of matrices of positive co-dimension.

**Remark.** The unitary group is connected, so if the conjecture fails then a transition occurs at which \( \mathcal{V}_1 \) is not smooth. We know that this happens, resulting in a bound state [IKS05], however in the three-chirality case, the degeneracy does not seem to
mark a transition in the topology of $\mathcal{V}_1$.

Specializing to one dimension, the manifold $\mathcal{V}_1$ is a union of topological circles. The map $\mu : \mathcal{V}_1 \rightarrow \mathbb{R}$ is evidently smooth, so it maps $\mathcal{V}_1$ to a union of intervals. In all catalogued cases, in fact the range of $\mu$ is an interval, so we have the following open question:

**Question 4.3.** Is it possible for the image of $\mu$ to be disconnected?

Because $\mu$ smoothly maps a union of circles to the real line, the Jacobian of the map $\mu$ must vanish at least twice on each circle. Let $\mathcal{W}$ denote the set of $z \in \mathcal{V}_1$ for which $\kappa(z) = 0$. The cardinality of $\mathcal{W}$ is not an invariant (compare, for example, the example in Section 4.1 with the first 4-chirality example on the web archive). This has the following interesting consequence. Again, because the unitary group $\mathcal{U}_k$ is connected, by interpolation there must be some $U$ for which there is a double degeneracy in the Jacobian of $\mu$. This means that the Taylor series for $\log y$ on $\mathcal{V}_1$ as a function of $\log x$ is missing not only its quadratic term but its cubic term as well. In a scaling window of size $n^{1/2}$ near the peaks, it is shown in [BP07] that the amplitudes are asymptotic to an Airy function. However, with a double degeneracy, the same method shows a quartic-Airy limit instead of the usual cubic-Airy limit. This may be the first combinatorial example of such a limit and will be discussed in forthcoming work.

Let $W = \{w^{(0)}, \ldots, w^{(t)}\}$ be a set of vectors in $\mathbb{R}^n$. Say that $W$ is rationally degenerate if the set of $t$-tuples $(r \cdot (w - w^{(0)}))_{w \in W}$ is not dense in $(\mathbb{R} \mod 2\pi)^t$ as $r$ varies.
over \(\mathbb{Z}^n\). Generic \(t\)-tuples are rationally nondegenerate because degeneracy requires a number of linear relations to hold over the \(2\pi\mathbb{Q}\). If \(W\) is rationally nondegenerate, then the distribution on \(t\)-tuples \((r \cdot (w - w^{(0)}))_{w \in W}\) when \(r\) is distributed uniformly over any cube of side \(M\) in \(\mathbb{Z}^d\) converges weakly to the uniform distribution on \((\mathbb{Z} \mod 2\pi)^t\). Let \(\chi(\alpha_1, \ldots, \alpha_t)\) denote the distribution of the square modulus of the sum of \(t\) complex numbers chosen independently at random with moduli \(\alpha_1, \ldots, \alpha_t\) and arguments uniform on \([-\pi, \pi]\). The following result now follows from the above discussion, Theorems 3.2 and 3.3, and Proposition 4.1.

**Proposition 4.4.** For any one-dimensional QRW, let \(Q, Z(r)\) and \(\kappa\) be as above. Let \(J\) be the image of \(V_1\) under \(\mu\). Let \(r\) be any point of \(J\) such that \(\kappa(z) \neq 0\) for all \(z \in Z(r)\) and \(W := (1/i) \log Z(r)\) is rationally nondegenerate. Then for any \(\epsilon > 0\) there exists an \(M\) such that if \(r(n)\) is a sequence of integer vectors with \(r(n)/n \to r\), the empirical distribution of \(n^d\) times the squared moduli of the amplitudes

\[
\{a(i, j, n, r(n) + \xi) : \xi \in \{0, \ldots, M - 1\}^{d+1}\}
\]

is within \(\epsilon\) of the distribution \(\chi(\alpha_1, \ldots, \alpha_t)\) where \(t = |Z(r)|\), \(\{z^{(j)}\}\) enumerates \(Z(r)\), and \(\alpha_j = |P_{ij}(z^{(j)})\kappa(z^{(j)})^{-1/2}|.\) If \(r \notin J\), then the empirical distribution converges to a point mass at zero.

\[\square\]

**Remark.** Rational nondegeneracy becomes more difficult to check when the size of \(Z(r)\) increases, which happens when the number of chiralities increases. If one weakens the conclusion to convergence to some nondegenerate distribution with support
in $I := \left[0, \sum |P_{ij}(z)^2 \kappa(z)^{-1}|\right]$, then one needs only that not all components of all differences $\log z - \log z'$ are rational, for $z, z' \in \mathbb{Z}(r)$. For the purpose of qualitatively explaining the plots, this is good enough, though the upper envelope may be strictly less than the upper endpoint of $I$ (and the lower envelope may be strictly greater than zero) if there is rational degeneracy.

Comparing to figure 2, we see that $J$ appears to be a proper subinterval of $[-1, 2]$, that there appears to be up to seven peaks which are local maxima of the probability profile. These include the endpoints of $J$ (cf. the last conclusion of Proposition 4.1) as well as several interior points, which we now understand to be places where the map $\mu$ folds back on itself. We now turn our attention to corroborating our understanding of the picture by computing the number and locations of the peaks.

### 4.1 Computations

Much of our computation is carried out symbolically in Maple. Symbolic computation is significantly faster when the entries of $U$ are rational, than when they are, say, quadratic algebraic numbers. Also, Maple sometimes incorrectly simplifies or fails to simplify expressions involving radicals. It is easy to generate quadratically algebraic orthogonal or unitary matrices via the Gram-Schmidt procedure. For rational matrices, however, we turn to a result we found in [LO91].

**Proposition 4.5.** The map $S \mapsto (I + S)(I - S)^{-1}$ takes the skew symmetric matrices over a field to the orthogonal matrices over the same field. To generate unitary
matrices instead, use skew-hermitian matrices $S$.

The map in the proposition is rational, so choosing $S$ to be rational, we obtain orthogonal matrices with rational entries. In our running example,

$$S = \begin{bmatrix}
0 & -3 & -1 & 3 \\
3 & 0 & 1 & -2 \\
1 & -1 & 0 & 2 \\
-3 & 2 & -2 & 0 \\
\end{bmatrix},$$

leading to the matrix $U$ of equation (2.1).

The example shows amplitudes for the transition from chirality 1 to chirality 1, so we need the polynomials $P_{11}$ and $Q$:

$$P_{11}(x, y) = (27 x - 15 y x^3 - 4 y x + 12 y^2 x^3 - 12 y + 4 y^2 x^2 + 9 y^2 - 17 y^3 x^2) x$$

$$Q(x, y) = -17 y^3 x^2 + 9 y^2 + 27 x - 12 y + 12 y^2 x^3 + 8 y^2 x^2 - 15 y x^3 - 4 y^3 x^3$$

$$-15 y^3 x + 12 y^2 x - 4 y x - 17 y x^2 + 9 y^2 x^4 - 12 y^3 x^4 + 27 y^4 x^3.$$

The curvature is proportional to the quantity

$$(-x Q_x - y Q_y) x Q_x y Q_y - x^2 y^2 (Q_y^2 Q_{xx} + Q_x^2 Q_{xy} - 2 Q_x Q_y Q_{xy}),$$

where subscripts denote partial derivatives. Evaluating this leads to $xy$ times a polynomial $K(x, y)$ that is about half a page in Maple 11. The command

```
Basis([[Q, K], plex (y, x))
```
leads to a Gröbner basis, the first element of which is an elimination polynomial $p(x)$, vanishing at precisely those $x$-values for which there is a pair $(x, y) \in \mathcal{V}$ for which $\kappa(x, y) = 0$. We may also verify that $Q$ is smooth by computing that the ideal generated by $[Q, Q_x, Q_y]$ has the trivial basis, [1].

To pass to the subset of roots of $p(x)$ that are on the unit circle, one trick is as follows. If $z = x + 1/x$ then $x$ is on the unit circle if and only if $z$ is in the real interval $[-2, 2]$. The polynomial defining $z$ is the elimination polynomial $q(z)$ for the basis $[p, 1 - zx + x^2]$. Applying Maple's built-in Sturm sequence evaluator to $q$ shows symbolically that there are six roots of $z$ in $[−2, 2]$. This leads to six conjugate pairs of $x$ values. The second Gröbner basis element is a polynomial linear in $y$, so each $x$ value has precisely one corresponding $y$ value. The $y$ value for $\mathfrak{x}$ is the conjugate of the $y$ value for $x$, and the function $\mu$ takes the same value at both points of a conjugate pair. Evaluating the $\mu$ function at all six places leads to floating point expressions approximately equal to

$$1.362766, 1.126013, 0.929248, 0.229537, -0.143835, -0.346306.$$
Figure 4: probability profile with peaks drawn as vertical lines

Drawing vertical lines corresponding to these six peak locations leads to figure 4.

Surprisingly, the largest peak appearing in the data plot appears to be missing from the set of analytically computed peak directions. Simultaneously, some of the analytically computed peaks appear quite small and it seems implausible that the probability profile blows up there. Indeed, this had us puzzled for quite a while. In order to doublecheck our work, we plotted $y$ against $x$, resulting in the plot in figure 5(a), which should be interpreted as having periodic boundary conditions because $x$ and $y$ range over a circle. This shows $\mathcal{V}_1$ to be the union of two circles, each embedded in $T^2$ so that the projection $\pi$ onto $x$ has degree 2. (Note: the projection onto $y$ has degree 1, and the homology class of the embedded circle is $(2, -1)$ in the
basis generated by the $x$ and $y$ axes.) We also plotted $\mu$ against $x$. To facilitate computation, we used Gröbner bases to eliminate $y$ from $Q$ and $xQ_x - \mu y Q_y$, enabling us to plot solutions to a single polynomial. The resulting plot is shown in figure 5(b).

![Graphs](image)

(a) $y$ versus $x$  
(b) $\mu$ versus $x$

Figure 5: Two interleaved circles and their images under the Gauss map

The last figure shows nicely how peaks occur at values where the map $\mu$ backtracks. The explanation of the appearance of the extra peak at $\mu \approx 0.7$ becomes clear if we compare plots at $n = 1,000$ and $n = 10,000$. At first glance, it looks as if the extra peak is still quite prominent, but in fact it has lowered with respect to the others. To be precise, the false peak has gone down by a factor of 10, from 0.004 to 0.0004, because its probabilities scaled as $n^{-1}$. The width of the peak also remained the same, indicating convergence to a finite probability profile. The real peaks, however, have gone down by factors of $10^{2/3}$, as is shown to occur in the Airy scaling windows near directions $\mathbf{r}$ where $\kappa(\mathbf{z}) = 0$ for some $\mathbf{z} \in Z(\mathbf{r})$. When the plot is vertically scaled so that the highest peak occurs at the same height in each picture, the width above half the maximum has shrunk somewhat, as must occur in an Airy scaling window,
Figure 6: As $n \rightarrow \infty$, one peak scales down more rapidly which has width $\sqrt{n}$. The location of the false peak is marked by a nearly flat spot in figure 5(b), at height around 0.7. The curve stays nearly horizontal for some time, causing the false peak to remain spread over a macroscopic rescaled region.

5 Two-dimensional QRW

In this section we consider two examples of QRW with $d = 2$, $k = 4$ and steps $v^{(1)} = (0, 0), v^{(2)} = (1, 0), v^{(3)} = (0, 1)$ and $v^{(4)} = (1, 1)$. To complete the specification
of the two examples, we give the two unitary matrices:

\[
U_1 := \frac{1}{2} \begin{bmatrix}
1 & 1 & -1 & 1 \\
1 & 1 & -1 & -1 \\
-1 & -1 & 1 & 1 \\
-1 & -1 & 1 & 1
\end{bmatrix} \quad (5.1)
\]

\[
U_2 := \frac{1}{2} \begin{bmatrix}
1 & 1 & -1 & 1 \\
1 & 1 & -1 & 1 \\
-1 & 1 & 1 & -1 \\
-1 & 1 & 1 & 1
\end{bmatrix} . \quad (5.2)
\]

Note that these are both Hadamard matrices; neither is the Hadamard matrix with the bound state considered in [Moo04], nor is either in the two-parameter family referred to as Grover walks in [WKKK08]. The second differs from the first in that the signs in the third row are reversed. Both are members of one-parameter families analyzed in [BBBP08], in Sections 4.1 and 4.3 respectively. The (arbitrary) names given to these matrices in [Bra07, BBBP08] are respectively $S(1/2)$ and $B(1/2)$. Intensity plots at time 200 for these two quantum walks, given in figure 7, reproduce those taken from [BBBP08] but with different parameter values (1/2 each time, instead of 1/8 and 2/3 respectively).

For the case of $U_1$ it is shown in [BBBP08, Lemma 4.3] that $\mathcal{V}_1$ is smooth. Asymptotics follow, as in Theorem 3.3 of the present paper, and an intensity plot of the asymptotics is generated that matches the empirical time 200 plot quite well. In the
Figure 7: Time 200 probability profiles for two quantum walks: the darkness at \((r, s)\) corresponds to the squared amplitude \(|a(1, 1, 200, r, s)|^2\).

In the case of \(U_2\), \(V_1\) is not smooth but [BBBP08, Theorem 3.5] shows that the singular points do not contribute to the asymptotics. Again, a limiting intensity plot follows from Theorem 3.3 of the present paper and matches the time 200 profile quite well.

It follows from Proposition 4.4 that the union of darkened curves where the intensity blows up is the algebraic curve where \(\kappa\) vanishes, and that this includes the boundary of the feasible region. The main result of this section is the identification of the algebraic curve. While this result is only computational, it is one of the first examples of computation of such a curve, the only similar prior example being the computation of the “Octic circle” boundary of the feasible region for so-called diabolo tilings, identified without proof by Cohn and Pemantle and first proved by [KO07] (see also [BP10]). The perhaps somewhat comical statement of the result is as follows.

**Theorem 5.1.** For the quantum walk with unitary coin flip \(U_2\), the curvature of the variety \(V_1\) vanishes at some \(z \in Z(r, s)\) if and only if \((r, s)\) is a zero of the polynomial

\(\ldots\)
\[ P_2 \text{ and satisfies } |r| + |s| < 3/4, \text{ where} \]
\[
P_2(r, s) := 1 + 14r^2 - 3126r^4 + 97752r^6 - 1445289r^8 + 12200622r^{10} - 64150356r^{12} +
220161216r^{14} - 504431361r^{16} + 774608490r^{18} - 785130582r^{20} + 502978728r^{22} -
184298359r^{24} + 29412250r^{26} + 14s^2 - 1284r^2s^2 - 113016r^4s^2 + 5220612r^6s^2 -
96417162r^8s^2 + 924427224r^{10}s^2 - 4865103360r^{12}s^2 + 14947388808r^{14}s^2 -
27714317286r^{16}s^2 + 30923414124r^{18}s^2 - 19802256648r^{20}s^2 + 6399721524r^{22}s^2 -
721963550r^{24}s^2 - 3126s^4 - 113016r^2s^4 + 7942218r^4s^4 - 68684580r^6s^4 - 666538860r^8s^4 +
15034322304r^{10}s^4 - 86727881244r^{12}s^4 + 226469888328r^{14}s^4 - 296573996958r^{16}s^4 +
183616180440r^{18}s^4 - 32546593518r^{20}s^4 - 8997506820r^{22}s^4 + 97752s^6 + 5220612r^2s^6 -
68684580r^4s^6 + 3243820496r^6s^6 - 25244548160r^8s^6 + 5976857720r^{10}s^6 -
147067477144r^{12}s^6 + 458758743568r^{14}s^6 - 749675452344r^{16}s^6 + 435217945700r^{18}s^6 -
16479111716r^{20}s^6 - 1445289s^8 - 96417162r^2s^8 - 666538860r^4s^8 - 25244548160r^6s^8 +
194515866042r^8s^8 - 421026680628r^{10}s^8 + 611623295476r^{12}s^8 -
331561483632r^{14}s^8 + 7820601831r^{16}s^8 + 72391117294r^{18}s^8 + 12200622r^{10} +
924427224r^2s^{10} + 15034322304r^4s^{10} + 5976857720r^6s^{10} - 421026680628r^8s^{10} +
421043188488r^{10}s^{10} - 1131276050256r^{12}s^{10} - 196657371288r^{14}s^{10} +
151002519894r^{16}s^{10} - 64150356s^{12} - 4865103360r^2s^{12} - 86727881244r^4s^{12} -
147067477144r^6s^{12} + 611623295476r^8s^{12} - 1131276050256r^{10}s^{12} + 586397171964r^{12}s^{12} -
231584205720r^{14}s^{12} + 220161216s^{14} + 14947388808r^2s^{14} + 226469888328r^4s^{14} +
458758743568r^6s^{14} - 331561483632r^8s^{14} - 196657371288r^{10}s^{14} - 231584205720r^{12}s^{14} -
504431361s^{16} - 27714317286r^2s^{16} - 296573996958r^4s^{16} - 749675452344r^6s^{16} +
\]
We check visually that the zero set of $P_2$ does indeed coincide with the curves of peak intensity for the $U_2$ QRW.

Before embarking on the proof, let us be clear about what is required. If $r$ is in the boundary of the feasible region, then $\kappa$ must vanish at the pre-images of $r$ in the unit torus. The boundary, $\partial G$, of the feasible region is therefore a component of a real algebraic variety, $W$. The variety $W$ is the image under the logarithmic Gauss map $\mu$ of the points of the unit torus where $Q$ and $\kappa$ both vanish. Computing this variety is easy in principle: two algebraic equations in $(x, y, z, r, s)$ give the conditions for $\mu(x, y, z) = (r, s)$ and two more give conditions for $Q(x, y, z) = \kappa(x, y, z) = 0;
algebraically eliminating \( \{x, y, z\} \) then gives the defining polynomial \( P_2 \) for \( W \). In fact, due to the number of variables and the degree of the polynomials, a straightforward Gröbner basis computation does not work and we need to use iterated resultants in order to get the computation to halt. The last step is to discard extraneous real zeros of \( P_2 \), namely those in the interior of \( G \) or \( G^c \), so as to arrive at a precise description of \( \partial G \).

**Proof.** To eliminate subscripts, we use the variables \((x, y, z)\) instead of \((x_1, x_2, y)\). The condition for \( z \in \mathbb{Z}(r, s) \) is given by the vanishing of two polynomials \( H_1 \) and \( H_2 \) in \((x, y, z, r, s)\), where

\[
H_1(x, y, z, r, s) := xQ_x - rzQ_z ;
\]

\[
H_2(x, y, z, r, s) := yQ_y - szQ_z .
\]

The curvature of \( \mathcal{V}_1 \) at \( z \) also vanishes when a single polynomial vanishes, which we will call \( L(x, y, z) \). We derive an explicit formulae for \( L \): For \((x, y, z) \in \mathcal{V}_1\), write \( x = e^{iX} \), \( y = e^{iY} \) and \( z = e^{iZ} \). By Proposition 4.1 we know that \( Q_z \neq 0 \) on \( \mathcal{V}_1 \), hence the parametrization of \( \mathcal{V}_1 \) by \( X \) and \( Y \) near a point \((x, y, z)\) is smooth and the partial derivatives \( Z_X, Z_Y, Z_{XX}, Z_{XY}, Z_{YY} \) are well defined. Implicitly differentiating \( Q(e^{iX}, e^{iY}, e^{iZ(X,Y)}) = 0 \) with respect to \( X \) and \( Y \) we obtain

\[
Z_X = \frac{-xQ_x}{zQ_z} \quad \text{and} \quad Z_Y = \frac{-yQ_y}{zQ_z},
\]
and differentiating again yields

\[
Z_{XX} = \frac{-ixz}{(zQ_z)^3} \left[ Q_x Q_z(zQ_z - 2xzQ_{xz} + xQ_x) + xz(Q_x^2 Q_{zz} + Q_z^2 Q_{xx}) \right] ;
\]

\[
Z_{YY} = \frac{-iyz}{(zQ_z)^3} \left[ Q_y Q_z(zQ_z - 2yzQ_{yz} + zQ_y) + yz(Q_y^2 Q_{zz} + Q_z^2 Q_{yy}) \right] ;
\]

\[
Z_{XY} = \frac{-ixyz}{(zQ_z)^3} \left[ zQ_z(zQ_{xy} - Q_x Q_{yz} - Q_y Q_{xz}) + Q_x Q_y Q_z + zQ_x Q_y Q_{zz} \right] .
\]

In any dimension, the Gaussian curvature vanishes exactly when the determinant of the Hessian vanishes of any parametrization of the surface as a graph over \(d - 1\) variables. In particular, the curvature vanishes when

\[
\det \begin{pmatrix} Z_{XX} & Z_{XY} \\ Z_{XY} & Z_{YY} \end{pmatrix}
\]

vanishes, and plugging in the computed values yields the polynomial

\[
L(x, y, z) := -xyzQ_x^2 Q_y^2 + zQ_z Q_x^2 Q_y - 2yzQ_x Q_y Q_{yz} + yQ_x Q_z Q_y^2 + yzQ_x Q_y Q_{zz} \\
+ yzQ_x Q_y Q_{yy} - 2xzQ_x Q_z Q_{xz} Q_y + 2xyQ_x Q_x Q_y Q_{yz} - 2xyzQ_x Q_y Q_{xz} Q_y \\
+ xQ_x^2 Q_y + xyQ_x^2 Q_y Q_{yy} + xQ_x^2 Q_z Q_y + yzQ_x Q_y Q_{xx} Q_y + xQ_x Q_y Q_{xx} Q_y \\
- 2xyzQ_x Q_y Q_{yy} + xyQ_x Q_y Q_{xy} Q_{yz} + xyQ_x Q_y Q_{xy} Q_{xz} + xyzQ_x Q_y Q_{xx} Q_y \\
- xyQ_x Q_{yz} + 2xyzQ_x Q_y Q_{yz} + 2xyzQ_x Q_y Q_{yy} - 2xyzQ_x Q_{yz} Q_{yy} \\
- 2xyzQ_x Q_y Q_{xyz} Q_{yz}.
\]

It follows that the curvature of \(\mathcal{V}_1\) vanishes for some \((x, y, z) \in Z(r, s)\) if and only if the four polynomials \(Q, H_1, H_2\) and \(L\) all vanish at some point \((x, y, z, r, s)\) with \((x, y, z) \in T^3\). Ignoring the condition \((x, y, z) \in T^3\) for the moment, we see that we
need to eliminate the variables \((x, y, z)\) from the four equations, leading to a one-dimensional ideal in \(r\) and \(s\). Unfortunately Gröbner basis computations can have very long run times, with published examples showing for example that the number of steps can be doubly exponential in the number of variables. Indeed, we were unable to get Maple to halt on this computation (indeed, on much smaller computations).

The method of resultants, however, led to a quicker elimination computation.

**Definition 5.2** (resultant). Let \(f(x) := \sum_{j=0}^{\ell} a_j x^j\) and \(g(x) := \sum_{j=0}^{m} b_j x^j\) be two polynomials in the single variable \(x\), with coefficients in a field \(K\). Define the resultant \(\text{result}(f, g, x)\) to be the determinant of the \((\ell + m) \times (\ell + m)\) matrix

\[
\begin{pmatrix}
  a_0 & b_0 \\
  a_1 & a_0 & b_1 & b_0 \\
  a_2 & a_1 & \ddots & b_2 & b_1 & \ddots \\
  \vdots & a_2 & \ddots & a_0 & \vdots & b_2 & \ddots & b_0 \\
  a_l & \vdots & a_1 & b_m & \vdots & \ddots & b_1 \\
  a_l & \vdots & a_2 & b_m & \vdots & b_2 & \ddots & \vdots \\
  \vdots & \vdots & \ddots & \vdots & \ddots & \ddots & \ddots & \vdots \\
  a_l & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & b_m \\
  & & & & & & b_m \\
\end{pmatrix}
\]

The crucial fact about resultants is the following fact, whose proof may be found in a number of places such as [CLO98, GKZ94]:

\[
\text{result}(f, g, x) = 0 \iff \exists x : f(x) = g(x) = 0. \quad (5.3)
\]

Iterated resultants are not quite as nice. For example, if \(f, g, h\) are polynomials in
$x$ and $y$, they may be viewed as polynomials in $y$ with coefficients in the field of rational functions, $K(x)$. Then $\mathsf{bresult}(f, h, y)$ and $\mathsf{bresult}(g, h, y)$ are polynomials in $x$, vanishing respectively when the pairs $(f, h)$ and $(g, h)$ have common roots. The quantity

$$R := \mathsf{bresult}(\mathsf{bresult}(f, h, y), \mathsf{bresult}(g, h, y), x)$$

will then vanish if and only if there is a value of $x$ for which $f(x, y_1) = h(x, y_1) = 0$ and $g(x, y_2) = h(x, y_2) = 0$. It follows that if $f(x, y) = g(x, y) = 0$ then $R = 0$, but the converse does not in general hold. A detailed discussion of this may be found in [BM07].

For our purposes, it will suffice to compute iterated resultants and then pass to a subvariety where a common root indeed occurs. We may eliminate repeated factors as we go along. Accordingly, we compute

$$R_{12} := \mathsf{Rad}(\mathsf{bresult}(Q, L, x))$$

$$R_{13} := \mathsf{Rad}(\mathsf{bresult}(Q, H_1, x))$$

$$R_{14} := \mathsf{Rad}(\mathsf{bresult}(Q, H_2, x))$$

where $\mathsf{Rad}(P)$ denotes the product of the first powers of each irreducible factor of $P$. Maple is kind to us because we have used the shortest of the four polynomials, $Q$, in each of the three first-level resultants. Next, we eliminate $y$ via

$$R_{124} := \mathsf{Rad}(\mathsf{bresult}(R_{12}, R_{14}, y))$$

$$R_{134} := \mathsf{Rad}(\mathsf{bresult}(R_{13}, R_{14}, y)).$$
Polynomials $R_{124}$ and $R_{134}$ each have several small univariate factors, as well as one large multivariate factor which is irreducible over the rationals. Denote the large factors by $f_{124}$ and $f_{134}$. Clearly the univariate factors do not contribute to the set we are looking for, so we eliminate $z$ by defining

$$R_{1234} := \mathcal{Rad}(\beta\text{result}(f_{124}, f_{134}, z)).$$

Maple halts, and we obtain a single polynomial in the variables $(r, s)$ whose zero set contains the set we are after. Let $\Omega$ denote the set of $(r, s)$ such that $\kappa(x, y, z) = 0$ for some $(x, y, z) \in \mathcal{V}$ with $\mu(x, y, z) = (r, s)$ [note: this definition uses $\mathcal{V}$ instead of $\mathcal{V}_1$.]

It follows from the symmetries of the problem that $\Omega$ is symmetric under $r \mapsto -r$ as well as $s \mapsto -s$ and the interchange of $r$ and $s$. Computing iterated resultants, as we have observed, leads to a large zero set $\Omega'$; the set $\Omega'$ may not possess $r$-$s$ symmetry, as this is broken by the choice of order of iteration. Factoring the iterated resultant, we may eliminate any component of $\Omega'$ whose image under transposition of $r$ and $s$ is not in $\Omega'$. Doing so, yields the irreducible polynomial $P_2$. Because the set $\Omega$ is algebraic and known to be a subset of the zero set of the irreducible polynomial $P_2$, we see that $\Omega$ is equal to the zero set of $P_2$.

Let $\Omega_0 \subseteq \Omega$ denote the subset of those $(r, s)$ for which as least one $(x, y, z) \in \mu^{-1}((r, s))$ with $\kappa(x, y, z) = 0$ lies on the unit torus. It remains to check that $\Omega_0$ consists of those $(r, s) \in \Omega$ with $|r| + |s| < 3/4$.

The locus of points in $\mathcal{V}$ at which $\kappa$ vanishes is a complex algebraic curve $\gamma$ given by the simultaneous vanishing of $Q$ and $L$. It is nonsingular as long as $\nabla Q$ and
\( \nabla L \) are not parallel, in which case its tangent vector is parallel to \( \nabla Q \times \nabla L \). Let 
\( \rho := xQ_x/(zQ_z) \) and \( \sigma := yQ_y/(zQ_z) \) be the coordinates of the map \( \mu \) under the
identification of \( \mathbb{C}P^2 \) with \( \{ (r, s, 1) : r, s \in \mathbb{C} \} \). The image of \( \gamma \) under \( \mu \) (and this
identification) is a nonsingular curve in the plane, provided that \( \gamma \) is nonsingular and
either \( d\rho \) or \( d\sigma \) is nonvanishing on the tangent. For this it is sufficient that one of
the two determinants \( \det M_\rho, \det M_\sigma \) does not vanish, where the columns of \( M_\rho \) are
\( \nabla Q, \nabla L, \nabla \rho \) and the columns of \( M_\sigma \) are \( \nabla Q, \nabla L, \nabla \sigma \).

Let \((x_0, y_0, z_0)\) be any point in \( \mathcal{V}_1 \) at which one of these two determinants does
not vanish. It is shown in [BBBP08, Proposition 2.1] that the tangent vector to \( \gamma \) at
\((x_0, y_0, z_0)\) in logarithmic coordinates is real; therefore the image of \( \gamma \) near \((x_0, y_0, z_0)\)
is a nonsingular real curve. Removing singular points from the zero set of \( P_2 \) leaves
a union \( \mathcal{U} \) of connected components, each of which therefore lies in \( \Omega_0 \) or is disjoint
from \( \Omega_0 \). The proof of the theorem is now reduced to listing the components, checking
that none crosses the boundary \( |r| + |s| = 3/4 \), and checking \( Z(r, s) \) for a single point
\((r, s)\) on each component (note: any component intersecting \( \{|r| + |s| > 1\} \) need not
be checked as we know the coefficients to be identically zero here).

We close by stating a result for \( U_1 \), analogous to Theorem 5.1. The proof is entirely
analogous as well and will be omitted.

**Theorem 5.3.** For the quantum walk with unitary coin flip \( U_1 \), the curvature of the
variety \( \mathcal{V}_1 \) vanishes at some \((x, y, z) \in Z(r, s)\) if and only if \( |r| \) and \( |s| \) are both at
most \( 2/3 \) and \((r, s)\) is a zero of the polynomial
$$P_1(r, s) := 132019 r^{16} + 2763072 s^2 r^{20} - 513216 s^2 r^{22} - 6505200 s^2 r^{18} + 256 s^2 r^2 + 8790436 s^2 r^{16} - 10639416 s^{10} r^8 + 39759700 s^{12} r^4 - 12711677 s^{10} r^4 + 4140257 s^{12} r^2 - 513216 s^{22} r^2 - 7492584 s^2 r^{14} + 2503464 s^{10} r^6 - 62208 s^{22} + 16 s^6 + 141048 r^{20} + 8790436 s^{16} r^2 + 2763072 s^{20} r^2 - 6505200 s^{18} r^2 - 40374720 s^{18} r^6 + 64689624 s^{16} r^4 - 33614784 s^{18} r^4 + 14725472 s^{10} r^{10} + 121508208 s^{16} r^8 - 1543 s^{10} - 23060 s^2 r^6 + 100227200 s^{10} r^{12} + 7363872 s^{20} r^4 - 176524 s^{18} r^6 + 121508208 s^8 r^{16} - 197271552 s^8 r^{14} - 13374107 s^8 r^6 + 1647627 s^8 r^4 + 18664050 s^8 r^8 - 227481984 s^{10} r^{14} - 19343 s^4 r^4 + 279234496 s^{12} r^{12} - 67173440 s^{14} r^4 - 7492584 s^{14} r^2 + 4140257 s^2 r^{12} + 291173 s^2 r^8 - 1449662 s^2 r^{10} + 7363872 s^4 r^{20} - 227481984 s^{14} r^{10} + 132019 s^{16} - 197271552 s^{14} r^8 - 59209 r^{14} - 1449662 s^{10} r^2 + 100227200 s^{12} r^{10} - 1543 r^{10} - 153035200 s^{14} r^6 - 13374107 s^6 r^8 + 3183044 s^6 r^6 + 39759700 s^4 r^{12} - 176524 s^{18} + 72718 s^6 r^4 + 1647627 s^4 r^8 - 62208 s^{22} + 141048 s^{20} - 1472 s^4 r^2 + 11664 s^{24} - 33614784 s^4 r^{18} + 128187648 s^{16} r^6 - 1472 s^2 r^4 - 67173440 s^4 r^{14} + 291173 s^8 r^2 + 64689624 s^4 r^{16} - 10639416 s^8 r^{10} - 59209 s^{14} + 72718 s^4 r^6 + 92321584 s^8 r^{12} - 56 r^8 + 92321584 s^{12} r^8 - 153035200 s^6 r^{14} - 23060 s^6 r^2 + 128187648 s^6 r^{16} - 40374720 s^6 r^{18} + 72282208 s^{12} r^6 + 14793 r^{12} + 11664 r^{24} + 14793 s^{12} + 16 r^6 + 2503464 s^6 r^{10} - 56 s^8 - 12711677 s^4 r^{10} + 72282208 s^6 r^{12}. $$
6 Next Steps

6.1 Higher dimensions

As with the development of the one-dimensional case in Section 2.2, the two-dimensional QRWs can be generalized beyond the Hadamard walk similarly. Our online database mentioned above includes several 2-dimensional walks. For example, we can take a walk with the same 4 chiralities as above, \{\( (0, 1), (0, -1), (1, 0), (-1, 0) \)\}, the unitary matrix

\[
U := \begin{array}{cccc}
57 & -12 & 30 & 14 \\
67 & 67 & 67 & 67 \\
204 & 17 & -30 & 366 \\
469 & 469 & 469 & 469 \\
-10 & 390 & 33 & 120 \\
469 & 469 & 469 & 469 \\
138 & 246 & -40 & 249 \\
469 & 469 & 469 & 469 \\
\end{array}
\]

and a starting distribution of the particle with amplitude \( \frac{1}{\sqrt{2}} \) in each of the first two chiralities. After 200 steps, we get the distribution in Figure 6.1, where as above, darker spots represent higher probabilities of the particle ending in that location.

Similarly, we can extend the process to 3 or more dimensions. For 3 dimensions, we choose the chiralities \{\( (0, 0, 1), (0, 0, -1), (0, 1, 0), (0, -1, 0), (1, 0, 0), (1, 0, 0), (-1, 0, 0) \)\} with a
Figure 9: The probability distribution of a 2-dimensional QRW after 200 steps.

starting state in the first chirality, and the unitary matrix

\[
\begin{pmatrix}
\frac{2}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\
\frac{1}{3} & \frac{2}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\
\frac{1}{3} & \frac{1}{3} & \frac{2}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\
\frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{2}{3} & \frac{1}{3} & \frac{1}{3} \\
\frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{2}{3} & \frac{1}{3} \\
\frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{2}{3}
\end{pmatrix}
\]

After twenty steps, we obtain the three-dimensional probability distribution Figure 10, where the size of the ball represents the probability it is at that point.
6.2 Multiple peaks

Finally, the QRW database has shown that the number of peaks for a given QRW with the same chiralities and initial state is not independent of the matrix, $U$. Therefore, we would like to investigate what controls the number of peaks. Say that the two QRWs have unitary matrices $U_1$ and $U_2$. One possible technique to compare the two is to use

![Figure 10: A 3-dimensional QRW after 20 steps](image_url)
the inverse of the map from skew-hermitian matrices to unitary matrices described above, in order to find 2 skew-hermitian matrices \( S_1 \) and \( S_2 \) which correspond to \( U_1 \) and \( U_2 \), respectively. Then, we can create a parameter \( t \) in a skew-hermitian matrix \( H \) such that at time \( t = 0 \), \( H = S_1 \), and at time \( t = 1 \), \( H = S_2 \). Through the forward map once again, this parameterization then describes a continuous family of unitary matrices, and therefore a family of QRWs which have a varying number of peaks. Upon further analysis, it should be possible to identify exact values of \( t \) where the QRW switches between numbers of peaks, representing critical QRWs with “double peaks” or other new phenomena. To date, these computations have been too complex to halt in Maple.
References


