QUANTUM RANDOM WALKS ON THE INTEGER LATTICE VIA GENERATING FUNCTIONS

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ABSTRACT

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We analyze several families of one and two-dimensional nearest neighbor Quantum Random Walks. Using a multivariate generating function analysis we give a simplified proof of a known phenomenon for two-chirality walks on the line, namely that the walk has linear speed rather than the diffusive behavior observed in classical random walks. We also demonstrate Airy phenomena between the regions of polynomial and exponential decay. For a three-chirality walk on the line we demonstrate similar behavior, with the addition of a bound state, in which the probability of finding the particle at the origin does not go to zero with time. For each of these walks on the line we obtain exact formulae for the leading asymptotic term of the wave function and the location probabilities. Analyzing two-dimensional walks we again find a region of polynomial decay which grows linearly with time. The limiting shape of the feasible region is, however, quite different. The limit region turns out to be an algebraic set, which we characterize as the rational image of a compact algebraic variety. We also compute the probability profile within the limit region, which is essentially a negative power of the Gaussian curvature of the same algebraic variety. We close with preliminary work concerning walks in higher dimensions.

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1 Introduction

In this thesis we will study methods to determine the asymptotics of multivariate sequences associated with Quantum Random Walks. A multivariate sequence is an array of numbers of the form:

$$\{a_{r_1,\ldots,r_d} : r_1, \ldots, r_d, \in \mathbb{Z}\}$$

which we will abbreviate as $\{a_{\mathbf{r}} : \mathbf{r} \in \mathbb{Z}^d\}$, where d will denote the dimension of the array unless otherwise stated. For $d \leq 3$ we will let r, s and t denote r_1, r_2 and r_3, respectively. The generating function for this sequence is the power series:

$$F(z_1, \ldots, z_d) := \sum_{z_i \in \mathbb{Z}\ \forall i} a_{r_1,\ldots,r_d} z_1^{r_1} \ldots z_d^{r_d}$$

which we abbreviate $F(\mathbf{z}) = \sum_{\mathbf{r} \in \mathbb{Z}^d} a_{\mathbf{r}} \mathbf{z}^{\mathbf{r}}$. When we create a power series, we will often first deal with it formally, without regard to its convergence. We will think of $F(\mathbf{z})$ simply as an element of $\mathbb{C}[[\mathbf{z}]]$ or of $\mathbb{C}((\mathbf{z})) := \mathbb{C}[[\mathbf{z}]][1/z]$ if negative indices are required. For $d \leq 3$ we let x, y and z denote z_1, z_2 and z_3, respectively.

Combinatorists have several methods for studying such arrays of numbers. These include, but are not limited to, the determination of associated recurrence relations, generating functions, asymptotics, and exact formulas for the elements of the array. While we will use each of these techniques as the need arises, our ultimate goal will be the determination of asymptotics. To establish asymptotics, the following notation will be important. If there exist $M \in \mathbb{R}^+$ and $N \in \mathbb{N}$ such that $n > N$ implies $|\frac{a_n}{b_n}| \leq M$ we say that $a_n = O(b_n)$. Alternatively if $\lim_{n\to\infty} \frac{a_n}{b_n} = 0$ we write that $a_n = o(b_n)$. Lastly if $\lim_{n\to\infty} \frac{a(n)}{b(n)} = 1$, we say that $a(n) \sim b(n)$, while noting that this is equivalent to "$a(n) = (1 + o(1)) \cdot b(n)$". In Chapter 2 we will see that asymptotics can often be even more useful than the determination of an exact formula.

For each array we study, there will be some narrative that accompanies it. If the array counts the elements of a sequence of sets, we will have $a_{\mathbf{r}} \in \mathbb{Z}^+$. If it is a sequence of probabilities, then each $a_{\mathbf{r}}$ will be in the interval $[0,1]$ and for each fixed t_0, we will have $\sum_{(r_1,\ldots,r_d)\in\mathbb{Z}^d} a_{(r_1,\ldots,r_d,t_0)} = 1$. It is also possible that $a_{\mathbf{r}} \in \mathbb{C}$, as will be the case with Quantum Random Walks.

Suppose the narrative is that a particle begins at the origin, moves to the right with probability p and stays still with probability $1-p$. Then if $a_{\mathbf{r}} = a_{r,s}$ designates the probability that the particle is at position r at time s, then it is immediate that $a_{\mathbf{r}} \in \mathbb{R}$ and $a_{r,s} = 0$ for $r \notin \{0, 1, \cdots, s\}$. The recurrence relation for this sequence would be $a_{r,s} = (1-p)a_{r,s-1} + pa_{r-1,s-1}$. Using this relation as well as the initial values above, we can derive the generating function $F(x,y) = \sum_{(r,s)\in(\mathbb{Z}^+)^2} a_{r,s}x^r y^s = \frac{1}{1-(1-p+px)y}$. The algebraic variety associated to this generating function is the set of points where its denominator vanishes. This variety, known as the singular variety, would thus be the set of points $\{(x,y) \in \mathbb{C}^2 : 1-(1-p+px)y = 0\}$. In many of the examples of interest to us, the generating function and singular variety will be necessary to derive formulas and asymptotics for the terms of the sequence. We will demonstrate a class of examples, including the Quantum Random Walk, in which the key contribution towards asymptotics comes from the Gaussian curvature of the singular variety.

In the case above, we can equate $a_{r,s}$ with the probability of getting exactly r heads from s coin flips. The binomial formula delivers $a_{r,s} = \binom{s}{r}p^r(1-p)^{s-r} = \binom{s}{r}(\frac{p}{1-p})^r(1-p)^s$. Then using Stirling's Formula: $n! \sim (\frac{n}{e})^n\sqrt{2\pi n}$, we obtain the asymptotic approximation:

$$a_{r,s} \sim \left[(1-p)\frac{s}{s-r}\right]^s \left[(\frac{p}{1-p})(\frac{s-r}{r})\right]^r \sqrt{\frac{s}{2\pi r(s-r)}}$$

The narrative above describes a variant of the classical random walk on the line in which the particle moves to the left and right with probabilities p and $1-p$, respectively. Variants of the classical random walk are used as the basis for algorithms for counting, sampling, and testing properties such as satisfiability of Boolean formulae or graph connectivity. The probability distribution of a particle undergoing a classical random walk converges to a normal distribution as time s increases. The particle's expected location is at the origin, and its standard deviation is $\frac{1}{2}\sqrt{s}$. As a result, $\Pr(x \in [-M\sqrt{s}, M\sqrt{s}]) \to 1$ uniformly in s as $M \to \infty$.

In contrast, in the Quantum Random Walk, it is not the particle's probability distribution that is directly affected by the coin flip, but its amplitude distribution, where probability will be the square of the norm of the amplitude. This fact will necessitate the introduction of an extra degree of freedom, called *chirality* or *spin* which will in turn lead to the phenomenon of quantum interference. This setup, detailed in Chapter 4, results in a walk on the line with linear speed, rather than the diffusive behavior of the classical walk. While it is yet to be determined whether a quantum computer can be constructed on a large enough scale, or whether such a computer could leverage the quadratic speedup of the Quantum Random Walk, it is evident that these walks merit study.

In Chapter 2 of this thesis we review known results concerning asymptotics of univariate and then multivariate generating functions. We interpret these results and apply them to easy examples. In Chapter 3 we supply further mathematical prerequisites for our results and applications in Chapters 4 and 5. In particular, we summarize results from Differential Geometry and Commutative Algebra that will be needed and are not known to combinatorists. In Section 4.1 we give an in depth introduction to Quantum Random Walks. We then demonstrate the application of Chapter 2 and Chapter 3 to QRWs on the line in Sections 4.2 and 4.4. Section 4.3 applies a method for demonstrating Airy behavior in the region between those of exponential decay and relatively uniform distribution. Chapter 5 develops and applies new theorems for the asymptotics of various QRWs on the plane and begins a discussion of QRWs in dimension greater than 2.

2 Combinatorial and Asymptotic Background

2.1 Univariate Asymptotics and Methods

In the case of the univariate generating $f(x) = \sum_{n=0}^{\infty} a_n x^n$, the concept of an asymptotic approximation is straightforward. One seeks a well known function $b(n)$ such that $\lim_{n\to\infty} \frac{a(n)}{b(n)} = 1$, which we have seen is denoted $a(n) \sim b(n)$. The rate of growth of the coefficients will be dictated by the singularities of f that are closest to the origin. This will be most apparent in the rational case.

2.1.1 Rational Functions

For any rational univariate generating function $f(x) = \frac{g(x)}{h(x)}$, with $\deg(g) = l$ and $\deg(h) = m$, by the fundamental theorem of algebra there will always exist unique $A, r_j \in \mathbb{C}$ (with the r_j in order of ascending modulus) such that $f(x) = \frac{Ag(x)}{\prod_{j=1}^{m}(1-x/r_j)}$. If the r_j are distinct, then with $\deg(p) = \max\{l-m, 0\}$ and $s_j \in \mathbb{C}$, $f(x)$ has the unique partial fraction decomposition $f(x) = p(x) + \sum_{j=1}^{m} \frac{s_j}{1-x/r_j}$ which expands formally to $p(x) + \sum_{j=1}^{m} \sum_{i=0}^{\infty} s_j (x/r_j)^i$. Then for $n > \deg(p)$, there is the exact formula $a_n = \sum_{j=1}^{m} s_j r_j^{-n}$ and the asymptotic estimate $a_n \sim s_1 r_1^{-n}$. If $|r_1| = |r_2| = \ldots = |r_p|$, the asymptotic estimate would be $a_n = \sum_{j=1}^{p} s_j r_j^{-n}$. Thus in this simplest case, the poles closest to the origin dictate asymptotics.

An example will help one develop a feel for the preference between an explicit formula and asymptotics. In the case of the famous fibonacci sequence, $a_0 = 0$, $a_1 = 1$ and $a_n = a_{n-1} + a_{n-2}$ for $n > 1$. To solve for $f(x) = \sum_{n=0}^{\infty} a_n x^n$ we multiply each side of the recurrence relation by x^n and sum over n beginning with $n = 2$. The left hand side of the equation becomes $\sum_{n=2}^{\infty} a_n x^n = f(x) - a_1 x - a_0 = f(x) - x$. The right hand side becomes $\sum_{n=2}^{\infty} a_{n-1} x^n + \sum_{n=2}^{\infty} a_{n-2} x^n = x(f(x) - a_0) + x^2 f(x) = (x + x^2) f(x)$. Equating the two sides and solving for $f(x)$ gives $f(x) = \frac{x}{1-x-x^2}$. In the form of the partial fraction decomposition above, $r_1 = \frac{-1+\sqrt{5}}{2}$, $r_2 = \frac{-1-\sqrt{5}}{2}$, $s_1 = \frac{1}{\sqrt{5}}$ and $s_2 = -\frac{1}{\sqrt{5}}$, so for all n, $a_n = \frac{1}{\sqrt{5}}\left[(\frac{2}{-1+\sqrt{5}})^n - (\frac{2}{-1-\sqrt{5}})^n\right] = \frac{1}{\sqrt{5}}\left[(\frac{1+\sqrt{5}}{2})^n - (\frac{1-\sqrt{5}}{2})^n\right]$. At this point one concerned with the number theoretic properties of the fibonacci numbers would want this formula. However, one concerned with the growth of the fibonacci numbers as $n \to \infty$ would prefer the asymptotic estimate $a_n \sim \frac{1}{\sqrt{5}}\left[\frac{1+\sqrt{5}}{2}\right]^n$. In this particular case, since for all n, $\frac{1}{\sqrt{5}}(\frac{1-\sqrt{5}}{2})^n < 1$, one can determine the n^{th} fibonacci number most efficiently by taking the asymptotic estimate and rounding to the nearest integer.

Now we suppose that the r_j are not distinct. In this case we show that asymptotics are dictated by the pole of highest multiplicity among those closest to the origin. We will use the fact, proven by induction and a simple substitution, that the coefficients of $(1 - x/r_j)^{-k}$ are given by the equation $a_n = \binom{n+k-1}{k-1} r_j^{-n}$. Again $f(x)$ has a partial fraction decomposition, now of the form $\sum_{j=1}^{t}\sum_{i=1}^{m_j} \frac{s_{ij}}{(1-x/r_j)^i}$ where f has t distinct roots and r_j has multiplicity m_j. The coefficients are then given by the formula: $a_n = \sum_{j=1}^{t}\sum_{i=1}^{m_j} s_{ij}\binom{n+i-1}{i-1} r_j^{-n}$. Now the leading terms are those that minimize $|r_j|$ and among those, maximize i. If there is a unique root r_{j_0} of minimal modulus and then of maximal multiplicity m_{j_0}, the coefficients have asymptotic approximation $a_n \sim s_{m_{j_0} j_0}\binom{n+m_{j_0}-1}{m_{j_0}-1} r_{j_0}^{-n}$

2.1.2 Analytic Methods

At first we assume $f(x)$ is rational with distinct simple poles and adopt the notation from the prior section. It is worth noting that if we were to expand $f(x)$ in a Laurent series around the pole $x = r_j$, the coefficient of $\frac{1}{x-r_j}$, also known as the *residue* of f at r_j, denoted $\mathrm{RES}\,(f, r_j)$, would be $-s_j r_j$. $\mathrm{RES}\,(f, r_j)$ can also be calculated as $\frac{g(r_j)}{h'(r_j)}$. Thus when the r_j are distinct, without calculating the partial fraction decomposition we determine $s_j = -\frac{\mathrm{RES}\,(f,r_j)}{r_j} = -\frac{g(r_j)}{r_j h'(r_j)}$.

If $f(x) = \sum_{n=1}^{\infty} a_n x^n$ is not rational we can still show that the singularities closest to the origin play a pivotal role. If the closest singularity to the origin r_1 has modulus R, then R will be the radius of convergence of the power series. Since R can be written as $\frac{1}{\limsup_{n\to\infty} |a_n|^{1/n}}$, we know there exists N such that for all $n > N$, $|a_n| < (\frac{1}{R} + \epsilon)^n$ while for infinitely many values of n, $|a_n| > (\frac{1}{R} - \epsilon)^n$.

As an example we consider the Catalan numbers. While this sequence is famous for having countless alternate definitions, we define a_n as the number of acceptable sequences of n left parentheses and n right parentheses such that for all $1 \leq j \leq n$, the j^{th} left parenthesis occurs before the j^{th} right parenthesis. In order to determine a recurrence relation, we let b_n denote the number of sequences of n left parenthesis and n right parenthesis such that for no $1 \leq j \leq n-1$ can one cut off the sequence after $2j$ parenthesis and have an acceptable sequence. In other words, one could say that b_n counts minimal acceptable sequence. It is important to note that every sequence counted by b_n begins with two left parenthesis and ends with two right parenthesis. If the second parenthesis had been a right, then the first two parenthesis would have been an acceptable sequence, while if the penultimate parenthesis had been a left, then the first $2n-2$ parenthesis would have been an acceptable sequence. Since every acceptable sequence has some j such that the first $2j$ parenthesis is a minimal acceptable sequence, we can write $a_n = \sum_{j=1}^{n} b_j \cdot a_{n-j}$. Meanwhile, if a minimal acceptable sequence sheds its first and last parentheses, the result is some (not necessarily minimal) acceptable sequence, so $b_n = a_{n-1}$. Making this substitution in the recurrence relation above we get $a_n = \sum_{j=1}^{n} a_{j-1} \cdot a_{n-j}$ as long as $n > 0$. In the language of generating functions, this implies that $f(x) = xf(x)^2 + 1$. (The 1 on the right hand side accounts for the $n = 0$ case and the extra x takes into account the fact that the a indices on the right side of the recurrence relation only sum to $n-1$.) Solving for $f(x)$ then gives $f(x) = \frac{1 \pm \sqrt{1-4x}}{2x}$, while the nonextraneous solution is $f(x) = \frac{1-\sqrt{1-4x}}{2x}$ as it is analytic at the origin. One can confirm this by rationalizing the numerator: $\frac{1-\sqrt{1-4x}}{2x} = \frac{2}{1+\sqrt{1-4x}}$. Using the binomial series expansion we get $f(x) = -\frac{1}{2}\sum_{k=1}^{\infty}\binom{k-3/2}{k}x^{k-1}4^k$ so $a_n = -\frac{1}{2}\binom{n-1/2}{n+1}4^{n+1}$. From a glance at the generating function, it is clear that $R = 1/4$, so we would immediately know that $a_n \sim p(n)4^n$ where $p(n)$ is subexponential.

2.1.3 Saddle Point Methods

The coefficients of a generating function can be written in terms of the Cauchy integral as

$$a_n = \frac{1}{2\pi i}\int_{\gamma} z^{-n-1}F(z)dz$$

where γ is a contour around the origin with winding number 1. Once the coefficients are expressed as integrals, one can attempt to apply the saddle point method, consisting of the following steps, enumerated in Section 3.2 of [Pem09]:

1. Rewrite the integrand as $e^{n\phi}$.
2. Locate the (discrete) set of zeroes of ϕ'.
3. See if γ can be deformed so as to minimize $\Re\{\phi\}$ at such a point.
4. Estimate the integral by integrating a Taylor series development of the integrand term by term.

If step 3 is successful, meaning that the modulus of the integrand falls steeply on either side of its maximum, then multiplying this maximum by the length of the interval where the modulus is near its maximum (or something slightly more fancy) will give a reasonable estimate for the integral. While generically this cannot be done, this situation is analogous to one which we will explore in several variables in Section 2.2, which is why we mention it here.

If step 3 cannot be achieved, but with the integrand rewritten as $\psi(z)\exp(-\lambda f(z))$ the function $\Re\{f\}$ is minimized at a point z_0 in the interior of γ, then Hayman's method [Hay56] can be employed. If furthermore ψ and f are smooth, and $\frac{\partial^2 f}{\partial z^2}|_{z_0} \neq 0$ then Hayman's method gives the estimate:

$$\int_\gamma \psi(z)\exp(-\lambda f(z)) \sim \psi(z_0)\sqrt{\frac{2\pi}{f''(z_0)}}\exp(-\lambda f(z_0))$$

2.2 Established Multivariate Results and Terminology

The subject of our attention henceforth will be a multivariate sequence with rational generating function $F(\mathbf{z}) = \frac{G(\mathbf{z})}{H(\mathbf{z})}$. To discuss the asymptotics of such a multivariate sequence takes a bit of terminology. In contrast to the univariate case in which the index can only approach infinity in a single direction, there are infinitely many directions to approach infinity in the multivariate case. We address this issue by letting the final coefficient r_d go to infinity while keeping r_j/r_d roughly fixed for each $1 \leq j \leq d-1$. Thus when we refer to a direction in which we seek asymptotics, we refer to the $(d-1)$-tuple $(r_1/r_d, \ldots, r_{d-1}/r_d)$. In contrast to the readily determined and understood results for univariate sequences, results in the multivariate case have proven significantly more elusive. In his survey of asymptotic results, Bender [Ben74] wrote: "Practically nothing is known about asymptotics for recursions in two variables even when a generating function is available. Techniques for obtaining asymptotics from bivariate generating functions would be quite useful." The earliest set of results after the publishing of this statement can be referred to collectively as GF-sequence methods. They involve dividing $\{a_{\mathbf{r}}\}$ into a sequence of $(d-1)$-dimensional arrays indexed by r_d. The other older results concern the algebraic extraction of individual diagonals and are appropriately referred to as the diagonal method. We utilize this method in Section 4.4 when our otherwise more powerful techniques fail us. Many of the more recent results involve the use of contour integration, including those in [BM93], [PW02], [PW04] and [PW08]. The last three of these serve as the launching off point for this thesis, and the remainder of this section draws heavily from [PW02] in particular. As the subsection titles below imply, the plan of [PW02] (when dealing with a d-variate generating function F) is to:

1. Use the multidimensional Cauchy integral formula to represent $a_{\mathbf{r}}$ as an integral over a d-dimensional torus inside $\mathbb{C}^d$

2. Expand the surface of integration across a point $\mathbf{z}$ (depending on the direction in which asymptotics may be computed) where F is singular, and use the residue theorem to represent

$a_{\mathbf{r}}$ as a $(d-1)$-dimensional integral of one-variable residues.

3. Put this in the form of an integral $\int \exp(\lambda f(\mathbf{z}))\psi(\mathbf{z})d\mathbf{z}$ for which the large-λ asymptotics can be read off from the theory of oscillating integrals.

2.2.1 Notation

Before moving on, we establish the terminology to be used throughout this section. Any notation which is not explicitly overruled by a later one will persist throughout this thesis. We denote the open domain of convergence of the power series as $\mathcal{D}$. We assume that $F = G/H$ converges in a neighborhood of the origin and can be analytically continued everywhere except a set $\mathcal{V}$ of complex dimension $d-1$ called the *singular variety*. In the cases of interest to us, we will be able to define $\mathcal{V}$ more simply as $\mathcal{V} = \{\mathbf{z} : H(\mathbf{z}) = 0\}$. For $\mathbf{z} \in \mathbb{C}^d$ we let $\mathbf{T}(\mathbf{z})$ denote the torus consisting of points $\mathbf{w}$ with $|w_j| = |z_j|$ for $1 \leq j \leq d$ and let $\mathbf{D}(\mathbf{z})$ denote the closed polydisk consisting of points $\mathbf{w}$ with $|w_j| \leq |z_j|$ for $1 \leq j \leq d$. It will be important that the domain $\mathcal{D}$ is a union of tori $\mathbf{T}(\mathbf{z})$ and is logarithmically convex, meaning that the set $\log\mathcal{D} := \{\mathbf{x} \in \mathbb{R}^d : (e^{x_1}, \ldots, e^{x_d}) \in \mathcal{D}\}$ is a convex subset of $\mathbb{R}^d$ as well as a subset closed under $\leq$ in the coordinatewise partial order. In the dimension two case we use (x, y) instead of (z_1, z_2) and (r, s) instead of (r_1, r_2). In dimension greater than 2 we use $\hat{\mathbf{z}}$ to denote $(z_1, \ldots, z_{d-1})$ in order to facilitate the decomposition $\mathbb{C}^d = \mathbb{C}^{d-1} \times \mathbb{C}$. Also we denote the partial derivative $\frac{\partial H}{\partial z_j}$ as H_j and in dimension 2 we use H_x and H_y. In addition to the notation $f \sim g$ introduced earlier, Pemantle [PW02] adds the notion of a function f being *rapidly decreasing* if $f(x) = O(x^{-N})$ for every N and the function f is *exponentially decreasing* if $f(x) = O(e^{-cx})$ for some $c > 0$. More generally, we write $f \sim \sum b_n g_n$ to mean that $f = \sum_{n=0}^{N} b_n g_n + o(g_N)$, where $b_n \in \mathbb{C}$ and $\{g_n\}$ is a series of functions such that $g_{n+1} = o(g_n)$ for each n.

2.2.2 The Cauchy Integral

The first step in determination of multivariate asymptotics is the use of Cauchy's integral formula:

$$a_{\mathbf{r}} = \left(\frac{1}{2\pi i}\right)^d \int_T \mathbf{w}^{-\mathbf{r}-1} F(\mathbf{w}) d\mathbf{w}$$

where T is a torus surrounding the critical point $\mathbf{z}$ of F that is relevant for $\mathbf{r}$. We then aim to rewrite $\mathbf{w}^{-\mathbf{r}-1}F(\mathbf{w})$ as $\exp(r_d f(\mathbf{w}))\psi(\mathbf{w})$ where ψ will be a residue in r_d of F/w_d while f is such that $\exp(r_d f) = (\mathbf{z}/\mathbf{w})^{\mathbf{r}}$.

2.2.3 Critical Points

As in the univariate case, the points of $\mathcal{V}$ closest to the origin will be the most important in the determination of asymptotics. In that light, we define a point $\mathbf{z} \in \mathcal{V}$ to be *minimal* if $\mathcal{V} \cap \mathbf{D}(\mathbf{z}) \subset \mathbf{T}(\mathbf{z})$. In this case, we call the torus $\mathbf{T}(\mathbf{z})$ a *minimal torus*. If the above condition holds with $\mathcal{V}$ replaced by a neighborhood of $\mathbf{z}$ in $\mathcal{V}$, then we call $\mathbf{z}$ *locally minimal*. Furthermore, depending on whether $|\mathcal{V} \cap \mathbf{D}(\mathbf{z})|$ is 1, finite, or infinite, we call $\mathbf{z}$ *strictly minimal*, *finitely minimal*, or *torally minimal*, respectively. While [PW02] deals strictly with the finitely minimal case, we generalize to the torally minimal case by Chapter 3 of this thesis.

If H vanishes to order 1 at $\mathbf{z}$, we call $\mathbf{z}$ a *simple pole* of F. At such a pole, ∇H does not vanish, so by reordering our indices if necessary, we guarantee that $H_d \neq 0$ at $\mathbf{z}$. Thus by the implicit function theorem there is a neighborhood of $\mathbf{z}$ where $\mathcal{V}$ may be parameterized by $z_d = g(z_1, \ldots, z_{d-1})$ for some analytic function g. We reserve the notation g to refer to this parametrization for the remainder of this chapter. Now on a neighborhood of $\hat{\mathbf{z}}$ we define

$$\psi(\hat{\mathbf{w}}) = -\lim_{w \to g(\hat{\mathbf{w}})} (w - g(\hat{\mathbf{w}})) \frac{F(\hat{\mathbf{w}}, w)}{w}.$$

Then for $\hat{\mathbf{w}} \in \mathbf{T}(\hat{\mathbf{z}})$ we write $w_j = z_j e^{i\theta_j}$. For fixed $\mathbf{r}$ with $r_d \neq 0$, we define a function f on a neighborhood of $\hat{\mathbf{z}}$ in $\mathbf{T}(\hat{\mathbf{z}})$ by:

$$f(\hat{\mathbf{w}}) = \log\left(\frac{g(\hat{\mathbf{w}})}{g(\hat{\mathbf{z}})}\right) + i\sum_{j=1}^{d-1} \frac{r_j}{r_d}\theta_j$$

As our integrals will be parameterized by θ, we compose each of f, g, and ψ with the map $M(\hat{\theta}) = M(\theta_1, \ldots, \theta_{d-1}) = (z_1 e^{i\theta_1}, \ldots, z_{d-1} e^{i\theta_{d-1}})$. We then define $\tilde{g} := g \circ M$, $\tilde{f} := f \circ M$ and $\tilde{\psi} := \psi \circ M$.

2.2.4 Oscillatory Integrals

Our first goal will be to show that the integrals we need to compute are in fact oscillatory, so that we may use the stationary phase method to evaluate them. We do so by showing that to calculate

$$I = \int_{\mathbf{T}} \exp(-r_d \tilde{f}(\theta)) \tilde{\psi}(\theta)) \mathbf{d}\theta \tag{2.1}$$

we need only integrate over a neighborhood $\tilde{\mathcal{N}}$ of $\mathbf{0}$ in $\mathbb{R}^{d-1}$, then showing that $\tilde{f}$ is analytic, Re $\tilde{f} \geq 0$, $\tilde{f}(\mathbf{0}) = 0$ and $\nabla \tilde{f}(\mathbf{0}) = \mathbf{0}$. The function $\tilde{f}$ is referred to as the *phase* of the integral and the plan is to show that asymptotics are dictated by the point where it is *stationary* when $\nabla \tilde{f}(\mathbf{0}) = \mathbf{0}$.

Our first goal is satisfied by the following lemma:

Lemma 2.1 (Lemma 4.1 of [PW02]). *Let $\mathbf{z}$ be a strictly minimal simple pole of $F = G/H$. Assume that $z_d H_d \neq 0$. For a neighborhood $\tilde{\mathcal{N}}$ of $\mathbf{0}$ in $\mathbb{R}^{d-1}$ define a quantity*

$$\Xi := (2\pi)^{1-d} \mathbf{z}^{-\mathbf{r}} \int_{\tilde{\mathcal{N}}} \exp(-r_d \tilde{f}(\hat{\theta})) \tilde{\psi}(\hat{\theta})) d\hat{\theta} \tag{2.2}$$

Then the quantity $|\mathbf{z}^{\mathbf{r}}||a_{\mathbf{r}} - \Xi|$ decreases exponentially as $\tilde{\mathcal{N}}$ remains fixed and $r \to \infty$

Proof: For $\epsilon \in (0, |z_d|)$, let T be the torus $\mathbf{T}(\mathbf{z})$ shrunk in the last coordinate by ϵ, that is, the set of $\mathbf{w}$ for which $|w_j| = |z_j|$, $j < d$ and $|w_d| = |z_d| - \epsilon$. Write Cauchy's formula as an iterated integral

$$a_{\mathbf{r}} = \left(\frac{1}{2\pi i}\right)^d \int_{\mathbf{T}(\hat{\mathbf{z}})} \hat{\mathbf{w}}^{-\hat{\mathbf{r}}-1} \left[\int_{\mathcal{C}_1} w_d^{-r_d} F(\mathbf{w}) \frac{dw_d}{w_d} \right] d\hat{\mathbf{w}} \tag{2.3}$$

Here $\mathcal{C}_1$ is the circle of radius $|z_d| - \epsilon$. Let $K \subset \mathbf{T}(\hat{\mathbf{z}})$ be a compact set not containing $\hat{\mathbf{z}}$. For each fixed $\hat{\mathbf{w}} \in K$, the function $F(\hat{\mathbf{w}}, \cdot)$ has a radius of convergence greater than $|z_d|$. Hence the inner integral in Equation 2.3 is $O(|z_d| + \delta)^{-r_d}$ for some $\delta > 0$. By continuity of the radius of convergence, we may integrate over K to see that $|\mathbf{z}^{\mathbf{r}}| \int_{K \times \mathcal{C}_1} \mathbf{w}^{-\mathbf{r}-\mathbf{1}} F(\mathbf{w}) d\mathbf{w}$ decreases exponentially. Thus if $\mathcal{N}$ is any neighborhood of $\hat{\mathbf{z}}$ in $\mathbf{T}(\hat{\mathbf{z}})$, the quantity

$$|\mathbf{z}^{\mathbf{r}}| \left| a_{\mathbf{r}} - \left(\frac{1}{2\pi i}\right)^d \int_{\mathcal{N}} \hat{\mathbf{w}}^{-\hat{\mathbf{r}}-\mathbf{1}} \left[\int_{\mathcal{C}_1} \frac{F(\mathbf{w})}{w_d^{r_d+1}} dw_d \right] d\hat{\mathbf{w}} \right|$$

decreases exponentially. Thus the problem is reduced to an integral over a neighborhood of $\hat{\mathbf{z}}$.

Near $\mathbf{z}$ there is a parametrization $w_d = g(\hat{\mathbf{w}})$ of $\mathcal{V}$. Let $\mathcal{C}_2$ be the circle of radius $|z_d| + \epsilon$. Then when $\mathcal{N}$ is sufficiently small compared to ϵ, the image of $\mathcal{N}$ under g is disjoint from $\mathcal{C}_2$. Fix such a neighborhood $\mathcal{N}$. For any $\hat{\mathbf{w}} \in \mathcal{N}$, the function $F(\hat{\mathbf{w}}, \cdot)$ has a single simple pole in the annulus bounded by $\mathcal{C}_1$ and $\mathcal{C}_2$, occurring at $g(\hat{\mathbf{w}})$. The residue in the last variable of F at $g(\hat{\mathbf{w}})$ is equal to

$$R(\hat{\mathbf{w}}) := -\psi(\hat{\mathbf{w}}) g(\hat{\mathbf{w}})^{-r_d} \tag{2.4}$$

where ψ is define in the Critical Point section above. Therefore, for each fixed $\hat{\mathbf{w}} \in \mathcal{N}$,

$$\int_{\mathcal{C}_1} \frac{F(\hat{\mathbf{w}})}{w_d^{r_d+1}} dw_d = \int_{\mathcal{C}_2} \frac{F(\hat{\mathbf{w}})}{w_d^{r_d+1}} dw_d - 2\pi i R(\hat{\mathbf{w}}).$$

But $|\mathbf{z}^{\mathbf{r}} \int_{\mathcal{C}_2} F(\mathbf{w}) dw_d / \mathbf{w}^{\mathbf{r}+\mathbf{1}}|$ is bounded by a constant multiple of $(1 + \epsilon/|z_d|)^{-r_d}$ (the constant depending on the maximum of F on $\mathcal{C}_2$) and hence $|\mathbf{z}^{\mathbf{r}}||a_{\mathbf{r}} - X|$ is exponentially decreasing where

$$X = (2\pi i)^{1-d} \int_{\mathcal{N}} \hat{\mathbf{w}}^{-\hat{\mathbf{r}}-\mathbf{1}} g(\hat{\mathbf{w}})^{-r_d} \psi(\hat{\mathbf{w}}) d\hat{\mathbf{w}} \tag{2.5}$$

$$= (2\pi i)^{1-d} \mathbf{z}^{-\mathbf{r}} \int_{\mathcal{N}} \frac{\hat{\mathbf{w}}^{-\hat{\mathbf{r}}}}{\hat{\mathbf{z}}^{-\hat{\mathbf{r}}}} \frac{d\hat{\mathbf{w}}}{\prod_{j=1}^{d-1} w_j} \left(\frac{g(\hat{\mathbf{w}})}{g(\hat{\mathbf{z}})}\right)^{-r_d} \psi(\hat{\mathbf{w}}) \tag{2.6}$$

Changing variables to $w_j = z_j e^{i\theta_j}$ and thus $dw_j = i w_j d\theta_j$ turns the quantity X into

$$(2\pi)^{1-d} \mathbf{z}^{-\mathbf{r}} \int_{\tilde{\mathcal{N}}} \prod_{j=1}^{d-1} e^{-i r_j \theta_j} \tilde{\psi}(\hat{\theta}) \left(\frac{g(\hat{\mathbf{w}})}{g(\hat{\mathbf{z}})}\right)^{-r_d} d\hat{\theta}$$

and plugging in the definitions of f and $\tilde{f}$ above yields

$$(2\pi)^{1-d} \mathbf{z}^{-\mathbf{r}} \int_{\tilde{\mathcal{N}}} \exp(-r_d \tilde{f}(\hat{\theta}) \tilde{\psi}(\hat{\theta}) d\hat{\theta}$$

which is none other than Ξ. $\square$

Now to use results for oscillating integrals, we need only show that $\nabla \tilde{f}(\mathbf{0}) = \mathbf{0}$ and $\Re(\tilde{f}) \geq 0$, as it is immediate that $\tilde{f}$ is analytic and $\tilde{f}(\mathbf{0}) = 0$. To facilitate this, for a given $\mathbf{z} \in \mathcal{V}$ with all nonzero coordinates, we define $\mathbf{dir}\,(\mathbf{z})$ to be the equivalence class of (complex) scalar multiples of the vector $(z_1 H_1, \ldots, z_d H_d)$. Given a direction $\mathbf{r}$ we will choose $\mathbf{z}$ so that $\mathbf{r} \in \mathbf{dir}\,(\mathbf{z})$ and refer to the set of all such $\mathbf{z}$ as $\mathrm{crit}(\mathbf{r})$ or $\Xi(\mathbf{r})$.

Given this choice of $\mathbf{z}$, we cite two results of [PW02], reproducing the proof of the second.

Lemma 2.2 (Lemma 2.1 of [PW02])**.** *Let $\mathbf{z}$ be a simple pole of F and suppose that $z_d H_d$ does not vanish there. If $\mathbf{z}$ is locally minimal then for all $j < d$, the quantity $z_j H_j/(z_d H_d)$ is real and nonnegative.* □

As a result, when $\mathbf{z}$ is a minimal pole of F with nonzero coordinates, $\mathbf{dir}\,(\mathbf{z})$ can be considered as a well defined element of $\mathbb{RP}^{d-1}$.

Lemma 2.3 (Lemma 4.2 of [PW02])**.** *The quantity $\tilde{f}(\mathbf{0})$ always vanishes. If $\mathbf{r} \in \mathbf{dir}\,(\mathbf{z})$, then $\nabla \tilde{f}(\mathbf{0}) = \mathbf{0}$ and the real part of $\tilde{f}$ has a strict minimum at $\mathbf{0}$.*

Proof: As mentioned above, the first part is immediate. To prove the second, we first note that if $\mathbf{r} \in \mathbf{dir}\,(\mathbf{z})$, then for each $1 \le j \le d$, $\frac{z_j H_j}{z_d H_d} = \frac{r_j}{r_d}$. Taking the partial derivative of the statement $H(z_1, \ldots, z_{d-1}, g(z_1, \ldots, z_{d-1})) = 0$ with respect to z_k, we get $H_k + \frac{\partial g}{\partial z_k} H_d = 0$ so $\frac{\partial g}{\partial z_k} = -\frac{H_k}{H_d}$. Then with $f(\hat{\mathbf{w}}) = \log\left(\frac{g(\hat{\mathbf{w}})}{g(\hat{\mathbf{z}})}\right) + i\sum_{j=1}^{d-1} \frac{r_j}{r_d}\theta_j$, we have $\frac{\partial f}{\partial \theta_k} = \frac{1}{g}\frac{\partial g}{\partial \theta_k} + i\frac{r_k}{r_d} = \frac{1}{g}\frac{\partial g}{\partial z_k}\frac{\partial z_k}{\partial \theta_k} + i\frac{r_k}{r_d} = -i\frac{z_k H_k}{z_d H_d} + i\frac{r_k}{r_d} = 0$. Lastly, we observe that $\Re\{\tilde{f}(\hat{\theta})\} = -\log|\tilde{g}(\hat{\theta})/z_d|$. By the strict minimality of $\mathbf{z}$, the modulus of $g(\hat{\mathbf{w}}) = \tilde{g}(\hat{\theta})$ is greater than $|z_d|$ for any $\hat{\mathbf{w}} \in \mathbf{T}(\hat{\mathbf{z}})$. □

From Lemma 2.3 above, $\mathbf{0}$ is a stationary point for the function $\tilde{f}$ as long as $\mathbf{r} \in \mathbf{dir}\,(\mathbf{z})$, so we can apply the theorem below from [PW02].

Theorem 2.4 (Theorem 5.4 of [PW02])**.** *Let f be a smooth complex-valued function on a neighborhood of $\mathbf{0}$ in $\mathbb{R}^d$ such that $\Re\{f\} \ge 0$ with equality only at $\mathbf{0}$. Suppose further that $\nabla f(\mathbf{0}) = \mathbf{0}$, and that the Hessian (matrix of second partials) of f has eigenvalues with positive real parts. Let $\mathcal{H}$ denote the Hessian determinant at $\mathbf{0}$. Then for $\psi \in C_0^\infty$, there is an asymptotic expansion*

$$\int \exp(-\lambda f(\mathbf{x}))\psi(\mathbf{x})d\mathbf{x} \sim \sum_{j \ge l} C_j \lambda^{-(j+d)/2}$$

where l is the degree of vanishing of ψ at $\mathbf{0}$. If $l = 0$ then $C_0 = \psi(\mathbf{0})(2\pi)^{d/2}\mathcal{H}^{-1/2}$. The choice of square root is determined by $\mathcal{H}^{-1/2} = \prod_{j=1}^{d} \mu_j^{-1/2}$ where μ_j are the eigenvalues of the Hessian and the principal square root is taken in each case.

PROOF: While we refer the reader to [PW02] for a full proof, we outline the proof here. First let $Q = \sum_{i,j=1}^{d} q_{i,j} z_i z_j$ be the quadratic form determined by the Hessian at the origin. Then change coordinates to make f exactly equal to Q, followed by a change of variables $\mathbf{y}(\mathbf{x})$ so that $Q(\mathbf{x}) = \sum_{j=1}^{d} y_j^2$, which is to say, normalize by $\mathcal{H}$. Next expand $\tilde{\psi}$ into monomials, before moving the region of integration to the real d-space. Evaluating the integral using further results for oscillatory integrals (see Chapter 2 of [Won89] for these) then yields the desired result. □

We note that the bulk of the results on the stationary phase method concern cases in which f is either real or purely imaginary. Using the strict minimality of $\Re\{f\}$ at 0, Pemantle and Wilson adjust for this discrepancy, creating an asymptotic expansion, necessary for some of the upcoming results.

Theorem 2.5 (Theorem 5.2 of [PW02]). *Let f be analytic and complex-valued on an interval $[0, B]$ and suppose that $k \geq 2$ is minimal such that $f^{(k)}(0) \neq 0$ (so in particular $f(0) = f'(0) = 0$). Assume that $f' \neq 0$ on $(0, B]$, and that $\Re\{f\}$ has a strict minimum at 0.*

Let m be minimal so that the real part of $f^{(m)}(0)$ does not vanish. Let $\psi \in C_0^\infty$, let l be minimal such that $\psi^{(l)}(0) \neq 0$, and denote $c_j := f^{(j)}(0)/j!$, $b_j := \psi^{(j)}(0)/j!$ and $b_j^* := \psi^{*(j)}(0)/j!$ where $\psi^* = (\psi \circ \eta) \cdot \eta'$ and η inverts the map $y(x) = f(x)^{1/k}$.

Then there is an asymptotic development

$$\int_0^B \exp(-\lambda f(x))\psi(x)dx \sim \sum_{j=l}^{\infty} A_+(k,j) b_j^* \lambda^{-(j+1)/k}. \tag{2.7}$$

$A_+(k,l)$ is defined as $\frac{1}{k}\Gamma(\frac{l+1}{k})$. The constant in the $O\left(\lambda^{-(N+1)/k}\right)$ term depends continuously (only) on the derivatives of f and ψ up to $(N+1)m/k - 1$.

□

2.2.5 Established Results

The established result of highest relevance to this thesis is Theorem 2.6 below. Many of our results will involve generalizing, reinterpreting and applying this result. Its proof follows from Theorem 2.4, once one identifies $\tilde{\psi}(\mathbf{0})$ as $G(\mathbf{0})/(z_d H_d)$.

Theorem 2.6 (Theorem 3.5 of [PW02])**.** *Let $F = G/H = \sum a_{\mathbf{r}} \mathbf{z}^{\mathbf{r}}$ have a strictly minimal, simple pole at $\mathbf{z}$. Suppose $z_d H_d$ does not vanish. If the Hessian of $\tilde{f}$ at $\mathbf{z}$ is nonsingular, then there is an expansion*

$$a_{\mathbf{r}} \sim \mathbf{z}^{-\mathbf{r}} \sum_{l \geq l_0} C_l r_d^{(1-d-l)/2}$$

where l_0 is the degree to which G vanishes on $\mathcal{V}$ near the point $\mathbf{z}$. When G does not vanish at $\mathbf{z}$ then $l_0 = 0$ and

$$C_0 = (2\pi)^{(1-d)/2} \mathcal{H}^{-1/2} \frac{G(\mathbf{z})}{z_d H_d}$$

where $\mathcal{H}$ is the determinant of the Hessian at $\mathbf{z}$.

□

The use of this theorem involves several intermediate steps. Given a generating function $F(\mathbf{z}) = G(\mathbf{z})/H(\mathbf{z})$, one must calculate $\tilde{f}$, $\tilde{\psi}$, and $\mathcal{H}$, as well as the critical point $\mathbf{z} \in \Xi(\mathbf{r})$. While the last calculation will persist in any general theorem, the first three are removed in the $d = 2$ case by Theorem 2.7. On the other hand, as Pemantle and Wilson put it in [PW02] "As we state more general theorems, it becomes cumbersome and in fact obfuscating to give formulae for the expansion coefficients directly in terms of derivatives of G and H." Another issue is the apparent designation of the d^{th} coordinate in the result. This persists in the following theorem, where the result does not appear to be symmetric in x and y. While the result is in fact canonical, we will not see this until we recast in terms of curvature in Section 5.2. Recall that in the $d = 2$ case we denote (z_1, z_2) as (x, y) and (r_1, r_2) as (r, s).

Theorem 2.7 (Theorem 3.1 of [PW02])**.** *Let $F = G/H$ be a meromorphic function of two variables, not singular at the origin. Define*

$$Q(x,y) = -x^2 H_x^2 y H_y - x H_x y^2 H_y^2 - x^2 y^2 (H_x^2 H_{yy} + H_y^2 H_{xx} - 2H_x H_y H_{xy}).$$

Then

$$a_{r,s} \sim \frac{G(x,y)}{\sqrt{2\pi}} x^{-r} y^{-s} \sqrt{\frac{-yH_y}{sQ}}$$

uniformly as (x,y) varies over a compact set of strictly minimal, simple poles of F on which Q and G are nonvanishing, and $(r,s) \in \mathbf{dir}\,(x,y)$.

Proof: While we refer the reader interested in an exact proof of Theorem 2.7 to [PW02], we observe that the key steps in its proof include the evaluation of $\tilde{f}''(0)$ (which is equivalent to $\mathcal{H}$ in the $d = 2$ case) in terms of the partial derivatives, as well as an application of a more general, two sided integral version of Theorem 2.5, which provides the uniform estimate. In the case of a strictly minimal simple pole where Q and G are nonvanishing, the leading asymptotic term is the $k = 2, l = 0$ term in Equation 2.7, for which $A_+(2,0) = \frac{1}{2}\Gamma(\frac{1}{2}) = \sqrt{\pi}/2$. While we do not demonstrate the complete evaluation of $\tilde{f}''(0)$ here, we will do so in the more general $d = 3$ case in Section 2.3 below. □

One can generalize either of the above theorems to the finitely minimal case using a partition of unity argument to develop the corollary below.

Corollary 2.8 (Corollary 3.7 of [PW02])**.** *Suppose $\mathbf{z}$ is a finitely minimal point of $\mathcal{V}$ with $\mathcal{V} \cap \mathbf{T}(\mathbf{z}) = \{\mathbf{z}_1, \ldots, \mathbf{z}_n\}$. Then*

$$a_{\mathbf{r}} \sim \sum_{j=1}^{n} E_j(\mathbf{r})$$

where $E_j(\mathbf{r})$ is the asymptotic expression given by the previous theorems with $\mathbf{z} = \mathbf{z}_j$. In other words, if there are finitely many points on $\mathcal{V} \cap \mathbf{T}(\mathbf{z})$, then sum the contributions as if each were strictly minimal.

□

2.3 Interpretation of Multivariate Results and Examples

Despite the comment by Pemantle and Wilson quoted in Section 2.2 concerning explicit results in terms of G and H, we find that for the $d = 3$ case, explicit results can facilitate the use of Theorem 2.6. Recall that in this case we denote (z_1, z_2, z_3) as (x, y, z) and (r_1, r_2, r_3) as (r, s, t).

Corollary 2.9. *Let $F = G/H$ be a meromorphic function of two variables, not singular at the origin. Then*

$$a_{r,s,t} \sim \frac{G(x,y,z)zH_z}{2\pi t\xi\sqrt{-Q(x,y,z)}}x^{-r}y^{-s}z^{-t}$$

uniformly as (x, y, z) varies over a compact set of strictly minimal, simple poles of $F(x, y, z)$ on which $Q(x, y, z)$ and $G(x, y, z)$ are nonvanishing, and $(r, s, t) \in \mathbf{dir}\,(x, y, z)$, where ξ is a root of unity consistent with the choice of square root of $\mathcal{H}$ and $Q(x, y, z)$ is defined as the symmetric polynomial

$$Q(x,y,z) := \frac{Q(x,z)Q(y,z) - R(x,y,z)^2}{(zH_z)^2}$$

with the polynomial Q in two variables defined as in the statement of Theorem 2.7 and $R(x, y, z)$ defined as

$$R(x,y,z) := xyz\left(zH_z(H_{xy}H_z - H_xH_{yz} - H_yH_{xz}) + H_xH_yH_z + zH_xH_yH_{zz}\right).$$

Proof: When $d = 3$ the Hessian determinant is:

$$\mathcal{H} = \det\begin{pmatrix} \frac{\partial^2 Z}{\partial X^2} & \frac{\partial^2 Z}{\partial X \partial Y} \\ \frac{\partial^2 Z}{\partial Y \partial X} & \frac{\partial^2 Z}{\partial Y^2} \end{pmatrix}$$

in which X, Y and Z represent the complex arguments of x, y and z, respectively. As (X, Y) varies over a neighborhood of $(0, 0) \in S^1 \times S^1$ we define h such that $H(e^{iX}, e^{iY}, e^{ih(X,Y)}) = 0$. Differentiating the statement $H(e^{iX}, e^{iY}, e^{ih(X,Y)}) = 0$ with respect to X results in the equation $ie^{iX}H_x + ie^{ih(X,Y)}H_zh_X = 0$. Recalling that $x = e^{iX}$ and $z = e^{ih(X,Y)}$, we get that $\frac{\partial Z}{\partial X} = h_X = -\frac{xH_x}{zH_z}$. Similarly $\frac{\partial Z}{\partial Y} = h_Y = -\frac{yH_y}{zH_z}$. Differentiating these statements with respect to X and Y, and making the proper substitutions using the above identities, we get

$$\begin{aligned}
\frac{\partial^2 Z}{\partial X^2} &= \frac{-ixz}{(zH_z)^3}\left(H_xH_z(zH_z - 2xzH_{xz} + xH_x) + xz(H_x^2H_{zz} + H_{xx}H_z^2)\right)\\
\frac{\partial^2 Z}{\partial X\partial Y} &= \frac{-ixyz}{(zH_z)^3}\left(zH_z(H_{xy}H_z - H_xH_{yz} - H_yH_{xz}) + H_xH_yH_z + zH_xH_yH_{zz}\right)\\
\frac{\partial^2 Z}{\partial Y^2} &= \frac{-iyz}{(zH_z)^3}\left(H_yH_z(zH_z - 2yzH_{yz} + yH_y) + yz(H_y^2H_{zz} + H_{yy}H_z^2)\right)\\
\frac{\partial^2 Z}{\partial X\partial Y} &= \frac{\partial^2 Z}{\partial Y\partial X}
\end{aligned}$$

Simplifying the expression for $\mathcal{H}$ using the above values proves the theorem. $\square$.

Before applying this corollary, we note the ease with which it can be generalized. In degree d, if we denote the argument of z_j as Z_j, then $\mathcal{H} = \det\left((\frac{\partial^2 Z_d}{\partial Z_j \partial Z_k})_{(j,k)}\right)$ and for $1 \le j,k \le d-1$

$$\begin{aligned}
\frac{\partial^2 Z_d}{\partial Z_j^2} &= \frac{-iz_jz_d}{(z_dH_d)^3}\left(H_jH_d(z_dH_d - 2z_jz_dH_{jd} + z_jH_j) + z_jz_d(H_j^2H_{dd} + H_{jj}H_d^2)\right)\\
\frac{\partial^2 Z_d}{\partial Z_j\partial Z_k} &= \frac{-iz_jz_kz_d}{(z_dH_d)^3}\left(z_dH_d(H_{jk}H_d - H_jH_{kd} - H_kH_{jd}) + H_jH_kH_d + z_dH_jH_kH_{dd}\right)
\end{aligned}$$

Now Theorem 2.6 can be readily applied in any dimension. We now do this in dimensions 3 and 4 to analogs of the Delannoy numbers. The Delannoy number $a_{r,s}$ is defined as the number of paths from the origin to the lattice point $(r,s) \in (\mathbb{Z}^+)^2$ using the steps $(1,0)$, $(0,1)$ and $(1,1)$. Notice that the deletion of the $(1,1)$ step would result in the binomial coefficients. Analyses of these numbers can be found throughout the literature.

We define the 3-Dimensional Delannoy number $a_{r,s,t}$ as the number of paths from the origin to the lattice point $(r,s,t) \in (\mathbb{Z}^+)^3$ using the steps $(1,0,0)$, $(0,1,0)$, $(0,0,1)$ and $(1,1,1)$. (There is no natural choice whether or not to include the $(1,1,0)$, $(1,0,1)$ and $(0,1,1)$ steps as well, so we choose to exclude them.) The generating function for this sequence is $\sum_{j=0}^{\infty}(x+y+z+xyz)^j$ where the term raised to the j^{th} power coincides with paths taking j steps. The sum converges formally in $\mathbb{C}[[x,y,z]]$ to $F = \frac{1}{1-(x+y+z+xyz)}$ since $x+y+z+xyz$ includes no constant coefficient. Also, F converges analytically in a neighborhood of the origin. Now $G(x,y,z) = 1$ and $H(x,y,z) = 1-(x+y+z+xyz)$, from which we determine that $Q(x,y,z) = (z + y + xz^2 + x + x^2z + x^2y +$

$yz^2 + y^2z + y^2z^2x + xy^2 + x^2yz^2 + x^2y^2z)xyz$. In dimension 3 the critical point equations become

$$H = 0 \tag{2.8}$$

$$K_1 := txH_x - rzH_z = 0 \tag{2.9}$$

$$K_2 := tyH_y - szH_z = 0 \tag{2.10}$$

Thus $\mathbf{z} = (x, y, z)$ is a critical point for the direction $\mathbf{r} = (1, 1) \iff$

$$1 - (x + y + z + xyz) = 0$$

$$tx(-1 - yz) - rz(-1 - xy) = 0$$

$$ty(-1 - xz) - sz(-1 - xy) = 0$$

We determine asymptotics along the main diagonal of this generating function, meaning the coefficients $a_{n,n,n}$ as $n \to \infty$. Thus $\frac{r}{t} = \frac{s}{t} = 1$. Using the method of Gröbner Bases described in detail in Section 3.1 we develop the three polynomial equations in three unknowns to the equivalent equations:

$$x^3 + 3x - 1 = 0$$

$$x - y = 0$$

$$x - z = 0$$

If we designate $\zeta = (4 + 4\sqrt{5})^{1/3}$, then the solution of the above equations closest to the origin (and thus minimal) is $\mathbf{z} = (\frac{\zeta}{2} - \frac{2}{\zeta}, \frac{\zeta}{2} - \frac{2}{\zeta}, \frac{\zeta}{2} - \frac{2}{\zeta})$. At this point $zH_z = -1 + \frac{1-\sqrt{5}}{4}\zeta^2 + \zeta \approx -.35562929$ and $Q = 54 - (6\sqrt{5} + \frac{9}{4})\zeta^2 + \frac{129-33\sqrt{5}}{4}\zeta \approx 25.39051888$ while $x^{-n}y^{-n}z^{-n} = x^{-3n} = (1 - 3x)^{-n} = (1 - \frac{3}{2}\zeta + \frac{6}{\zeta})^{-n} \approx 29.9007868^n$. Thus $a_{n,n,n} \sim \frac{1.791980746}{2\pi n} \cdot 29.9007868^n$.

To confirm this estimate we calculate the actual values of $a_{n,n,n}$ for various values of n. We note that if a path from the origin to (n, n, n) includes exactly j steps of the flavor $(1, 0, 0)$, then it must include exactly j $(0, 1, 0)$ and $(0, 0, 1)$ steps as well, and exactly $n - j$ $(1, 1, 1)$ steps, while

n	Actual $a_{n,n,n}$	Asymptotic Prediction	Percent Error
1	7	8.528	21.83%
10	$1.595 \cdot 10^{13}$	$1.629 \cdot 10^{13}$	2.13%
100	$1.053 \cdot 10^{145}$	$1.055 \cdot 10^{145}$	0.21%
1000	$1.373 \cdot 10^{1472}$	$1.373 \cdot 10^{1472}$	0.02%
10000	$1.911 \cdot 10^{14753}$	$1.911 \cdot 10^{14753}$	0.01%

Table 1: Comparison of Asymptotic Predictions versus Actual Values for the 3-Dimensional Delannoy Numbers

these steps can occur in any order. Thus we can calculate $a_{n,n,n}$ as $\sum_{j=0}^{n} \binom{n+2j}{j,\,j,\,j,\,n-j}$. Comparing the actual values to our predicted asymptotics gives us the following table:

The table ends with $n = 10000$ as the actual calculation gets cumbersome. While it only takes Maple .6 seconds to calculate $a_{1000,1000,1000}$, it takes 50.6 seconds and then 537.5 seconds to calculate $a_{4000,4000,4000}$ and $a_{10000,10000,10000}$, respectively. In comparison, once the initial determinations of $\mathbf{z}$ and Q are made, the asymptotic estimate can be calculated almost instantaneously. This difference in computation time highlights the usefulness of such an asymptotic expression. Further highlighting this fact, our asymptotic analysis could quickly be generalized to diagonals other than the main diagonal, while our calculation of the actual values is highly dependent on the use of the main diagonal. A more thorough exploration of results for the 3-Dimensional Delannoy numbers, including analysis of alternate diagonals, is done as an example in Section 3.1 below.

One could argue that the most important calculation for these asymptotics was the growth rate of 29.9007868^n. Only the determination of $\mathbf{z}$ and not the more involved interpretation of $\mathcal{H}$ was necessary for this. Similarly, without directly interpreting $\mathcal{H}$ in the case of $d = 4$ we can calculate that for the 4-Dimensional Delannoy numbers $a_{n,n,n,n} \sim a \cdot 259.9769802^n$ for constant a. While it is true that the growth rate is always important; the determination of the remaining constant is more important than we suggest above. For example, in the case of the Quantum Random Walk, for many of the directions of interest to us we will have $|\mathbf{z}| = 1$ for the minimal critical points, and the determination of the factor a above will be paramount. In fact, we will find that a is a multiple of the curvature of the variety $\mathcal{V}$ at $\mathbf{z}$, further linking our field of study to differential geometry, while elucidating our results.

3 Algebraic and Geometric Background

3.1 Gröbner Bases

Determining asymptotics for $a_{\mathbf{r}}$ requires determining the set of relevant critical points $\text{crit}(\mathbf{r})$ by solving the equations $(z_1H_1, \ldots, z_dH_d)||(r_1, \ldots, r_d)$ and $H(\mathbf{z}) = 0$ for fixed $\mathbf{r}$. We can rephrase the equations as d polynomial equations: $z_jH_jr_d - z_dH_dr_j\,\forall\,1 \leq \jmath \leq d-1$ and $H(\mathbf{z}) = 0$. While we could focus on numerical methods to determine the solution to several equations in several variables, there are certain advantages to working algebraically. While we are interested in $\mathbf{z} \in \Xi(\mathbf{r})$ as an input to $\mathbf{z}^{-\mathbf{r}}G(x,y)\sqrt{\frac{-yH_y}{sQ}}$ (or its equivalent for $d \neq 2$), if we keep track of our solutions in terms of the ideals of polynomials that annihilate them, we can take advantage of algebraic simplifications. Over the last twenty years, the field of computational algebra has blossomed, providing algorithms to manipulate these ideals and easily determine ideal membership. Our reliance on these algorithms will be focused on the use of Maple's algorithm for determining a Gröbner basis. In order to define a Gröbner basis, however, we must first define several concepts related to term orders. Below k will represent the field of rationals numbers, though as much of the below applies to arbitrary characteristic zero fields, we use the notation k instead of $\mathbb{Q}$. For an ideal $I \subset k[\mathbf{z}] = k[z_1, \ldots, z_d]$ generated by the set of polynomials $\{f_1, \ldots, f_n\} \subset k[\mathbf{z}]$, the algebraic variety in k^n where every element of I vanishes will be denoted $V(I)$. The definitions and propositions below are due to [CLO98].

A *monomial ordering* on $k[\mathbf{z}]$ is any relation $>$ on the set of monomials z^α in $k[\mathbf{z}]$ (or equivalently on the exponent vectors $\alpha \in \mathbb{Z}^d_{\geq 0}$) satisfying:

1. $>$ is a total (linear) ordering relation. That is, the terms appearing within any polynomial f can be uniquely listed in increasing or decreasing order under $>$;

2. $>$ is compatible with multiplication in $k[\mathbf{z}]$, in the sense that if $\mathbf{z}^\alpha > \mathbf{z}^\beta$ and $\mathbf{z}^\gamma$ is a monomial, then $\mathbf{z}^\alpha\mathbf{z}^\gamma = \mathbf{z}^{\alpha+\gamma} > \mathbf{z}^{\beta+\gamma} = \mathbf{z}^\beta\mathbf{z}^\gamma$;

3. $>$ is a well-ordering. That is, every nonempty collection of monomials has a smallest element under $>$.

In the *lexicographic* term order, $\mathbf{z}^\alpha > \mathbf{z}^\beta$ if and only if for some $j \leq d$, $\alpha_j > \beta_j$ while $\alpha_k = \beta_k$ for all $k < j$. The lexicographic Gröbner basis has the property that when the associated ideal I is zero-dimensional, the first element of the basis is a polynomial $f \in k[z_d]$. This f is called the *elimination polynomial* for z_d and can be extremely helpful in identifying the points of $V(I)$. Similarly, the j^{th} element of the basis is a polynomial $f_j \in k[z_{d-j+1}, \ldots, z_d]$ which can be used along with the prior f_k's with $k \leq j$ to identify the z_{d-j+1} coordinates of the points in $V(I)$. While this is highly desirable, simplifying future computations, this algorithm can be rather time-intensive. Alternatively, we may consider a *total degree order* in which $\alpha > \beta$ if either the degree of α is greater than the degree of β, or their degrees are equal while $\alpha > \beta$ in the reverse version of the lexicographic order (where $z_1 > z_2 \ldots > z_d$). While Gröbner bases delivered by Maple with respect to this ordering may not be as helpful, the bases can be determined much more quickly.

Before moving on, we make a note on the importance of a term ordering. When $d = 1$ and we deal in $k[z]$, simple division requires the notion of an ordering. The ordering of monomials by degree is essential to the division algorithm, as well as to the notion of a remainder. Dividing $p(z)$ by $q(z)$ we find that $p = aq + r$; it must be that $r < q$ in order for this result to be unique. Thus the important concept of degree in $k[z]$ is really a simple term ordering.

Given any monomial order $>$ and polynomial $f \in k[\mathbf{z}]$ we denote the leading term of f with respect to $>$ as LT (f). For any ideal $I \subset k[\mathbf{z}]$ we define its associated Gröbner basis as follows. A **Gröbner basis** for the ideal I with respect to the monomial order $>$ is a basis $\{g_1, \ldots, g_k\}$ for I with the property that for any nonzero $f \in I$, $\mathrm{LT}(f)$ is divisible by $\mathrm{LT}(g_i)$ for some i. The basis is **reduced** if no monomial of g_i is divisible by $\mathrm{LT}(g_j)$ for any distinct i and j. As reduced Gröbner bases are unique (via Proposition 6 in Section 2.7 of [CLO98]) they can be used to determine if two ideals I and J are equivalent. More importantly (for our purposes), reduced Gröbner bases are algorithmically computable, and they have been implemented in Maple's Groebner package via the command `Basis` $([p_1, \ldots, p_k]$, `order`).

In the examples of interest to us, there will be finitely many solutions to the critical point equations. Consequently, the following theorem (whose proof can be found in [CLO92]) will be extremely useful. Most importantly, it guarantees the existence of z_d's elimination polynomial as the first element of the lexicographic Gröbner basis.

Theorem 3.1 (Theorem 6 of Chapter 5, Section 3 of [CLO92])**.** *Let I be an ideal in $\mathbb{Q}[\mathbf{z}]$. The following conditions are equivalent:*

1. *The set $V(I)$ of common solutions to all polynomials in I is a finite subset of $\mathbb{C}^d$.*
2. *$\mathbb{C}[\mathbf{z}]/I$ is a finite dimensional vector space over $\mathbb{C}$.*
3. *Given a monomial order, there are finitely many monomials not divisible by a leading term of the Gröbner basis for I.*

Furthermore, if these conditions are met, then there is a univariate polynomial in I whose roots are precisely the values of z_d of the last coordinates of the roots $\mathbf{z}$ of I.

As an example of the use of a Gröbner basis, we consider the critical point equations for the 3-Dimensional Delannoy numbers introduced in Section 2.3. As this is a relatively simple set of equations (judged both by number of equations, as well as by the equations' degrees) we ask Maple for a Gröbner basis in the lexicographic order. We do this with the command $GB =$ `Basis` $([1-(x+y+z+xyz), x(-1-yz)-z(-1-xy), y(-1-xz)-z(-1-xy)], \texttt{plex}(z,y,x))$. The triple (z, y, x) at the end of this command designates the order of the variables, meaning we ask Maple to let $z_1 = z$, $z_2 = y$ and $z_3 = x$. Thus we can expect that if the output is of the form $\{g_1, g_2, g_3\}$, then $g_1 \in \mathbb{Q}[x]$, $g_2 \in \mathbb{Q}[x, y]$ and $g_3 \in \mathbb{Q}[x, y, z]$. This is what we receive, with the Maple output $GB = [-1 + 3x + x^3, x - y, x - z]$. If we refer to the three solutions of $g_1 = -1 + 3x + x^3 = 0$ as x_1, x_2 and x_3, then $V(I) = \{(x_1, x_1, x_1), (x_2, x_2, x_2), (x_3, x_3, x_3)\}$. While useful enough to help us with the analysis of the 3-Dimensional Delannoy numbers in Section 2.3, this analysis does not include the exploitation of algebraic simplification promised above. If we further exploit the machinery described above, we can determine the value of $A = \frac{(GzH_z)^2}{-Q}$ and our desired result will be $\frac{\sqrt{A}}{2\pi\xi t}x^{-r}y^{-s}z^{-t}$. The key here is that we force a new variable Z to be equal to $-\frac{1}{Q}$ by requiring that the polynomial $ZQ+1$ vanishes. We then force an additional variable A to be equal to $\frac{(GzH_z)^2}{-Q} = Z(GzH_z)^2$ by requiring that $A - Z(GzH_z)^2$ vanishes. Now to find the asymptotics in the direction $(\lambda t, \mu t, t)$, we enter the Maple command: `Basis` $([H, K_1, K_2, QZ+1, A - Z(zH_z)^2]$, `plex`$(z, y, x, Z, A))$ with K_1 and K_2 defined by Equations (2.9) and (2.10). As we order A last in our lexicographic term order, the first polynomial in our Gröbner basis output will be an elimination polynomial for A. The polynomial Maple outputs is $f_1(\lambda,\mu)(A\lambda\mu+\lambda+\mu+1)A^2 + f_2(\lambda,\mu)A + (\mu-\lambda+1)(\mu-\lambda-1)(\mu+\lambda-1)$ where $f_1(a,b) = b^6+4b^5+4ab^5-12ab^4+8ab^3-10b^3a^3+8b^3a^2-10b^3+8ab^2+8a^3b^2-36a^2b^2-12a^4b+8ba^2-12ba+4a^5b+8ba^3+4b+1+a^6+4a^5+4a-10a^3$ and $f_2(a,b) = -3b^5-ab^4-b^4-ab^3+4b^3+4b^3a^2+4a^2b^2+4ab^2+4a^3b^2+4b^2+4ba^2-ba-ba^3-b-a^4b+4a^3+4a^2-a^4-a-3a^5-3$. One interested in a general solution of the form $a_{\lambda t,\mu t,t} \sim f(\lambda,\mu,t)$ could find the roots of this degree three polynomial. We simply notice here that for the direction we solved in Section 2.3, we would have $\lambda = \mu = 1$, in which case the minimal polynomial would be $1 - 18A + 81A^2 + 27A^3$. With $\rho = (292 + 4\sqrt{5})^{1/3}$, the solution $A = -\frac{\rho}{6} - \frac{22}{3\rho} - 1$ delivers the asymptotics developed in Section 2.3 with $a_{t,t,t} \sim \frac{\sqrt{-A}}{2\pi t}x^{-t}y^{-t}z^{-t}$.

3.2 Resultants

According to [CLO98], given two polynomials $f, g \in k[x]$ of positive degree with $f = a_0x^l + \cdots + a_l,\ a_0 \neq 0,\ l > 0$ and $g = b_0x^m + \cdots + b_m,\ b_0 \neq 0,\ m > 0$, the *resultant* of f and g, denoted $Res(f, g)$ is the determinant of the $(l + m) \times (l + m)$ matrix

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

in which the blank entries are filled with zeroes, the first m columns have first nonzero entry a_0 and the remaining l columns have first nonzero entry b_0. To stress the dependence on x (when more than one variable is involved) we will denote the resultant as $Res(f, g, x)$. We note that $Res(f, g)$ is an integer polynomial in the coefficients of f and g. However, the property of resultants most relevant to our interests is that $Res(f, g) = 0 \iff f$ and g have a nontrivial common factor in $k[x]$. This is the result of Proposition 1.7 of [CLO98].

Supposing that $f, g \in k[x, y]$ we can view f and g as elements of $k(y)[x]$. Then the resultant of f and g gives a polynomial in y whose roots are the y_j values for which there exist x_j such that $f(x_j, y_j) = g(x_j, y_j) = 0$. We can generalize to determine solutions of more than 2 equations in more than 2 unknowns, with a word of caution. Let $f, g, h \in k[x, y, z]$. Suppose there exists a triple $\mathbf{z} := (x', y', z')$ such that $f(\mathbf{z}) = g(\mathbf{z}) = h(\mathbf{z}) = 0$. Then $Res(Res(f, g, x), Res(f, h, x), y)$ will vanish when $z = z'$. However, the vanishing of the iterated resultant does not imply a solution to the equation $f = g = h = 0$. That is to say, the method of iterated resultants may deliver extraneous roots. We see this as follows.

Suppose we wish to determine when $f = g = h = 0$. We let $r_1 = Res(f, g, x)$ and $r_2 = Res(f, h, x)$. Thus, $r_1(y', z') = 0 \Rightarrow \exists x_1'$ such that $f(x_1', y', z') = g(x_1', y', z') = 0$ and $r_2(y', z') = 0 \Rightarrow \exists x_2'$ such that $f(x_2', y', z') = h(x_2', y', z') = 0$. It need not be the case that $x_1' = x_2'$. Thus if there are some $\overline{y}$ and $\overline{z}$ such that $r_1(\overline{y}, \overline{z}) = r_2(\overline{y}, \overline{z}) = 0$, there need not be some $\overline{x}$ such that $f(\overline{x}, \overline{y}, \overline{z}) = g(\overline{x}, \overline{y}, \overline{z}) = h(\overline{x}, \overline{y}, \overline{z}) = 0$. If, however, there is a triple $(\underline{x}, \underline{y}, \underline{z})$ at which f,g, and h all vanish, then it will be the case that both r_1 and r_2 vanish at the pair $(\underline{y}, \underline{z})$.

We make two final notes on resultants which will make our work easier. As we are only concerned with points of vanishing, we may discard repeated factors and units. Thus if $r_1 = 3p_1p_2^2$ and $r_2 = 2q_1^3$, for polynomials p_1, p_2 and q_1, we need only consider $Res(p_1p_2, q_1)$. Also when we are concerned with vanishing on $\mathcal{V}_1$ we can remove factors of x, y and z.

3.3 Differential Geometry

For a smooth orientable hypersurface $\mathcal{V} \subset \mathbb{R}^{d+1}$, the Gauss map $\mathfrak{n}$ sends each point $p \in \mathcal{V}$ to a consistent choice of normal vector. We may identify $\mathfrak{n}(p)$ with an element of S^d. For a given patch $P \subset \mathcal{V}$ containing p, let $\mathfrak{n}[P] := \cup_{q \in P} \mathfrak{n}(q)$, and denote the area of a patch P in either $\mathcal{V}$ or S^d as $A[P]$. Then the **Gauss-Kronecker** curvature of $\mathcal{V}$ at p is defined as

$$\mathcal{K} := \lim_{P \to p} \frac{A(\mathfrak{n}[P])}{A[P]} . \tag{3.1}$$

When d is odd, the antipodal map on S^d has determinant -1, whence the particular choice of unit normal will influence the sign of $\mathcal{K}$, which is therefore only well defined up to sign. When d is even, we take the numerator to be negative if the map $\mathfrak{n}$ is orientation reversing and we have a well defined signed quantity. Clearly, $\mathcal{K}$ is equal to the Jacobian of the Gauss map at the point p. For computational purposes, it is convenient to have a formula for the curvature of the graph of a function from $\mathbb{R}^d$ to $\mathbb{R}$.

Proposition 3.2. *Suppose that in a neighborhood of the point p, the smooth hypersurface $\mathcal{V} \subseteq \mathbb{R}^{d+1}$ is the graph of a function h mapping the origin to p; that is, in some neighborhood of the origin, $\mathcal{V} = \{(\mathbf{x}, \tau) : \tau = h(\mathbf{x})\}$. Let $\nabla := \nabla h(\mathbf{0})$ and $\mathcal{H} := \det \left(\frac{\partial h}{\partial u_i \partial u_j}(\mathbf{0}) \right)_{1 \leq i,j \leq d}$ denote respectively the gradient and Hessian determinant of h at the origin. Then the curvature of $\mathcal{V}$ at the origin is given by*

$$\mathcal{K} = \frac{\mathcal{H}}{\sqrt{1 + |\nabla|^2}^{\,2+d}} .$$

The square root is taken to be positive and in case d is odd, the curvature is with respect to a unit normal in the direction in which the dependent variable increases.

First Proof: Let $\mathbf{X} : \mathbf{U} \subseteq \mathbb{R}^{\mathbf{d}} \to \mathbb{R}^{\mathbf{d+1}}$ denote the parameterizing map defined by

$$\mathbf{X}(\mathbf{u}) := (u_1, \ldots, u_d, h(u_1, \ldots, u_d))$$

on a neighborhood U of the origin. Let π be the restriction to $\mathcal{V}$ of projection of $\mathbb{R}^{d+1}$ onto the first d coordinates, so π inverts $\mathbf{X}$ on U. Define a vector

$$\mathbf{N}(\mathbf{u}) := \left(\frac{\partial h}{\partial u_1}, \ldots, \frac{\partial h}{\partial u_d}, -1\right)$$

normal to $\mathcal{V}$ at $\mathbf{X}(\mathbf{u})$ and let $\hat{\mathbf{N}}$ denote the corresponding unit normal $\mathbf{N}/|\mathbf{N}|$. Observe that $|\mathbf{N}| = \sqrt{1+|\nabla h|^2}$, and in particular, that $|\mathbf{N}(\mathbf{0})| = \sqrt{1+|\nabla|^2}$. The Jacobian of π at the point p is, up to sign, the cosine of the angle between the z_{d+1} axis and the normal to the tangent plane to $\mathcal{V}$ at p. Thus

$$|J(\pi(p))| = \frac{|\hat{\mathbf{N}} \cdot e_{d+1}|}{|\hat{\mathbf{N}}||e_{d+1}|} = \frac{1/|\mathbf{N}(\mathbf{0})|}{1 \cdot 1} = \frac{1}{\sqrt{1+|\nabla|^2}} . \tag{3.2}$$

The Gaussian curvature at the point p is, by definition, the Jacobian of the map $\hat{\mathbf{N}} \circ \pi$ at p. Using J to denote the Jacobian, write $\hat{\mathbf{N}}$ as $|\cdot| \circ \mathbf{N}$ and apply the chain rule to see that

$$\mathcal{K} = J(\pi(p)) \cdot J(\mathbf{N})(\mathbf{0}) \cdot J(|\cdot|)(\mathbf{N}(\mathbf{0})) \; = \frac{1}{\sqrt{1+|\nabla|^2}} \cdot J(\mathbf{N})(\mathbf{0}) \cdot J(|\cdot|)(\nabla, -1) . \tag{3.3}$$

Here, $|\cdot|$ is considered as a map from $\mathbb{R}^d \times \{-1\}$ to S^d; at the point $\mathbf{y}$, its differential is an orthogonal projection onto the plane orthogonal to $(\mathbf{y}, -1)$ times a rescaling by $|(\mathbf{y}, -1)|^{-1}$, whence

$$J(|\cdot|)(\mathbf{y}) = \sqrt{1+|\mathbf{y}|^2}^{\,-1} \sqrt{1+|\mathbf{y}|^2}^{\,-d} . \tag{3.4}$$

Because $\mathbf{N}$ maps into the plane $z_{d+1} = -1$ we may compute $J(\mathbf{N})$ from the partial derivatives $\partial N_i / \partial x_j = \partial^2 h / \partial x_i \partial x_j$, leading to $J(\mathbf{N})(\mathbf{0}) = \mathcal{H}$. Putting this together with (4.3) gives

$$J(\hat{\mathbf{N}})(\mathbf{0}) = \frac{\mathcal{H}}{\sqrt{1+|\nabla|^2}^{\,d+1}} \tag{3.5}$$

and using (3.3) and (3.2) gives

$$\mathcal{K} = \frac{\mathcal{H}}{\sqrt{1+|\nabla|^2}^{\,d+2}} ,$$

proving the proposition. □

Second Proof: We reuse the notation from the first proof. Additionally, for each $1 \le j \le d$ we abbreviate by denoting the partial derivative h_{u_j} as h_j and the vector $\mathbf{X}_{u_j}$ with 1 in its j^{th} position, h_j in its $(d+1)^{th}$ position, and 0 in its remaining positions as $\mathbf{X}_j$.

We first note that $\lim_{P\to p} A(P)$ can be represented by the square root of the determinant of the matrix whose coefficients are the coefficients of the first fundamental form. That is to say that the denominator of $\mathcal{K}$ is $\sqrt{\det((<\mathbf{X}_j, \mathbf{X}_k>)_{j,k})}$ where $<,>$ represents the standard inner product.

In order to determine the value of the numerator of $\mathcal{K}$, we again make the choice of normal vector $\hat{\mathbf{N}}$ defined in the first proof. As with $\mathbf{X}$ we abbreviate the vector derivative of $\hat{\mathbf{N}}$ with respect to u_j as $\hat{\mathbf{N}}_j$. We can now calculate the area of an infinitesimal patch in S^d (i.e. $\lim_{P\to p} A(\mathcal{G}(P))$) as the determinant of the matrix whose coefficients are the coefficients of the second fundamental form, divided by the square root of the determinant of the matrix whose coefficients are the coefficients of the first fundamental form. That is to say that the numerator of $\mathcal{K}$ is $\det((<\hat{\mathbf{N}}_j, \mathbf{X}_k>)_{j,k})$. Thus now:

$$\mathcal{K} = \frac{\det((<\hat{\mathbf{N}}_j, \mathbf{X}_k>)_{j,k})}{\det((<\mathbf{X}_j, \mathbf{X}_k>)_{j,k})}$$

To evaluate the numerator we first note that since $<\hat{\mathbf{N}}, \mathbf{X}_j> = 0$, by integration by parts $<\hat{\mathbf{N}}_j, \mathbf{X}_k> = -<\hat{\mathbf{N}}, \mathbf{X}_{j,k}>$ for all pairs $1 \le j,k \le d$. Concurrently, for all pairs $1 \le j,k \le d$ we have $\mathbf{X}_{j,k} = (0,...,0,h_{j,k})$, so $-<\hat{\mathbf{N}}, \mathbf{X}_{j,k}> = \frac{h_{j,k}}{\sqrt{1+|\nabla|^2}}$. Thus the numerator of $\mathcal{K}$ can be rewritten as $(1+|\nabla|^2)^{-d/2}\mathcal{H}$.

Evaluating the denominator, we note that $<\mathbf{X}_j, \mathbf{X}_j> = 1+h_j^2$, while for $j \ne k$, $<\mathbf{X}_j, \mathbf{X}_k> = h_j h_k$. Thus, we wish to calculate $\det((\delta_{j,k} + h_j h_k)_{j,k})$, where δ is the Kronecker delta function. We do this by row reduction by first noting that at p there is some j such that $h_j \ne 0$. We know this in the general case of a regular surface (regularity being a necessary requirement of a surface before we discuss its Gauss-Kronecker curvature) and we know this in the application to generating functions as $\mathbf{X}$ is a smooth parametrization. Without loss of generality we assume that h_1 is nonzero at p. As demonstrated below, if we subtract $\frac{h_k}{h_1} \cdot$ (row 1) from row k for each $k \in \{2,...,d\}$ we get a matrix with identical determinant whose first row is unchanged and whose

j^{th} row has $-\frac{h_j}{h_1}$ in the first column, a 1 on the main diagonal and 0's elsewhere.

$$\det \begin{pmatrix} 1+h_1^2 & h_1h_2 & h_1h_3 & \dots & h_1h_d \\ h_1h_2 & 1+h_2^2 & h_2h_3 & \dots & h_2h_d \\ h_1h_3 & \vdots & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \vdots \\ h_1h_d & h_2h_d & \dots & & 1+h_d^2 \end{pmatrix} = \det \begin{pmatrix} 1+h_1^2 & h_1h_2 & h_1h_3 & \dots & h_1h_d \\ -h_2/h_1 & 1 & 0 & \dots & \dots \\ -h_3/h_1 & 0 & 1 & 0 & \dots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ -h_d/h_1 & 0 & \dots & \dots & 1 \end{pmatrix}$$

The determinant of this latter matrix is easy to calculate as only d elements of the symmetric group $\mathcal{S}_d$ make nonzero contributions. The contributors are the identity (meaning the product of the diagonal entries) which contributes $1+h_1^2$ and the single transpositions $(1,j)$ (in cycle notation) which each contribute $(-1)\cdot(-\frac{h_j}{h_1}h_1h_j) = h_j^2$. Thus the determinant is $1+|\nabla|^2$. Putting together our results for the numerator and denominator of $\mathcal{K}$ completes the proof. □

We pause to record two special cases, the first following immediately from $\nabla h(\mathbf{0}) = \mathbf{0}$. If Q is a homogeneous quadratic form, we let $||Q||$ denote the determinant of the Hessian matrix of Q; to avoid confusion, we point out that the diagonal elements a_{ii} of this matrix are twice the coefficient of x_i^2 in Q. The determinant will be the same when the coefficients of $||Q||$ are computed with respect to any orthonormal basis.

Corollary 3.3. *Let $\mathcal{P}$ be the tangent plane to $\mathcal{V}$ at p and let $\mathbf{v}$ be a unit normal. Suppose that $\mathcal{V}$ is the graph of a smooth function h over $\mathcal{P}$, that is,*

$$\mathcal{V} = \{p + \mathbf{u} + h(\mathbf{u})\mathbf{v} : \mathbf{u} \in U \subseteq \mathcal{P}\}\,.$$

Let Q be the quadratic part of h, that is, $h(\mathbf{u}) = Q(\mathbf{u}) + O(|\mathbf{u}|^3)$. Then the curvature of $\mathcal{V}$ at p is given by

$$\mathcal{K} = ||Q||\,.$$

□

Corollary 3.4 (curvature of the zero set of a polynomial)**.** *Suppose* $\mathcal{V}$ *is the set* $\{\mathbf{x} : H(\mathbf{x}) = 0\}$ *and suppose that* p *is a smooth point of* $\mathcal{V}$*, that is,* $\nabla H(p) \neq \mathbf{0}$*. Let* ∇ *and* Q *denote respectively the gradient and quadratic part of* H *at* p*. Let* $Q_\perp$ *denote the restriction of* Q *to the hyperplane* $\nabla_\perp$ *orthogonal to* ∇*. Then the curvature of* $\mathcal{V}$ *at* p *is given by*

$$\mathcal{K} = \frac{||Q_\perp||}{|\nabla|^d} \, . \tag{3.6}$$

Proof: Replacing H by $|\nabla|^{-1}H$ leaves $\mathcal{V}$ unchanged and reduces to the case $|\nabla H(p)| = 1$; we therefore assume without loss of generality that $|\nabla| = 1$. Letting $\mathbf{u}_\perp + \lambda(\mathbf{u})\nabla$ denote the decomposition of a generic vector $\mathbf{u}$ into components in $\langle\nabla\rangle$ and $\nabla_\perp$, the Taylor expansion of H near p is

$$H(p + \mathbf{u}) = \nabla \cdot \mathbf{u} + Q_\perp(\mathbf{u}) + R$$

where $R = O(|\mathbf{u}_\perp|^3 + |\lambda(\mathbf{u})||\mathbf{u}_\perp|)$. Near the origin, we solve for λ to obtain a parametrization of $\mathcal{V}$ by $\nabla_\perp$:

$$\lambda(\mathbf{u}) = Q_\perp(\mathbf{u}) + O(|\mathbf{u}|^3) \, .$$

The result now follows from the previous corollary. $\square$

4 Introduction to Quantum Random Walks

In this chapter we analyze several aspects of the Quantum Random Walk on the line, as well as give details of the setup for these walks in any dimension. In Section 4.1 we give a detailed description of these walks, and prove facts that will be useful for the remainder of this thesis. In Section 4.2 we determine asymptotics for the 2-Chirality walk on $\mathbb{Z}$ applicable everywhere outside neighborhoods of the points $\frac{r}{s} = \frac{1 \pm c}{2}$ with c a parameter of the unitary coin flip operator. Section 4.3 gives asymptotics for the neighborhoods missing in Section 4.2. Lastly, Section 4.4 determines asymptotics for a 3-Chirality walk on the line.

4.1 Description of QRWs and Key Lemmas

4.1.1 Background on QRWs

The classical random walk is a well-understood system with many important applications to computer science. Well-known examples of algorithms based on random walks include algorithms for counting, sampling, and testing properties such as satisfiability of Boolean formulae or graph connectivity. One of the most basic and useful random walks is a simple random walk on $\mathbb{Z}$. Here, a single particle moves on the one-dimensional integer lattice. At each step the particle moves one position to the left or right with equal probability. As the time t increases, the probability distribution describing the particle's location can be approximated increasing well by a normal distribution. The particle's expected location is at the origin, and its standard deviation is $\frac{1}{2}\sqrt{t}$, so its distribution is $O(\sqrt{t})$ in probability. That is to say that $\Pr\left(x \in [-M\sqrt{t}, M\sqrt{t}]\right) \to 1$ uniformly in t as $M \to \infty$.

Throughout the last century mankind has developed an increasing appreciation for the fact that Newton's laws alone do not describe our world. Among man's most recent attempts to harness the power of his quantum reality has been the field of quantum information theory, bringing with it the potential to devise instruments of extraordinary power [NC00]. For example, in 1994 Peter

Shor [Sho97] discovered an algorithm to factor numbers on a quantum computer in a number of steps which is polynomial in the length of the number to factored. This problem is not known to be solvable in polynomial time on a classical computer. Similarly, in [Gro96], Lov Grover determined a quantum mechanical algorithm reducing the time for searching a database of N entries from $O(N)$ steps to $O(\sqrt{N})$ steps. Algorithms such as these have brought researchers from a variety of scientific fields to focus on quantum information theory.

With the application of the classical random walk to information theory, as well as the growing promise of quantum information theory, it is clearly of interest to define the Quantum Random Walk. This was first done by Y. Aharanov, L. Davidovich and N. Zagury [ADZ93] who introduced the Quantum Random Walk and first discussed differences with the classical random walk due to quantum interference. Shortly thereafter, David Meyer [Mey96] pointed out that the simple classical random walk described above does not translate into a quantum framework. Semigroup operators, such as the combination $\frac{1}{2}\sigma_+ + \frac{1}{2}\sigma_-$ of shifts defining the classical simple random walk, are positive operators of norm 1 over the classical state space $l_1(\mathbb{Z})$, but fail to be unitary over the quantum space $l_2(\mathbb{Z})$. In fact, it is easy to verify that the only translation-invariant positive real operators on $l_2(\mathbb{Z})$ are trivial (powers of the shift operator).

In order to construct unitary operators that disperse the position of a particle, it is necessary to introduce an extra degree of freedom, known as *chirality*. At any position on the lattice the particle's chirality takes either the value R (for RIGHT) or L (for LEFT). The elementary states are thus $\mathbb{Z} \times \Sigma$ where $\Sigma := \{R, L\}$, and the state space is $l_2(\mathbb{Z} \times \Sigma) = l_2(\mathbb{Z}) \otimes l_2(\Sigma)$. While this is the convention established by Ambainis *et al.* in [ABN$^+$01], we will refer to particles in the LEFT and RIGHT positions with the vector notation $\binom{1}{0}$ and $\binom{0}{1}$, respectively. We will denote the unit basis vector of $l_2(\mathbb{Z}) \otimes l_2(\Sigma)$ at position i with LEFT chirality as $e(i, L)$ and we define $e(i, R)$ analogously. We will order this basis as

$$\ldots e(i-1, L), e(i-1, R), e(i, L), e(i, R), e(i+1, L), e(i+1, R) \ldots .$$

Ambainis *et al.* focus on the Hadamard walk. This is based on the Hadamard transformation, a unitary operator on $l_2(\Sigma)$ whose matrix with respect to the standard basis is

$$U_{\sqrt{\frac{1}{2}}} := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

We then extend this transformation to $l_2(\mathbb{Z}) \otimes l_2(\Sigma)$ as $I \otimes U_{\sqrt{\frac{1}{2}}}$ where I is the identity, resulting in a transformation which acts as the block diagonal matrix:

$$\begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \\ \cdots & U_{\sqrt{\frac{1}{2}}} & 0 & 0 & \cdots \\ \cdots & 0 & U_{\sqrt{\frac{1}{2}}} & 0 & \cdots \\ \cdots & 0 & 0 & U_{\sqrt{\frac{1}{2}}} & \cdots \\ & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

We then define a translation operator $\tilde{T}$ which shifts a particle with chirality R to the right one step and shifts a particle with chirality L to the left one step. More formally, we have

$$\tilde{T} : e(i, L) \mapsto e(i-1, L),\ \tilde{T} : e(i, R) \mapsto e(i+1, R)$$

and in the basis described above,

$$\tilde{T} = \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\ \dots & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \dots \\ \dots & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \dots \\ \dots & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & \dots \\ & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

in which every fourth diagonal alternates in 0's and 1's and all other entries are 0. We then define the operator $\tilde{W}$ as $\tilde{W} = \tilde{T}(I \otimes U_{\sqrt{\frac{1}{2}}})$. As each of $\tilde{T}$ and $I \otimes U_{\sqrt{\frac{1}{2}}}$ are unitary, $\tilde{W}$ is unitary as well. This unitary composition of operators represents one step of the Hadamard walk.

In the quantum framework, the state of the system is any element $\psi \in l_2(\mathbb{Z} \times \Sigma)$. If the state is ψ and we choose to measure the location (and chirality, which are simultaneously measurable), then the experiment ends and the probability of finding the particle at location i with chirality ξ is given by

$$p(i, \xi) := |\psi(i, \xi)|^2 .$$

The quantity $\psi(i, \xi)$ is called the *amplitude* of the particle to be in state (i, ξ). Execution of s steps of the QRW corresponds to acting on the state space by $\tilde{W}^s$. The most general question we can ask about QRW is the chance of finding it in state ξ after s steps, given that it started in state ξ_0. By linearity, it suffices to answer this for elementary states, and by translation invariance, our study may be reduced to the analysis of the quantities $\psi_{\xi_0,\xi}(r, s)$, defined to be the amplitude to be in state (r, ξ) at time s given the starting state $(0, \xi_0)$. We let

$$p_{\xi_0,\xi}(r,s) := |\psi_{\xi_0,\xi}(r,s)|^2$$

be the corresponding probabilities, and

$$P_{\xi_0}(r,s) = p_{\xi_0,L}(r,s) + p_{\xi_0,R}(r,s)$$

be the total probability of translating r units after time s, starting from chirality ξ_0.

The first rigorous analysis of the QRW on the line, resulting in asymptotics for the Hadamard walk, was done in [ABN$^+$01]. Their work spurred on much related analysis, including that in [AAKV01], [Kem05], [CFG02], and [MBSS02]. Furthermore, new methods have been developed by [CIR03], simplifying analysis and results, as well as by [Kon05a], allowing certain generalizations to unitary transformations. We believe our methods to be simpler than those employed in the above, and our methods will allow for ease of generalization, with extension to the unitary case in Section 4.2, new regions of asymptotics in Section 4.3, extension to 3 chiralities in Section 4.4 and generalization to dimensions greater than 1 in Chapter 5. We discuss further work by other authors in higher dimensions and multiple chiralities in the sections in which we present our results.

In the years since Ambainis *et al.* first successfully analyzed this walk, papers have begun to emerge offering new methods to transfer the results of the Quantum Random Walk to quantum computing. For example, in [SKW03] the authors introduce a quantum search algorithm based on the architecture of the Quantum Random Walk that attains an algorithmic speed-up over classical algorithms. Additionally, in [Amb05] Ambainis constructs a quantum walk algorithm for element distinctness. In the wake of such developments, it is more clear than ever that much benefit can come from a firm understanding of Quantum Random Walks.

4.1.2 Generating Functions for QRWs and Key Lemmas

In this section we work in as much generality as possible so that the lemmas we prove will be applicable for the remainder of this thesis. In that context, the Quantum Random Walk is a model for the motion of a single quantum particle evolving in $\mathbb{Z}^d$ under a time and translation invariant Hamiltonian for which the probability profile of a particle after one time step, started from a known location, is supported on the set of neighbors. Let $d \geq 1$ be the spatial dimension, so $d+1$ will be the dimension of our generating functions going forward. Let $E = \{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(k)}\} \subseteq \mathbb{Z}^d$ be a set of finite cardinality k. When E is the set of signed standard basis vectors we call this a *nearest neighbor* QRW; for example in one dimension, a nearest neighbor walk like that described above has $E = \{(1), (-1)\}$, while in two dimensions, a nearest neighbor walk has $E = \{(0,1), (0,-1), (1,0), (-1,0)\}$.

Let U be a unitary matrix of size k. The set $\mathbb{Z}^d \times E$ indexes the set of pure states of the QRW with parameters k, E and U. Let $\mathrm{Id} \otimes U$ denote the operator that sends $(\mathbf{r}, \mathbf{v}^{(j)})$ to $(\mathbf{r}, U\mathbf{v}^{(j)})$, that is, it leaves the location unchanged but operates on the chirality by U. Let σ denote the operator that sends $(\mathbf{r}, \mathbf{v}^{(j)})$ to $(\mathbf{r} + \mathbf{v}^{(j)}, \mathbf{v}^{(j)})$, that is, it translates the location according to the chirality and does not change the chirality. The product $\sigma \cdot (\mathrm{Id} \otimes U)$ is the operator we call QRW with parameters k, E and U. Let us denote this by $\mathcal{Q}$.

For $1 \leq i, j \leq k$ and $\mathbf{r} \in \mathbb{Z}^k$,

$$\psi_n^{(i,j)}\mathbf{r} := \langle e_{\mathbf{0},i} | \mathcal{Q}^n | e_{\mathbf{r},j} \rangle$$

denotes the amplitude at time n for a particle starting at location $\mathbf{0}$ in chirality i to be in location $\mathbf{r}$ and chirality j. As before, let $\mathbf{z}$ denote $(z_1, \ldots, z_{d+1})$ and define

$$F^{(i,j)}(\mathbf{z}) := \sum_{n,\mathbf{r}} \psi_n^{(i,j)}(\mathbf{r}) z_1^{r_1} \cdots z_d^{r_d} z_{d+1}^n \tag{4.1}$$

which denotes the spacetime generating function for n-step transitions from chirality i to chirality j and all locations. Let $\mathbf{F}(\mathbf{z})$ denote the matrix $(F^{(i,j)})_{1 \leq i,j \leq k}$. Let M denote the diagonal matrix whose entries are the monomials $\{\mathbf{z}^{\mathbf{r}} : \mathbf{r} \in E\}$. When $d = 2$ we use (x, y, z) for (z_1, z_2, z_3) and (r, s) for $\mathbf{r}$; for a two-dimensional nearest neighbor QRW, therefore, the notation becomes

$$F^{(i,j)}(x, y, z) = \sum_{n,r,s} \psi_n^{(i,j)}(r, s) x^r y^s z^n$$

and

$$M = \begin{pmatrix} x & 0 & 0 & 0 \\ 0 & x^{-1} & 0 & 0 \\ 0 & 0 & y & 0 \\ 0 & 0 & 0 & y^{-1} \end{pmatrix} .$$

We can now derive an explicit expression for $\mathbf{F}$ via the elementary enumerative technique known as the transfer matrix method [Sta97, GJ83]. We do so for the nearest neighbor walk with $d = 2$, though the explanation in higher dimensions is analogous, with slight variations for walks that are not nearest neighbor. The interpretation of the entries of the product $(MU)^n$ is as follows. The (ξ_0, ξ)-entry sums the weights of paths $\xi_0, \xi_1, \ldots, \xi_n$ with $\xi_n = \xi$, with the weight of each path given by the product over each of the n consecutive pairs (ξ_j, ξ_{j+1}) of $(MU)_{\xi_j, \xi_{j+1}}$. This product is equal to the product of $U_{\xi_j, \xi_{j+1}}$ times $x^r y^s$ where r is the number of times $(1, 0)$ appears in $\xi_0, \ldots, \xi_{n-1}$ minus the number of times $(-1, 0)$ appears and s is the number of times $(0, 1)$ appears in $\xi_0, \ldots, \xi_{n-1}$ minus the number of times $(0, -1)$ appears. But the sum over paths of $U_{\xi_j, \xi_{j+1}}$ with a given value of (r, s) is the amplitude of the wave function to be at $((r, s), \xi)$ if the elementary state $((0, 0), \xi_0)$ is chosen at time zero. Therefore, $(MU)^n$ is a matrix whose (ξ_0, ξ)-entry is the generating function whose $x^r y^s$ coefficient is $\psi_{\xi_0, \xi}(r, s, n)$. Multiplying by z^n and summing over z establishes the following proposition:

Proposition 4.1.

$$\mathbf{F}(x, y, z) = \sum_{n=0}^{\infty} z^n (MU)^n = (I - zMU)^{-1} .$$

Proof: Let $\mathbf{A}$ denote the matrix zMU. Since $\mathbf{A}$ contains no entries with nonzero $x^0 y^0 z^0$ coefficient, the sum $\sum_{k \geq 0} \mathbf{A}^k$ converges in the (matrices over the) formal power series ring. The limit $\mathbf{B}$ clearly satisfies $(I - \mathbf{A})\mathbf{B} = \mathbf{B}(I - \mathbf{A}) = I$. $\square$

In general the (i, j)-entry of the matrix, $F^{(i,j)}$, may therefore be written as a rational function

G/H where

$$H = \det(I - z_{d+1} M U) \,.$$

The following result is easy but crucial. It is valid in any dimension $d \geq 1$. Let $\mathbf{T}_d$ denote the unit torus in $\mathbb{C}^d$.

Proposition 4.2 (torality)**.** *The denominator H of the spacetime generating function for a Quantum Random Walk has the property that*

$$(z_1, \ldots, z_d) \in \mathbf{T}_d \text{ and } H(\mathbf{z}) = 0 \implies |z_{d+1}| = 1 \,. \tag{4.2}$$

Proof: If $(z_1, \ldots, z_d) \in \mathbf{T}_d$ then M is unitary, hence MU is unitary. The zeros of $\det(I - z_{d+1} MU)$ are the reciprocals of eigenvalues of MU, which are therefore complex numbers of unit modulus. □

The next result, which will be just as crucial towards Theorem 5.9, is due to Yuliy Baryshnikov.

Proposition 4.3. *Let H be any polynomial and let $\mathcal{V}$ denote the pole variety, namely the set $\{\mathbf{z} : H(\mathbf{z}) = 0\}$. Let $\mathcal{V}_1 := \mathcal{V} \cap \mathbf{T}_{d+1}$. Assume the torality hypothesis* (4.2)*. Let $p \in \mathcal{V}_1$ be any point for which $\nabla H(p) \neq \mathbf{0}$. Then $\mathcal{V}_1$ is a smooth d-dimensional manifold in a neighborhood of p.*

Proof: We will show that $\partial H / \partial z_{d+1}(p) \neq 0$. It follows by the implicit function theorem that there is an analytic function $g : \mathbb{C}^d \to \mathbb{C}$ such that for $\mathbf{z}$ in some neighborhood of p, $H(\mathbf{z}) = 0$ if and only if $z_{d+1} = g(z_1, \ldots, z_d))$. Restricting $(z_1, \ldots, z_d)$ to the unit torus, the torality hypothesis implies $z_{d+1} = 1$, whence $\mathcal{V}_1$ is locally the graph of a smooth function.

To see that $\partial H / \partial z_{d+1}(p) \neq 0$, first change coordinates to $z_j = p_j \exp(i\theta_j)$ and $z_{d+1} = p_{d+1} \exp(i\sigma)$. Letting $\tilde{H} := H \circ \exp$, the new torality hypothesis is $(\theta_1, \ldots, \theta_d) \in \mathbb{R}^d$ and $H(\theta_1, \ldots, \theta_d, \sigma) = 0$ implies $\sigma \in \mathbb{R}$. We are given $\nabla \tilde{H}(\mathbf{0}) \neq \mathbf{0}$ and are trying to show that $\partial \tilde{H} / \partial \sigma(\mathbf{0}) \neq 0$.

Consider first the case $d = 1$ and let $\theta := \theta_1$. Assume for contradiction that $\partial \tilde{H} / \partial \sigma(0, 0) = 0 \neq \partial \tilde{H} / \partial \theta(0, 0)$. Let $\tilde{H}(\theta, \sigma) = \sum_{j,k \geq 0} b_{j,k} \theta^j \sigma^k$ be a series expansion for $\tilde{H}$ in a neighborhood of

$(0,0)$. We have $b_{0,0} = 0 \neq b_{1,0}$. Let ℓ be the least positive integer for which $b_{0,\ell} \neq 0$; such an integer exists (otherwise $\tilde{H}(0,\sigma) \equiv 0$, contradicting the new torality hypothesis) and is at least 2 by the vanishing of $\partial H/\partial\sigma(0,0)$. Then there is a Puiseux expansion for the curve $\{\tilde{H} = 0\}$ for which $\sigma \sim (b_{1,0}\theta/b_{0,\ell})^{1/\ell}$. This follows from [BK86] although it is quite elementary in this case: as $\sigma, \theta \to 0$, the power series without the $(1,0)$ and $(0,\ell)$ terms sums to $O(|\theta|^2 + |\theta\sigma| + |\sigma|^{\ell+1}) = o(|\theta| + |\sigma|^\ell)$ (use Hölder's inequality); in order for $\tilde{H}$ to vanish, one must therefore have $b_{1,0}\theta + b_{0,\ell}\sigma^\ell = o(|\theta| + |\sigma|^\ell)$, from which $\sigma \sim (b_{1,0}\theta/b_{0,\ell})^{1/\ell}$ follows. The only way the new torality hypothesis can now be satisfied is if $\ell = 2$ and $b_{1,0}\theta/b_{0,\ell}$ is always positive; but θ may take either sign, so we have a contradiction.

Finally, if $d > 1$, again we must have $b_{0,\ldots,0,\ell} \neq 0$ in order to avoid $\tilde{H}(0,\ldots,0,\sigma) \equiv 0$. Let $\mathbf{r} \in \mathbb{R}^d$ be any vector not orthogonal to $\nabla\tilde{H}(\mathbf{0})$ and let $G(\theta,\sigma) := \tilde{H}(r_1\theta,\ldots,r_d\theta,\sigma)$. Then $\partial G/\partial\theta(0,0) \neq 0 = \partial G/\partial\sigma(0,0)$ and the new torality hypothesis holds for G; a contradiction then results from the above analysis for the case $d = 1$. $\square$

4.2 Initial Asymptotics for QRWs on $\mathbb{Z}$

In this section we begin our analyses of QRWs by recovering the results of [ABN$^+$01]. Our analysis via generating functions is simpler than their work, allowing the generalization to multiple chiralities and higher dimensions in the coming chapters. We further simplify our analysis of the walk on $\mathbb{Z}$ by making the walk aperiodic. The most convenient way to do this is to choose steps $\{0, 1\}$, replacing the $\{-1, 1\}$ steps in [ABN$^+$01]. In order to facilitate comparison of our results to those in [ABN$^+$01], we need to avoid using the same notation for different quantities. Hence we replace their $\{L, R\}$ with $\{\uparrow, \downarrow\}$, their rescaled location parameter α with λ, and so forth, as outlined in the upcoming paragraph.

Define the chirality space $\Sigma := \{\uparrow, \downarrow\}$, where a particle with chirality $\downarrow$ will shift to the right with each increase in time by one unit. Formally, we replace $\tilde{T}$ by T, defined by

$$T(e(i, \uparrow)) = e(i, \uparrow),\ T(e(i, \downarrow)) = e(i + 1, \downarrow)\,.$$

Given a unitary operator U on $l_2(\Sigma)$, our QRW operator is defined by

$$W := T(I \otimes U)\,.$$

In particular, the Hadamard Quantum Random Walk is

$$W_{\sqrt{\frac{1}{2}}} := T(I \otimes U_{\sqrt{\frac{1}{2}}})\,.$$

A particle at position n at time t in the QRW defined by [ABN$^+$01] corresponds to a particle at position $r := \frac{n+t}{2} \in \mathbb{Z}^+$ at time $s = t$ in our model; note that $|n| \leq t$ and $n \equiv t (\mod 2)$. Furthermore, just as $\alpha = \frac{n}{t}$ represents the location, rescaled linearly by time within the framework of Ambainis *et al.*, we use the rescaled location parameter

$$\lambda := \frac{r}{s} = \frac{\alpha + 1}{2}\,.$$

Again, the information of interest for a QRW is the value of $p_{\xi_0,\xi}(r, s) := |\psi_{\xi_0,\xi}(r, s)|^2$ for any time s and any state of a system (r, ξ) that began in state $(0, \xi_0)$. Comparing to [ABN$^+$01]:

- Our λ is their $(1+\alpha)/2$;
- Our $\psi_{\downarrow\downarrow}(r,s)$ is their $\psi_R(2r-s,s)$;
- Our $\psi_{\downarrow\uparrow}(r,s)$ is their $\psi_L(2r-s,s)$;

4.2.1 Statement of results

The Hadamard QRW may be generalized by allowing the quantum coin flip matrix U to be any unitary operator on the two dimensional chirality space $l_2(\Sigma)$. The unitary group of rank 2 may be parameterized by three unit circle parameters $e^{i\alpha}, e^{i\beta}, e^{i\gamma}$ and a real parameter $c \in [0,1]$:

$$U_{\alpha,\,\beta,\,\gamma,\,c} = \begin{pmatrix} ce^{i\alpha} & \sqrt{1-c^2}e^{i\beta} \\ \sqrt{1-c^2}e^{i\gamma} & -ce^{i(\beta+\gamma-\alpha)} \end{pmatrix} .$$

All our results are stated in this generality, which we refer to as a general unitary nearest-neighbor QRW on $\mathbb{Z}^1$. The behavior of this QRW is the same as the behavior of the Hadamard QRW (in which $c = \sqrt{\frac{1}{2}}$), except that the parameter c controls the size of the rescaled interval in which the particle may be found. Specifically, define

$$J := \left[\frac{1-c}{2}, \frac{1+c}{2}\right] . \tag{4.3}$$

We assume throughout that the parameter c is not one or zero, since these correspond respectively to propagation of the initial chirality and strict alternation of chiralities, hence to deterministic motion to the right and a mixture of no motion.

Corresponding to Theorems 1 and 2 of [ABN$^+$01], we have the following two results.

Theorem 4.4 (rapid decay beyond J)**.** *Consider the quantities $p_{\xi_0,\xi}$ for a general unitary QRW with $0 < c < 1$. For each compact $K \subseteq J^c$ and each integer $N > 0$ there is a $C > 0$ such that for any chiralities ξ_0 and ξ,*

$$p_{\xi_0,\xi}(r,s) \leq Cs^{-N}$$

whenever $\lambda = r/s \in K$.

Remark. Rapid decay may be improved to exponential decay by an argument that is not too complicated but involves moving a contour in two complex dimensions.

Theorem 4.5 (asymptotics inside the interval J)**.** *Given a general unitary walk with transformation U, let $\lambda := \frac{r}{s}$. Then there are phase functions $\rho_{\xi_0,\xi}(r,s)$ described in Equation* (4.20) *below, such that*

$$p_{\downarrow\downarrow}(r,s) \sim \frac{2}{\pi}\frac{\lambda\sqrt{1-c^2}}{(1-\lambda)s\sqrt{-((1-c^2)-4\lambda+4\lambda^2)}}\cos^2(\rho_{\downarrow\downarrow}(r,s)) \tag{4.4}$$

$$p_{\uparrow\uparrow}(r,s) \sim \frac{2}{\pi}\frac{(1-\lambda)\sqrt{1-c^2}}{\lambda s\sqrt{-((1-c^2)-4\lambda+4\lambda^2)}}\cos^2(\rho_{\uparrow\uparrow}(r,s)) \tag{4.5}$$

$$p_{\downarrow\uparrow}(r,s) \sim \frac{2}{\pi}\frac{\sqrt{1-c^2}}{s\sqrt{-((1-c^2)-4\lambda+4\lambda^2)}}\cos^2(\rho_{\downarrow\uparrow}(r,s)) \tag{4.6}$$

$$p_{\uparrow\downarrow}(r,s) \sim \frac{2}{\pi}\frac{\sqrt{1-c^2}}{s\sqrt{-((1-c^2)-4\lambda+4\lambda^2)}}\cos^2(\rho_{\uparrow\downarrow}(r,s)) \tag{4.7}$$

uniformly as λ varies over any compact subset of the interior of J.

Remark. The computations will be the most transparent when the parameters α, β and γ are zero. These parameters have no physical significance and in any case, the result for nonzero α, β, γ is easily deduced from the case $\alpha = \beta = \gamma = 0$. The same is not the case for the parameter c. We will therefore begin the proofs by assuming that the coin flip operator U is real, hence in the orthogonal group, parameterized by c:

$$U_{\text{Re}} := \begin{pmatrix} c & \sqrt{1-c^2} \\ \sqrt{1-c^2} & -c \end{pmatrix}.$$

In fact this parameterizes the anti-special orthogonal group (determinant = -1). This slightly unusual choice is due to the fact that $U_{\sqrt{\frac{1}{2}}}$ happens to have determinant -1.

These results of Theorem 4.5 for $p_{\downarrow\downarrow}(r,s)$ and $p_{\downarrow\uparrow}(r,s)$ are depicted below in Figure 1 for the Hadamard Walk.

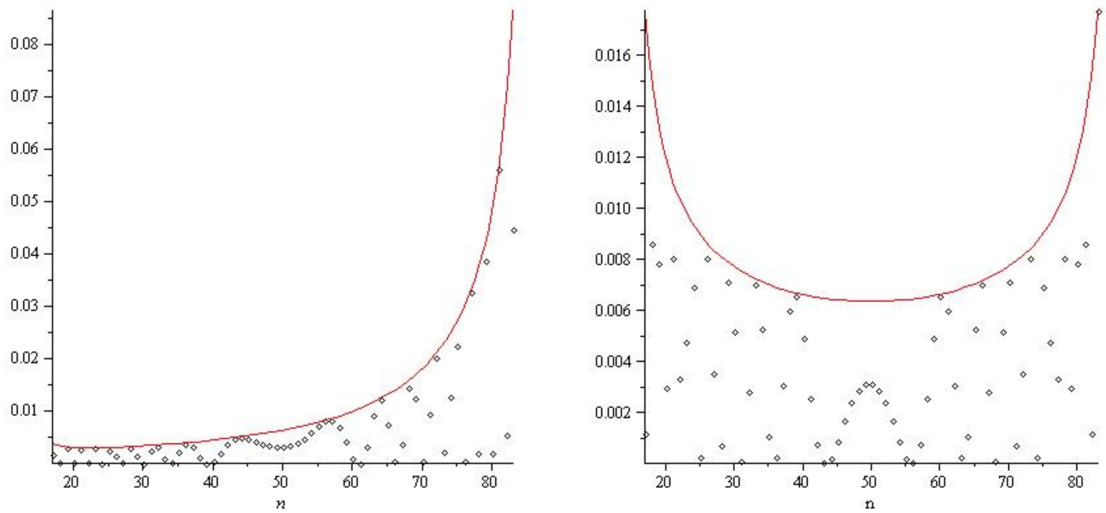

Figure 1: Time $n = 100$ probability values by location ($p_{\downarrow,\downarrow}$ on left and $p_{\downarrow,\uparrow}$ on right) and their upper envelope obtained by dropping the $\cos^2(\rho)$ term.

4.2.2 Determination and Preliminary Analysis of Generating Functions

As the generating functions of this section have degree two, we denote (z_1, z_2) as (x, y) with the exponents of x and y denoting position and time, respectively. With steps of $\{0, 1\}$, in the notation introduced in Section 4.1, we have $E = \{(0), (1)\}$ so

$$M = \begin{pmatrix} 1 & 0 \\ 0 & x \end{pmatrix} .$$

Then by Proposition 4.1, we have $\mathbf{F}(x, y) = (I - yMU)^{-1} = \frac{1}{H}\mathbf{G}$. Where

$$\mathbf{G}(x, y) = \begin{pmatrix} 1 + ce^{(\beta+\gamma-\alpha)i}xy & e^{\beta i}xy\sqrt{1-c^2} \\ e^{\gamma i}y\sqrt{1-c^2} & 1 - ce^{\alpha i}y \end{pmatrix} \tag{4.8}$$

and

$$H(x, y) = 1 - ce^{\alpha i}y + ce^{(\beta+\gamma-\alpha)i}xy - e^{(\beta+\gamma)i}xy^2 . \tag{4.9}$$

In the case that $U = U_c$ is real, this specializes to

$$\mathbf{G}_c = \begin{pmatrix} 1+cxy & xy\sqrt{1-c^2} \\ y\sqrt{1-c^2} & 1-cy \end{pmatrix},$$

$$H_c = 1 - cy + cxy - xy^2 \,.$$

To see why the only physically relevant parameter is c, observe that

$$H_{c,\alpha,\beta,\gamma}(x,y) = H_c\left(e^{i(\beta+\gamma-2\alpha)}x, e^{i\alpha}y\right) \tag{4.10}$$

while the entries of $\mathbf{G}_{c,\alpha,\beta,\gamma}(x,y)$ are equal to unit complex multiples of $\mathbf{G}_c(e^{i(\beta+\gamma-2\alpha)}x, e^{i\alpha}y)$. It follows that the coefficients of the generating function $F_{c,\alpha,\beta,\gamma}$ have the same magnitudes as the coefficients of F_c.

For comparison to the literature, we specialize further to the Hadamard case ($c = \sqrt{1/2}$) and record:

$$\mathbf{G}_{\sqrt{\frac{1}{2}}}(x,y) = \begin{pmatrix} 1+\frac{xy}{\sqrt{2}} & \frac{xy}{\sqrt{2}} \\ \frac{y}{\sqrt{2}} & 1-\frac{y}{\sqrt{2}} \end{pmatrix}$$

$$H_{\sqrt{\frac{1}{2}}}(x,y) = 1 - \frac{1-x}{\sqrt{2}}y - xy^2 \,.$$

For the remainder of this section, we omit subscripts when referring to the real case, which from above we see is all we need consider to derive all desired asymptotics. Furthermore, by making additional substitutions in our generating functions, we see that we need only consider certain combinations of chiralities in our analysis. For example, as $F_{\uparrow,\uparrow}(\frac{1}{x}, -xy) = \frac{1-cy}{1+cxy-cy-xy^2} = F_{\downarrow,\downarrow}(x,y)$, for any positive integers r and s we see that $\psi_{\downarrow,\downarrow}(r,s) = (-1)^s\psi_{\uparrow,\uparrow}(s-r,s)$. Thus $p_{\downarrow,\downarrow}(r,s) = p_{\uparrow,\uparrow}(s-r,s)$, meaning that the graphs of $p_{\downarrow,\downarrow}$ and $p_{\uparrow,\uparrow}$ are mirror images of each other with respect to the line $\lambda = \frac{1}{2}$. Similarly, $F_{\uparrow,\downarrow}(\frac{1}{x}, -xy) = \frac{-xy\sqrt{1-c^2}}{1+cxy-cy-xy^2} = -F_{\downarrow,\uparrow}(x,y)$, so for any $(r,s) \in (\mathbb{Z}^+)^2$ we observe that $\psi_{\downarrow,\downarrow}(r,s) = (-1)^{s+1}\psi_{\uparrow,\uparrow}(s-r,s)$ and $p_{\downarrow,\downarrow}(r,s) = p_{\uparrow,\uparrow}(s-r,s)$. Thus the graphs of $p_{\downarrow,\uparrow}$ and $p_{\uparrow,\downarrow}$ are mirror images of each other with respect to the line $\lambda = \frac{1}{2}$. As

$F_{\downarrow,\uparrow}(x,y) = xF_{\uparrow,\downarrow}(x,y)$, we also see that $p_{\downarrow,\uparrow}(r+1,s) = p_{\uparrow,\downarrow}(r,s)$, implying that $F_{\uparrow,\downarrow}$ and $F_{\downarrow,\uparrow}$ have identical asymptotics. Thus any asymptotic formula for either $p_{\downarrow,\uparrow}(r,s)$ or $p_{\uparrow,\downarrow}(r,s)$ should be symmetric with respect to the line $\lambda = \frac{1}{2}$. While we will not yet exploit these symmetries in our analysis, they will limit the number of graphs that we must provide under full disclosure. Also, these symmetries will be helpful with the analysis in Section 4.3.

In general, the geometry of $\mathcal{V} = \{\mathbf{z} : H(\mathbf{z}) = 0\}$ can be complicated and asymptotic results depend greatly on the geometric classification of $\mathcal{V}$; see [PW02, PW04, PW08]. In the case of the one-dimensional QRW, the geometry of $\mathcal{V}$ is simple enough that asymptotics can be handled by the methods for smooth critical points found in [PW02]. The following propositions establish these geometric facts.

Proposition 4.6. *For QRWs on $\mathbb{Z}^1$ with matrix U_c for $0 < c < 1$, the quantity H_y is nonvanishing on $\mathcal{V}_1$.*

PROOF: Solving $H = 0, H_y = 0$, using the Maple command `Basis([H, diff(H,y)], plex(x,y))`, shows that there are precisely two pairs (x, y) where both polynomials vanish; the possible values of y are not on the unit circle except in the degenerate case $c = 1$. □

Proposition 4.7. *For the general unitary QRW on $\mathbb{Z}^1$, if $(x,y) \in \mathcal{V}$, then $|x| = 1$ if and only if $|y| = 1$.*

PROOF: The forward direction is a direct result of Proposition 4.2. Conversely, solving

$$H(x,y) := 1 - cy + cxy - xy^2 = 0$$

for x gives

$$x = \frac{cy - 1}{y(c-y)} = \frac{c - y^{-1}}{c - y}.$$

If $|y| = 1$, then $|y^{-1}| = 1$ and since $c \in \mathbb{R}$, it follows that $|c - y^{-1}| = |c - y|$. Thus $|y| = 1 \implies |x| = 1$. □

4.2.3 New Asymptotics for Torally Minimal Points when $d = 2$

As we show in the following section, for any λ in the interior of J, the set of critical points $\Xi(r, s)$ for this direction will consist of torally minimal points. We therefore seek a result that is as similar to Theorem 2.7 as possible, but handles the case of torally minimal points.

Before stating one, we note that while in dimension $d > 2$, $\mathbf{dir}\,(\mathbf{z}) = (z_1 H_1, \ldots, z_d H_d)$, in dimension 2 we define $\mathbf{dir}$ as the ratio of the two coordinates of the associated vector. That is $\mathbf{dir}\,(x_0, y_0) = \frac{yH_y}{xH_x}|_{x=x_0, y=y_0}$. Also for $a, b \in \mathbb{R}^+$, we define $D_{a,b} = \{(x, y) \in \mathbb{C}^2 : |x| \leq a,\ |y| \leq b\}$ and $T_{a,b} = \{(x, y) \in \mathbb{C}^2 : |x| = a,\ |y| = b\}$. Also, we remind the reader of the definition of Q from Section 2.2:

$$Q(x, y) = -x^2 H_x^2 y H_y - x H_x y^2 H_y^2 - x^2 y^2 (H_x^2 H_{yy} + H_y^2 H_{xx} - 2 H_x H_y H_{xy} \tag{4.11}$$

We can now state a variation of Theorem 2.7 and adapt the proof of Theorem 2.7 to this scenario.

Theorem 4.8. *For fixed $a, b > 0$ suppose that the following conditions hold:*

1. $\mathcal{V} \cap D_{a,b} = \mathcal{V} \cap T_{a,b}$;
2. $|x| = a \iff |y| = b$ *on* $\mathcal{V}$;
3. *For each x the set $\{y_1(x), \ldots, y_k(x)\}$ of values for which $H(x, y) = 0$ is finite;*
4. H_y *is nonvanishing on* $\mathcal{V} \cap T_{a,b}$.

Then the following two conclusions hold.

1. *If λ is not in the image under* $\mathbf{dir}$ *of $\mathcal{V} \cap T_{a,b}$, then $a^r b^s a_{rs}$ is rapidly decreasing. Specifically, as λ varies over a compact set disjoint from the range of* $\mathbf{dir}$, *for every integer $N > 0$ there is a $C > 0$ such that $a^r b^s a_{rs} \leq C s^{-N}$.*
2. *Conversely, let Λ be a compact subset of the range of* $\mathbf{dir}$ *such that for any $\lambda \in \Lambda$, the set $\Xi(\lambda)$ of points $(x, y) \in \mathcal{V} \cap T_{a,b}$ for which* $\mathbf{dir}\,(x, y) = \lambda$ *is finite and neither Q nor G vanishes*

there. Then

$$a_{r,s} \sim \sum_{(x,y)\in\Xi(r/s)} \frac{G(x,y)}{\sqrt{2\pi}} x^{-r} y^{-s} \sqrt{\frac{-yH_y}{sQ(x,y)}} \tag{4.12}$$

as $r, s \to \infty$, uniformly as r/s varies over Λ.

PROOF: We prove the second conclusion first. The proof of Theorem 2.7 begins with the localization step (Lemma 2.1) and it is this step which requires alteration in order to prove the second conclusion of Theorem 4.8. Instead, we substitute the following lemma:

Lemma 4.9. *Given r, s, let $\{(x_l(r/s), y_l(r/s) : 1 \leq l \leq L\}$ enumerate $\Xi(r/s)$ and let $\mathcal{N}_l$ be a small neighborhood of x_l. Then*

$$a_{rs} = \frac{1}{2\pi} \sum_l \int_{\mathcal{N}_l} x^{-r-1} y^{-s-1} \sum_l \frac{G(x, y_l(x))}{(\partial H/\partial y)(x, y_l(x))}\, dx + O(a^{-r} b^{-s} s^{-N}) \tag{4.13}$$

for every N, uniformly for $\lambda \in \Lambda$.

Assuming this for the moment, the remainder of the proof follows the proof of Theorem 2.7 (the full proof can be found in [PW02]) so closely that we merely indicate the numbers of the corresponding results. Changing variables to $x = ae^{i\theta}$, we write $x^{-r}y^{-s}$ as $\exp(-sf_l(\theta))$ near each $(x_l, y_l) \in \Xi(r/s)$ and rewrite (4.13) as

$$a_{rs} \sim \frac{1}{2\pi} a^{-r} b^{-s} \sum_l \int_{\mathcal{N}'_l} \exp(-sf(\theta))\psi(\theta)\, d\theta$$

where $\mathcal{N}'_l$ is a neighborhood around each critical θ and f and ψ are defined in Section 2.2. The summand is an integral near a stationary phase point; in the present case the exponent f is purely imaginary, so we may use a standard result to evaluate this, such as [Ste93, Proposition 3 of CH. VIII], rather than the complex phase version found in Theorem 2.4. The application of the formula for $\frac{\partial^2 Z}{\partial X^2}$ in the proof of Corollary 2.9 to the $d = 2$ case (in which we replace Z and z by Y and y, respectively) finishes the computation in the case at hand, finishing the proof of the second conclusion of Theorem 4.8.

The first conclusion then follows from the fact that there are, in the case $\lambda \notin J$, no stationary phase points. Thus the sum is empty and the result follows (and in fact one may halt the derivation in the lemma at (4.16)). Finally, the uniformity in both conclusions is a consequence of the fact that estimates such as Theorem 2.4 and [Ste93, Proposition VIII.3] are uniform under these conditions. □

Proof of Lemma 4.9: The following successive estimates for a_{rs} copy the reasoning in the proof of Lemma 2.1, though they occur in a different order due to differing geometry. We will write down the estimates and then see what is needed to justify them in our case.

$$a_{rs} = \left(\frac{1}{2\pi}\right)^2 \int_{C_a} \int_{C_{b-\epsilon}} x^{-r-1} y^{-s-1} F(x,y)\, dy\, dx\,. \tag{4.14}$$

$$= \left(\frac{1}{2\pi}\right)^2 \left[\int_{C_a} \int_{C_{b+\epsilon}} x^{-r-1} y^{-s-1} F(x,y)\, dy\, dx \right. \tag{4.15}$$
$$\left. - \int_{C_a} \left(\int_{C_{b+\epsilon}} - \int_{C_{b-\epsilon}} \right) x^{-r-1} y^{-s-1} F(x,y)\, dy\, dx \right].$$

$$= \frac{1}{2\pi} \int_{C_a} x^{-r-1} \sum_j y_j^{-s-1} \mathrm{Res}(F; y = y_j)\, dx + O(a^{-r}(b+\epsilon)^{-s})\,. \tag{4.16}$$

$$= \frac{1}{2\pi} \int_{C_a} x^{-r-1} \sum_j y_j^{-s-1} \frac{G(x, y_j(x))}{(\partial H/\partial y)(x, y_j(x))} + O(a^{-r}(b+\epsilon)^{-s})\, dx\,. \tag{4.17}$$

The first of these is Cauchy's integral formula. It is valid as long as F is analytic on $D_{a,b-\epsilon}$, which is guaranteed by hypothesis (1). The second is true whenever F is analytic on the torus $T_{a,b+\epsilon}$ as well, which is guaranteed by hypothesis (2). The third equation is true as long as $F(x,\cdot)$ has finitely many poles on the annulus $b-\epsilon < |y| < b+\epsilon$ for every $x \in C_a$. This is guaranteed by hypothesis (3). The fourth of these is true as long as the poles of $H(x,\cdot)$ are simple for x outside a set of measure zero, which is guaranteed by hypothesis (4).

Finally, to arrive at (4.13), we establish that

$$\eta := \frac{G}{\partial H/\partial y}\, dx$$

pulls back to a smooth form on the smooth manifold $\mathcal{V} \cap T_{a,b}$. In fact, smoothness of the form and the manifold follow from hypothesis (4) and the implicit function theorem. It now follows by [Ste93, Proposition 1 of Ch. VIII], using a partition of unity, that the integral is rapidly decreasing away from the critical points $\Xi(r/s)$, reducing (4.17) to (4.13). □

4.2.4 Location of the critical points for QRW

We show that for λ in the interval

$$J := \left[\frac{1}{2}(1-c), \frac{1}{2}(1+c)\right] ,$$

asymptotics are determined by a pair of critical points on the unit torus via Theorem 4.8, while for λ outside the closure of this interval, asymptotics are determined by a single critical point on a different torus via Theorem 2.7. This is established in the following lemmas.

Lemma 4.10.

$$(x(\lambda), y(\lambda)) \in T_{1,1} \iff \lambda \in J = \left[\frac{1}{2}(1-c), \frac{1}{2}(1+c)\right] .$$

Proof: First assume $(x(\lambda), y(\lambda)) \in T_{1,1}$. By Proposition 4.7, this is equivalent to $|y| = 1$. If we let X and Y be the arguments of x and y respectively, then implicit differentiation of the equation

$$e^{iX} = \frac{1 - ce^{iY}}{e^{iY}(e^{iY} - c)}$$

results in the logarithmic derivative

$$\frac{dY}{dX} = -\frac{1}{\frac{ce^{iY}}{1-ce^{iY}} + 1 + \frac{e^{iY}}{e^{iY}-c}} = -\left(1 + \frac{c^2 - 1}{-cy^{-1} + 2 - cy}\right) .$$

When (x, y) is on the unit torus, this expression simplifies to $\frac{dY}{dX} = -\left(1 + \frac{c^2-1}{2 - 2c \cdot \cos(Y)}\right)$. We now observe that

$$\frac{dY}{dX} = \frac{d(\log y)}{d(\log x)} = -\frac{x\partial H/\partial x}{y \partial H/\partial y} = -\frac{1}{\mathbf{dir}\,(x, y)} = -\frac{1}{1/\lambda} = -\lambda$$

by the definition of **dir**. Thus $\lambda = 1 + \frac{c^2-1}{2-2c \cdot \cos(Y)}$. It is not hard from here to check that as y varies over the unit circle, λ is decreasing in $\mathrm{Re}\,\{y\}$, so that the minimum value of λ is $\lambda(1) = (1-c)/2$, while the maximum is $\lambda(-1) = (1+c)/2$. Thus

$$(x(\lambda), y(\lambda)) \in T_{1,1} \Rightarrow \lambda \in J := \left[\frac{1}{2}(1-c), \frac{1}{2}(1+c)\right] .$$

For the other direction, we choose $\lambda \in J$ and solve for all possible points $(x(\lambda), y(\lambda))$. These are points $(x, y) \in \mathcal{V}$ at which the logarithmic normal vector (xH_x, yH_y) is parallel to (r, s) where $r/s = \lambda$. Thus (x, y) satisfies the two equations:

$$H(x, y) = 0 \tag{4.18}$$

$$K(x, y) := sxH_x - ryH_y = 0 \tag{4.19}$$

Then the Maple command `Basis([H,K], plex(y,x))` results in a reduced Gröbner basis whose first polynomial is the polynomial satisfied by x over $\mathbb{Z}[r, s]$:

$$s^2c^2x - xs^2 - 2rc^2xs + sc^2rx^2 + rc^2s + 4rxs + 2r^2c^2x - c^2r^2x^2 - r^2c^2 - 4r^2x\,.$$

Dividing by s^2 and recalling that $\lambda = \frac{r}{s}$ yields

$$\lambda(1-\lambda)c^2x^2 - [(1-c^2) - (4-2c^2)\lambda + (4-2c^2)\lambda^2]\,x + \lambda(1-\lambda)c^2\,.$$

Viewed as a polynomial in x, the roots are conjugate (possibly equal) if and only if the discriminant is nonpositive, which happens exactly when $\lambda \in J$. The product of the roots is the ratio of the constant to the quadratic coefficient, in this case 1, therefore $\lambda \in J$ implies the two conjugate roots are on the unit circle, hence by Proposition 4.7, $|x| = |y| = 1$ for all critical points. $\square$

To sum up:

Proposition 4.11. *The torus $T_{1,1}$ is a minimal torus and the image of* **dir** *on $\mathcal{V} \cap T_{1,1}$ is J.*

Proof: In order for $T_{1,1}$ to be a minimal torus, it is necessary and sufficient to show the following two conditions:

1. $\mathcal{V} \cap \{|x| < 1, |y| < 1\} = \varnothing$

2. $\mathcal{V} \cap (\{|x| < 1, |y| = 1\} \cup \{|x| = 1, |y| < 1\}) = \varnothing$.

Condition (1) follows from the absolute convergence of $F(\alpha, \beta)$ for every pair of positive real $\alpha, \beta < 1$. Condition (2) follows from Proposition 4.7. $\square$

4.2.5 Proofs of Theorems 4.4 and 4.5

Observe first, using the relation (4.10) and the subsequent discussion, that it suffices to prove both theorems in the real case, $U = U_c$. Thus we assume throughout this section that $\alpha = \beta = \gamma = 0$.

PROOF OF THEOREM 4.4: This is immediate from the first conclusion of Theorem 4.8 with $a = b = 1$, once one observes that the hypothesis are satisfied. The first hypothesis was verified in Proposition 4.11, the second in Proposition 4.7, the third follows whenever H has no factor $P(x)$, and the fourth was Proposition 4.6. □

PROOF OF THEOREM 4.5: Fix λ in the interior of J. By Proposition 4.11, $T_{1,1}$ is a minimal torus containing two conjugate critical points, (x, y) and $(\overline{x}, \overline{y})$. These satisfy the hypotheses of Theorem 4.8, whence the conclusion (4.12) holds.

Recalling that $G_{\downarrow\downarrow}(x, y) = 1-cy$, and observing that the two summands in (4.12) are conjugates, we see that

$$\psi_{\downarrow\downarrow}(r, s) \sim 2\text{Re}\left\{\frac{1-cy}{\sqrt{2\pi}} x^{-r} y^{-s} \sqrt{\frac{-yH_y}{sQ(x,y)}}\right\}$$

where Q is given in (4.11). Letting

$$\rho_{\xi_0,\xi}(r, s) := \text{Arg}\left(\frac{G_{\xi_0,\xi}}{\sqrt{2\pi}} x^{-r} y^{-s} \sqrt{\frac{-yH_y}{sQ(x,y)}}\right), \tag{4.20}$$

allows us to rewrite this as

$$p_{\downarrow\downarrow}(r, s) \sim \frac{2}{\pi} \cos^2 \rho_{\downarrow\downarrow}(r, s) \left|(1-cy)^2 \frac{-yH_y}{sQ(x,y)}\right| .$$

Instead of solving for x and y and plugging into expressions for H_y and Q, the computations are simplified by finding directly the minimal polynomial for $w := (1-cy)^2 \frac{-yH_y}{sQ(x,y)}$.

Recalling that (x, y) satisfies $H(x, y) = K(x, y) = 0$, we introduce a variable $z := 1/(sQ)$ so that w may be expressed as the solution to the following four polynomial equations.

$$\begin{aligned} H &= 0 \\ K &= 0 \\ szQ - 1 &= 0 \\ w + (1-cy)^2(yH_y)z &= 0 \end{aligned}$$

To obtain a polynomial in w alone, we use the `Basis` command with term order `plex(x,y,z,w)`, resulting in the polynomial

$$r^2s^2(1-c^2) - (s(1+c)-2r)(s(1-c)-2r)(s-r)^2w^2 \,.$$

We divide by s^2 and rewrite in terms of λ:

$$\lambda^2(1-c^2) + 4\left(\frac{1+c}{2} - \lambda\right)\left(\lambda - \frac{1-c}{2}\right)(1-\lambda)^2s^2w^2 \,.$$

We are actually interested in $|w|$, but since the above expression may be written as $A + Bw^2$ for positive real A and B, we see that $|w|$ is the positive square root of A/B, in other words,

$$|w| = \frac{\sqrt{1-c^2}\lambda}{(1-\lambda)s\sqrt{-((1-c^2) - 4\lambda + 4\lambda^2)}} \,.$$

This proves Equation (4.4). The computations for the other three cases are slight variations, the only difference being the value of $G_{\xi_0,\xi}(x,y)$. Because $G_{\uparrow\downarrow}(x,y) = y\sqrt{1-c^2}$ has the same magnitude as $G_{\downarrow\uparrow}(x,y) = xy\sqrt{1-c^2}$, the formulae for $p_{\uparrow\downarrow}$ and $p_{\downarrow\uparrow}$ will differ only in the phase term. The minimal polynomial for $-G_{\uparrow\downarrow}^2 yH_y/(sQ)$ in terms of r and s turns out to be Aw^2+Bw+C where

$$\begin{aligned} A &= 4rc^2(s-r)\left(\frac{s(c+1)}{2} - r\right)\left(\frac{s(c-1)}{2} + r\right) \\ B &= 4(1-c^2)(2r-s)\left(\frac{s(c+1)}{2} - r\right)\left(\frac{s(c-1)}{2} + r\right) \\ C &= rc^2(1-c^2)(s-r) \end{aligned}$$

Dividing each of these by s^2, and letting $\lambda = \frac{r}{s}$ we get $A'w^2 + B'w + C'$, where

$$\begin{aligned} A' &= 4\lambda c^2(1-\lambda)\left(\frac{c+1}{2} - \lambda\right)\left(\frac{c-1}{2} + \lambda\right)s^2 \\ B' &= 4(1-c^2)(2\lambda - 1)\left(\frac{c+1}{2} - \lambda\right)\left(\frac{c-1}{2} + \lambda\right)s \\ C' &= \lambda c^2(1-c^2)(1-\lambda) \end{aligned}$$

Then since $B'^2 - 4A'C' < 0$ for $\lambda \in J$, we have that

$$|w| = |\frac{-B' \pm \sqrt{B'^2 - 4A'C'}}{2A'}| = \sqrt{\frac{B'^2}{4A'^2} + \frac{-B'^2 + 4A'C'}{4A'^2}} = \sqrt{\frac{C'}{A'}} = \frac{\sqrt{1-c^2}}{s\sqrt{-((1-c^2) - 4\lambda + 4\lambda^2)}}$$

The minimal polynomial for $-G^2_{\uparrow\uparrow} y H_y / Q$ in terms of λ turns out to be:

$$(1-\lambda)^2(1-c^2) + 4\left(\frac{1+c}{2} - \lambda\right)\left(\lambda - \frac{1-c}{2}\right)\lambda^2 s^2 w^2 .$$

Again we are interested in $|w|$, and the above expression may be written as $A + Bw^2$ for positive real A and B, so $|w|$ is the positive square root of A/B. Thus

$$|w| = \frac{\sqrt{1-c^2}(1-\lambda)}{\lambda s\sqrt{-((1-c^2) - 4\lambda + 4\lambda^2)}} .$$

This completes the proof of Theorem 4.5. □

4.3 Airy Behavior for QRWs on $\mathbb{Z}$

The results of the prior section relied on the asymptotic estimation of an integral of the form:

$$\int \exp(-r_d \tilde{f}(\theta))\tilde{\psi}(\theta))\mathbf{d}\theta \tag{4.21}$$

using the stationary phase method when the stationary points of $\tilde{f}$ (which are the saddle points for the integral) are isolated. We summed the contributions from two isolated conjugate saddle points (at each of which $\tilde{f}$ vanished to order 2) to determine the asymptotic estimate. As $\lambda \to \frac{1\pm c}{2}$, however, the saddle points coalesce into a single point at which $\tilde{f}$ vanishes to order 3. Consequently, our previous results do not hold in neighborhoods of the points $\lambda = \frac{1\pm c}{2}$. In this section we demonstrate this coalescence, then we review and apply a result for the asymptotics of integrals with coalescing saddle points.

4.3.1 Statement of Results

As mentioned in Section 4.2, we need only forecast asymptotics in a neighborhood of the direction $\lambda = \frac{r}{s} = \frac{1-c}{2}$ for each of our four pairs of chiralities, due to the symmetries of our distributions.

Theorem 4.12 (Asymptotics near $\lambda = \frac{1-c}{2}$)**.** *Given a general unitary walk with transformation U_c, let $\delta = \frac{s}{r} - \frac{2}{1-c}$. Then as $s \to \infty$ and $\delta \to 0$ the probabilities for the directions $\lambda = \frac{r}{s}$ are given by the following asymptotic formula:*

$$p_{\xi_0,\xi}(r,s) \sim \left(\frac{d\theta}{dt}\right)^2 |\frac{Airy(r^{2/3}\gamma^2)}{r^{1/3}} F^0_{\xi_0,\xi} + \frac{Airy'(r^{2/3}\gamma^2)}{r^{2/3}} \cdot F^1_{\xi_0,\xi}|^2 \tag{4.22}$$

where

$$F^0_{\downarrow,\downarrow} \equiv 1 \qquad F^1_{\downarrow,\downarrow} \equiv 0 \tag{4.23}$$

$$F^0_{\uparrow,\uparrow} = \frac{\delta(1-c)+(1+c)}{1-c} \qquad F^1_{\uparrow,\uparrow} \equiv 0 \tag{4.24}$$

$$F^0_{\uparrow,\downarrow} = \frac{\delta(1-c)+2c}{2c}\sqrt{\frac{1+c}{1-c}} \qquad F^1_{\uparrow,\downarrow} = \frac{(1+c)^{1/6}}{2c^{5/6}}\sqrt{\frac{\delta(1-c)(1+c)+4c}{1-c}} \tag{4.25}$$

$$F^0_{\downarrow,\uparrow} = F^0_{\uparrow,\downarrow} \qquad F^1_{\downarrow,\uparrow} = -F^1_{\uparrow,\downarrow} \tag{4.26}$$

$$\gamma \sim \sqrt{\delta(1-c)(1+c)}[c(1+c)]^{-1/6} \tag{4.27}$$

and

$$\left(\frac{d\theta}{dt}\right)^2 \sim \frac{2(1+c)^{1/3}(1-c)^2}{c^{1/6}[\delta(1-c)+(c+1)]\sqrt{\delta(1-c)(1+c)+4c}}$$

with $Airy(x)$ *the function defined for* $x \in \mathbb{R}$ *as* $Airy(x) := \frac{1}{\pi}\int_0^\infty \cos(\frac{t^3}{3}+xt)dt$.

We again demonstrate our results pictorially, this time with a graph of the $U_{1/2}$ walk's actual probabilities (for the $(\downarrow,\downarrow)$ chirality on the left and $(\downarrow,\uparrow)$ chirality on the right) versus our predictions in the range of the point $\frac{r}{s} = \frac{1-c}{2} = \frac{1}{4}$ for time $s = 1000$. One can see that the prediction is best when δ is smallest, which in Figure 2 is when the location is closest to 250.

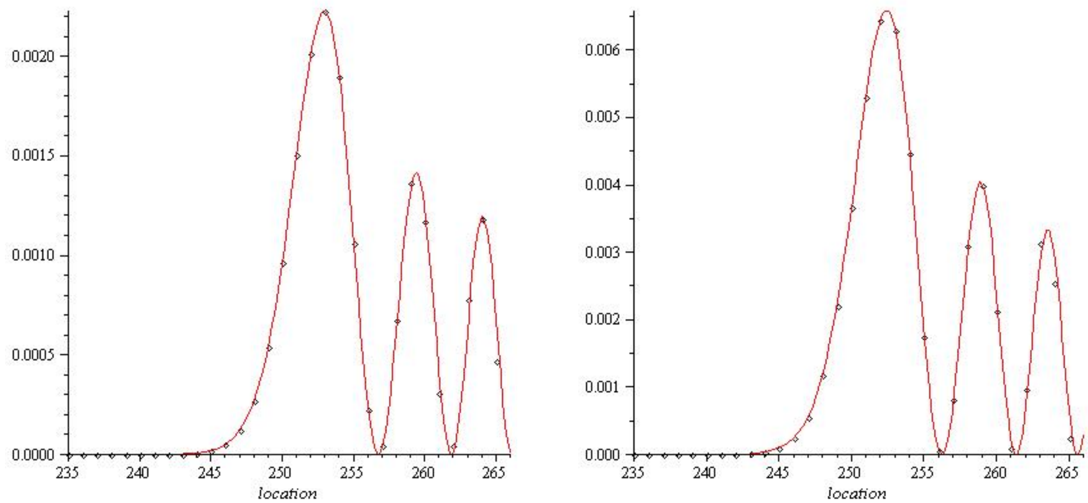

Figure 2: Time $n = 1000$ probability values by location ($p_{\downarrow,\downarrow}$ on left and $p_{\downarrow,\uparrow}$ on right) for the $U_{1/2}$ walk and our asymptotic prediction.

4.3.2 Proof of Theorem 4.12

We employ the method detailed in Chapter 9 (titled Uniform Asymptotic Expansions) of [BH86]. This method determines an asymptotic approximation for an integral such as ours in the neighborhood of a point where two simple saddle points coalesce into a saddle point of order 2. The "order" of a saddle point is the degree to which the derivative of the phase $\tilde{f}$ vanishes. A "simple" saddle point is one of order 1. While in the case of a single saddle point we defined $\tilde{f}$ so that it vanished along with its derivative, this is not necessary.

Before utilizing the methods of [BH86], we determine the explicit integral representations of our coefficients and demonstrate the coalescence of our simple saddle points into a saddle point of order 2.

Lemma 4.13. *For the nearest neighbor QRW on the line with unitary coinflip U_c, given initial chirality ξ_0 and final chirality ξ, the norm of the amplitude $a_{\xi_0,\xi}(r,s)$ is given by the equation:*

$$|a_{\xi_0,\xi}(r,s)| = \frac{1}{2\pi}|\int_{\mathcal{C}} \tilde{\psi}_{\xi_0,\xi}(\theta) \exp\left[-r\left(\log\left(\frac{1-ce^{i\theta}}{e^{i\theta}(e^{i\theta}-c)}\right) + i\frac{s}{r}\theta\right)\right] d\theta| \tag{4.28}$$

where $\mathcal{C}$ is a contour circling the origin with winding number 1 containing the critical points $\mathbf{z} \in \Xi(\mathbf{r})$ while:

$$\tilde{\psi}_{\uparrow,\uparrow}(\theta) := 1 \tag{4.29}$$

$$\tilde{\psi}_{\uparrow,\uparrow}(\theta) := \frac{e^{i\theta}(1-c)(1+c)}{(1-ce^{i\theta})(e^{i\theta}-c)} \tag{4.30}$$

$$\tilde{\psi}_{\uparrow,\downarrow}(\theta) = \frac{e^{i\theta}}{1-ce^{i\theta}}\sqrt{1-c^2} \tag{4.31}$$

$$\tilde{\psi}_{\downarrow,\uparrow}(\theta) = \frac{1}{e^{i\theta}-c}\sqrt{1-c^2} \tag{4.32}$$

Proof: To simplify our calculations we reorder the variables x and y (from the generating function of QRWs on $\mathbb{Z}$) as $\mathbf{z} = (y, x)$. Thus the function g defined in Section 2.2 is the function such that $H(y, g(y)) = 0\ \forall y$. From the proof of Proposition 4.7, we obtain $g(y) = \frac{1-cy}{y(y-c)}$. Also, we maintain the original associations between $\mathbf{r}$ and $\mathbf{z}$ so that $\mathbf{r}$ is now (s, r). Thus $r_d = r$. Our result now follows from the proof of Lemma 2.1, once one determines $\tilde{f}$ and $\tilde{\psi}$ and omits the localization step.

In Section 2.2 we defined $\tilde{f}$ so that the point $\theta = 0$ coincided with the sole critical point $\mathbf{z} \in \Xi(\mathbf{r})$, and hence the sole saddle point for the integral. With two critical points we define $\tilde{f}$ so that $\theta = 0$ corresponds to $y = 1$, a natural choice as the critical points will correspond to additive inverses for θ. This is a translate of the phase used in Section 2.2, and as we use the same contour of integration, the value of the integral is unaffected. To distinguish this setting from that of Section 2.2, as well as to borrow from the notation of [BH86], we rename this new phase w. In this context, $w(\theta) = \log\left(\frac{g(\exp(i\theta))}{g(1)}\right) + i\frac{s}{r}\theta = \log\left(g(\exp(i\theta))\right) + i\frac{s}{r}\theta = \log\left(\frac{1-ce^{i\theta}}{e^{i\theta}(e^{i\theta}-c)}\right) + i\frac{s}{r}\theta$.

In contrast, the calculation of $\tilde{\psi}$ will be slightly more involved, and as it depends on both the numerator and denominator of the generating function, it will vary depending on the initial and final chirality. From the definition of $\tilde{\psi}$ in Section 2.2, centering at $y = 1$ we have

$$\begin{aligned}
\tilde{\psi}_{\downarrow,\downarrow}(\theta) &= -\lim_{x\to g(e^{i\theta})} \left(x - g(e^{i\theta})\right) \frac{1-ce^{i\theta}}{[1-ce^{i\theta}+xe^{i\theta}(c-e^{i\theta})]x} \\
&= -\lim_{x\to g(e^{i\theta})} \left(x - \frac{1-ce^{i\theta}}{e^{i\theta}(e^{i\theta}-c)}\right) \frac{\frac{1-ce^{i\theta}}{e^{i\theta}(e^{i\theta}-c)}}{[\frac{1-ce^{i\theta}}{e^{i\theta}(e^{i\theta}-c)} - x]x} \\
&= -\lim_{x\to g(e^{i\theta})} \frac{1}{x} \cdot \frac{1-ce^{i\theta}}{e^{i\theta}(e^{i\theta}-c)} \\
&= 1
\end{aligned}$$

Making the analogous calculation for the other combinations of chiralities completes the proof. $\Box$.

With this integral representation, it is a direct computation to show that the methods of [BH86] apply to our integral.

Lemma 4.14. *For the nearest neighbor QRW on the line with unitary coinflip U_c, the integral*

$$I(r) := \int_{\mathcal{C}} \exp(-rw(\theta))\tilde{\psi}(\theta)d\theta \tag{4.33}$$

has 2 simple saddle points $\alpha_\pm$ which coalesce into a saddle point of order 2 precisely when $\frac{r}{s} = \frac{1\pm c}{2}$. Furthermore, there is a simply connected domain D_1 containing the contour $\mathcal{C}$ and the points $\theta = \alpha_\pm$.

Proof: We begin by solving the critical point equations via Gröbner bases with the Maple command `Basis([H,K], plex(x,y))`. This results in a reduced Gröbner basis whose first polynomial is the polynomial satisfied by y over $\mathbb{Z}[r,s]$. Making the substitution $s = r\lambda$ in this polynomial and dividing by the coefficient of y^2 results in the minimal polynomial: $y^2 + \frac{\lambda(1+c^2)-2}{c(1-\lambda)}y + 1 = 0$. Whether or not this equation's solutions have unit modulus, they will be multiplicative inverses, as the coefficients of y^2 and y^0 are both 1. Furthermore, this equation has a single solution of order 2 if and only if $\lambda = \frac{1\pm c}{2}$. We focus on the point $\lambda = \frac{1-c}{2}$; the calculations for $\lambda = \frac{1+c}{2}$ are analogous.

Making the substitution $\frac{s}{r} = 1/\lambda = \frac{2}{1-c} + \delta$ and solving for y results in the two solutions:

$$y_\pm = \frac{[2+\delta(1-c)](c^2+1) - 2(1-c) \pm (1-c)\sqrt{\delta(1-c)(1+c)[\delta(1-c)(1+c)+4c]}}{2c[(1+c)+\delta(1-c)]} \tag{4.34}$$

which coalesce in a neighborhood of $\delta = 0$ only when $\delta = 0$, in which case $y_+ = y_- = 1$. Using the equation $x = g(y)$ we obtain a unique value of x to correspond with each of y_+ and y_-. We now define $\alpha_+ = i\log(y_+)$ and $\alpha_- = i\log(y_-) = -i\log(y_+)$. We complete the proof by showing that the integral has simple saddle points at $\alpha_\pm$ when δ is in a neighborhood of 0 and that these points coalesce into a saddle point of order 2 when $\delta = 0$. (Note: When we take the log of a number $z \in \mathbb{C}$ we always let $\log(z)$ denote the principal logarithm with discontinuity when $Arg(z) = \pi$.)

By taking derivatives we see that $w_\theta(\alpha_+) = w_\theta(\alpha_-) = 0$, while

$$w_{\theta\theta}(i\log(y_+)) = -w_{\theta\theta}(i\log(y_-)) = \frac{(1-c)(1+c)(1-y_+)(1+y_+)y_+c}{(y_+-c)^2(y_+c-1)^2}. \tag{4.35}$$

To simplify this, we note that if we refer to the minimal polynomial of $y_\pm$ as $y^2 + Ay + 1$, then $(y_+-1)(y_++1) = -2 - Ay_+$ and $(y_+-c)(y_+c-1) = -y_+(Ac+1+c^2)$. Then

$$\frac{y_+(y_+-1)(y_++1)}{(y_+-c)^2(y_+c-1)^2} = \frac{y_+(-2-Ay_+)}{y_+^2(Ac+1+c^2)^2} = \frac{-2y_-A}{(Ac+1+c^2)^2}.$$

Now substituting the values of y_+ and y_- as well as $A = \frac{\lambda(1+c^2)-2}{c(1-\lambda)}$ and simplifying we get

$$w_{\theta\theta}(i\log(y_+)) = \frac{[\delta(1-c)+(c+1)]\sqrt{\delta(1+c)(1-c)[\delta(1-c)(1+c)+4c]}}{(1+c)(1-c)^2} \tag{4.36}$$

which only vanishes in a neighborhood of $\delta = 0$ when $\delta = 0$.

Differentiating once more, we see that

$$w_{\theta\theta\theta}(0)|_{\delta=0} = \frac{2i(1+c)c}{(1-c)^3} \tag{4.37}$$

which is nonvanishing in our interval $c \in (0,1)$. This completes the proof. □

We are now free to employ the methods of [BH86], the first step of which is a conformal change of variables $t = v(\theta)$ designed to simplify the phase w of the integral. We denote the inverse of the map v as $u = v^{-1}$ so that $\theta = u(t)$. These changes of variables are defined implicitly by the equation

$$w(\theta) = -\left(\frac{t^3}{3} - \gamma^2 t\right) + \rho = \phi(t) \tag{4.38}$$

in which γ and ρ are constants, yet to be determined.

Equation 4.38 defines three potential maps u, none of which is clearly conformal. Theorem 4.15 below, cited from [CFU57], isolates the correct conformal map:

Theorem 4.15. *For each $\alpha_\pm$ in D_1, the transformation* (4.38) *has just one branch which defines a conformal map of some disc D_α containing $\alpha_\pm$. On this branch the points $\theta = \alpha_+$ and $\theta = \alpha_-$ correspond respectively to $t = \gamma$ and $t = -\gamma$.*

□

We adopt the notation $\hat{D}_\alpha$ for the image $u(D_\alpha)$ from [BH86]. Now with the conformal maps u and v so defined, we determine the values of ρ and γ. First we note that as desired, the new phase ϕ has isolated simple saddle points at $t = \pm\gamma$ when $\gamma \neq 0$ and a single saddle point of order 2 when $\gamma = 0$.

By differentiating (4.38) with respect to t, we obtain

$$\frac{d\theta}{dt} = \frac{\gamma^2 - t^2}{w_\theta(\theta)}. \tag{4.39}$$

Since $\frac{d\theta}{dt}$ must be finite and nonzero for all $t \in \hat{D}_\alpha$ (or equivalently all $\theta \in D_\alpha$) so that u may be conformal, it must be as Theorem 4.15 prescribes that

$$t = \pm\gamma \text{ when } \theta = \alpha_\pm. \tag{4.40}$$

Making the correspondence (4.40) in Equation (4.38) provides the following expressions for γ and ρ.

$$\frac{4\gamma^3}{3} = w(\alpha_+) - w(\alpha_-) \tag{4.41}$$

$$\rho = \frac{1}{2}[w(\alpha_+) + w(\alpha_-)] \tag{4.42}$$

As our phase function w is odd and α_+ and α_- are additive inverses in our case, the above equations simplify to:

$$\begin{aligned} \frac{4\gamma^3}{3} &= 2w(\alpha_+) \\ &= 2\log\left(\frac{1-cy_-}{y_-(y_- - c)}\right) + 2\log(y_-)\left(\frac{2}{1-c} + \delta\right) \\ &= 2\log\left(\frac{1-cy_-}{1-cy_+}\right) + 2\log(y_-)\left(\frac{2c}{1-c} + \delta\right) \end{aligned}$$

and

$$\rho = 0. \tag{4.43}$$

Substituting the values of y_+ and y_- from (4.34) into the equation in γ above and expanding into a power series in δ at the origin, we obtain

$$\gamma^3 = -\frac{(1-c)^{3/2}}{\sqrt{c(1+c)}}\delta^{3/2} + o(\delta^{3/2}) \tag{4.44}$$

so that

$$\gamma = -\frac{\sqrt{\delta(1-c)}}{[c(1+c)]^{1/6}}\zeta_3 + o(\delta^{1/2}) \tag{4.45}$$

for some third root of unity ζ_3.

Thus we have three possible values of γ when $\alpha_+ \neq \alpha_-$. In [BH86] the authors resolve this ambiguity by developing contours $\mathcal{C}_1$, $\mathcal{C}_2$, and $\mathcal{C}_3$, each beginning and ending at ∞, such that for $t \in \mathcal{C}_j$, they have $\frac{\pi}{3}(4-2j) < \mathrm{Arg}(t) < \frac{\pi}{3}(6-2j)$. For each of the three possible choices of γ in Equation (4.41) the regular branch of $u(t)$ promised by Theorem 4.15 maps $\mathcal{C} \cap D_\alpha$ onto a contour asymptotically equivalent to one of $\mathcal{C}_1 \cap \hat{D}_\alpha$, $\mathcal{C}_2 \cap \hat{D}_\alpha$, or $\mathcal{C}_3 \cap \hat{D}_\alpha$. The authors show it is correct to choose the determination of γ leading to an image contour asymptotically equivalent to $\mathcal{C}_1 \cap \hat{D}_\alpha$. Furthermore, they demonstrate that this choice of γ is that satisfying the equation:

$$\frac{1}{2}\operatorname{Arg}\Delta\theta + \frac{1}{2}\operatorname{Arg}(w_\theta(\theta_0)) - \frac{2\pi}{3} < \operatorname{Arg}(\gamma) < \frac{1}{2}\operatorname{Arg}\Delta\theta + \frac{1}{2}\operatorname{Arg}(w_\theta(\theta_0)) - \frac{\pi}{3} \pmod{\pi} \tag{4.46}$$

where $\theta = \theta_0$ is the preimage of $t = 0$ and $\Delta\theta$ is an increment directed from $\theta = \theta_0$ to the contour $\mathcal{C}$.

In the following lemma we demonstrate $\zeta_3 = 1$ will always be our desired third rooty of unity.

Lemma 4.16. *For any δ in a neighborhood of the origin, letting $\zeta_3 = 1$ gives the choice of γ satisfying Equation* (4.46)*. Thus $\gamma = -\frac{\sqrt{\delta(1-c)}}{[c(1+c)]^{1/6}} + o(\delta^{1/2})$.*

Proof: To facilitate the proof we refer to our original form for the oscillatory integral, taking a step back from (2.1) to the integral with f and ψ in terms of $\hat{\mathbf{w}}$. In this case $\hat{\mathbf{w}} = y = \hat{y}e^{i\theta} = e^{i\theta}$. The contour of integration is then the unit circle when $\delta \leq 0$ (in which case $|y_+| = |y_-| = 1$) and while it must be deformed in the case that $\delta > 0$, the contour still circles the origin. In light of the fact that y_0 is clearly 1, Δy will be a negative real increment, so $\operatorname{Arg}(\Delta y) = \pi$. We next differentiate $w(y(\theta))$ to get $w_\theta = \frac{dw}{dy}\frac{dy}{d\theta}$. For $y = 1$ we find $\frac{dw}{d\theta} = i\delta$ and $\frac{dy}{d\theta} = i$, so $w_y(1) = \delta$. Thus for $\delta < 0$, $\operatorname{Arg}(w_y(y_0)) = \pi$ while for $\delta > 0$, $\operatorname{Arg}(w_y(y_0)) = 0$. Substituting into Equation (4.46) for $\delta < 0$, we have:

$$\frac{\pi}{2} + \frac{\pi}{2} - \frac{2\pi}{3} < \operatorname{Arg}(\gamma) < \frac{\pi}{2} + \frac{\pi}{2} - \frac{\pi}{3} \pmod{\pi}$$

so the argument of γ is within $\pi/6$ of the argument of a purely imaginary number. As $\zeta_3 = 1$ ensures that $\gamma \in \mathbb{R}^- i$, it is the appropriate choice. Substituting into Equation (4.46) for $\delta > 0$, we have:

$$0 + \frac{\pi}{2} - \frac{2\pi}{3} < \operatorname{Arg}(\gamma) < 0 + \frac{\pi}{2} - \frac{\pi}{3} \pmod{\pi}$$

so the argument of γ is within $\pi/6$ of the argument of a real number. As $\zeta_3 = 1$ ensures that $\gamma \in \mathbb{R}^-$, it is the appropriate choice. □

With γ and ρ now defined, we note that when $\alpha_+ \neq \alpha_-$ so that $\gamma \neq 0$, by applying L'Hopital's rule in Equation (4.39) we obtain

$$\left(\frac{d\theta}{dt}\right)^2 |_{t=\pm\gamma \ or \ \theta=\alpha_\pm} = \frac{\mp 2\gamma}{w_{\theta\theta}(\alpha_\pm)} \tag{4.47}$$

which is finite and nonzero. In our case we have

$$\frac{d\theta}{dt}|_{\theta=\alpha_+} = \sqrt{-\frac{2\gamma}{w_{\theta\theta}(\alpha_+)}} \sim \sqrt{\frac{2(1+c)^{1/3}(1-c)^2}{c^{1/6}[\delta(c-1)-(c+1)]\sqrt{\delta(1-c)(1+c)+4c}}} \tag{4.48}$$

while $\frac{d\theta}{dt}|_{\theta=\alpha_-} = \frac{d\theta}{dt}|_{\theta=\alpha_+}$ as $w_{\theta\theta}(\alpha_-) = -w_{\theta\theta}(\alpha_+)$. We will denote this common value simply as $\frac{d\theta}{dt}$.

When $\delta = 0$, so that $\alpha_+ = \alpha_-$ and $\gamma = 0$, L'Hopital's rule must be applied twice and the result is

$$\left(\frac{d\theta}{dt}\right)^3 |_{t=0 \ or \ \theta=\alpha_+} = \frac{-2}{w_{\theta\theta\theta}(\alpha_+)} \tag{4.49}$$

which is also finite and nonzero. In our case, when $\delta = 0$ we have

$$\frac{d\theta}{dt} = -\frac{1-c}{[(1+c)c]^{1/3}} i. \tag{4.50}$$

which has equal norm to the limit as $\delta \to 0$ in our original expression for $\frac{d\theta}{dt}$. Thus when we seek the value of $|\frac{d\theta}{dt}|$ going forward, we may always use the formula for the $\delta \neq 0$ case.

We are now free to apply the transformation (4.38) to the integral (4.33) to obtain

$$I(r) = \int_{\mathcal{C}_1 \cap \hat{D}_\alpha} G_0(t) \exp\{-r\phi(t)\} dt + \mathcal{E} \tag{4.51}$$

with

$$G_0(t) := \tilde{\psi}(u(t)) \frac{d\theta}{dt} \tag{4.52}$$

which is regular in $\hat{D}_\alpha$, while $\mathcal{E}$ is asymptotically negligible, being by assumption exponentially smaller than I itself.

We next expand G_0 to facilitate the derivation of a uniform expansion. Specifically, we exploit the fact that when the integrand vanishes near a critical point, the contribution to asymptotics from that point is diminished. Thus we write:

$$G_0(t) := a_0 + a_1 t + (t^2 - \gamma^2) H_0(t) \tag{4.53}$$

(with a_0, a_1 and H to be determined) so that as long as H_0 is regular in $\hat{D}_\alpha$, the last term of (4.53) vanishes at the two saddle points $t = \pm\gamma$. We can then determine a_0 and a_1 by assuming H_0 to be regular and setting $t = \pm\gamma$ in (4.53) to get

$$a_0 := \frac{G_0(\gamma) + G_0(-\gamma)}{2} \tag{4.54}$$

$$a_1 := \frac{G_0(\gamma) - G_0(-\gamma)}{2\gamma} \tag{4.55}$$

With a_0 and a_1 so determined, it is shown in [BH86] that $H_0 = \frac{G_0(t) - a_0 - a_1 t}{t^2 - \gamma^2}$ is regular in $\hat{D}_\alpha$ as desired.

Then inserting (4.53) into (4.51) we obtain

$$I(r) \sim \exp\{r\rho\} \int_{\mathcal{C}_1 \cap \hat{D}_\alpha} \exp\{-r(\frac{t^3}{3} - \gamma^2 t)\}(a_0 + a_1 t)dt + R_0(r) \tag{4.56}$$

where $R_0(r) = \exp\{r\rho\} \int_{\mathcal{C}_1 \cap \hat{D}_\alpha} (t^2 - \gamma^2) H_0(t) \exp\{-r(\frac{t^3}{3} - \gamma^2 t)\} dt$.

We rewrite the first integral in (4.56) by first replacing $\mathcal{C}_1 \cap \hat{D}_\alpha$ with $\mathcal{C}_1$ itself (introducing an asymptotically negligible error) then using the alternate characterization of the Airy function:

$$Ai(x) = \frac{1}{2\pi i} \int_{\mathcal{C}_1} \exp(sx - s^3/3)ds = \frac{2}{\pi} \int_{-\infty}^{\infty} \cos(\frac{\tau^3}{3} + \tau x)d\tau \tag{4.57}$$

in order to express the integral in terms of $Ai(x)$ and its derivative $Ai'(x)$. To determine R_0 we integrate by parts and introduce another asymptotically negligible error by ignoring the boundary terms. The result is the expansion;

$$I(r) \sim 2\pi i \exp\{r\rho\} \left[\frac{a_0}{r^{1/3}} Ai(r^{2/3}\gamma^2) + \frac{a_1}{r^{2/3}} Ai'(r^{2/3}\gamma^2) \right] + R_1(r) \tag{4.58}$$

with

$$R_1(r) = \frac{\exp\{r\rho\}}{r} \int_{\mathcal{C}_1 \cap \hat{D}_\alpha} G_1(t) \exp\{-r(\frac{t^3}{3} - \gamma^2 t)\} dt$$

and $G_1(t) = \frac{d}{dt}H_0$. We observe that $R_1(r)$ is an integral of the form (4.51) multiplied by r^{-1}. Thus the above process can be applied repeatedly, after $N+1$ applications arriving at the asymptotic expansion

$$I(r) \sim 2\pi i \exp\{r\rho\}\left[\frac{Ai(r^{2/3}\gamma^2)}{r^{1/3}}\sum_{n=0}^{N}\frac{a_{2n}}{r^n} + \frac{Ai'(r^{2/3}\gamma^2)}{r^{2/3}}\sum_{n=0}^{N}\frac{a_{2n+1}}{r^n}\right] + R_N(r) \tag{4.59}$$

with $R_N(r) = r^{-(N+1)}\exp\{r\rho\}\int_{\mathcal{C}_1\cap\hat{D}_\alpha} G_{N+1}(t)\exp\{-r(\frac{t^3}{3} - \gamma^2 t)\}dt$.

In Theorem 9.2.2 of [BH86] the authors show that the above formal procedure yields an asymptotic expansion of $I(r)$ that is uniformly valid for δ small. In addition, they point out that the Airy function provides a smooth transition in the algebraic order of I in r which is $r^{-1/2}$ for separated simple saddle points and $r^{-1/3}$ for a single saddle point of order 2.

Thus, in particular, we have the asymptotic formula

$$I(r) \sim 2\pi i \exp\{r\rho\}\left[\frac{a_0}{r^{1/3}}Ai(r^{2/3}\gamma^2) + \frac{a_1}{r^{2/3}}Ai'(r^{2/3}\gamma^2)\right].$$

As $\rho = 0, |a(r,s)| = |\frac{I(r)}{2\pi}|$ and $p(r,s) = |a(r,s)|^2$, we seek to simplify the asymptotic expression

$$p(r,s) \sim |\frac{a_0}{r^{1/3}}Ai(r^{2/3}\gamma^2) + \frac{a_1}{r^{2/3}}Ai'(r^{2/3}\gamma^2)|^2. \tag{4.60}$$

We begin by simplifying a_0 and a_1 below:

$$a_0 = \frac{\tilde{\psi}_{\xi_0\xi}(\alpha_+)\frac{d\theta}{dt} + \tilde{\psi}_{\xi_0\xi}(\alpha_-)\frac{d\theta}{dt}}{2} = \frac{\tilde{\psi}_{\xi_0\xi}(\alpha_+) + \tilde{\psi}_{\xi_0\xi}(\alpha_-)}{2}\frac{d\theta}{dt} \tag{4.61}$$

and similarly

$$a_1 = \frac{\tilde{\psi}_{\xi_0\xi}(\alpha_+) - \tilde{\psi}_{\xi_0\xi}(\alpha_-)}{2\gamma}\frac{d\theta}{dt}.$$

Remark. In the above we facilitate the application of [BH86] by writing $G_0(\pm\gamma) = \tilde{\psi}(u(\pm\gamma))\frac{d\theta}{dt}|_{t=\pm\gamma}$ simply as $\tilde{\psi}(\alpha_\pm)\frac{d\theta}{dt}$ and avoiding the direct use of the new variable t.

If we let $F^0_{\xi_0,\xi} = \left[\frac{\tilde{\psi}_{\xi_0,\xi}(\alpha_+)+\tilde{\psi}_{\xi_0,\xi}(\alpha_-)}{2}\right]$ and $F^1_{\xi_0,\xi} = \left[\frac{\tilde{\psi}_{\xi_0,\xi}(\alpha_+)-\tilde{\psi}_{\xi_0,\xi}(\alpha_-)}{2\gamma}\right]$, then Equation (4.60) becomes

$$p(r,s) \sim |\frac{d\theta}{dt}|^2 \cdot |\frac{Ai(r^{2/3}\gamma^2)}{r^{1/3}}F^0_{\xi_0,\xi} + \frac{Ai'(r^{2/3}\gamma^2)}{r^{2/3}}F^1_{\xi_0,\xi}|^2. \tag{4.62}$$

As $\frac{d\theta}{dt}$ and γ are calculated above, it only remains to determine F^0 and F^1.

Since $\tilde{\psi}_{\downarrow,\downarrow} \equiv 1$, we obtain $F^0_{\downarrow,\downarrow} = 1$ and $F^1_{\downarrow,\downarrow} = 0$ with no work. Also, as $\tilde{\psi}_{\uparrow,\uparrow}$ is an even function, $F^1_{\uparrow,\uparrow}$ will be 0 as well, while $F^0_{\uparrow,\uparrow} = \tilde{\psi}_{\uparrow,\uparrow}(\alpha_+)$. As $\tilde{\psi}_{\uparrow,\downarrow}(\theta) = \tilde{\psi}_{\downarrow,\uparrow}(-\theta)$, we know that $F^0_{\downarrow,\uparrow} = F^0_{\uparrow,\downarrow}$ and $F^1_{\downarrow,\uparrow} = -F^1_{\uparrow,\downarrow}$. Thus we have reduced our number of calculations from 8 to 3. Using the notation from above we have

$$F^0_{\uparrow,\uparrow} = \frac{(1-c)(1+c)}{(1-y_-c)(1-y_+c)} = \frac{(1-c)(1+c)}{1+c^2+cA} = \frac{\delta(1-c)+(1+c)}{1-c}$$

and

$$F^0_{\uparrow,\downarrow} = \frac{1}{2}\frac{y_- + y_+ - 2c}{(1-y_-c)(1-y_+c)}\sqrt{1-c^2} = \frac{1}{2}\frac{-A-2c}{1+c^2+cA}\sqrt{1-c^2} = \frac{\delta(1-c)+2c}{2c(1-c)}\sqrt{1-c^2}$$

while

$$F^1_{\uparrow,\downarrow} = \frac{\sqrt{1-c^2}}{2\gamma}\left[\frac{y_-}{1-y_-c} - \frac{1}{y_- - c}\right] = \frac{\sqrt{1-c^2}}{2\gamma}\cdot\frac{y_-^2-1}{(1-y_c)(y_- - c)} = \frac{\sqrt{1-c^2}}{2\gamma}\cdot\frac{-2y_+ - A}{Ac+1+c^2}.$$

Making substitutions for y_+, A, and γ gives the estimate $F^1_{\uparrow,\downarrow} \sim \frac{(1+c)^{1/6}\cdot\sqrt{\delta(1-c)(1+c)+4c}}{2c^{5/6}\sqrt{1-c}}$ and completes the proof of the theorem. □

4.4 The Three-Chirality QRW on $\mathbb{Z}$

In this section we include a brief discussion of a three-chirality walk on the line. In this walk, (first studied in [Kon05b]) the particle either moves one step to the left or right, or stays still with each time step, thus

$$M := \begin{pmatrix} x & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & x^{-1} \end{pmatrix}.$$

The matrix

$$U^3_{\text{Had}} := \frac{1}{3}\begin{pmatrix} 1 & -2 & -2 \\ -2 & 1 & -2 \\ -2 & -2 & 1 \end{pmatrix}$$

is used as the unitary coin flip operator. We will denote the three chiralities R, M and L.

While the walk behaves very similarly to the 2 chirality walks above in most regions, including exponential decay outside an interval, and relatively uniform oscillation in another, it also includes a *bound state*, that is, a particular ratio $\lambda' = r/s$ just that $\lim_{s\to\infty} a_{\lambda' s,s} \neq 0$. We give a simplified proof of the results found in [Kon05b]). For example, the existence of a potential bound state is immediate from the factoring of the generating function $\hat{H}_3 := (1+y)(-3y^2x + y + 4yx + yx^2 - 3x)$ as the first factor depends only on y with unit root. While we require Theorem 5.9 as $\mathcal{V}_1$ is not smooth, we include our asymptotics here along with the above results for walks on the line. We also show that Theorem 5.9 cannot prescribe asymptotics for the bound state; we use an alternate technique to determine these asymptotics.

4.4.1 Statement of Results

Theorem 4.17. *For the three-chirality Quantum Random Walk with unitary matrix* $U = U^3_{\text{Had}}$*, let* $J = (-\sqrt{1/3}, 0) \cup (0, \sqrt{1/3})$ *and* $\lambda = \frac{r}{s}$*. Let* $p_{\mathbf{r}} := p_{r,s}$ *denote the probability to be at position* r *at time* s*. Then as* $|\mathbf{r}| \to \infty$*, uniformly over* $\hat{\mathbf{r}}$ *in a compact subset of the interior of* J*, there are phase functions* $\rho_{\xi_0,\xi}(r,s)$ *defined in Equation* (4.83)*, such that*

$$p_{R,R}(r,s) \sim \frac{1}{2\pi s} \cdot \frac{(1+\lambda)^3}{(1-\lambda)\sqrt{2-6\lambda^2}} \cos^2(\rho_{R,R}(r,s)) \tag{4.63}$$

$$p_{R,M}(r,s) \sim \frac{1}{\pi s} \cdot \frac{(1+\lambda)^2}{\sqrt{2-6\lambda^2}} \cos^2(\rho_{R,M}(r,s)) \tag{4.64}$$

$$p_{R,L}(r,s) \sim \frac{1}{2\pi s} \cdot \frac{(1+\lambda)(1-\lambda)}{\sqrt{2-6\lambda^2}} \cos^2(\rho_{R,L}(r,s)) \tag{4.65}$$

$$p_{M,R}(r,s) \sim \frac{1}{\pi s} \cdot \frac{(1+\lambda)^2}{\sqrt{2-6\lambda^2}} \cos^2(\rho_{M,R}(r,s)) \tag{4.66}$$

$$p_{M,M}(r,s) \sim \frac{2}{\pi s} \cdot \frac{(1+\lambda)(1-\lambda)}{\sqrt{2-6\lambda^2}} \cos^2(\rho_{M,M}(r,s)) \tag{4.67}$$

$$p_{M,L}(r,s) \sim \frac{1}{\pi s} \cdot \frac{(1-\lambda)^2}{\sqrt{2-6\lambda^2}} \cos^2(\rho_{M,L}(r,s)) \tag{4.68}$$

$$p_{L,R}(r,s) \sim \frac{1}{2\pi s} \cdot \frac{(1+\lambda)(1-\lambda)}{\sqrt{2-6\lambda^2}} \cos^2(\rho_{L,R}(r,s)) \tag{4.69}$$

$$p_{L,M}(r,s) \sim \frac{1}{\pi s} \cdot \frac{(1-\lambda)^2}{\sqrt{2-6\lambda^2}} \cos^2(\rho_{L,M}(r,s)) \tag{4.70}$$

$$p_{L,L}(r,s) \sim \frac{1}{2\pi s} \cdot \frac{(1-\lambda)^3}{(1+\lambda)\sqrt{2-6\lambda^2}} \cos^2(\rho_{L,L}(r,s)) \tag{4.71}$$

When $\lambda \notin J \cup \{0\}$ *then for every integer* $N > 0$ *there is a* $C > 0$ *such that* $\Pr(\mathbf{r}) \le C|\mathbf{r}|^{-N}$ *with* C *uniform as* $\mathbf{r}$ *ranges over a neighborhood* $\mathcal{N}$ *of* $\mathbf{r}$ *whose closure is disjoint from the closure of* J*.*

Theorem 4.18. *For the three-chirality Quantum Random Walk with unitary matrix $U = U^3_{\text{Had}}$, define $p_{\mathbf{r}}$ as above. Then the particle appears at the origin with the probabilities:*

$$\lim_{s\to\infty} p_{R,R}(0,s) = \frac{1}{6} \tag{4.72}$$

$$\lim_{s\to\infty} p_{R,M}(0,s) = \frac{5-2\sqrt{6}}{3} \tag{4.73}$$

$$\lim_{s\to\infty} p_{R,L}(0,s) = \frac{49-20\sqrt{6}}{6} \tag{4.74}$$

$$\lim_{s\to\infty} p_{M,R}(0,s) = \frac{5-2\sqrt{6}}{3} \tag{4.75}$$

$$\lim_{s\to\infty} p_{M,M}(0,s) = \frac{2}{3} \tag{4.76}$$

$$\lim_{s\to\infty} p_{M,L}(0,s) = \frac{5-2\sqrt{6}}{3} \tag{4.77}$$

$$\lim_{s\to\infty} p_{L,R}(0,s) = \frac{49-20\sqrt{6}}{6} \tag{4.78}$$

$$\lim_{s\to\infty} p_{L,M}(0,s) = \frac{5-2\sqrt{6}}{3} \tag{4.79}$$

$$\lim_{s\to\infty} p_{L,L}(0,s) = \frac{1}{6} \tag{4.80}$$

We once again demonstrate our results pictorially, this time with a graph of the walk's actual probabilities versus the predicted upper envelope (calculated by dropping the $\cos^2$ term from our asymptotic prediction) for (ξ_0, ξ) equal to each of (L, L), (L, M), and (L, R). With time $t = 400$, we use a shifted walk beginning at the point $r = 401$. We note that as the prediction of Theorem 4.17 holds for λ in a compact subset of J, we refer to Theorem 4.18 for $r = 401$.

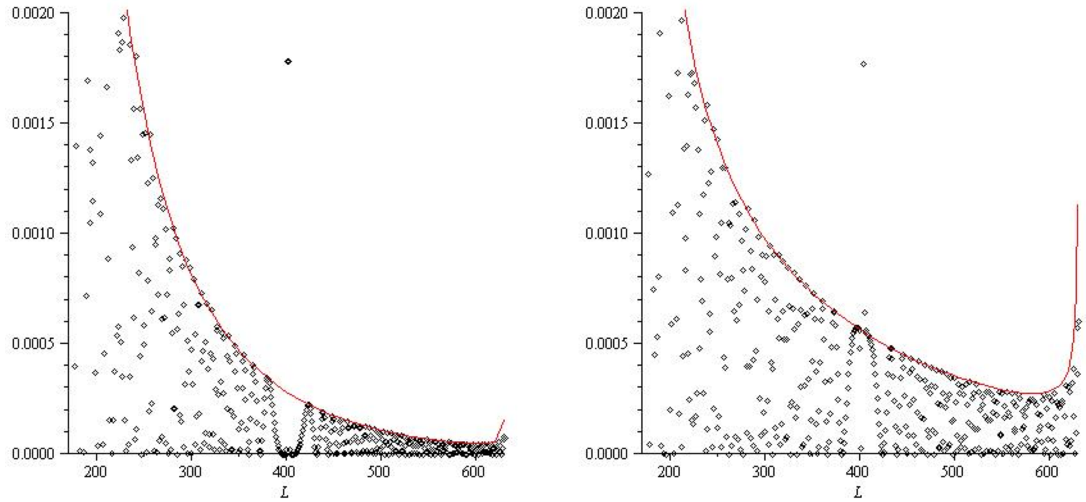

Figure 3: Time $t = 400$ probability values by location ($p_{L,L}$ on left and $p_{L,D}$ on right) for the three chirality walk on the line and our asymptotic prediction of the upper envelope. The asymptotic values of $p_{L,L}(401, 400)$ and $p_{L,M}(401, 400)$ predicted by Theorem 4.18 are $\frac{1}{6}$ and $\frac{5-2\sqrt{6}}{3} \approx .0168$, respectively. The actual values of $p_{L,L}(401, 400)$ and $p_{L,M}(401, 400)$, too large to appear in these viewing windows, are ≈ 0.1675 and $\approx .0255$, respectively. As $\rho_{L,M}(0, s)$ is close to 0, it will take much longer for $p_{L,M}(0, s)$ to converge than for the other states pictured above.

4.4.2 Proof of Theorem 4.17

We define $\mathbf{G}, \mathbf{F}, x, y, X, Y, r, s, H$ and λ as earlier in this chapter, with one exception. To clear denominators we define $\hat{H} := -3x \det(I - yMU_{\text{Had}}^3)$. (We also include a factor of $-3x$ in $\mathbf{G}$ as not to affect asymptotics.) As this gives $\hat{H} = (1+y)(-3y^2x + y + 4yx + yx^2 - 3x)$, it will be convenient to define $H = -3y^2x + y + 4yx + yx^2 - 3x$. While $\hat{H}_y$ will vanish on the unit torus, we still aim to use a result like that of Theorem 4.8. To this end, we turn to Theorem 5.9 of the following chapter, while also making an adjustment to account for the factoring of $\hat{H}$. For the purpose of the following discussion we note that the image of $\mathbf{dir}\,(\mathcal{V}_1)$ is a subset of the set $\mathbf{K}$ from Theorem 5.9, while the result of Theorem 5.9 is a generalization to dimension d of the result for Theorem 4.8. We will be more thorough and specific in our exploration of these connections in the next chapter.

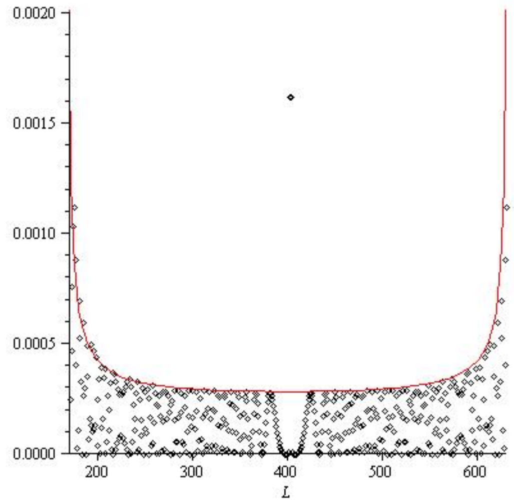

Figure 4: Time $t = 400$ probability values by location ($p_{L,R}$) for the three chirality walk on the line and our asymptotic prediction of the upper envelope. The asymptotic value of $p_{L,R}(401, 400)$ predicted by Theorem 4.18 is $\frac{49-20\sqrt{6}}{6} \approx .0017$

Our current modification is the treatment of the $(1 + y)$ factor in $\hat{H}$ as a locally smooth factor, which we do as follows. Using the fact that $\cos(X) = \frac{1}{2}(x + 1/x)$ for x on the unit torus, we factor $\hat{H}$ as $\hat{H} = 2xy(1 + y)(\cos(X) - 3\cos(Y) + 2)$. We then write $\mathcal{V}_1 = C_1 \cup C_2$ where $C_1 = \{(x, y) : |x| = |y| = 1,\ \cos(X) - 3\cos(Y) = 2\}$ and $C_2 = \{(x, y) : |x| = 1,\ y = -1\}$. Then every $(x, y) \in C_2$ can only contribute towards asymptotics in the direction $\lambda = -\frac{dY}{dX} = 0$, which is the image of the Gauss map of C_2. As C_2 is a flat plane, Gaussian curvature vanishes there, so we may effectively ignore C_2 as we apply Theorem 5.9. Our modified result will then have an extra factor of $y + 1$ in the denominator of its asymptotic estimate, and we can now deal with H instead of $\hat{H}$.

Next we accommodate the fact that C_1 is not smooth. That is to say, ∇H vanishes on C_1. As the lexicographic Gröbner Basis for the ideal generated by H, H_x and H_y is $\{y - 1, x - 1\}$, we see that the gradient of H vanishes on C_1 precisely at the point $(1, 1)$. The use of an additional Gröbner basis shows that this point is the only one on C_1 where H_y vanishes. Theorem 5.9 can then handle this case, delivering a result like that of Theorem 4.8, under the appropriate conditions. In this case those conditions are met on account of the facts that $\mathbf{dir}\,(1,1) \notin J$ and while H does vanish to degree 2 at $(x,y) = (1,1)$, $\mathbf{G}$ vanishes at this point as well. The second of these we observe as

$$\mathbf{G} := \begin{pmatrix} -3x+y+yx+y^2 & 2yx(-y+x) & -2yx^2(y-1) \\ 2y(-y+x) & -3x+y+yx^2+y^2x & -2y(-1+yx)x \\ -2y(y-1) & -2y(-1+yx) & (-3+y+yx+y^2x)x \end{pmatrix}$$

vanishes at $(x,y) = (1,1)$, while we establish the first in the following lemma.

Lemma 4.19. $\mathbf{dir}\,(1,1) \notin J$

Before proving the lemma we also note that the factoring of $\hat{H}$ and the vanishing of ∇H on C_1 do not combine to create a problem greater than the sum of their parts. To be more specific, another Gröbner Basis computation shows that the gradient of $\hat{H}$ also only vanishes on $C_1 \cup C_2$ at the point $(1,1)$.

Proof of Lemma 4.19: We recall that $(x,y) \in C_1$ precisely when

$$3\cos(Y) = 2 + \cos(X). \tag{4.81}$$

Differentiating this equation implicitly with respect to X gives the other critical point equation:

$$-\lambda = \frac{dY}{dX} = \frac{\sin(X)}{3\sin(Y)} \tag{4.82}$$

Squaring this equation results in $\lambda^2 = \frac{1-\cos^2(X)}{9(1-\cos^2(Y))}$. Substituting the value of $\cos(Y)$ given by Equation (4.81) results in the equation $\lambda^2 = \frac{1+\cos(X)}{1+5\cos(X)}$. Thus as $(x,y) \to (1,1) \in C_1$, the direction λ associated to (x,y) can only go to $\pm\sqrt{1/3} \notin J$. □

Another advantage of using Theorem 5.9 instead of a result like Theorem 4.8 is that we only need to show $\mathbf{dir}\,(C_1 \setminus (1,1)) = J \cup \{0\}$ as opposed to proving a version of Proposition 4.11. The only other major hypothesis of Theorem 5.9 is a result of Proposition 4.2.

Proposition 4.20. $\mathbf{dir}\,(C_1 \setminus (1,1)) = J \cup \{0\}$.

PROOF: The inclusion $\mathbf{dir}\,(C_1 \setminus (1,1)) \subset J \cup \{0\}$ follows immediately from the fact $\lambda^2 = \frac{1+\cos(X)}{5+\cos(X)}$, which we demonstrated in the proof of Lemma 4.19. For the inclusion $J \cup \{0\} \subset \mathbf{dir}\,(C_1 \setminus (1,1))$, we choose $\lambda \in J \cup \{0\}$ and solve for all possible points $(x(\lambda), y(\lambda))$, by letting $K = sxH_x - ryH_y$ and using the Maple command $GB = \texttt{Basis}\ ([H,K],\ \texttt{plex}(y,x))$. The first basis element is the minimal polynomial for x. Letting $\lambda = \frac{r}{s}$ and discarding the solution $x = 1$ we get

$$x = \frac{5\lambda^2 - 1 \pm 2\lambda\sqrt{6\lambda^2 - 2}}{1 - \lambda^2}.$$

When $\lambda \in J \cup \{0\}$, $6\lambda^2 - 2 < 0$ and the solutions are conjugate complex units. By Proposition 4.2 the y coordinates are also units, completing the proof. $\square$

It now remains only to mimic the last step in the proof of 4.5. With an extra factor of $1 + y$ in each denominator, we have that for each pair $(\xi_0, \xi) \in \{L, M, R\}^2$ and $r/s \in J$,

$$p_{\xi_0\xi}(r,s) \sim \frac{2}{\pi}\cos^2 \rho_{\xi_0\xi}(r,s) \left| G^2_{\xi_0\xi} \frac{-yH_y}{s(1+y)^2 Q(x,y)} \right|$$

where

$$\rho_{\xi_0,\xi}(r,s) := \operatorname{Arg}\left(\frac{G_{\xi_0,\xi}}{\sqrt{2\pi}} x^{-r} y^{-s} \sqrt{\frac{-yH_y}{s(1+y)^2 Q(x,y)}} \right). \tag{4.83}$$

Again we solve for the minimal polynomial of the bulk of this expression:

$$w := G^2_{\xi_0\xi} \frac{-yH_y}{s(1+y)^2 Q(x,y)}.$$

Recalling that (x,y) satisfies $H(x,y) = K(x,y) = 0$, we introduce a variable $z := 1/((1+y)^2 sQ)$ so that when $\xi_0 = \xi = R$, w may be expressed as the solution to the following four polynomial equations.

$$\begin{aligned} H &= 0 \\ K &= 0 \\ (1+y)^2 szQ - 1 &= 0 \\ w + (-3x + y + yx + y^2)^2 (yH_y) z &= 0 \end{aligned}$$

To obtain a polynomial in w alone, we use the `Basis` command with term order $\texttt{plex}(\texttt{x}, \texttt{y}, \texttt{z}, \texttt{w})$, resulting in the polynomial

$$32s^4(3r^2 - s^2)(r - s)^2w^2 - (r + s)^6.$$

With $\lambda = r/s$, we find that

$$|w_{R,R}| = \frac{(1 + \lambda)^3}{4(1 - \lambda)s\sqrt{2 - 6\lambda^2}}.$$

We repeat this process for each pair $(\xi_0, \xi) \in \{L, M, R\}^2$, noting that $|G_{\xi_0,\xi}| = |G_{\xi,\xi_0}|$ in each of our cases, as x and y are units. When the minimal polynomial of $w_{\xi_0,\xi}$ is of the form $Aw^2 + Bw + C$ with $B \neq 0$, we find that $|w_{\xi_0,\xi}| = \sqrt{C/A}$, as is shown at the end of Section 4.2. Theorem 4.17 follows. $\square$

4.4.3 Proof of Theorem 4.18

As Gaussian curvature vanishes on C_2, Theorem 5.9 will not be able to deliver asymptotics in the direction $\lambda = 0$. Alternatively, we use the Hautus-Klarner-Furstenberg method for diagonal extraction; we borrow the description of this method from Section 2.4 of [Pem09], particularly the proof of its Theorem 2.8. This method requires a rational power series, versus the Laurent series above, so we now use

$$M := \begin{pmatrix} x^2 & 0 & 0 \\ 0 & x & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

giving us a walk with asymptotics in the direction $\lambda = 1$ equal to those of our original walk in the direction $\lambda = 0$.

Given a generating function $F(x, y) = \frac{G(x,y)}{H(x,y)} = \sum_{r,s \geq 0} a_{rs} x^r y^s$, the method will deliver the univariate generating function $h(z) := \sum_{n \geq 0} a_{nn} z^n$ as follows. Since F converges in a neighborhood of the origin, for $|y|$ sufficiently small, the function $F(z, y/z)$ converges absolutely for z in some annulus $A(y)$. If we treat y as a constant and view $F(z, y/z)$ as a Laurent series expansion with respect to z in the annulus $A(y)$, then the constant term of this series will be $h(y)$. Thus by Cauchy's integral formula,

$$h(y) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{G(z, y/z)}{zH(z, y/z)} dz$$

where $\mathcal{C}$ is any circle around the origin in $A(y)$. Then by the Residue Theorem

$$h(y) = \sum_j \text{RES} \left(\frac{G(z, y/z)}{zH(z, y/z)}; a_j \right)$$

where the a_j are the poles inside the inner circle of the annulus. These are the poles that converge to 0 as $y \to 0$.

We demonstrate the use of this method in the calculation of $\lim_{s \to \infty} p_{L,M}(0, s)$ and note that Maple's `residue` command may be used to automate the process. In this case

$$\frac{G_{L,M}(z, w/z)}{zH_{L,M}(z, w/z)} = \frac{2w(wz - 1)}{z(w + 1)[-wz^2 + (3w^2 - 4w + 3)z - w]} = \frac{2(1 - wz)}{z(w + 1)(z - a_+)(z - a_-)}$$

where $a_\pm = \frac{3w^2-4w+3\pm(w-1)\sqrt{9w^2-6w+9}}{2w}$. We then use the method of partial fractions to write $\frac{G_{L,M}(z,w/z)}{zH_{L,M}(z,w/z)} = \frac{A_0}{z} + \frac{A_1}{z-a_+} + \frac{A_2}{z-a_-}$. Since $z = 0$ and $z = a_+$ are the poles that go to 0 with w, $h(w)$ is the sum of their residues. Setting $z = 0$ and $z = a_+$ we find in turn that $A_0 = \frac{2}{a_+a_-(w+1)}$ and $A_1 = \frac{2}{a_+(w+1)(a_+-a_-)} - \frac{2w}{(w+1)(a_+-a_-)}$. Thus $h(w) = \sum_{n\geq 0} a_{nn}w^n = \frac{2}{a_+a_-(w+1)} + \frac{2}{a_+(w+1)(a_+-a_-)} - \frac{2w}{(w+1)(a_+-a_-)}$. Using the fact that $a_+a_- = 1$ and otherwise simplifying, we find $h(w) = \frac{w-3+\sqrt{9w^2-6w+9}}{(w+1)\sqrt{9w^2-6w+9}}$. Now as $w = -1$ is the pole of h closest to the origin and it is a simple pole, we know $\lim_{n\to\infty} a_{nn} = \mathrm{RES}\,(h(w);-1) = h(w)(w+1)|_{w=-1} = \frac{3-\sqrt{6}}{3}$. Thus $\lim_{s\to\infty} p_{L,M}(0,s) = \left(\frac{3-\sqrt{6}}{3}\right)^2 = \frac{5-2\sqrt{6}}{3}$. Repeating this process for each pair of chiralities proves the theorem. $\square$

Remark. Alternatively, we could prove the above by using results of [PW04], adapted for torally minimal multiple points. This approach, however, would be less self-contained. Also, their theorem as written does not cover this case, though in fact their results hold in this case, as seen in the later work [BP08]. We make this note as their methods are significantly more robust than the diagonal method employed above. That being said, in this case the diagonal method lets us quickly reproduce the results from [Kon05b].

5 QRWs on $\mathbb{Z}^d$

In this chapter we provide the first results for several families of two-dimensional Quantum Random Walks, determining new, more transparent asymptotic results for multivariate generating functions along the way. In our QRWs on the plane, the feasible region (the region where probabilities do not decay exponentially with time) grows linearly with time, as is the case with one-dimensional QRWs. The limiting shape of the feasible region is, however, quite different. The limit region turns out to be an algebraic set, which we characterize as the rational image of a compact algebraic variety. We explicitly determine the boundary of this region using algebraic methods. We also compute the probability profile within the limit region, which is essentially a negative power of the Gaussian curvature of the same algebraic variety. Our methods are based on analysis of the space-time generating function, following the methods of [PW02]. We also give asymptotics for the Hadamard QRW on the plane, as well as preliminary results for walks in dimension $d > 2$. Throughout this chapter, d will designate the dimension of the integer lattice for the walk, and thus one less than the dimension of the associated generating function. This is in contrast to the first three chapters, in which d designated the dimension of the generating function.

5.1 An Introduction to QRWs on the plane

Published work on Quantum Random Walks in dimensions two and higher began around 2002 (see [MBSS02]). Most studies, including the most recent and broad study [KWKK08], are concerned to a great extent with localization; this phenomenon is not generic in quantum random walk models and among the models we discuss, it is only present in the Hadamard walk of Section 5.5. The analyses we have seen range from analytic derivations without complete proofs to numerical studies. As far as we know, no rigorous analysis of two-dimensional QRW has been published. The question of describing the behavior of two-dimensional QRW was brought to the attention of Robin Pemantle and Yuliy Baryshnikov by Cris Moore (personal communication). In the next two sections, we answer this question by proving theorems about the limiting shape of the feasible region (the region where probabilities do not decay exponentially with time) for two-dimensional QRW, and by giving asymptotically valid formulae for the probability amplitudes at specific locations within this region.

As in dimension $d = 1$, our analyses begin with the space-time generating function: a multivariate rational function which may be derived without too much difficulty. This approach pays its greatest dividends in dimension two and higher. While alternative techniques become exceedingly complicated here, we can continue to use the methods introduced in [PW02, PW04, PW08] and reviewed in Section 2.2 allowing nearly automatic transfer from rational generating functions to asymptotic formulae for their coefficients. Based on these results, analyses of any instance of a

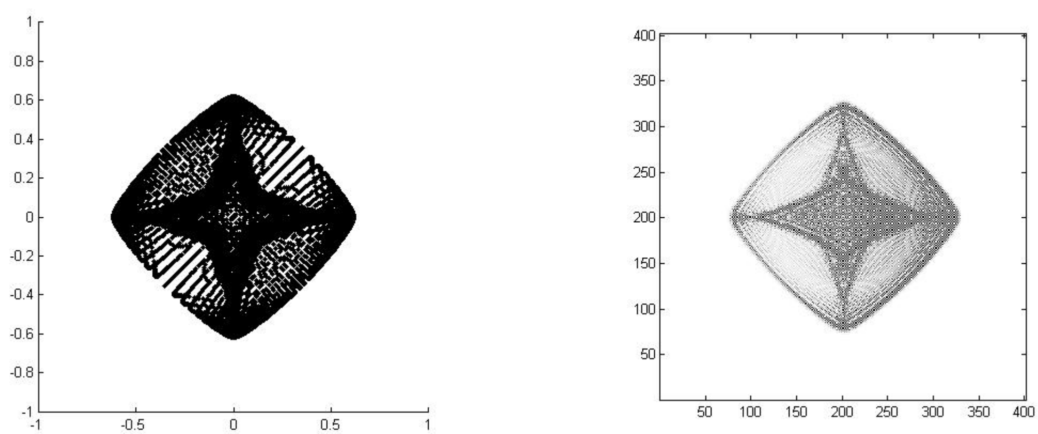

Figure 5: Fixed-time empirical plot (on right for time 200) versus theoretical limit (on left)

two-dimensional QRW becomes relatively easy, although in some cases new versions of the results under weaker hypotheses were required. Empirically computed probability profiles such as are shown on the right in Figure 5 are explained by algebraic computations, leading to limit shapes as shown on the left. We computed probability profiles for a number of instances of two-dimensional QRW. The pictures, which appear scattered throughout the upcoming sections, are quite varied.

Not only did we find these pictures visually intriguing, but they pointed toward some refinements of the theoretical work in Section 2.2, which we now describe, beginning with a more detailed description of the two plots.

On the right is depicted the probability distribution for the location of a particle after 200 steps of a Quantum Random Walk on the planar integer lattice; the particular instance of QRW is a nearest neighbor walk ($E = \{(0,1),(0,-1),(1,0),(-1,0)\}$) whose unitary matrix is discussed in Section 5.3. Greater probabilities are shown as darker shades of grey. The feasible region, where probabilities are not identically zero, is the diamond with vertices at the midpoints of the 400×400 square. The region where probabilities are not extremely close to zero appears to be a slightly rounded, smaller diamond.

In [Bra07], Wil Brady computed an asymptotically valid formula for the probability amplitudes associated with some instances of QRW. As $n \to \infty$, the probabilities become exponentially small outside of a certain algebraic set $\mathbf{\Xi}$, but are $\Theta(n^{-2})$ inside of $\mathbf{\Xi}$. Theorem 4.5 of [Bra07] proves such a shape result for a different instance of two-dimensional QRW and conjectures it for this one, giving the believed characterization of Ξ as an algebraic set. The plot on the left side in Figure 5 is a picture of this characterization, constructed by parameterizing Ξ by patches in the flat torus $T_0 := (\mathbb{R}/2\pi\mathbb{Z})^2$ and then depicting the patches by showing the image of a grid embedded in the torus.

When the plot was constructed, it was intended only to exhibit the overall shape. Nevertheless, it is visually obvious that significant internal structure is duplicated as well. Identical dark regions in the shape of a Maltese cross appear inside each of the two figures. To explain this, we consider the map $\Phi : \mathbf{T} \to \mathbb{R}^2$ whose image produces the region Ξ. Let $\mathcal{V}$ denote the pole variety of the generating function F for a given QRW, that is, the complex algebraic hypersurface on which the denominator H of F vanishes. Let $\mathcal{V}_1$ denote the intersection of $\mathcal{V}$ with the unit torus $\mathbf{T}$. It is easy to solve for the third coordinate z as a local function of x and y on $\mathcal{V}_1$ and thereby obtain a piecewise parametrization

$$(\alpha, \beta) \mapsto \left(e^{i\alpha}, e^{i\beta}, e^{i\phi(\alpha,\beta)}\right)$$

of $\mathcal{V}_1$ by patches in $\mathbb{R}^2$. Theorem 5.7 extends the results of [PW02] to show that each point $\mathbf{z}$ of $\mathcal{V}_1$ produces a polynomially decaying contribution to the probability profile for movement at velocity (r, s) which is the image of $\mathbf{z}$ under the logarithmic Gauss map $\mathfrak{n}$ of the surface $\mathcal{V}_1$ at $\mathbf{z}$:

$$\mathfrak{n}(\mathbf{z}) := \left(x\frac{\partial H}{\partial x}, y\frac{\partial H}{\partial y}, z\frac{\partial H}{\partial z}\right) .$$

Formally, $\mathfrak{n}$ maps into the projective space $\mathbb{RP}^2$, but we map this to $\mathbb{R}^2$ by taking the projection $\pi(r, s, t) := (r/t, s/t, 1)$. In other words, the plot is the image of the grid $(\mathbb{Z}/100\mathbb{Z})^2$ under the following composition of maps:

$$(\mathbb{Z}/100\mathbb{Z})^2 \xrightarrow{\iota} S^1 \times S^1 \xrightarrow{(1,1,\phi)} \mathcal{V} \xrightarrow{\mathfrak{n}} \mathbb{RP}^2 \xrightarrow{\pi} \mathbb{R}^2 . \tag{5.1}$$

The intensity of an image of a uniform grid of dots is proportional to the inverse of the Jacobian of the mapping. The Jacobian of the composition is the product of the Jacobians of the factors, the most significant factor being the Gauss map, $\mathfrak{n}$. Its Jacobian is just the Gaussian curvature (in logarithmic coordinates). The darkest regions therefore correspond to the places where the curvature of $\log \mathcal{V}_1$ vanishes. Alignment of this picture with the empirical amplitudes can only mean that the formulae for asymptotics of generating functions given in [PW02] blow up when the Gaussian curvature of $\log \mathcal{V}_1$ vanishes. This observation allowed us to produce new expressions for the quantities in the conclusions of theorems in [PW02], where lengthy polynomials were replaced by quantities involving Gaussian curvatures.

To summarize, in the next three sections we will:

1. Prove (In Theorem 5.18), the shape conjecture from [Bra07]; further instances of this are proved in Theorems 5.11 and 5.16.

2. Reformulate (in Theorems 5.7 and 5.9) the main result in [PW02] to clarify the relation

between the asymptotics of a multivariate rational generating function and the curvature of the pole variety in logarithmic coordinates.

3. Algebraically determine the directions associated with the subvariety on which curvature vanishes.

The next two sections of this thesis are rather lengthy, and as such we give the following additional guidance as towards its organization. Below we summarize relevant background information concerning Quantum Random Walks on the plane. We then supplement the background given in Section 2.2 and Chapter 3 with additional background on notions of Laurent polynomials, the multivariate Cauchy formula, and certain standard applications of the stationary phase method to the evaluation of oscillating integrals. Section 5.2 contains general results on rational multivariate asymptotics, clarifying the role of curvature, which, along with its application to QRW limit theorems, is at the core of this thesis. In particular, Theorem 5.7 gives a new formulation of the main result of [PW02], while Theorem 5.9 proves a version of these results in situations where the geometry of $\mathcal{V}_1$ is more complicated than can be handled by the methods of [PW02]. Finally, Section 5.3 applies these results to a collection of instances of two-dimensional nearest neighbor QRW in which the unitary matrices are elements of one-parameter families named $S(p), A(p)$ and $B(p)$, $0 < p < 1$. This results in Theorems 5.11, 5.16 and 5.18 respectively. The QRW in Figure 5 has unitary matrix $B(1/2)$, while the following figures show examples of the $S(1/2)$ and $A(5/9)$ Quantum Random Walks.

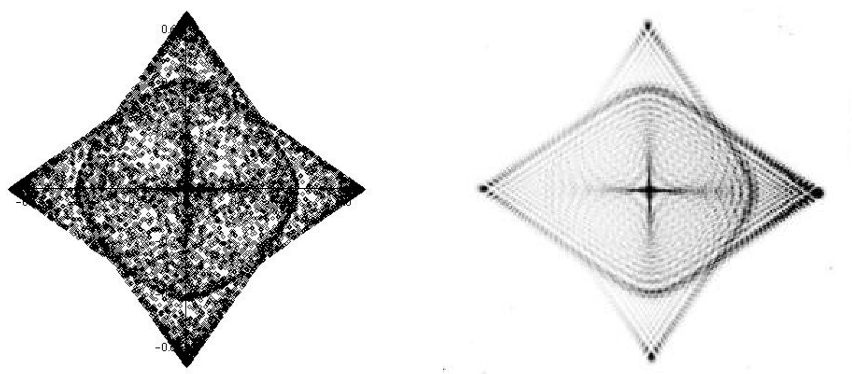

Figure 6: Limiting region (left) and Probabilities at time 200 (right) for the $S(1/2)$ QRW

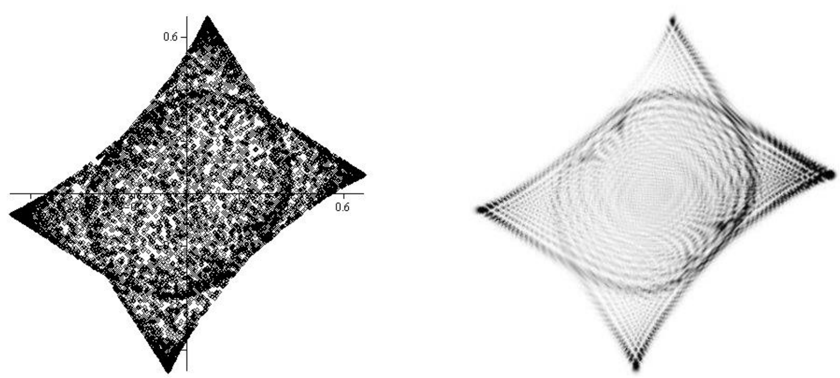

Figure 7: Limiting region (left) and Probabilities at time 200 (right) for the $A(5/9)$ QRW

We define each of d, U, F and M as in Section 4.1, using the transfer matrix method [Sta97, GJ83] to determine the explicit expression

$$\mathbf{F}(\mathbf{z}) = (I - z_{d+1}MU)^{-1} . \tag{5.2}$$

for the generating function defined as

$$F^{(i,j)}(x, y, z) = \sum_{n,r,s} \psi_n^{(i,j)}(r, s) x^r y^s z^n$$

where we will use

$$M = \begin{pmatrix} x & 0 & 0 & 0 \\ 0 & x^{-1} & 0 & 0 \\ 0 & 0 & y & 0 \\ 0 & 0 & 0 & y^{-1} \end{pmatrix}$$

as we will focus on nearest neighbor QRWs. As before, the (i, j)-entry of the matrix, $F^{(i,j)}$, may be written as a rational function G/H where

$$H = \det(I - z_{d+1}MU) .$$

A **Hadamard** matrix is one whose entries are all ± 1. There is more than one rank-4 unitary matrix that is a constant multiple of a Hadamard matrix, but for some reason the "standard Hadamard" QRW in two dimensions is the QRW whose unitary matrix is

$$U_{\text{Had}} := \frac{1}{2} \begin{pmatrix} 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ -1 & -1 & -1 & 1 \end{pmatrix} .$$

This is referred to by Konno [IKK04, KWKK08] as the "Grover walk" because of its relation to the quantum search algorithm of L. Grover. Shown on the right in Figure 8 is a plot of the probability profile for the position of a particle performing a standard Hadamard QRW for 200 time steps. This is the only two-dimensional QRW we are aware of for which even a nonrigorous analysis had previously been carried out. On the left, in Figure 8, is the analogous plot of the region of non-exponential decay. We give asymptotics for certain regions of this walk's probability distribution in Section 5.5.

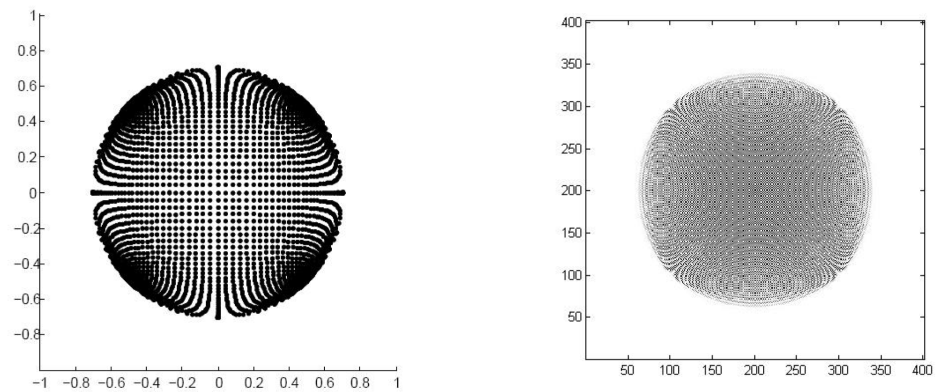

Figure 8: Limit Prediction (left) and Exact Probabilities at time 200 for Moore's Hadamard QRW

Another 4×4 unitary Hadamard matrix reflects the symmetries of $(\mathbb{Z}/(2\mathbb{Z}))^2$ rather than $\mathbb{Z}/(4\mathbb{Z})$:

$$\tilde{U}_{\text{Had}} := \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & -1 & 1 & 1 \end{pmatrix} .$$

This matrix also goes by the name of $S(1/2)$ and is a member of the first family of QRW that we will analyze. There is no reason to stick with Hadamard matrices. Varying U further produces a number of other probability profiles including the families $S(p)$, $A(p)$ and $B(p)$ analyzed in Section 5.3.

5.2 The Connection Between Curvature and Asymptotics

We begin this section by giving necessary background on amoebas and Cauchy's formula, in addition to oscillatory integrals. While there is some overlap with Section 2.2, the following refines those descriptions for use in the theorems to come. We refer the reader to Chapter 3 for further background.

5.2.1 Amoebae and Cauchy's formula

Let $F = G/H$ be a quotient of Laurent polynomials, with pole variety $\mathcal{V} := \{\mathbf{z} : H(\mathbf{z}) = 0\}$. Let $\text{Log} : (\mathbb{C}^*)^{d+1} \to \mathbb{R}^{d+1}$ denote the log-modulus map, defined by

$$\text{Log}\,(\mathbf{z}) := (\log |z_1|, \ldots, \log |z_{d+1}|)\,.$$

The **amoeba** of H is defined to be the image under Log of the variety $\mathcal{V}$. To each component B of the complement of this amoeba in $\mathbb{R}^{d+1}$ corresponds a Laurent series expansion of F. When F is the $(d+1)$-variable spacetime generating function of a d-dimensional QRW, we will be interested in the component B_0 containing a translate of the negative z_{d+1}-axis; this corresponds to the Laurent expansion that is an ordinary series in the time variable and a Laurent series in the space variables. For QRW, the point $\mathbf{0}$ is always on the boundary of B_0. In general, all components of the complement of any amoeba are convex. For further details and properties of amoebas, see [GKZ94, Chapter 6].

For any $\mathbf{r} \in \mathbb{R}^{d+1}$, let $\hat{\mathbf{r}}$ denote the unit vector $\mathbf{r}/|\mathbf{r}|$. Two important hypotheses that will be satisfied for QRW are as follows.

$$\text{The function } \mathbf{r} \cdot \mathbf{x} \text{ is maximized over } \overline{B_0} \text{ at a specified point } \mathbf{x}_*\,; \tag{5.3}$$

we will be primarily concerned with those $\hat{\mathbf{r}}$ for which this maximizing point is the origin, and we denote by $\mathbf{K}$ the set of $\hat{\mathbf{r}}$ for which this holds: thus for $\hat{\mathbf{r}} \in \mathbf{K}$ and $\mathbf{x} \in \overline{B_0}$, $\mathbf{r} \cdot \mathbf{x} \leq 0$ with equality when $\mathbf{x} = \mathbf{0}$. Secondly, we assume that the set $\mathbf{W} = \mathbf{W}(\mathbf{r})$ of $\mathbf{z} = \exp(\mathbf{x} + i\mathbf{y})$ such that

$$H(\mathbf{z}) = 0 \text{ and } \nabla_{\log} H(\mathbf{z}) \parallel \hat{\mathbf{r}} \tag{5.4}$$

is finite. The set $\mathbf{W}(\mathbf{r})$ depends on $\mathbf{r}$ only through $\hat{\mathbf{r}}$. We introduce the notation $\nabla_{\log} H(\mathbf{z})$ to denote the gradient of $H \circ \exp$ evaluated at $\log(\mathbf{z})$ and note that at $\mathbf{z} \in \mathbf{W}$, $\nabla_{\log} H(\mathbf{z}) = (z_1 \partial H/\partial z_1, \ldots, z_{d+1} \partial H/\partial z_{d+1})$. It is immediate from (5.4) that $\nabla_{\log} H(\mathbf{z})$ is a multiple of the real vector $\hat{\mathbf{r}}$.

Before we proceed we point out a condition under which (5.4) is always satisfied. Suppose that $\mathcal{V}_1$ is smooth off a finite set E, and we let $\mathbf{r}$ be some direction such that hypothesis (5.4) fails. The set $\mathbf{W}(\mathbf{r})$ is algebraic, so if it is infinite it contains a curve, which is a curve of constancy for the logarithmic Gauss map. This implies that the Jacobian of the logarithmic Gauss map vanishes on the curve, which is equivalent to vanishing Gaussian curvature at every point of the curve. Thus, if we restrict $\mathbf{r}$ to the subset of $\mathcal{V}_1$ where $\mathcal{K} \neq 0$, then hypothesis (5.4) is automatically satisfied.

The coefficients $a_{\mathbf{r}}$ of the Laurent series corresponding to B_0 may be computed via Cauchy's integral formula. Define the flat torus $T_0 := (\mathbb{R}/(2\pi\mathbb{Z}))^{d+1}$. The following proposition is well known.

Proposition 5.1 (Cauchy's Integral Formula)**.** *For any* $\mathbf{u}$ *interior to* B_0*,*

$$a_{\mathbf{r}} = \left(\frac{1}{2\pi}\right)^{d+1} \exp(-\mathbf{r} \cdot \mathbf{u}) \int_{T_0} \exp(-i\mathbf{r} \cdot \mathbf{y}) F \circ \exp(\mathbf{u} + i\mathbf{y})\, d\mathbf{y}\,. \tag{5.5}$$

Corollary 5.2. *Let* $\lambda := \lambda(\hat{\mathbf{r}}) := \sup\{\hat{\mathbf{r}} \cdot \mathbf{x} : \mathbf{x} \in B_0\}$*. For any* $\lambda' < \lambda$*, the estimate*

$$|a_{\mathbf{r}'}| = o(\exp(-\lambda' |\mathbf{r}'|))$$

holds uniformly as $\mathbf{r}' \to \infty$ *in some cone with* $\mathbf{r}$ *in its interior.*

Proof: Pick $\mathbf{u}$ interior to B_0 such that $\mathbf{r} \cdot \mathbf{u} > \lambda'$. There is some $\epsilon > 0$ and some cone $\mathbf{K}$ with $\mathbf{r}$ in its interior such that $\mathbf{r}' \cdot \mathbf{u} \geq \lambda' + \epsilon$ for all $\mathbf{r}' \in \mathbf{K}$. The function F is bounded on the torus $\exp(\mathbf{u} + i\mathbf{y})$, and the corollary follows from Cauchy's formula. □

NOTE: We allow for the possibility that hypothesis (5.4) holds for no points with modulus 1. In the asymptotic estimate (5.13) below, the sum will be empty and we will be able to conclude that $a_{\mathbf{r}} = O(|\mathbf{r}|^{-(d+1)/2})$, as opposed to $\Theta(|\mathbf{r}|^{-d/2})$ in the more interesting regime; we will not be able to conclude that $a_{\mathbf{r}}$ decays exponentially, as it does when $\mathbf{r} \notin \overline{\mathbf{K}}$. This will correspond to the case where in fact $\mathbf{r} \in \overline{\mathbf{K}} \setminus \mathbf{K}$.

5.2.2 Oscillating integrals

Let $\mathcal{M}$ be an oriented d-manifold, let $\phi : \mathcal{M} \to \mathbb{R}$ be a smooth function and let A be a smooth d-form on $\mathcal{M}$. Say that $p_* \in \mathcal{M}$ is a **critical point** for ϕ if $d\phi(p_*) = 0$. Equivalently, in coordinates, p_* is critical if the gradient vector $\nabla\phi(p_*)$ vanishes. At a critical point, $\phi(p) - \phi(p_*)$ is a smooth function of p which vanishes to order at least 2 at $p = p_*$. Say that a critical point p_* for ϕ is **quadratically nondegenerate** if the quadratic part is nondegenerate; in coordinates, this means that the Hessian matrix

$$\mathcal{H}(\phi; p_*) := \left(\frac{\partial^2 \phi}{\partial x_i \partial x_j}(p_*) \right)_{1 \le i,j \le k}$$

has nonzero determinant. It is well known (e.g., [BH86, Won89]) that the integral

$$\int_{\mathcal{M}} \exp(i\lambda\phi(\mathbf{y}))A(\mathbf{y})\, d\mathbf{y}$$

can be asymptotically estimated via a stationary phase analysis. The following formulation is adapted from [Ste93].

If $p \mapsto (x_1, \ldots, x_d)$ is a local right-handed coordinatization, we denote by $\eta[p, d\mathbf{x}]$ the value $A(p)$ for the function A such that $\eta = A(p)\, d\mathbf{x}$. If the real matrix M has nonvanishing real eigenvalues, we denote a signature function $\sigma(M) := n_+(M) - n_-(M)$ where $n_+(M)$ (respectively $n_-(M)$) denotes the number of positive (respectively negative) eigenvalues of M. Given ϕ and η as above, and a critical point p_* for ϕ, we claim that the quantity $\mathcal{F}$ defined by

$$\mathcal{F}(\phi, \eta, p_*) := e^{-i\pi\sigma/4} \left|\det \mathcal{H}(\phi; p_*)\right|^{-1/2} \eta[p_*, d\mathbf{x}] \tag{5.6}$$

does not depend on the choice of coordinatization. To see this, note that the symmetric matrix $\mathcal{H}$ has nonzero real eigenvalues, whence $i\mathcal{H}$ has purely imaginary eigenvalues and the quantity $e^{-i\pi\sigma/4}|\det \mathcal{H}(\phi; p_*)|^{-1/2}$ is a $-1/2$ power of $\det(i\mathcal{H})$, in particular, the product of the reciprocals of the principal square roots of the eigenvalues. Up to the sign choice, this is invariant because a change of coordinates with Jacobian J at p_* divides $\eta[p_*, d\mathbf{x}]$ by J and $\mathcal{H}(\phi; p_*)$ by J^2. Invariance of the sign choice follows from connectedness of the special orthogonal group, implying that any two right-handed coordinatizations are locally homotopic and the sign choice, being continuous, must be constant.

Lemma 5.3 (nondegenerate stationary phase integrals)**.** *Let ϕ be a smooth function on a d-manifold $\mathcal{M}$ and let η be a smooth, compactly supported d-form on $\mathcal{M}$. Assume the following hypotheses.*

1. *The set $\mathbf{W}$ of critical points of ϕ on the support of η is finite and non-empty.*

2. *ϕ is quadratically nondegenerate at each $p_* \in \mathbf{W}$.*

Then

$$\int_{\mathcal{M}} \exp(i\lambda\phi)\, \eta = \left(\frac{2\pi}{\lambda}\right)^{d/2} \sum_{p_* \in \mathbf{W}} e^{i\lambda\phi(p_*)} \mathcal{F}(\phi, \eta, p_*) + O\left(\lambda^{-(d+1)/2}\right) . \tag{5.7}$$

Remarks. The stationary phase method actually gives an infinite asymptotic development for this integral. In our application, the contributions of order $\lambda^{-d/2}$ will not cancel, in which case (5.7) gives an asymptotic formula for the integral. The remainder term (see [Ste93]) is bounded by a polynomial in the reciprocals of $|\nabla\phi|$ and $\det \mathcal{H}$ and partial derivatives of ϕ (to order two) and η (to order one); it follows that the bound is uniform if ϕ and η vary smoothly with (1) and (2) always holding.

Proof: Let $\{\mathcal{N}_\alpha\}$ be a finite cover of $\mathcal{M}$ by open sets containing at most one critical point of ϕ, with each $\mathcal{N}_\alpha$ covered by a single chart map and no two containing the same critical point. Let

$\{\psi_\alpha\}$ be a partition of unity subordinate to $\{\mathcal{N}_\alpha\}$. Write

$$I := \int_{\mathcal{M}} \exp(i\lambda\phi)\,\eta$$

as $\sum_\alpha I_\alpha$ where

$$I_\alpha := \int_{\mathcal{N}_\alpha} \exp(i\lambda\phi)\,\eta\,\psi_\alpha\,.$$

According to [Ste93, Proposition 4 of VIII.2.1], when $\mathcal{N}_\alpha$ contains no critical point of ϕ then I_α is rapidly decreasing, i.e, $I_\alpha(\lambda) = o(\lambda^{-N})$ for every N. According to [Ste93, Proposition 6 of VIII.2.3], when $\mathcal{N}_\alpha$ contains a single nondegenerate critical point p_* for ϕ then, using the fact that $\psi_\alpha(p_*) = 1$,

$$I_\alpha = \left(\frac{2\pi}{\lambda}\right)^{d/2} A(p_*) \prod_{j=1}^{d} \mu_j^{-1/2} + O\left(\lambda^{-d/2-1}\right)$$

where $\eta = A(\mathbf{x})d\mathbf{x}$ in the local chart map, $\{\mu_j\}$ are the eigenvalues of $i\mathcal{H}$ in this chart map, and the principal $-1/2$ powers are chosen. Summing over α then proves the lemma. □

As a corollary, we derive the asymptotics for the Fourier transform of a smooth d-form on an oriented d-manifold immersed in $\mathbb{R}^{d+1}$. Let $\mathcal{M}$ be such a manifold and let $\mathcal{K}(p)$ denote the curvature of $\mathcal{M}$ at p. If η is a smooth, compactly supported d-form on $\mathcal{M}$, denote $\eta[p] = \eta[p, d\mathbf{x}]$ with respect to the immersion coordinates, and define the Fourier transform $\hat{\eta}$ by

$$\hat{\eta}(\mathbf{r}) := \int_{\mathcal{M}} e^{i\hat{\mathbf{r}}\cdot\mathbf{x}} \cdot \eta\,.$$

Corollary 5.4. *Let K be a compact subset of the unit sphere. Assume that for $\hat{\mathbf{r}} \in K$, the set $\mathbf{W}$ of critical points for the phase function $\hat{\mathbf{r}} \cdot \mathbf{x}$ is finite (possibly empty), and all critical points are quadratically nondegenerate. For $\mathbf{x} \in \mathbf{W}$, let $\tau(\mathbf{x})$ denote the index of the critical point, that is, the difference between the dimensions of the positive and negative tangent subspaces for the function $\hat{\mathbf{r}} \cdot \mathbf{x}$. Then*

$$\hat{\eta}(\mathbf{r}) = \left(\frac{2\pi}{|\mathbf{r}|}\right)^{d/2} \sum_{\mathbf{x}_* \in \mathbf{W}} e^{i\mathbf{r}\cdot\mathbf{x}_*} \eta[\mathbf{x}_*] \mathcal{K}(\mathbf{x}_*)^{-1/2} e^{-i\pi\tau(\mathbf{x}_*)/4} + O\left(\lambda^{-(d+1)/2}\right)$$

uniformly as $|\mathbf{r}| \to \infty$ with $\hat{\mathbf{r}} \in K$.

Proof: Plugging $\phi = \hat{\mathbf{r}} \cdot \mathbf{x}$ into Lemma 5.3, and comparing with (5.6) we see that we need only to verify for each $\mathbf{x}_* \in \mathbf{W}$ that

$$e^{-i\pi\sigma/4} \left|\det \mathcal{H}(\phi; \mathbf{x}_*)\right|^{-1/2} \eta[\mathbf{x}_*, d\mathbf{x}] = \eta[\mathbf{x}_*] \left|\mathcal{K}(\mathbf{x}_*)\right|^{-1/2} e^{-i\pi\tau(\mathbf{x}_*)/4}.$$

With the immersed coordinates, $\sigma = \tau$, and this amounts to verifying that

$$|\det \mathcal{H}(\phi; \mathbf{x}_*)| = |\mathcal{K}(\mathbf{x}_*)|.$$

Let $\mathcal{P}$ denote the tangent space to $\mathcal{M}$ at $\mathbf{x}_*$ and let $u_1, \ldots, u_d$ be an orthonormal basis for $\mathcal{P}$. Let v be the unit vector in direction $\hat{\mathbf{r}}$, which is orthogonal to $\mathcal{P}$ because $\mathbf{x}_*$ is critical for ϕ. In this coordinate system, express $\mathcal{M}$ as a graph over $\mathcal{P}$. Thus locally,

$$\mathcal{M} = \{\mathbf{x}_* + \mathbf{u} + h(\mathbf{u})v : \mathbf{u} \in \mathcal{P}\}$$

for some smooth function h with $h(\mathbf{0})$ and $\nabla h(\mathbf{0})$ vanishing. Let Q denote the quadratic part of h. By Corollary 3.3, we have $\mathcal{K}(\mathbf{x}_*) = ||Q||$. But

$$\phi(\mathbf{x}_* + \mathbf{u} + h(\mathbf{u})v) = \phi(\mathbf{x}_*) + h(\mathbf{u})$$

whence $\mathcal{H}(\phi; \mathbf{x}_*) = Q$, completing the verification. □

5.2.3 Results on multivariate generating functions: when $\mathcal{V}$ is smooth on the unit torus

In this section, we state general results on asymptotics of coefficients of rational multivariate generating functions. These results extend previous work of [PW02] in two ways: the hypotheses are generalized to remove a finiteness condition, and the conclusions are restated in terms of Gaussian curvature. Our two theorems concern reductions of the $(d+1)$-variable Cauchy integral to something more manageable; the second theorem is an extension of the first.

We give some notation and hypotheses that are assumed throughout this section. Let $F = G/H$ be the quotient of Laurent polynomials in $d+1$ variables $\mathbf{z} := (z_1, \ldots, z_{d+1})$ and let B_0 be a component of the complement of the amoeba of H containing a translate of the negative z_{d+1}-axis (see Section 5.2.1). Assume $\mathbf{0} \in \partial B_0$ and let $F = \sum_{\mathbf{r}} a_{\mathbf{r}} \mathbf{z}^{\mathbf{r}}$ be the Laurent series corresponding to B_0. Let $\mathcal{V}$ denote the set $\{\mathbf{z} \in \mathbb{C}^{d+1} : H(\mathbf{z}) = 0\}$ and $\mathcal{V}_1 := \mathcal{V} \cap T$ denote the intersection of $\mathcal{V}$ with the unit torus. Let $E := \mathcal{V}_1 \cap \{\mathbf{z} : \nabla H(\mathbf{z}) = \mathbf{0}\}$ denote the singular set of $\mathcal{V}_1$. Let $\mathbf{K} := \mathbf{K}(\mathbf{0})$ denote the cone of $\hat{\mathbf{r}}$ for which the maximality condition (5.3) is satisfied with $\mathbf{x}_* = \mathbf{0}$ and let $\mathcal{N}$ be any compact subcone of the interior of $\mathbf{K}$ such that (5.4) holds for $\hat{\mathbf{r}} \in \mathcal{N}$ (finitely many critical points).

We start with the definition/construction of the residue form in the case of a generic rational function $F = P/Q$ with singular variety $\mathcal{V}_Q$.

Proposition 5.5 (residue form)**.** *There is a unique d-form η, holomorphic everywhere ∇Q does not vanish such that $\eta \wedge dQ = P\, d\mathbf{z}$. We call it the residue form for F on $\mathcal{V}_Q$ and denote it by* $\mathrm{RES}\,(F\, d\mathbf{z})$.

Remark. To avoid ambiguous notation, for the remainder of this section we denote the usual residue at a simple pole a of a univariate function f by

$$\texttt{residue}(f; a) = \lim_{z \to a} (z - a) f(z)\,.$$

Proof: To prove uniqueness, let η_1 and η_2 be two solutions. Then $(\eta_1 - \eta_2) \wedge dQ = 0$. The inclusion $\iota : \mathcal{V}_Q \to \mathbb{C}^d$ induces a map ι^* that annihilates any form ξ with $\xi \wedge dQ = 0$. Hence $\eta_1 = \eta_2$ when they are viewed as forms on $\mathcal{V}_Q$.

To prove existence, suppose that $(\partial Q / \partial z_{d+1})(\mathbf{z}) \neq 0$. Then the form

$$\eta := \frac{P}{\partial Q / \partial z_{d+1}}\, dz_1 \cdots dz_d \tag{5.8}$$

is evidently a solution. One has a similar solution assuming $\partial Q / \partial z_j$ is nonvanishing for any other j. The form is therefore well defined and nonsingular everywhere that ∇Q is nonzero. □

From the previous proposition, $\mathrm{RES}\,(F\, d\mathbf{z})$ is holomorphic wherever $\nabla H \neq 0$, and in particular, on $\mathcal{V}_1 \setminus E$.

Lemma 5.6. *Let $F, G, H, \mathcal{V}, B_0, \mathcal{V}_1$ and E be as stated in the beginning of this section. Assume torality* (4.2) *and suppose that the singular set E is empty. Then $a_{\mathbf{r}}$ may be computed via the following holomorphic integral.*

$$a_{\mathbf{r}} = \left(\frac{1}{2\pi i}\right)^d \int_{\mathcal{V}_1} \mathbf{z}^{-\mathbf{r}-\mathbf{1}} \mathrm{RES}\left(F\, d\mathbf{z}\right). \tag{5.9}$$

PROOF: As a preliminary step, we observe that the projection $\pi : \mathcal{V} \to \mathbb{C}^d$ onto the first d coordinates induces a fibration of $\mathcal{V}_1$ with discrete fiber of cardinality $2d$, everywhere except on a set of positive codimension. To see this, first observe (cf. (5.2)) that the polynomial H has degree $2d$ in the variable z_{d+1}. Let $Y \subseteq \mathcal{V}$ be the subvariety on which $\partial H/\partial z_{d+1}$ vanishes. Then on the regular set $U := T \setminus \pi(Y)$, the inverse image of π contains $2d$ points and there are distinct, locally defined smooth maps $y_1(\mathbf{x}), \ldots, y_{2d}(\mathbf{x})$ that are inverted by π. The fibration

$$\pi^{-1}[U] \xrightarrow{\pi} U$$

is the aforementioned fibration with fiber cardinality $2d$.

Next, we apply Cauchy's integral formula with $\mathbf{u} = -e_{d+1}$. Let S_1 and S_2 denote the circles in $\mathbb{C}^1$ of respective radii e^{-1} and $1 + s$, and let $T_j := \mathbf{T}_d \times S_j$ for $j = 1, 2$. By (4.2), neither T_1 nor T_2 intersects $\mathcal{V}$, so beginning with the integral formula and integrating around T_1, we have

$$\begin{aligned} a_{\mathbf{r}} &= \left(\frac{1}{2\pi i}\right)^{d+1} \int_{T_1} \mathbf{z}^{-\mathbf{r}-\mathbf{1}} F(\mathbf{z})\, d\mathbf{z} \\ &= \left(\frac{1}{2\pi i}\right)^{d+1} \left[\int_{T_1} \mathbf{z}^{-\mathbf{r}-\mathbf{1}} F(\mathbf{z}) d\mathbf{z} - \int_{T_2} \mathbf{z}^{-\mathbf{r}-\mathbf{1}} F(\mathbf{z}) d\mathbf{z}\right] + \left(\frac{1}{2\pi i}\right)^{d+1} \int_{T_2} \mathbf{z}^{-\mathbf{r}-\mathbf{1}} F(\mathbf{z}) d\mathbf{z}\,. \end{aligned}$$

Expressing the integral over T_j as an iterated integral over $\mathbf{T}_d \times S_j$ shows that the quantity in square brackets is

$$\int_{\mathbf{T}_d} \left[\int_{S_1} \mathbf{z}^{-\mathbf{r}-\mathbf{1}} F(\mathbf{z})\, dz_{d+1} - \int_{S_2} \mathbf{z}^{-\mathbf{r}-\mathbf{1}} F(\mathbf{z})\, dz_{d+1}\right] d\mathbf{z}_{\dagger} \tag{5.10}$$

where $\mathbf{z}_{\dagger}$ denotes $(z_1, \ldots, z_d)$. The inner integral is the integral in z_{d+1} of a bounded continuous function of $(\mathbf{z}_{\dagger}, z_{d+1})$, so it is a bounded function of $\mathbf{z}_{\dagger}$. We may always write the inner integral as a sum of residues. In fact, when $\mathbf{z}_\dagger \in U$ it is the sum of $2d$ simple residues, and since $\mathbf{T}_d \setminus U$ has measure zero, we may rewrite (5.10) as

$$2\pi i \int_U \left[\sum_{k=1}^{2d} \mathbf{z}^{-\mathbf{r}-\mathbf{1}} \texttt{residue}(F(\mathbf{z}_\dagger, \cdot); y_k(\mathbf{z}_\dagger)) \right] d\mathbf{z}_\dagger \, . \tag{5.11}$$

On U, we have seen from (5.8) that

$$\text{RES}\,(F\,d\mathbf{z})(\mathbf{z}) = \pi^* \left[\texttt{residue}\,(F(\mathbf{z}_\dagger, \cdot); z_{d+1})\, d\mathbf{z}_\dagger \right] (\pi(\mathbf{z}))\, ,$$

hence, from the fibration, (5.11) becomes

$$2\pi i \int_{\pi^{-1}[U]} \mathbf{z}^{-\mathbf{r}-\mathbf{1}} \text{RES}\,(F\,d\mathbf{z})\, .$$

Because the complement of $\pi^{-1}[U]$ in $\mathcal{V}_1$ has measure zero, we have shown that

$$a_{\mathbf{r}} = \left(\frac{1}{2\pi i} \right)^d \int_{\mathcal{V}_1 \setminus E} \mathbf{z}^{-\mathbf{r}-\mathbf{1}} \text{RES}\,(F\,d\mathbf{z}) + \left(\frac{1}{2\pi i} \right)^{d+1} \int_{T_2} \mathbf{z}^{-\mathbf{r}-\mathbf{1}} F(\mathbf{z}) d\mathbf{z}\, . \tag{5.12}$$

The integral over T_2 is $O((1+s)^{-r_d})$; because s is arbitrary, sending $s \to \infty$ shows this integral to be zero. We have assumed that E is empty, so (5.12) becomes the desired conclusion (5.9). $\Box$

The next theorem has the Quantum Random Walk as its main target, however it is valid for a general class of rational Laurent series, provided we assume the hypotheses of Lemma 5.6, namely torality (4.2) and smoothness ($E = \emptyset$). Under these hypotheses, the image of $\mathcal{V}_1$ under $\mathbf{z} \mapsto (\log \mathbf{z})/i$ is a smooth co-dimension-one submanifold $\mathcal{M}$ of the flat torus; we let $\mathcal{K}(\mathbf{z})$ denote the curvature of $\mathcal{M}$ at the point $(\log \mathbf{z})/i$. Of primary interest is the regime of sub-exponential decay, which is governed by critical points on the unit torus. We therefore let $\mathbf{K}$ denote the set of directions $\hat{\mathbf{r}}$ for which $\hat{\mathbf{r}} \cdot \mathbf{x}$ is maximized at $\mathbf{x} = \mathbf{0}$ on the closure $\overline{B_0}$ of the component of the amoeba complement in which we are computing a Laurent series. We also assume (5.4) (finiteness of $\mathbf{W}(\hat{\mathbf{r}})$) for each $\hat{\mathbf{r}} \in \mathbf{K}$. Observing that $\mathbf{z} = \exp(i\mathbf{x}) \in \mathbf{W}$ if and only if $\mathbf{x}$ is critical for the function $\mathbf{r} \cdot \mathbf{x}$ on $\mathcal{M}$, we may define $\tau(\mathbf{z})$ to be the signature of the critical point $(\log \mathbf{z})/i$ (the dimension of positive space minus dimension of negative space) for the function $\hat{\mathbf{r}} \cdot \mathbf{x}$ on $\mathcal{M}$.

Theorem 5.7. *Under the above hypotheses, let $\mathcal{N}$ be a compact subset of the interior of* $\mathbf{K}$ *such that the curvatures $\mathcal{K}(\mathbf{z})$ at all points $\mathbf{z} \in \mathbf{W}(\hat{\mathbf{r}})$ are nonvanishing for all $\hat{\mathbf{r}} \in \mathcal{N}$. Then as $|\mathbf{r}| \to \infty$, uniformly over $\hat{\mathbf{r}} \in \mathcal{N}$,*

$$a_{\mathbf{r}} = \left(\frac{1}{2\pi|\mathbf{r}|}\right)^{d/2} \sum_{\mathbf{z}\in\mathbf{W}} \mathbf{z}^{-\mathbf{r}} \frac{G(\mathbf{z})}{|\nabla_{\log} H(\mathbf{z})|} \frac{1}{\sqrt{|\mathcal{K}(\mathbf{z})|}} e^{-i\pi\tau(\mathbf{z})/4} + O\left(|\mathbf{r}|^{-(d+1)/2}\right) \tag{5.13}$$

provided that $\nabla_{\log} H$ is a positive multiple of $\hat{\mathbf{r}}$ (if it is a negative multiple, the estimate must be multiplied by -1). When $\hat{\mathbf{r}} \notin \overline{\mathbf{K}}$ then $a_{\mathbf{r}} = o(\exp(-c|\mathbf{r}|))$ for some positive constant c, which is uniform if $\hat{\mathbf{r}}$ ranges over a compact subcone of the complement of $\overline{\mathbf{K}}$.

Proof: The conclusion in the case where $\mathbf{r} \notin \overline{K}$ follows from Corollary 5.2. In the other case, assume $\mathbf{r} \in \mathcal{N}$ and apply Lemma 5.6 to express $a_{\mathbf{r}}$ in the form (5.9):

$$a_{\mathbf{r}} = \left(\frac{1}{2\pi i}\right)^d \int_{\mathcal{V}_1} \mathbf{z}^{-\mathbf{r}} \mathrm{RES}\left(F \frac{d\mathbf{z}}{\mathbf{z}}\right).$$

The chain of integration is a smooth d-dimensional submanifold of the unit torus in $\mathbb{R}^{d+1}$, so when we apply the change of variables $\mathbf{z} = \exp(i\mathbf{y})$, the chain of integration becomes a smooth submanifold $\mathcal{M}$ of the flat torus T_0, hence locally an immersed d-manifold in $\mathbb{R}^{d+1}$. We have $d\mathbf{z} = i\mathbf{z}\, d\mathbf{y}$, so $F(\mathbf{z})d\mathbf{z}/\mathbf{z} = i^d\, F \circ \exp(\mathbf{y})\, d\mathbf{y}$ and functoriality of RES implies that

$$\mathrm{RES}\left(F \frac{d\mathbf{z}}{\mathbf{z}}\right) = \mathrm{RES}\left(F \circ \exp\, d\mathbf{y}\right).$$

After the change of coordinates, therefore, the integral becomes

$$a_{\mathbf{r}} = (2\pi)^{-d}\hat{\eta}(\mathbf{r}) = \left(\frac{1}{2\pi}\right)^d \int_{\mathcal{M}} e^{-i\mathbf{r}\cdot\mathbf{y}}\, \eta$$

where $\eta := \mathrm{RES}\,(F \circ \exp\, d\mathbf{y})$. By hypothesis, η is smooth and compactly supported, so if we apply Corollary 5.4 and divide by $(2\pi)^d$ we obtain

$$a_{\mathbf{r}} = \left(\frac{1}{2\pi|\mathbf{r}|}\right)^{d/2} \sum_{\mathbf{z}\in\mathbf{W}} \mathbf{z}^{-\mathbf{r}} \eta[\mathbf{z}]\, |\mathcal{K}(\mathbf{z})|^{-1/2}\, e^{-i\pi\tau(\mathbf{z})/4} + O\left(|\mathbf{r}|^{-(d+1)/2}\right).$$

Finally, we evaluate $\eta[\mathbf{z}]$ in a coordinate system in which the $(d+1)^{st}$ coordinate is $\hat{\mathbf{r}}$. We see from (5.8) that

$$\eta = \frac{G(\mathbf{z})}{\partial H/\partial \hat{\mathbf{r}}(\mathbf{z})} dA$$

where $d\hat{\mathbf{r}} \wedge dA = d\mathbf{z}$. Because the gradient of H is in the direction $\hat{\mathbf{r}}$, this boils down to $\eta = G(\mathbf{z})/|\nabla_{\log} H(\mathbf{z})|$ at the point $\mathbf{z}$, finishing the proof. □

5.2.4 Results on multivariate generating functions: when $\mathcal{V}$ contains noncontributing cone points

In this section, we generalize Theorem 5.7 to allow ∇H to vanish at finitely many points of $\mathcal{V}$. The key is to ensure that the contribution to the Cauchy integral near these points does not affect the asymptotics. This will be a consequence of an assumption about the degrees of vanishing of G and H at points of E. We begin with some estimates in the vein of classical harmonic analysis. Suppose η is a smooth p-form on a smooth cone in $\mathbb{R}^{d+1}$; the term "smooth" for cones means smooth except at the origin. We say η is **homogeneous of degree** k if in local coordinates it is a finite sum of forms $A(\mathbf{z})\, dz_{i_1} \wedge \cdots \wedge dz_{i_p}$ with A homogeneous of degree $k-p$, that is, $A(\lambda \mathbf{z}) = \lambda^{k-p} A(\mathbf{z})$. A smooth p-form η on a smooth cone is said to have leading degree α if

$$\eta = \eta^\circ + \sum_{i_1,\ldots,i_p} O(|\mathbf{z}|^{\alpha-p+1}\, dz_{i_1} \wedge dz_{i_p}) \tag{5.14}$$

with η° homogeneous of degree α. The following lemma is a special case of the big-O lemma from [BP08]. That lemma requires a rather complicated topological construction from [ABG70]; we give a self-contained proof, due to Phil Gressman, for the special case required here.

Lemma 5.8. *Let $\mathcal{V}_0$ be a smooth $(d-1)$-dimensional manifold in S^d and let $\mathcal{V}$ denote the cone over $\mathcal{V}_0$ in $\mathbb{R}^{d+1}$. Let η be a compactly supported d-form of leading degree $\alpha > 0$ on $\mathcal{V}$. Then*

$$\int_{\mathcal{V}} e^{i\mathbf{r}\cdot\mathbf{z}} \eta = O(|\mathbf{r}|^{-\alpha})\,.$$

Proof: Assume without loss of generality that η is supported on the unit polydisk $\{\mathbf{z} : |\mathbf{z}| \le 1\}$, where $|\mathbf{z}| := \sqrt{\sum_{j=1}^{d+1} |z_j|^2}$ is the usual Euclidean norm on $\mathbb{C}^{d+1}$. The union of the interiors of the annuli

$$B_n := \{\mathbf{z} : 2^{-n-2} \le |\mathbf{z}| \le 2^{-n}\}$$

is the open unit polydisk, minus the origin. Let $\theta_n : B_0 \to B_n$ denote dilation by 2^{-n} and let $\eta_n := \theta_n^* \eta|_{B_0}$ be the pullback to B_0 from B_n of the form η. Let η° denote the homogeneous part of η, that is, the unique form satisfying (5.14). The forms η_n are asymptotically equal to $2^{-\alpha n}\eta^\circ$ in the following sense: for each L, the partial derivatives of $2^{\alpha n}\eta_n$ up to order L converge to the corresponding partial derivatives of η°, uniformly on B_0. Let χ_n be smooth functions, compactly supported on the interior of B_0, and with partial derivatives up to any fixed order bounded uniformly in n. Then for any $N > 0$ there is an estimate

$$\int_{B_0} e^{i\mathbf{r}\cdot\mathbf{z}} \chi_n(\mathbf{z}) \cdot (2^{\alpha n}\eta_n(\mathbf{z})) = O\left(|\mathbf{r}|^{-N}\right) \tag{5.15}$$

uniformly in n. This is a standard result, an argument for which may be found in [Ste93, Proposition 4 of Section VIII.2], noting that uniform bounds on the partial derivatives of coefficients of $\chi_n\eta_n$ up to a sufficiently high order L suffice to prove Stein's Proposition 4 for the class η_n, uniformly in n. To make the O-notation explicit, we rewrite (5.15) as

$$\int_{B_0} e^{i\mathbf{r}\cdot\mathbf{z}} \chi_n(\mathbf{z})\eta_n(\mathbf{z}) \le g_N(|\mathbf{r}|)\, 2^{-\alpha n}\, |\mathbf{r}|^{-N} \tag{5.16}$$

for some functions $g_N(x)$ each going to zero as $x \to \infty$.

Next, let $\{\psi_n : n \ge 0\}$ be a partition of unity subordinate to the cover $\{B_n\}$. We may choose ψ_n so that $0 \le \psi_n \le 1$ and so that the partial derivatives of ψ_n up to a fixed order L are bounded by $C_L 2^n$ where C_L does not depend on n. We estimate $\int_{B_n} e^{i\mathbf{r}\cdot\mathbf{z}}\psi_n\eta$ in two ways. First, using $|\psi_n| \le 1$ and $\eta(\mathbf{z}) = O(|\mathbf{z}|^{\alpha-d}\, dz_{i_1} \cdots dz_{i_d})$, we obtain

$$\left| \int_{B_n} e^{i\mathbf{r}\cdot\mathbf{z}}\psi_n\eta \right| \le C\, 2^{-nd} \sup_{\mathbf{z}\in B_n} |\mathbf{z}|^{\alpha-d} \le C'\, 2^{-n\alpha} \tag{5.17}$$

for some constants C, C' independent of n. On the other hand, pulling back by θ_n, we observe that the partial derivatives of $\theta_n^*\psi_n$ up to order L are bounded by C_L independently of n. Using (5.16), for any $N > 0$ we choose $L = L(N)$ appropriately to obtain

$$\begin{aligned} \left| \int_{B_n} e^{i\mathbf{r}\cdot\mathbf{z}} \psi_n \eta \right| &= \left| \int_{B_0} e^{i(\mathbf{r}/2^n)\cdot\mathbf{z}} (\theta_n^* \psi_n) \cdot (2^{\alpha n} \eta_n) \right| \\ &\leq g_N \left(\frac{|\mathbf{r}|}{2^n} \right) 2^{-\alpha n} \left(\frac{|\mathbf{r}|}{2^n} \right)^{-N} \end{aligned}$$

for all n, N, where g_N are real functions going to zero at infinity.

Let $n_0(\mathbf{r})$ be the least integer such that $2^{-n_0} \leq 1/|\mathbf{r}|$. Our last estimate implies that for $n = n_0 - j < n_0$,

$$\begin{aligned} \left| \int_{B_n} e^{i\mathbf{r}\cdot\mathbf{z}} \psi_n \eta \right| &\leq 2^{-\alpha n} g_N \left(\frac{|\mathbf{r}|}{2^n} \right) \left(\frac{|\mathbf{r}|}{2^n} \right)^{-N} \\ &= 2^{-\alpha n_0} \left[2^{\alpha j} g_N \left(2^j \frac{|\mathbf{r}|}{2^{n_0}} \right) \left(2^j \frac{|\mathbf{r}|}{2^{n_0}} \right)^{-N} \right] . \end{aligned}$$

Once $N > \alpha$, the quantity in the square brackets is summable over $j \geq 1$, giving

$$\sum_{n < n_0} \left| \int_{B_n} e^{i\mathbf{r}\cdot\mathbf{z}} \psi_n \eta \right| = O\left(2^{-\alpha n_0}\right) .$$

On the other hand, (5.17) is summable over $n \geq n_0$, so we have

$$\sum_{n \geq n_0} \left| \int_{B_n} e^{i\mathbf{r}\cdot\mathbf{z}} \psi_n \eta \right| = O\left(2^{-\alpha n_0}\right) .$$

The last two estimates, along with $|\mathbf{r}| = \Theta(2^{n_0})$, prove the lemma. □

Given an algebraic variety $\mathcal{V} := \{H = 0\}$, let p be an isolated singular point of $\mathcal{V}$. Let $H^\circ = H_p^\circ$ denote the leading homogeneous term of H at p, namely the homogeneous polynomial of some degree m such that $H(p + \mathbf{z}) = H^\circ(\mathbf{z}) + O(|\mathbf{z}|^{m+1})$; the degree m will be the least degree of any term in the Taylor expansion of H near p. The **normal cone** to $\mathcal{V}$ at p is defined to be the set of all normals to the homogeneous variety $\mathcal{V}_p := \{\mathbf{z} : H_p^\circ(p + \mathbf{z}) = 0\}$. We remark that $\mathbf{r}$ is in the normal cone to $\mathcal{V}$ at p if and only if $\mathbf{r} \cdot \mathbf{z}$ has (a line of) critical points on $\mathcal{V}_p$.

Theorem 5.9. *Let $F, G, H, \mathcal{V}, B_0, \mathcal{V}_1$ and E be as stated at the beginning of this section. Assume torality* (4.2)*. Suppose that the singular set E is finite and that for each $p \in E$, the following hypotheses are satisfied.*

1. *The residue form η has leading degree $\alpha > d/2$ at p.*

2. *The cone $\mathcal{V}_p$ is projectively smooth and $\mathbf{r}$ is not in the normal cone to $\mathcal{V}$ at p.*

Then a conclusion similar to that of Theorem 5.7 holds, namely the sum (5.13) *over the points $\mathbf{z}_j \notin E$ where $\nabla H \parallel \mathbf{r}$ gives the asymptotics of $a_{\mathbf{r}}$ up to a correction that is $o(|\mathbf{r}|^{-d/2})$.*

PROOF: By [Tou68, Cor. 2"], condition (2) implies that the function $H(p + \mathbf{z})$ is bi-analytically conjugate to the function H_p°, that is, locally there is a bi-analytic change of coordinates Ψ_p such that $H_p^\circ \circ \Psi_p = H(p + \mathbf{z})$. Now for each $p \in E$, let U_p be a neighborhood of p in $\mathcal{V}$ sufficiently small so that it contains no other $p' \in E$, contains no $\mathbf{y}_j$, and so that the bi-analytic map Ψ_p is defined on U_p. Let U_0 be a neighborhood of the complement of the union of the sets U_p. Using a partition of unity subordinate to $\{U_p, U_0\}$, we replicate the beginning of the proof of Theorem 5.7 to see that it suffices to show

$$\int_{U_p} e^{i\mathbf{r}\cdot\mathbf{y}} \text{RES}\,(F\,d\mathbf{x}) = o(|\mathbf{r}|^{-d/2})\,.$$

Changing coordinates via Ψ_p gives an integral of a smooth, compactly supported form η on the cone $\mathcal{V}_p$ which is homogeneous of order $\alpha > d/2$. Lemma 5.8 estimates the integral to be $O(|\mathbf{r}|^{-\alpha})$, which completes the proof. $\square$

5.3 Application to 2-D Quantum Random Walks

As before, we let $\mathbf{F} = (F^{(i,j)})_{1\leq i,j\leq k}$ where

$$F^{(i,j)}(x,y,z) = \sum_{r,s,t} a^{(i,j)}_{r,s,t} x^r y^s z^t$$

and $a^{(i,j)}_{r,s,t}$ is the amplitude for finding the particle at location (r,s) at time t in chirality j if it started at the origin at time zero in cardinality i. Each entry $F^{(i,j)}$ has some numerator $G^{(i,j)}$ and the same denominator $H = \det(I - zMU)$. In addition, we denote the image of the Gauss map of $\mathcal{V}_1 \setminus E$ as $\mathcal{G}$. We note that $\hat{\mathbf{r}} \in \mathcal{G}$ precisely when

$$\text{There is some } \mathbf{z} \text{ in the unit torus for which } H(\mathbf{z}) = 0 \text{ and } \nabla_{\log} H(\mathbf{z}) \parallel \hat{\mathbf{r}}\,. \tag{5.18}$$

In fact, we can make the stronger statement:

Lemma 5.10. $\mathcal{G} \subset \mathbf{K}$.

Proof of Lemma 5.10: Let $\mathbf{z}$ satisfy (5.18) for some $\hat{\mathbf{r}}$. Because $\mathcal{V}$ is smooth at $\mathbf{z}$, a neighborhood of $\mathbf{z}$ (or a patch including $\mathbf{z}$) in $\mathcal{V}$ is mapped by the coordinatewise Log map to a support patch to B_0 which is normal to $\hat{\mathbf{r}}$. This patch lies entirely outside B_0 by the convexity of amoeba complements. In the limit we see the following. If we take the real version of the complex tangent plane to $\mathcal{V} \in \mathbb{C}^{d+1}$ at $\mathbf{z}$ and map by the coordinatewise log map, the result is a support hyperplane to B_0 which again, lies completely outside B_0 (except at $\operatorname{Log}|\mathbf{z}|$) by convexity. Now when $\hat{\mathbf{r}} \in \mathcal{G}$, Equation (5.18) is satisfied with $\mathbf{z} \in \mathcal{V}_1$. Thus $\operatorname{Log}|\mathbf{z}| = \mathbf{0}$ and $\hat{\mathbf{r}} \in \mathbf{K}$. The desired conclusion follows. □

We apply the results of Section 5.2 to several one-parameter families of two-dimensional QRWs. Each analysis requires us to verify properties of the corresponding family of generating functions.

5.3.1 S_p

We begin by introducing a family $S(p)$ of orthogonal matrices with $p \in (0,1)$:

$$S(p) = \begin{pmatrix} \frac{\sqrt{p}}{\sqrt{2}} & \frac{\sqrt{p}}{\sqrt{2}} & \frac{\sqrt{1-p}}{\sqrt{2}} & \frac{\sqrt{1-p}}{\sqrt{2}} \\ -\frac{\sqrt{p}}{\sqrt{2}} & \frac{\sqrt{p}}{\sqrt{2}} & -\frac{\sqrt{1-p}}{\sqrt{2}} & \frac{\sqrt{1-p}}{\sqrt{2}} \\ \frac{\sqrt{1-p}}{\sqrt{2}} & -\frac{\sqrt{1-p}}{\sqrt{2}} & -\frac{\sqrt{p}}{\sqrt{2}} & \frac{\sqrt{p}}{\sqrt{2}} \\ -\frac{\sqrt{1-p}}{\sqrt{2}} & -\frac{\sqrt{1-p}}{\sqrt{2}} & \frac{\sqrt{p}}{\sqrt{2}} & \frac{\sqrt{p}}{\sqrt{2}} \end{pmatrix}.$$

The matrix $S(1/2)$ is the alternative Hadamard matrix referred to earlier as $\tilde{U}_{\text{Had}}$. A probability profile was shown in Figure 6; here is a picture for another parameter value, namely 1/8. The following theorem, conjectured in [Bra07], shows why similarity of the pictures is not a coincidence.

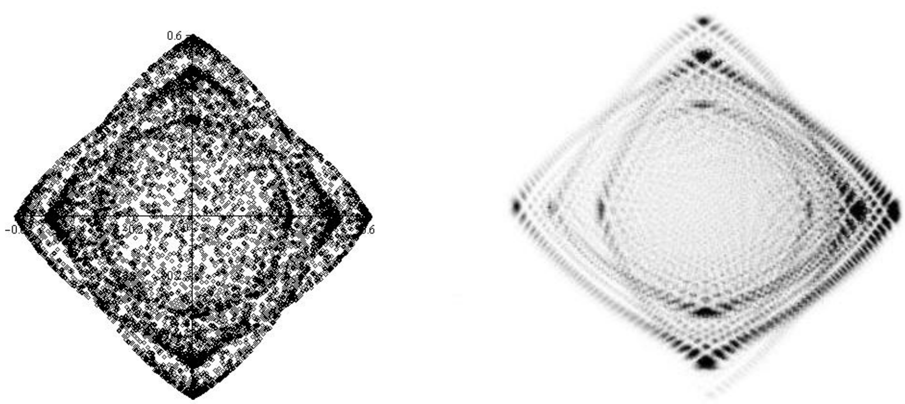

Figure 9: Limiting region (left) and Probabilities at time 200 (right) for the $S(1/8)$ QRW

Theorem 5.11. *For the Quantum Random Walk with unitary matrix $U = S(p)$, let $\mathcal{G}'$ be a compact subset of the interior of $\mathcal{G}$ such that the curvatures $\mathcal{K}(\mathbf{z})$ at all points $\mathbf{z} \in \mathbf{W}(\hat{\mathbf{r}})$ are nonvanishing for all $\hat{\mathbf{r}} \in \mathcal{G}'$. Fix chiralities i, j, let $G := G^{(i,j)}$, and let $a_{\mathbf{r}} := a_{r,s,t}$ denote the* *amplitude to be at position (r, s) at time t. Then as $|\mathbf{r}| \to \infty$, uniformly over $\hat{\mathbf{r}} \in \mathcal{G}'$,*

$$a_{\mathbf{r}} = (-1)^{\delta} \frac{1}{2\pi|\mathbf{r}|} \sum_{\mathbf{z} \in \mathbf{W}} \mathbf{z}^{-\mathbf{r}} \frac{G(\mathbf{z})}{|\nabla_{\log} H(\mathbf{z})|} \frac{1}{\sqrt{|\mathcal{K}(\mathbf{z})|}} e^{-i\pi\tau(\mathbf{z})/4} + O\left(|\mathbf{r}|^{-3/2}\right) \tag{5.19}$$

where $\delta = 1$ if $\nabla_{\log} H$ is a negative multiple of $\hat{\mathbf{r}}$ (so as to change the sign of the estimate) and zero otherwise. When $\hat{\mathbf{r}} \in [-1, 1]^2 \setminus \mathcal{G}$ then for every integer $N > 0$ there is a $C > 0$ such that $\Pr(\mathbf{r}) \le C|\mathbf{r}|^{-N}$ with C uniform as $\mathbf{r}$ ranges over a neighborhood $\mathcal{N}$ of $\mathbf{r}$ whose closure is disjoint from the closure of $\mathcal{G}$.

Before proving this theorem we interpret its implication for the probability profile. The probability of finding the particle at (r, s) in the given chiralities at the given time is equal to $|a_{\mathbf{r}}|^2$. We only care about $a_{\mathbf{r}}$ up to a unit complex multiple, so we don't care whether δ is zero or one, but we must keep track of phase factors inside the sum because these affect the interference of terms from different $\mathbf{z} \in \mathbf{W}$. In fact, the nearest neighbor QRW has periodicity (because all possible steps are odd); the manifestation of this is that $\mathbf{W}$ consists of conjugate pairs. When $r + s$ and t have opposite parities the summands in the formula for $a_{\mathbf{r}}$ cancel. Otherwise the probability amplitude $|a_{\mathbf{r}}|^2$ will be $\Theta(t^{-2})$, uniformly over compact regions avoiding critical values in the range of the logarithmic Gauss map but blowing up at these values.

Proof of Theorem 5.11: As $\mathcal{G} \subset \mathbf{K}$ by Lemma 5.10, the result when $\hat{\mathbf{r}} \in \mathcal{G}'$ is immediate once we have shown that for any $S(p)$, its generating function satisfies the hypotheses of Theorem 5.7. We establish this in the lemma below.

Lemma 5.12. *Let $H := H^{(p)} = \det(I - zM(x, y)S(p))$. Then for $0 < p < 1$, $\nabla H \neq 0$ on T_3. Consequently, $\mathcal{V}_1 := \mathcal{V}_H \cap T_3$ is smooth.*

Theorem 5.7 will not be helpful in proving the case when $\hat{\mathbf{r}} \in [-1, 1]^2 \setminus \mathcal{G}$. To prove this condition we present the following lemma, which is a generalization of [Ste93, Proposition 4 of Section VIII.2].

Lemma 5.13. *Let $\mathcal{M}$ be a compact d-manifold. Suppose α is smooth and that f is a smooth* *real-valued function with no critical points in* $\mathcal{M}$*. Then*

$$I(\lambda) = \int_{\mathcal{M}} e^{i\lambda f(x)} \alpha(x) dx = O(\lambda^{-N}) \tag{5.20}$$

as $\lambda \to \infty$*, for every* $N \geq 0$*.*

We see below that $\mathcal{V}_1$ is compact as it is a four-cover of the two-torus. In the calculation of $a_{\mathbf{r}}$, we have $f(\mathbf{y}) = -\hat{\mathbf{r}} \cdot \mathbf{y}$ and $\lambda = |\mathbf{r}|$. Thus a direction $\hat{\mathbf{r}}$ is not in $\mathcal{G}$ precisely when $f(\mathbf{y})$ has no critical points in $\mathcal{V}_1$. Uniform exponential decay of amplitudes for $\mathbf{r}$ bounded outside the image of the Gauss map follows. Thus Theorem 5.11 is proved, pending the proofs of the lemmas. □

We now prove the above lemmas in reverse order.

Proof of Lemma 5.13 : As $\mathcal{M}$ is compact it admits a finite open cover $\{U_i\}_{i \in I}$ with subordinate partition of unity $\{\phi_i\}_{i \in I}$. We decompose the integral

$$\begin{aligned} I(\lambda) &= \int_{\mathcal{M}} e^{i\lambda f(x)} \alpha(x) dx \\ &= \int_{\mathcal{M}} e^{i\lambda f(x)} \alpha(x) \sum_{i \in I} \phi_i(x) dx \\ &= \sum_{i \in I} \int_{\mathcal{M}} e^{i\lambda f(x)} \alpha(x) \phi_i(x) dx \\ &= \sum_{i \in I} \int_{U_i} e^{i\lambda f(x)} \alpha(x) \phi_i(x) dx \end{aligned}$$

We will show that for each $i \in I$, $\int_{U_i} e^{i\lambda f(x)} \alpha(x) \phi_i(x) dx$ is rapidly decreasing (the requirement above for $I(\lambda)$). As the cover U_i is finite, this will give us the desired result.

For a given $i \in I$, we let $\psi(x) := \alpha(x)\phi_i(x)$ which is then smooth with compact support. For each x_0 in the support of $\psi(x)$, there is a unit vector ξ and a small ball $B(x_0)$, centered at x_0, such that $\xi \cdot (\nabla f)(x) \geq c > 0$ for some real c uniformly for all $x \in B(x_0)$. We then decompose the integral $\int_{U_i} e^{i\lambda f(x)} \psi(x) dx$ as a finite sum

$$\sum_k \int e^{i\lambda f(x)} \psi_k(x) dx$$

where each ψ_k is smooth and has compact support in one of these balls. It then suffices to prove the corresponding estimate for each summand. Now choose a coordinate system $x_1, \ldots, x_d$ so that x_1 lies along ξ. Then

$$\int e^{i\lambda f(x)}\psi_k(x)dx = \int \left(\int e^{i\lambda f(x_1,\ldots,x_d)}\psi_k(x_1, ..., x_d)dx_1 \right) dx_2 \ldots dx_d$$

Now by [Ste93, Proposition 1 of Section VIII.2] the inner integral is rapidly decreasing, giving us the desired conclusion. □

For the next two proofs, we clear denominators to obtain the following explicit polynomial: $H = (x^2y^2+y^2-x^2-1+2xyz^2)z^2-2xy-\sqrt{2p}z(xy^2-y-x+z^2y-z^2x+z^2xy^2+z^2x^2y-x^2y)$. We make the substitution $\alpha = \sqrt{2p}$ to facilitate the use of Gröbner Bases, which require polynomials as inputs. Use the notation H_x for $\frac{\partial H}{\partial x}$, and similarly with y and z.

Proof of Lemma 5.12:

Using the Maple command $\texttt{Basis}([\texttt{H}, \texttt{H}_\texttt{x}, \texttt{H}_\texttt{y}, \texttt{H}_\texttt{z}], \texttt{plex}(\texttt{x}, \texttt{y}, \texttt{z}, \alpha)$ we get a Gröbner Basis with first term $z\alpha^2(\alpha^2-1)(\alpha^2-2) = 2zp(2p-1)(2p-2)$. Thus to show that $S(p)$ results in a variety whose intersection with T is smooth for $p \in (0, 1)$, we need only consider the case when $p = 1/2$. In this case $\alpha = 1$ and the Gröbner Basis for the ideal where $(H, \nabla H) = \mathbf{0}$ is $(-z+z^5, z^3+2y-z, -z-z^3+2x)$. Here B_1 vanishes on the unit circle for $z = \pm 1, \pm i$. However, for $z = \pm 1$, B_2 vanishes only when $y = 0$ and for $z = \pm i$, B_3 vanishes only when $x = 0$. Thus ∇H does not vanish on T_3. □

Further analysis of the limit shape for $S(p)$

Proposition 5.14. *For each pair (x, y), there are four distinct values z_1, z_2, z_3, z_4 such that $(x, y, z_i) \in \mathcal{V}_1$ for $i \in 1, 2, 3, 4$. Consequently, the projection $(x, y, z) \mapsto (x, y)$ is a smooth four-covering of T_2 by $\mathcal{V}_1$.*

Proof: Since H has degree four in z, it has at most four z values for each pair (x, y). Thus for each (x, y) there are at most four z values on $\mathcal{V}_1$. Recall from Proposition 4.2 that all solutions to

$H(x, y, z) = 0$ for a given (x, y) in the unit torus have $|z| = 1$ as well. Hence, if ever there are fewer than four z values for a given (x, y), then there are fewer than four solutions to $H(x, y, \cdot) = 0$ and the implicit function theorem must fail. Consequently, $\frac{\partial H}{\partial z} = 0$. This cannot be true, however, by the following argument. We have ruled out $H_x = H_y = H_z = 0$ on $\mathcal{V}_1$, so if $H_z = 0$, then the point (x, y, z) contributes toward asymptotics in the direction $(r, s, 0)$ for some $(r, s) \neq (0, 0)$. The particle moves at most one step per unit time, so this is impossible. $\square$

To facilitate discussions of subsets of the unit torus, we let (α, β, γ) denote the respective arguments of (x, y, z), that is, $x = e^{i\alpha}, y = e^{i\beta}, z = e^{i\gamma}$. We may think of α, β and γ as belonging to the flat torus $(\mathbb{R}/2\pi\mathbb{Z})^3$.

Proposition 5.15. *$\mathcal{V}_1$ can be decomposed into connected components as $\mathcal{V}_1 = A \amalg B \amalg C \amalg D$, where A, B, C and D will be the components containing the γ values $0, \pi/2, \pi$ and $3\pi/2$, respectively.*

Proof: Let $\chi := \{(x, y, z) : z^4 = -1\}$. We begin by establishing that $|\mathcal{V}_1 \cap \chi| = 8$ with two points for each of the fourth roots of -1. Furthermore, $-\pi/4 \leq \gamma \leq \pi/4$ on A, $\pi/4 \leq \gamma \leq 3\pi/4$ on B, $3\pi/4 \leq \gamma \leq 5\pi/4$ on C, and $5\pi/4 \leq \gamma \leq 7\pi/4$ on D. These observations suffice to prove the proposition, because the smooth variety $\mathcal{V}_1$ cannot have its intersection with a stratum $\{(\alpha, \beta, \gamma) : \gamma = c\}$ that is pinched down to a point; the only possibility is therefore that these values of γ are extreme values on components of $\mathcal{V}_1$.

To check the first of these statements, use the identities $\cos\gamma = (z + z^{-1})/2$, $\sin\gamma = (z - z^{-1})/(2i)$, as well as the analogous identities for α and β, to write the equation of $\mathcal{V}$ in terms of α, β and γ. We find that $H(x, y, z) = 0$ if and only if

$$0 = L(\alpha, \beta, \gamma) := 2\sin\gamma\cos\gamma - \sqrt{2p}(\sin\beta\cos\gamma + \cos\alpha\sin\gamma) + \cos\alpha\sin\beta \,. \tag{5.21}$$

Substituting $\gamma = \pi/4$ results in

$$1 - (\sin\beta + \cos\alpha)\sqrt{p} + \cos\alpha\sin\beta = 0 \,.$$

Verifying that $\sin\beta = \sqrt{p}$ is not a solution, and dividing by $\sin\beta - \sqrt{p}$, we find that

$$\cos\alpha = \frac{1-\sqrt{p}\sin\beta}{\sin\beta - \sqrt{p}}\,.$$

The right-hand side is in $[-1,1]$ only when $\sin\beta = \pm 1$. Thus when $\gamma = \pi/4$, the pair (α,β) is either $(\pi,\pi/2)$ or $(0,3\pi/2)$.

To check the remaining statements, we introduce the following set of isometries for $\mathcal{V}_1$. Define

$$\begin{aligned}
\phi_A(\alpha,\beta,\gamma) &:= (-\alpha,-\beta,-\gamma)\\
\phi_B(\alpha,\beta,\gamma) &:= \left(\beta+\frac{\pi}{2},\alpha+\frac{\pi}{2},\gamma+\frac{\pi}{2}\right)\\
\phi_C(\alpha,\beta,\gamma) &:= (\alpha+\pi,\beta+\pi,\gamma+\pi)\\
\phi_D(\alpha,\beta,\gamma) &:= \left(\beta+\frac{3\pi}{2},\alpha+\frac{3\pi}{2},\gamma+\frac{3\pi}{2}\right)
\end{aligned}$$

Verifying that ϕ_A, ϕ_B and ϕ_C (and hence ϕ_D which is equal to $\phi_C \circ \phi_B$) are isometries is a simple exercise in trigonometry using Equation 5.21, which we will omit. Each isometry inherits its name from the region it proves isometric with A. Using these isometries, we see that γ is equal to $3\pi/4$, $5\pi/4$ and $7\pi/4$ exactly twice on $\mathcal{V}_1$. □

We remark upon the existence of an additional eight-fold isometry within each connected component: $\phi_1(\alpha,\beta,\gamma) := (\alpha,\beta+\pi,-\gamma)$, $\phi_2(\alpha,\beta,\gamma) := (-\alpha,\beta,\gamma)$ and $\phi_3(\alpha,\beta,\gamma) := (\alpha,\pi-\beta,\gamma)$. These symmetries manifest themselves in the plots in figures 6 and 9 as follows. The image is clearly the superposition of two pieces, one horizontally oriented and one vertically oriented. Each of these two is the image of the Gauss map on two of the regions A,B,C,D, and each of these four regions maps to the plot in a 2 to 1 manner on the interior, folding over at the boundary. To verify this, we observe that if p_0 contributes to asymptotics in the direction (r,s) then $\phi_A(p_0),\phi_B(p_0),\phi_C(p_0),\phi_D(p_0),\phi_1(p_0),\phi_2(p_0)$ and $\phi_3(p_0)$ contribute to asymptotics in the directions $(r,s)(s,r),(r,s),(s,r),(-r,-s),(-r,s)$ and $(r,-s)$, respectively. Thus while the image of the Gauss map is two overlapping leaves, the Gauss map of A and C contribute to one leaf, while the Gauss map of B and D contribute to the other.

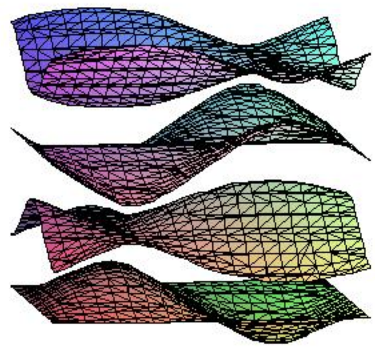

Figure 10: The variety $\mathcal{V}_1$ for $p = 1/2$

We end the analysis with a few observations on the way in which the plots were generated. Our procedure was as follows. Solving for $\sin\gamma$ in (5.21), we obtained

$$\sin\gamma = \sin\beta\,\frac{\sqrt{2p}\,\cos\gamma - \cos\alpha}{2\cos\gamma - \sqrt{2p}\,\cos\alpha}\,. \tag{5.22}$$

Squaring (5.21) and making the substitution $\sin^2\gamma = 1 - \cos^2\gamma$, we found that

$$\left(1-\cos^2\gamma\right)\left(2\cos\gamma - \sqrt{2p}\,\cos\alpha\right)^2 - \left(1-\cos^2\beta\right)\left(\sqrt{2p}\,\cos\gamma - \cos\alpha\right)^2 = 0$$

which we used to get the four solutions for γ in terms of α and β. We then let α and β vary over a grid embedded in the 2-torus and solved for the four values of γ to obtain four points in $\mathcal{V}_1$; this is the composition of the first two maps in (5.1). Differentiation of $H(e^{i\alpha}, e^{i\beta}, e^{i\gamma}) = 0$ shows that the projective direction (r, s, t) corresponding to a point (α, β, γ) is given by $r/t = -\partial\gamma/\partial\alpha$, $s/t = -\partial\gamma/\partial\beta$. Implicit differentiation of (5.21) then gives four explicit values for $(r/t, s/t)$ in terms of α and β. This is the composition of the last two maps in (5.1), with the parametrization of $\mathbb{RP}^2$ by $(r/t, s/t)$ corresponding to the choice of a planar rather than a spherical slice.

5.3.2 A_p

We now present a second family of orthogonal matrices $A(p)$ below. In order for the matrices to be real, we restrict p to the interval $(0, 1/\sqrt{3})$.

$$A(p) = \begin{pmatrix} p & p & p & \sqrt{1-3p^2} \\ -p & p & -\sqrt{1-3p^2} & p \\ p & -\sqrt{1-3p^2} & -p & p \\ -\sqrt{1-3p^2} & -p & p & p \end{pmatrix}$$

This family intersects the family $S(p)$ in one case, namely $A(1/2) = S(1/2)$; for any $(p, p') \in (0,1)^2$ other than $(1/2, 1/2)$, we have $A(p) \neq S(p')$. The following theorem follows from Lemma 5.13 along with a new lemma, namely Lemma 5.17 below, analogous to Lemma 5.12.

Theorem 5.16. *If $0 < p < 1/\sqrt{3}$ then Theorem 5.11 holds for the unitary matrix $A(p)$ in place of the matrix $S(p)$.* □

Lemma 5.17. *Let $H := H^{(p)} = \det(I - zM(x,y)A(p))$. Then for $0 < p < 1/\sqrt{3}$, $\nabla H \neq 0$ on T_3. Consequently, $\mathcal{V}_1 := \mathcal{V}_H \cap T_3$ is smooth.*

Proof of Lemma 5.17: We clear our denominator by setting $H := (-xy)\det(I - MA(p)z)$, now to get

$$H = 2(x-1)(x+1)(y^2+1)z^2p^2 - (-y-x+xy^2+z^2y-x^2y+z^2xy^2-z^2x+z^2x^2y)zp + (yz^2-x)(xz^2+y)\,.$$

As no $\sqrt{1-p^2}$ term appears, we can determine a Gröbner Basis without making a substitution. The Maple command $\mathtt{Basis([H, H_x, H_y, H_z], plex(x, y, z, p)}$ delivers a Basis with first term $p^3z(2p+1)(8p^2-3)(2p^2-1)(2p-1)$. The roots of the first four factors fall outside of the interval $(0, 1/\sqrt{3})$ while the root of the last factor corresponds to the matrix $S(1/2)$ for which we know $\mathcal{V}_1$ is smooth from the discussion above. □

Again we use Theorem 5.7 to correctly predict asymptotics for individual directions. We show probability profiles for a number of parameter values.

Figure 11: The profile for $A(1/6)$ shows how the QRW approaches degeneracy at the endpoints $p \rightarrow 0, 1$

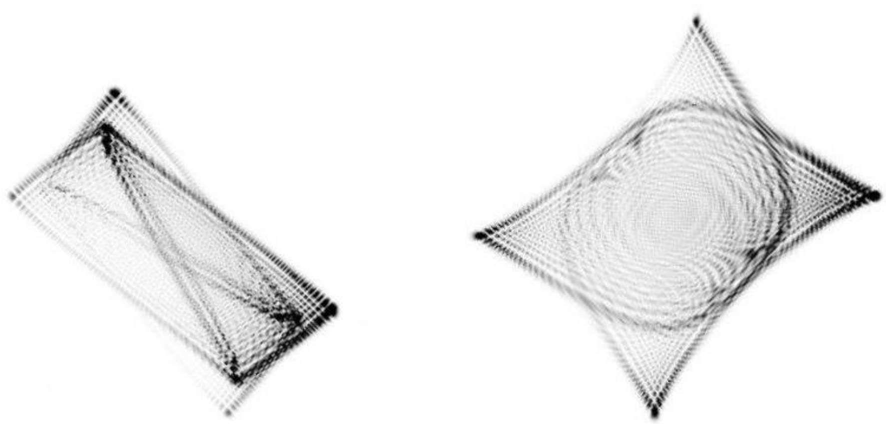

Figure 12: As p increases from 1/3 to 5/9, the direction of the tilt switches

5.3.3 B_p

To demonstrate the application of Theorem 5.9 we introduce a third family of orthogonal matrices, $B(p)$, with $p \in (0,1)$.

$$B(p) = \begin{pmatrix} \frac{\sqrt{p}}{\sqrt{2}} & \frac{\sqrt{p}}{\sqrt{2}} & \frac{\sqrt{1-p}}{\sqrt{2}} & \frac{\sqrt{1-p}}{\sqrt{2}} \\ -\frac{\sqrt{p}}{\sqrt{2}} & \frac{\sqrt{p}}{\sqrt{2}} & -\frac{\sqrt{1-p}}{\sqrt{2}} & \frac{\sqrt{1-p}}{\sqrt{2}} \\ -\frac{\sqrt{1-p}}{\sqrt{2}} & \frac{\sqrt{1-p}}{\sqrt{2}} & \frac{\sqrt{p}}{\sqrt{2}} & -\frac{\sqrt{p}}{\sqrt{2}} \\ -\frac{\sqrt{1-p}}{\sqrt{2}} & -\frac{\sqrt{1-p}}{\sqrt{2}} & \frac{\sqrt{p}}{\sqrt{2}} & \frac{\sqrt{p}}{\sqrt{2}} \end{pmatrix}$$

We have already seen a walk generated by such a matrix, as Figure 5 depicted the walk generated by $B(1/2)$. We note that $B(p)$ is almost identical to $S(p)$ with the one exception being the multiplication of the third row by -1. As was the case with the $S(p)$ walks we can see strong similarities between the image of the Gauss map and the probability profile for various values of p.

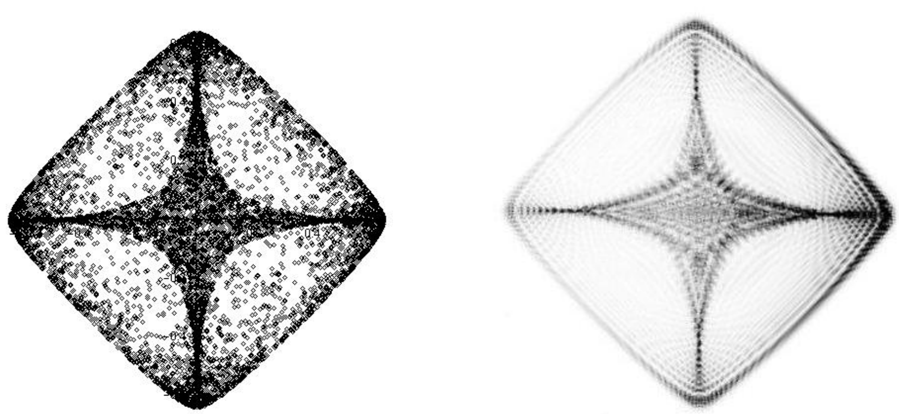

Figure 13: The image of the Gauss map alongside the probability profile for the $B(2/3)$ walk

In contrast to the cases of $S(p)$ and $A(p)$, we will not be able to apply Theorem 5.7 because $\mathcal{V}_1$ is not smooth.

Theorem 5.18. *For the Quantum Random Walk with unitary matrix $U = B(p)$, let $\mathcal{G}'$ be a compact subset of the interior of $\mathcal{G}$ such that the curvatures $\mathcal{K}(\mathbf{z})$ at all points $\mathbf{z} \in \mathbf{W}(\hat{\mathbf{r}})$ are nonvanishing for all $\hat{\mathbf{r}} \in \mathcal{G}'$. Then as $|\mathbf{r}| \to \infty$, uniformly over $\hat{\mathbf{r}} \in \mathcal{G}'$,*

$$a_{\mathbf{r}} = \pm\frac{1}{2\pi|\mathbf{r}|}\sum_{\mathbf{z}\in\mathbf{W}} \mathbf{z}^{-\mathbf{r}}\frac{G(\mathbf{z})}{|\nabla_{\log}H(\mathbf{z})|}\frac{1}{\sqrt{|\mathcal{K}(\mathbf{z})|}}e^{-i\pi\tau(\mathbf{z})/4} + O\left(|\mathbf{r}|^{-3/2}\right) . \tag{5.23}$$

When $\hat{\mathbf{r}} \in [-1,1]^2 \setminus \mathcal{G}$ then for every integer $N > 0$ there is a $C > 0$ such that $\Pr(\mathbf{r}) \leq C|\mathbf{r}|^{-N}$ with C uniform as $\mathbf{r}$ ranges over a neighborhood $\mathcal{N}$ of $\mathbf{r}$ whose closure is disjoint from the closure of $\mathcal{G}$.

Proof: First, we apply Lemma 5.13 with the lemma being applicable as we will see below that $\mathcal{V}_1 := \mathcal{V}_H \cap T_3$ is a two-fold cover of T_2 and thus compact. The conclusion when $\hat{\mathbf{r}} \in [-1,1]^2 \setminus \mathcal{G}$ follows. We get the conclusion in the case where $\hat{\mathbf{r}} \in \mathcal{G}'$ by verifying the hypotheses of Theorem 5.9 in the following lemmas.

Lemma 5.19. *Let $H := H^{(p)} = \det(I - zM(x,y)B(p))$. Then for $0 < p < 1$, the set $E = \{(x,y,z) : (H, \nabla H) = 0\}$ consists only of the four points $(x,y,z) = \pm(1,1,\sqrt{p/2} \pm i\sqrt{1-p/2})$.*

Lemma 5.20. *For any $0 < p < 1$ we have the following conclusions for each $p_0 \in E$ for the generating function associated to the unitary matrix $U = B(p)$.*

1. *The residue form η has leading degree $\alpha > d/2$ at p_0.*

2. *The cone $\mathcal{V}_{p_0}$ is projectively smooth and $\mathbf{r}$ is not in the normal cone to $\mathcal{V}$ at p_0.*

Proof of Lemma 5.19: The proof of Lemma 5.19 is similar to the corresponding proofs in the two previous examples, so we give only a sketch. Computing H from (5.2) and the subsequent formula yields

$$\begin{aligned} H &= 2xy(z^4+1) - (x+y+xy^2+x^2y)(z^3+z)\sqrt{2p} + (4pxy+x^2+x^2y^2+1+y^2)z^2 \\ &= xyz^2 \cdot [4p+ \\ & \quad 2(z^2+z^{-2}) - \left((x+x^{-1})+(y+y^{-1})\right)(z+z^{-1})\sqrt{2p} + (x+x^{-1})(y+y^{-1})\Big] , \end{aligned} \tag{5.24}$$

Treating p as a parameter and computing a Gröbner basis of $\{H, H_x, H_y, H_z\}$ with term order $\texttt{plex}(x, y, z)$ one obtains $\{x^3 - x, y - x, z(x^2 - 1), z^2 - 2x\sqrt{p}z + 2x^2\}$. Removing the extraneous roots when one of x, y or z vanishes, what remains is $\pm(1, 1, z)$ where z solves $z^2 - 2\sqrt{p}z + 2 = 0$. $\square$

Proof of Lemma 5.20: Condition (1) follows from the fact that for each $p_0 \in E$, the numerator $G^{(p)}(x, y, z)$ vanishes as well as the denominator $H^{(p)}$ which only vanishes to order 1. To prove (2), we compute the local geometry of $\{H = 0\}$ near the four points found in the previous lemma. We will do this for the points with positive $(x, y) = (1, 1)$; the case $(x, y) = (-1, -1)$ is similar. Substituting $x = 1 + u, y = 1 + v, z = z_0 + w$ into H and then reducing modulo $z_0^2 - 2\sqrt{p}z_0 + 2$, we find that the leading homogeneous term in the variables $\{u, v, w\}$ is $4[\sqrt{p}(1-p)(u^2+v^2)-(2-p)w^2]$. For $0 < p < 1$, this is the cone over a nondegenerate ellipse and therefore smooth. The dual cone is the set of (r, s, t) with $r^2 + s^2 = \frac{2-p}{(1-p)\sqrt{p}}t^2$. The minimum value of $\frac{2-p}{(1-p)\sqrt{p}}$ on $[0, 1]$ is greater than 4, while the vectors (r, s, t) inside the image of the Gauss map all have $r^2 + s^2 < 4t^2$, whence $\mathbf{r}$ is never in the normal cone to $\mathcal{V}$ at p_0. $\square$

Beginning with (5.25), we see that $(x, y, z) \in \mathcal{V}_1 \iff$

$$2\cos^2\gamma - (\cos\alpha + \cos\beta)\sqrt{2p}\cos\gamma + \cos\alpha\cos\beta + p - 1 = 0\,. \tag{5.25}$$

Thus for given α and β, the four values of γ are given explicitly by

$$\gamma = \pm\arccos\left[\frac{(\cos\alpha + \cos\beta)\sqrt{2p} \pm \sqrt{2p\,(\cos\alpha + \cos\beta)^2 - 8\cos\alpha\cos\beta - 8p + 8}}{4}\right]\,. \tag{5.26}$$

We then differentiate 5.25 with respect to α and β to obtain the partial derivatives

$$\frac{\partial\gamma}{\partial\alpha} = \frac{\sin\alpha}{\sin\gamma}\cdot\frac{\cos\beta - \cos\gamma\sqrt{2p}}{(\cos\alpha + \cos\beta)\sqrt{2p} - 4\cos\gamma}$$

and

$$\frac{\partial\gamma}{\partial\beta} = \frac{\sin\beta}{\sin\gamma}\cdot\frac{\cos\alpha - \cos\gamma\sqrt{2p}}{(\cos\alpha + \cos\beta)\sqrt{2p} - 4\cos\gamma}\,.$$

Remark. The fact that we can solve explicitly for γ with this family allows us to more clearly depict the connection between curvature and asymptotics. Using Proposition 3.2 and (5.26), we let Maple evaluate ∇ as well as

$$\mathcal{H} = \begin{bmatrix} \frac{\partial^2 \gamma}{\partial \alpha^2} & \frac{\partial^2 \gamma}{\partial \alpha \partial \beta} \\ \frac{\partial^2 \gamma}{\partial \beta \partial \alpha} & \frac{\partial^2 \gamma}{\partial \alpha^2} \end{bmatrix}$$

We then plot $\mathcal{K}$ against $-\frac{\partial \gamma}{\partial \alpha}$ and $-\frac{\partial \gamma}{\partial \beta}$ as (α, β) varies over the two-dimensional torus.

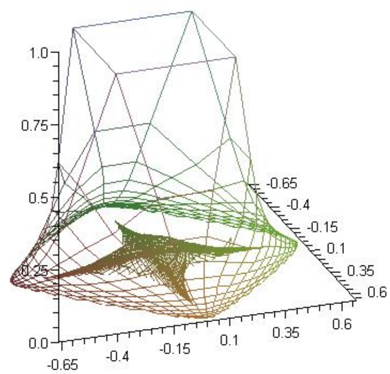

Figure 14: A graph of curvature versus direction for the $B(1/2)$ walk

In the above picture we see the expected cross within a diamond region where curvature is low, though the view is obstructed by regions of higher curvature.

To remedy this problem we restrict our view of the $\mathcal{K}$ axis to focus on the smallest values of $\mathcal{K}$ which in turn contribute to the largest probabilities. The resulting picture thus predicts the regions that will appear darkest in the probability profile.

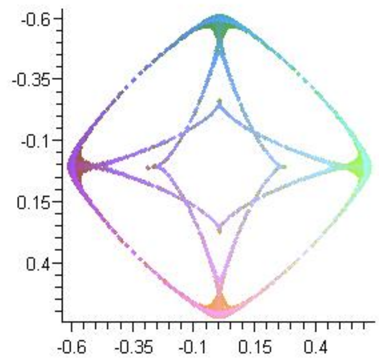

Figure 15: A graph of the areas of lowest curvature and hence highest probabilities for the $B(1/2)$ walk

5.4 Resultants for boundary of region of subexponential decay

Our goal is to determine for which $\hat{\mathbf{r}}$ it is the case that $\mathcal{K}$ vanishes. For $U = B(1/2)$ our result is

Theorem 5.21. *For the Quantum Random Walk with unitary coin flip $U = B(1/2)$, the curvature of the variety $\mathcal{V}_1$ vanishes at some $\mathbf{z} \in \Xi(u, v)$ if and only if $(u, v) = (k_1/t, k_2/t)$ is a zero of the polynomial P_1 and satisfies $|u| + |v| < 3/4$ where*

$P_1(u, v) = 1 + 14u^2 - 3126u^4 + 97752u^6 - 1445289u^8 + 12200622u^{10} - 64150356u^{12}+$

$220161216u^{14} - 504431361u^{16} + 774608490u^{18} - 785130582u^{20} + 502978728u^{22}-$

$184298359u^{24} + 29412250u^{26} + 14v^2 - 1284u^2v^2 - 113016u^4v^2 + 5220612u^6v^2-$

$96417162u^8v^2 + 924427224u^{10}v^2 - 4865103360u^{12}v^2 + 14947388808u^{14}v^2 - 27714317286u^{16}v^2+$

$30923414124u^{18}v^2 - 19802256648u^{20}v^2 + 6399721524u^{22}v^2 - 721963550u^{24}v^2 - 3126v^4-$

$113016u^2v^4 + 7942218u^4v^4 - 68684580u^6v^4 - 666538860u^8v^4 + 15034322304u^{10}v^4-$

$86727881244u^{12}v^4 + 226469888328u^{14}v^4 - 296573996958u^{16}v^4 + 183616180440u^{18}v^4-$

$32546593518u^{20}v^4 - 8997506820u^{22}v^4 + 97752v^6 + 5220612u^2v^6 - 68684580u^4v^6+$

$3243820496u^6v^6 - 25244548160u^8v^6 + 59768577720u^{10}v^6 - 147067477144u^{12}v^6+$

$458758743568u^{14}v^6 - 749675452344u^{16}v^6 + 435217945700u^{18}v^6 - 16479111716u^{20}v^6-$

$1445289v^8 - 96417162u^2v^8 - 666538860u^4v^8 - 25244548160u^6v^8 + 194515866042u^8v^8-$

$421026680628u^{10}v^8 + 611623295476u^{12}v^8 - 331561483632u^{14}v^8 + 7820601831u^{16}v^8+$

$72391117294u^{18}v^8 + 12200622v^{10} + 924427224u^2v^{10} + 15034322304u^4v^{10} + 59768577720u^6v^{10}-$

$421026680628u^8v^{10} + 421043188488u^{10}v^{10} - 1131276050256u^{12}v^{10} - 196657371288u^{14}v^{10}+$

$151002519894u^{16}v^{10} - 64150356v^{12} - 4865103360u^2v^{12} - 86727881244u^4v^{12}-$

$147067477144u^6v^{12} + 611623295476u^8v^{12} - 1131276050256u^{10}v^{12} + 586397171964u^{12}v^{12}-$

$231584205720u^{14}v^{12} + 220161216v^{14} + 14947388808u^2v^{14} + 226469888328u^4v^{14}+$

$458758743568u^6v^{14} - 331561483632u^8v^{14} - 196657371288u^{10}v^{14} - 231584205720u^{12}v^{14}-$

$504431361v^{16} - 27714317286u^2v^{16} - 296573996958u^4v^{16} - 749675452344u^6v^{16}+$

$7820601831u^8v^{16} + 151002519894u^{10}v^{16} + 774608490v^{18} + 30923414124u^2v^{18} +$

$183616180440u^4v^{18} + 435217945700u^6v^{18} + 72391117294u^8v^{18} - 785130582v^{20} -$

$19802256648u^2v^{20} - 32546593518u^4v^{20} - 16479111716u^6v^{20} + 502978728v^{22} +$

$6399721524u^2v^{22} - 8997506820u^4v^{22} - 184298359v^{24} - 721963550u^2v^{24} + 29412250v^{26}.$

Before proving the theorem, we verify the importance of $P_1(u,v)$ by comparing the points of vanishing of P_1 to the probability profile for the walk below.

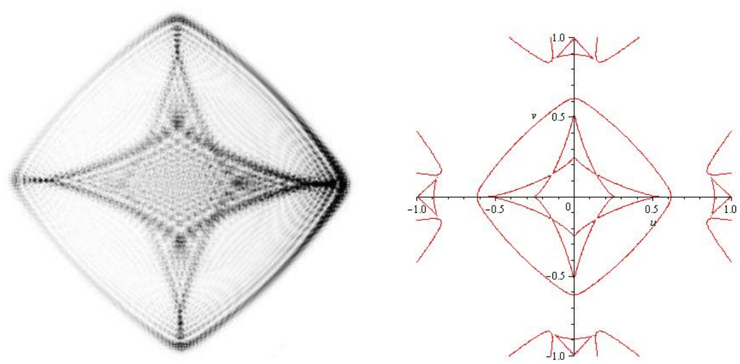

Figure 16: The probability profile for the $B(1/2)$ walk alongside the graph of $P_1(u,v) = 0$

PROOF:

From Theorem 5.11 and the definition of $\mathbf{W}(\hat{\mathbf{r}})$, $\mathbf{z} \in \mathcal{V}_1$ contributes to asymptotics in the direction $\hat{\mathbf{r}}$ if and only if $H(\mathbf{z}) = 0$ and $\nabla_{\log} H(\mathbf{z}) \parallel \hat{\mathbf{r}}$. Letting $u = k_1/t$ and $v = k_2/t$ we see $\mathbf{z} \in \mathbf{W}(\hat{\mathbf{r}})$ if and only if $H(\mathbf{z}) = K_1(\mathbf{z}) = K_2(\mathbf{z}) = 0$, where $K_1 := uzH_z - xH_x$ and $K_2 := vzH_z - yH_y$. Lemma 5.22 gives a final polynomial whose vanishing indicates that curvature vanishes as well.

Lemma 5.22. *Gaussian curvature vanishes at $\mathbf{z} \in \mathcal{V}_1$ if and only if $L(\mathbf{z}) = 0$ with*

$$L(x, y, z) := \frac{Q(x, z)Q(y, z) - R(x, y, z)^2}{(zH_z)^2}$$

with the polynomial Q in two variables defined as in the statement of Theorem 2.7 and $R(x, y, z)$ defined as

$$R(x, y, z) := xyz\left(zH_z(H_{xy}H_z - H_xH_{yz} - H_yH_{xz}) + H_xH_yH_z + zH_xH_yH_{zz}\right).$$

PROOF OF LEMMA 5.22: From Proposition 3.2, $\mathcal{K} = 0 \iff \mathcal{H} = 0$. From the proof of Corollary 2.9, $\mathcal{H} = 0 \iff L(x, y, z) = 0$. □

We now need only determine when $K_1 = K_2 = L = 0$ on $\mathcal{V}_1$ with $U = B(1/2)$ to prove Theorem 5.21. For $U = B(1/2)$ we define $H := H_B = -2xy \det(I - zMB(1/2))$ to clear denominators. The multiplication by $-2xy$ does not affect the torality property as $H = 0 \iff \det(I - zMB(1/2)) = 0$ for $x, y \in T_1$. We omit the value of L (determined using Lemma 5.22) and have:

$$H = -2xy + zx + xzy^2 - 2xz^2y + zy - z^2 - z^2y^2 + z^3y + zx^2y - z^2x^2 - z^2x^2y^2 + z^3x^2y + z^3x + z^3xy^2 - 2z^4xy$$

$$K_1 = uz(x + xy^2 - 4zxy + y - 2z - 2zy^2 + 3z^2y + x^2y - 2zx^2 - 2zx^2y^2 + 3z^2x^2y + 3z^2x + 3z^2y^2x - 8z^3yx) - x(-2y + z + zy^2 - 2z^2y + 2zxy - 2z^2x - 2z^2y^2x + 2z^3yx + z^3 + z^3y^2 - 2z^4y)$$

$$K_2 = vz(x + xy^2 - 4zxy + y - 2z - 2zy^2 + 3z^2y + x^2y - 2zx^2 - 2zx^2y^2 + 3z^2x^2y + 3z^2x + 3z^2y^2x - 8z^3yx) - y(-2x + 2zxy - 2z^2x + z - 2z^2y + z^3 + zx^2 - 2z^2x^2y + z^3x^2 + 2z^3yx - 2z^4x)$$

We then determine for which u and v we have $H = K_1 = K_2 = L = 0$ by eliminating each of x, y, and z, one at a time, using resultants. We streamline this process by renaming these polynomials with $p_1 := H$, $p_2 := L$, $p_3 := K_1$ and $p_4 := K_2$. We eliminate x by defining $res_{12} := Res(p_1, p_2, x)$, $res_{13} := Res(p_1, p_3, x)$, and $res_{14} := Res(p_1, p_4, x)$. We then omit repeated factors from each of these polynomials, effectively dividing them by $z^6y^2(zy-1)^2(z-y)^2(4z^{10} - 4z^{14}y^6 - 12z^{11}y^7 - 4z^2y^2 + 40z^{13}y^3 + 40z^{13}y^5 - 16z^{14}y^4 - 12z^{12}y^6 + z^4 - 16z^2y^4 + 40z^3y^3 + z^{12}y^8 - 12z^4y^2 - 12z^5y - 118z^4y^4 + 108z^5y^3 - 28z^6y^2 + 4z^6 + 4y^4 - 12z^{12}y^2 + 40z^3y^5 - 12z^4y^6 + 108z^5y^5 - 184z^6y^4 + 4z^7y + 132z^7y^3 - 28z^6y^6 + 132z^7y^5 + 4z^{16}y^4 - 40z^8y^2 - 196z^8y^4 + 132z^9y^3 - 4z^2y^6 - 12z^{11}y - 4z^{14}y^2 - 12z^5y^7 + z^4y^8 + 4z^{10}y^8 + 4z^9y - 28z^{10}y^2 - 40z^8y^6 + 132z^9y^5 - 184z^{10}y^4 + 108z^{11}y^3 - 28z^{10}y^6 + 108z^{11}y^5 - 118z^{12}y^4 + 4z^9y^7 + 4z^7y^7 - 6z^8y^8 + 4z^6y^8 - 6z^8 + z^{12}$, z and $z(2vy^2z^6 + z^5y - z^5y^3 - 4z^5vy - 4z^5vy^3 + z^4vy^4 + 6z^4vy^2 + z^4v - vz^2 - 6vz^2y^2 - z^2vy^4 + zy - zy^3 + 4vzy + 4zvy^3 - 2vy^2)$, respectively, and referring to the results as p_{12}, p_{13} and p_{14}, respectively. We have used H in each of these calculations to simplify our work, as H is the simplest of our four initial polynomials.

We now eliminate y by defining $res_{124} := Res(p_{12}, p_{14}, y)$ and $res_{134} := Res(p_{13}, p_{14}, y)$. Omitting repeated factors from these polynomials, we effectively divide by $16z^34(z-1)^2(z+1)^2(z^4 +$

$1)^6(z^2 - z + 1)^3(z^2 + z + 1)^3$ and $16z^{28}(z^2 + z + 1)^2(z^2 - z + 1)^2(z - 1)^4(z + 1)^4(z^4 + 1)^4$, respectively, and refer to the results as p_{124} and p_{134}, respectively. We then eliminate z by defining $res_{1234} = Res(p_{124}, p_{134}, z)$.

From the section on resultants, we know that res_{1234} may contain extraneous factors. One way to remove many of these is by exploiting the known symmetry of $\Omega := \{(u, v) | \exists \mathbf{z} \in \mathcal{V} \text{ with } K_1(\mathbf{z}) = K_2(\mathbf{z}) = L(\mathbf{z}) = 0\}$. (Note: this definition uses $\mathcal{V}$ instead of $\mathcal{V}_1$.) As a result of the work in the prior two sections we know that Ω is symmetric with respect to the u and v axes, as well as the line $u = v$. Thus we may eliminate any factor of res_{1234} whose image under these symmetries is not also a factor. Doing so yields the irreducible polynomial $P_1(u, v)$. As the set Ω is algebraic and known to be a subset of the zero set of an irreducible polynomial P_1, we see that Ω is the zero set of P_1.

Let $\Omega_0 \subset \Omega$ denote the subset of those (u, v) for which at least one $(x, y, z) \in \Xi(u, v)$ with $L(x, y, z) = 0$ lies on the unit torus. It remains to check that Ω_0 consists of those $(u, v) \in \Omega$ with $|u| + |v| < 3/4$.

The locus of points in $\mathcal{V}$ at which L vanishes is a complex algebraic curve γ given by the simultaneous vanishing of H and L. It is nonsingular as long as ∇H and ∇L are not parallel, in which case its tangent vector is parallel to $\nabla H \times \nabla L$. Let $\rho := xH_x/(zH_z)$ and $\sigma := yH_y/(zH_z)$ be the coordinates of the map **dir** under the identification of $\mathbb{CP}^2$ with $\{(u, v, 1) : u, v \in \mathbb{C}\}$. The image of γ under **dir** (and this identification) is a nonsingular curve in the plane, provided that γ is nonsingular and either $d\rho$ of $d\sigma$ 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 $\det M_\rho$ are ∇H, ∇L, $\nabla \rho$ and the columns of M_σ are ∇H, ∇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. By Lemma 2.2 the tangent vector to γ at (x_0, y_0, z_0) in logarithmic coordinates is real; therefore the image of γ near (x_0, y_0, z_0) is a nonsingular real curve. Removing singular points from the zero set of P_1 leaves a union $\mathcal{U}$ of connected components, each of which therefore lies in Ω_0 or is disjoint from Ω_0. The proof of the theorem is now reduced to listing the components, checking that none crosses the boundary $|u| + |v| = 3/4$, and checking $\Xi(u, v)$ for a single point (u, v) on each component. (Note: any component intersecting $\{|u| + |v| > 1\}$ need not be checked as we know the coefficients to be identically zero here.) □

We state an analogous result for $U = S(1/2)$. While we again demonstrate the result pictorially, we omit the proof as it is completely analogous to that of Theorem 5.21.

Theorem 5.23. *For the Quantum Random Walk with unitary coin flip $U = S(1/2)$, the curvature of the variety $\mathcal{V}_1$ vanishes at some $\mathbf{z} \in \Xi(u, v)$ if and only if $(u, v) = (k_1/t, k_2/t)$ is a zero of the polynomial P_2 and satisfies $|u| + |v| \leq 2/3$ where*

$$\begin{aligned}
P_2(u,v) = {} & 132019u^{16} + 2763072v^2u^{20} - 513216v^2u^{22} - 6505200v^2u^{18} + 256v^2u^2 + 8790436v^2u^{16} \\
& -10639416v^{10}u^8 + 39759700v^{12}u^4 - 12711677v^{10}u^4 + 4140257v^{12}u^2 - 513216v^{22}u^2 - \\
& 7492584v^2u^{14} + 2503464v^{10}u^6 - 62208v^{22} + 16v^6 + 141048u^{20} + 8790436v^{16}u^2 + 2763072v^{20}u^2 - \\
& 6505200v^{18}u^2 - 40374720v^{18}u^6 + 64689624v^{16}u^4 - 33614784v^{18}u^4 + 14725472v^{10}u^{10} + \\
& 121508208v^{16}u^8 - 1543v^{10} - 23060v^2u^6 + 100227200v^{10}u^{12} + 7363872v^{20}u^4 - 176524u^{18} + \\
& 121508208v^8u^{16} - 197271552v^8u^{14} - 13374107v^8u^6 + 1647627v^8u^4 + 18664050v^8u^8 - \\
& 227481984v^{10}u^{14} - 19343v^4u^4 + 279234496v^{12}u^{12} - 67173440v^{14}u^4 - 7492584v^{14}u^2 + \\
& 4140257v^2u^{12} + 291173v^2u^8 - 1449662v^2u^{10} + 7363872v^4u^{20} - 227481984v^{14}u^{10} + 132019v^{16} - \\
& 197271552v^{14}u^8 - 59209u^{14} - 1449662v^{10}u^2 + 100227200v^{12}u^{10} - 1543u^{10} - 153035200v^{14}u^6 - \\
& 13374107v^6u^8 + 3183044v^6u^6 + 39759700v^4u^{12} - 176524v^{18} + 72718v^6u^4 + 1647627v^4u^8 - \\
& 62208u^{22} + 141048v^{20} - 1472v^4u^2 + 11664v^{24} - 33614784v^4u^{18} + 128187648v^{16}u^6 - 1472v^2u^4 - \\
& 67173440v^4u^{14} + 291173v^8u^2 + 64689624v^4u^{16} - 10639416v^8u^{10} - 59209v^{14} + 72718v^4u^6 + \\
& 92321584v^8u^{12} - 56u^8 + 92321584v^{12}u^8 - 153035200v^6u^{14} - 23060v^6u^2 + 128187648v^6u^{16} - \\
& 40374720v^6u^{18} + 72282208v^{12}u^6 + 14793u^{12} + 11664u^{24} + 14793v^{12} + 16u^6 + 2503464v^6u^{10} - \\
& 56v^8 - 12711677v^4u^{10} + 72282208v^6u^{12}.
\end{aligned}$$

□

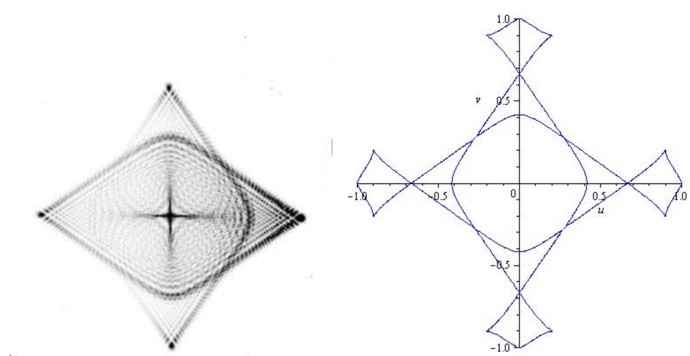

Figure 17: The probability profile for the $S(1/2)$ walk alongside the graph of $P_2(u,v)=0$

5.5 Asymptotics for the Hadamard Walk on $\mathbb{Z}^2$

The walk based on the Hadamard matrix U_{Had} mentioned in Section 5.1 distinguishes itself from the other walks on $\mathbb{Z}^2$ in several ways. Its high level of symmetry greatly simplifies its study, which is likely why it is the only walk on $\mathbb{Z}^2$ we are aware of to be studied using methods alternative to our own. This symmetry allows us to surpass a result like Theorems 5.11, 5.16 and 5.18 to determine a general asymptotic formula holding for any direction in a compact subset of the interior of the Gauss map image, with the exception of those directions in a neighborhood of the origin. (Note: while the origin is in the image of the Gauss map, asymptotics for the origin have contribution by points of vanishing curvature. In this case, as with the three-chirality walk on the line, the result is a probability of finding the particle at the origin which does not go to 0 with time.)

In our discussion of this walk, we again denote $\mathbf{z}$ as (x, y, z), and $\mathbf{r}$ as (r, s, t). When $|x| = |y| = |z| = 1$, we let $x = e^{i\alpha}$, $y = e^{i\beta}$ and $z = e^{i\gamma}$. In addition we denote the relative direction coordinates r/t and s/t as λ and μ, respectively. As explained in Section 5.3, with this notation the critical point equations become $H = 0, \lambda = -\partial\gamma/\partial\alpha$ and $\mu = -\partial\gamma/\partial\beta$. Lastly, we denote the chiralities R, L, U and D, respectively, with a particle in the R chirality being sent one lattice point to the right with each time step, and so forth.

While we can apply Theorem 5.9 as $|E| = 2$, we instead apply a slight variation to account for the decomposition of $\mathcal{V}_1$ into two very different components. One of these components consists of the two flat planes $z = \pm 1$, $|x| = |y| = 1$ while the other supports the asymptotics we seek for $\hat{\mathbf{r}} \in \mathcal{G}'$ below. For $z = \pm 1$ and either x or y not equal to z, $\mathbf{z}$ contributes toward asymptotics in the direction $\lambda = \mu = 0$, though as curvature vanishes at these points, we cannot determine asymptotics in this direction with a theorem like 5.9. In theory one could use the Hautus-Klarner-Furstenberg method for diagonal extraction to determine $\lim_{t\to\infty} p(0,0)$ as in the proof of Theorem 4.18, however as one iterates the use of this method, it becomes cumbersome and even intractable.

5.5.1 Statement of Results

Theorem 5.24. *For the Quantum Random Walk with unitary matrix $U = U_{\text{Had}}$, let $\mathcal{G}'$ be a compact subset of the interior of the punctured disk $\{(\lambda, \mu) : 0 < \lambda^2 + \mu^2 < 1/2\}$ where $\lambda = r/t$ and $\mu = s/t$. Let $p_{\mathbf{r}} := p_{r,s,t}$ denote the probability to be at position (r, s) at time t. Then as $|\mathbf{r}| \to \infty$, uniformly over $\hat{\mathbf{r}} \in \mathcal{G}'$, there are phase functions $\rho_{\xi_0,\xi}(r, s, t)$ defined in Equation (5.45), such that*

$$p_{R,R}(r,s,t) \sim \frac{1}{\pi^2 t^2} \cdot \frac{(\lambda+\mu+1)(\lambda-\mu+1)}{(\lambda+\mu-1)(\lambda-\mu-1)} \cos^2(\rho_{R,R}(r,s,t)) \tag{5.27}$$

$$p_{R,L}(r,s,t) \sim \frac{1}{\pi^2 t^2} \cos^2(\rho_{R,L}(r,s,t)) \tag{5.28}$$

$$p_{R,U}(r,s,t) \sim \frac{1}{\pi^2 t^2} \cdot \frac{\lambda+\mu+1}{\lambda+\mu-1} \cos^2(\rho_{R,U}(r,s,t)) \tag{5.29}$$

$$p_{R,D}(r,s,t) \sim \frac{1}{\pi^2 t^2} \cdot \frac{\lambda-\mu+1}{\lambda-\mu-1} \cos^2(\rho_{R,D}(r,s,t)) \tag{5.30}$$

$$p_{L,L}(r,s,t) \sim \frac{1}{\pi^2 t^2} \cdot \frac{(\lambda+\mu-1)(\lambda-\mu-1)}{(\lambda+\mu+1)(\lambda-\mu+1)} \cos^2(\rho_{L,L}(r,s,t)) \tag{5.31}$$

$$p_{L,U}(r,s,t) \sim \frac{1}{\pi^2 t^2} \cdot \frac{\lambda-\mu-1}{\lambda-\mu+1} \cos^2(\rho_{L,U}(r,s,t)) \tag{5.32}$$

$$p_{L,D}(r,s,t) \sim \frac{1}{\pi^2 t^2} \cdot \frac{\lambda+\mu-1}{\lambda+\mu+1} \cos^2(\rho_{L,D}(r,s,t)) \tag{5.33}$$

$$p_{U,U}(r,s,t) \sim \frac{1}{\pi^2 t^2} \cdot \frac{(\lambda+\mu+1)(\lambda-\mu-1)}{(\lambda+\mu-1)(\lambda-\mu+1)} \cos^2(\rho_{U,U}(r,s,t)) \tag{5.34}$$

$$p_{U,D}(r,s,t) \sim \frac{1}{\pi^2 t^2} \cos^2(\rho_{U,D}(r,s,t)) \tag{5.35}$$

$$p_{D,D}(r,s,t) \sim \frac{1}{\pi^2 t^2} \cdot \frac{(\lambda+\mu-1)(\lambda-\mu+1)}{(\lambda+\mu+1)(\lambda-\mu-1)} \cos^2(\rho_{D,D}(r,s,t)) \tag{5.36}$$

and for all pairs of chiralities ξ_0, ξ, $p_{\xi_0,\xi} \cos^{-2}(\rho_{\xi_0,\xi}) = p_{\xi,\xi_0} \cos^{-2}(\rho_{\xi,\xi_0})$. When $\lambda^2 + \mu^2 > 1/2$ then for every integer $N > 0$ there is a $C > 0$ such that $\Pr(\mathbf{r}) \leq C|\mathbf{r}|^{-N}$ with C uniform as $\mathbf{r}$ ranges over a neighborhood $\mathcal{N}$ of $\mathbf{r}$ whose closure is disjoint from the closure of $\mathcal{G}'$.

We once more demonstrate our results pictorially, this time with a graph of the walk's actual probabilities versus the predicted upper envelope (calculated by dropping the $\cos^2$ term from the asymptotic prediction) for (ξ_0, ξ) equal to each of (U, U), (U, D), (U, R) and (U, L). With time $t = 100$, we use a shifted walk beginning at the point $(r, s) = (101, 101) \in \mathbb{Z}^2$. We note that as the prediction holds for (λ, μ) in a compact subset of $\mathcal{G}'$, it does not hold for $(\frac{r-101}{100})^2 + (\frac{s-101}{100})^2$ near

0 or 1/2.

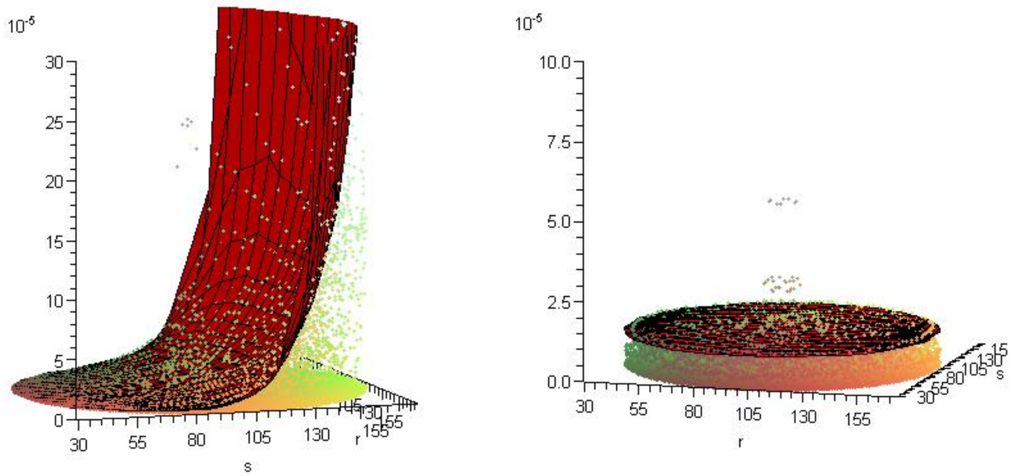

Figure 18: Time $t = 100$ probability values by location ($p_{U,U}$ on left and $p_{U,D}$ on right) for the Hadamard walk on $\mathbb{Z}^2$ and the asymptotic prediction of the upper envelope.

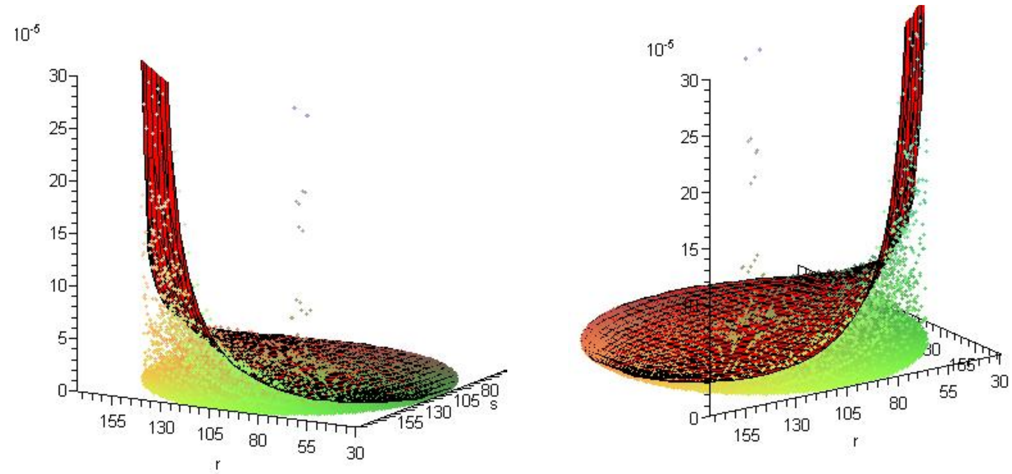

Figure 19: Time $t = 100$ probability values by location ($p_{U,R}$ on left and $p_{U,L}$ on right) for the Hadamard walk on $\mathbb{Z}^2$ and the asymptotic prediction of the upper envelope.

5.5.2 Proof of Theorem 5.24

We begin by letting $\hat{H} := xy \det (I - zM(x,y)U_{\text{Had}})$ where the xy suits to clear the denominator. Using the fact that $\cos(\alpha) = \frac{1}{2}(x+1/x)$ for x on the unit torus, we factor $\hat{H}$ as $\hat{H} = xyz(z-1)(z+1)(\cos(\alpha) + \cos(\beta) - 2\cos(\gamma))$. We can then write $\mathcal{V}_1 = C_1 \cup C_2$ where $C_1 = \{\mathbf{z} : |x| = |y| = |z| = 1,\ \cos(\alpha) + \cos(\beta) = 2\cos(\gamma)\}$ and $C_2 = \{\mathbf{z} : |x| = |y| = 1,\ z = \pm 1\}$. Determining a Gröbner Basis in Maple for the polynomials $\hat{H}$, $\hat{H}_x$, $\hat{H}_y$ and $\hat{H}_z$, results in the set $GB := \{-z + 3z^3 - 3z^5 + z^7, 3z + 2z^2y - 2y - 4z^3 + z^5, z^5 + 2z^2x - 4z^3 - 2x + 3z, x - 5z + y + 8z^3 - 3z^5 - 4yzx + xy^2 + x^2y\}$. While the first basis element factors to $z(z-1)^3(z+1)^3$, all the elements but the last vanish when $z = 1$. With this substitution, the final basis element becomes $x + y - 4yx + xy^2 + x^2y = 2xy(\cos(\alpha) + \cos(\beta) - 2)$ which vanishes on the unit torus precisely when $x = y = 1$. We similarly find that when $z = -1$, $\nabla\hat{H}$ vanishes if and only if $x = y = -1$. Thus $E = \{(1,1,1), (-1,-1,-1)\} = C_1 \cap C_2$.

Our first goal is to show that we can use the variety C_1 as if it were $\mathcal{V}_1$ and treat $(z-1)(z+1)$ as a locally smooth factor. This works so long as we only prescribe asymptotics for directions in the set $\pi \circ \mathfrak{n}(C_1) \setminus \pi \circ \mathfrak{n}(C_2)$ where the maps π and $\mathfrak{n}$ are those used in Equation (5.1). The composition of these is what we refer to as the Gauss map for the sake of simplicity, while in actuality, $\mathfrak{n}$ is the logarithmic Gauss map. We meet this goal with the following two lemmas.

Lemma 5.25. $\pi \circ \mathfrak{n}(C_1 \setminus E) = \{(\lambda, \mu) : 0 \leq \lambda^2 + \mu^2 < \frac{1}{2}\}$

Lemma 5.26. $\pi \circ \mathfrak{n}(C_2) = \{(0, 0)\}$

Proof of Lemma 5.26: If $\mathbf{z} \in C_2 \setminus E$, then each of $\hat{H}$, $\hat{H}_x$, and $\hat{H}_y$ vanish due to the $(z-1)(z+1)$ factor in $\hat{H}$. As $\mathbf{z} \notin E$, it must be that $\hat{H}_z$ does not vanish. So $(x\hat{H}_x, y\hat{H}_y, z\hat{H}_z)$ is parallel to the vector $(0, 0, 1)$. While $(x\hat{H}_x, y\hat{H}_y, z\hat{H}_z)$ vanishes at $\mathbf{z} = \pm(1, 1, 1)$, the limit of $(x\hat{H}_x, y\hat{H}_y, z\hat{H}_z)$ as $\mathbf{z} \to \pm(1, 1, 1)$ in C_2 is a vector parallel to $(0, 0, 1)$. Thus the component C_2 of $\mathcal{V}_1$ can only affect asymptotics in a neighborhood of the direction $(\lambda, \mu) = (0, 0)$. Furthermore, as all $\mathbf{z} \in C_2$ have the same normal, $\mathcal{K} \equiv 0$ on this component, so Theorem 5.9 will not prescribe asymptotics for the direction $(\lambda, \mu) = (0, 0)$. □

Proof of Lemma 5.25: We recall that $\mathbf{z} \in C_1$ precisely when

$$\cos(\gamma) = \frac{\cos(\alpha) + \cos(\beta)}{2}. \tag{5.37}$$

Differentiating this equation implicitly with respect to each of α and β gives the remaining two critical point equations:

$$-\lambda = \frac{\partial \gamma}{\partial \alpha} = \frac{\sin(\alpha)}{2\sin(\gamma)} \tag{5.38}$$

$$-\mu = \frac{\partial \gamma}{\partial \beta} = \frac{\sin(\beta)}{2\sin(\gamma)} \tag{5.39}$$

Squaring, then summing these formulas results in the equation:

$$\lambda^2 + \mu^2 = \frac{2 - (\cos^2(\alpha) + \cos^2(\beta))}{4(1 - \cos^2(\gamma))}.$$

Substituting the value of $\cos(\gamma)$ given by Equation (5.37) results in the equation:

$$\lambda^2 + \mu^2 = \frac{2 - (\cos^2(\alpha) + \cos^2(\beta))}{4 - (\cos^2(\alpha) + 2\cos(\alpha)\cos(\beta) + \cos^2(\beta))}. \tag{5.40}$$

Some simple calculus then shows that $\lambda^2 + \mu^2 \leq 1/2$ for $\mathbf{z} \in C_1$. This shows that the image of the Gauss map is contained within this circle.

Before considering the reverse inclusion, we note the significance of excluding E when taking the image of the Gauss map. Taking E as a subset of C_1 we find that $\pi \circ \mathfrak{n}$ is undefined at E. We find this by observing that

$$\lim_{\alpha=0,\beta\to 0,\gamma=\arccos(\frac{\cos(\alpha)+\cos(\beta)}{2})} \frac{\sin(\alpha)}{2\sin(\gamma)} = 0$$

while

$$\lim_{\alpha=\beta=\gamma\to 0} \frac{\sin(\alpha)}{2\sin(\gamma)} = \frac{1}{2}$$

Thus $\frac{\sin(\alpha)}{2\sin(\gamma)}$ is undefined when $\mathbf{z} = (1,1,1)$. Similarly $\frac{\sin(\alpha)}{2\sin(\gamma)}$ is undefined at $(-1,-1,-1)$ as well. This guarantees that E does not contribute toward asymptotics in the directions such that $0 < \lambda^2 + \mu^2 < 1/2$, as required by Theorem 5.9.

For the reverse inclusion, we will see when we solve the critical point equations that $\exists \mathbf{z}$ such that $\mathbf{dir}\,(\mathbf{z})\,||\,(\lambda t, \mu t, t)$ precisely when $0 \leq \lambda^2 + \mu^2 < 1/2$. $\square$

Thus we can treat C_1 as if it were $\mathcal{V}_1$, treat the $(z-1)(z+1) = 2iz\sin(\gamma)$ term as a locally smooth factor (which will appear in the denominator of the asymptotic formula) and get an asymptotic formula that holds for (λ, μ) in any compact subset $\mathcal{G}' \subset \{(\lambda,\mu) : 0 < \lambda^2 + \mu^2 < \frac{1}{2}\}$.

Our next task is to solve the critical point equations, before substituting the result into the expression

$$a_{\mathbf{r}} \sim \frac{1}{2\pi|\mathbf{r}|} \sum_{\mathbf{z}\in\mathbf{W}} \mathbf{z}^{-\mathbf{r}} \frac{G(\mathbf{z})}{|\nabla_{\log} H(\mathbf{z})|} \frac{1}{2iz\sin(\gamma)\sqrt{|\mathcal{K}(\mathbf{z})|}} e^{-i\pi\tau(\mathbf{z})/4}.$$

Again the eventual goal is an expression for $p_{\mathbf{r}} = |a_{\mathbf{r}}|^2$, simplifying our calculations. In the case of the Hadamard walk on $\mathbb{Z}^2$, the critical point equations are much more easily manipulated in terms of α, β and γ, rather than x, y, and z. As a result Maple's Groebner package has difficulty doing the work for us (as it had done for walks on $\mathbb{Z}$) but we can make progress by hand, while relying on Maple for simplification.

Now substituting from Equation (5.38) into Equation (5.39) we get $\sin(\beta) = \frac{\mu}{\lambda}\sin(\alpha)$. If we let $a = \sin^2(\alpha)$, then squaring the prior equation results in $\sin^2(\beta) = \frac{\mu^2}{\lambda^2}a$, while squaring Equation (5.38) we get $\sin^2(\gamma) = \frac{a}{4\lambda^2}$. Substituting the new expressions for $\sin^2(\beta)$ and $\sin^2(\gamma)$ into a squared Equation (5.37) results in the equation:

$$4(1 - \frac{a}{4\lambda^2}) = 1 - a \pm 2\sqrt{(1-a)(1 - \frac{\mu^2}{\lambda^2}a} + 1 - \frac{\mu^2}{\lambda^2}a$$

Solving for $a = \sin^2(\alpha)$, we get

$$\sin^2(\alpha) = 0, \ \frac{4\lambda^2 B(\lambda,\mu)}{A(\lambda,\mu)}$$

where $A(\lambda,\mu) := (\lambda+\mu+1)(\lambda+\mu-1)(\lambda-\mu+1)(\lambda-\mu-1)$ and $B(\lambda,\mu) := 1 - 2(\lambda^2+\mu^2)$. We note first that the solution $\sin(\alpha) = 0$ for all (λ,μ) is degenerate as it corresponds to the points $\mathbf{z} \in E$ where $\nabla\hat{H}$ vanishes. It will also be of interest that for $B \geq 0$, A only vanishes at the points $(\lambda,\mu) = (\pm\frac{1}{2}, \pm\frac{1}{2})$.

Combining the solution for $\sin^2(\alpha)$ with our earlier observations, we get the complete list of possible sines and then cosines for the critical points:

$$(\sin(\alpha), \sin(\beta), \sin(\gamma)) = \pm\left(2\sqrt{\frac{\lambda^2 B}{A}}, 2\frac{\mu}{\lambda}\sqrt{\frac{\lambda^2 B}{A}}, -\frac{1}{\lambda}\sqrt{\frac{\lambda^2 B}{A}}\right)$$

$$(\cos(\alpha), \cos(\beta), \cos(\gamma)) = \frac{1}{\sqrt{A}}\left(\pm(3\lambda^2+\mu^2-1), \pm(\lambda^2+3\mu^2-1), \pm(\lambda^2-\mu^2)\right)$$

Substitution of these possible solutions into Equation (5.37) reveals that the nonextraneous solutions are

$$(\cos(\alpha), \cos(\beta), \cos(\gamma)) = \pm\frac{1}{\sqrt{A}}\left(3\lambda^2+\mu^2-1, -(\lambda^2+3\mu^2-1), \lambda^2-\mu^2\right) \tag{5.41}$$

We thus get four contributing critical points for each direction, as each of the two triples of cosine values can correspond with either triple of sine values. We note that when $\lambda^2+\mu^2 = 1/2$, $\sqrt{A}$ becomes $2\lambda^2 - 1/2$ and $(\cos(\alpha), \cos(\beta), \cos(\gamma))$ becomes $\pm(1,1,1)$, corresponding to the points of E. As there are no other obstructions when $B \geq 0$, it is when $B > 0$ that $(\lambda,\mu) \in \pi \circ \mathfrak{n}(C_1 \setminus E)$. If we refer to one of the critical points as $\mathbf{z}_1 = (x_1, y_1, z_1)$, then the other critical points are

$(-x_1,-y_1,-z_1),(\overline{x_1},\overline{y_1},\overline{z_1})$ and $(-\overline{x_1},-\overline{y_1},-\overline{z_1})$. As a consequence, $e^{-i\pi\tau(\mathbf{z})/4}$ is equal for each of these critical points, so the expression for $p_{\mathbf{r}}$ becomes

$$p_{\mathbf{r}} \sim |\frac{1}{2\pi|\mathbf{r}|}\sum_{\mathbf{z}\in\mathbf{W}} \mathbf{z}^{-\mathbf{r}} \frac{G(\mathbf{z})}{|\nabla_{\log} H(\mathbf{z})|} \frac{1}{2iz\sin(\gamma)\sqrt{|\mathcal{K}(\mathbf{z})|}}|^2 \tag{5.42}$$

We now express each component of this formula in terms of λ, μ and t. As we have seen in Section 3.3, when $d = 2$,

$$\mathcal{K} = \frac{\frac{\partial^2\gamma}{\partial\alpha^2}\cdot\frac{\partial^2\gamma}{\partial\beta^2} - (\frac{\partial^2\gamma}{\partial\alpha\partial\beta})^2}{\left[1+(\frac{\partial\gamma}{\partial\alpha})^2+(\frac{\partial\gamma}{\partial\beta})^2\right]^2} \tag{5.43}$$

For each of Equation (5.38) and Equation (5.39), we take partial derivatives, then make substitutions for the values of λ and μ to get $\frac{\partial^2\gamma}{\partial\alpha^2} = -\lambda\cot(\alpha) - \lambda^2\cot(\gamma)$, $\frac{\partial^2\gamma}{\partial\beta^2} = -\mu\cot(\beta) - \mu^2\cot(\gamma)$ and $\frac{\partial^2\gamma}{\partial\alpha\partial\beta} = -\lambda\mu\cot(\gamma)$, so

$$\mathcal{K} = \frac{\lambda\mu(\cot(\alpha)\cot(\beta) + \lambda\cot(\beta)\cot(\gamma) + \mu\cot(\alpha)\cot(\gamma))}{(1+\lambda^2+\mu^2)^2}.$$

Substituting the values of the critical points, we find that for any of the four critical points:

$$\mathcal{K} = \frac{-A}{4(1+\lambda^2+\mu^2)^2}.$$

Also, $|\mathbf{r}| = \sqrt{r^2+s^2+t^2} = t\sqrt{\lambda^2+\mu^2+1}$ and $|\nabla_{\log} H(\mathbf{z})| = \sqrt{x^2H_x^2+y^2H_y^2+z^2H_z^2} = \epsilon z H_z\sqrt{\lambda^2+\mu^2+1}$ where ϵ is a unit ensuring that the represented norm is a positive real, and $H = \hat{H}/(z^2-1)$. A simple calculation shows that $zH_z \pmod{H} = 4ixyz\sin(\gamma)$. Combining this information, we get that

$$|\mathbf{r}|\cdot|\nabla_{\log} H(\mathbf{z})|\cdot\sqrt{\mathcal{K}} = -2\epsilon txyz\sin(\gamma)\sqrt{A}.$$

Now recalling that $\sin^2(\gamma) = B/A$ and substituting these results into Equation (5.42) we get

$$p_{\mathbf{r}} \sim |\sum_{\mathbf{z}\in\mathbf{W}} \mathbf{z}^{-\mathbf{r}} \frac{G(\mathbf{z})}{8\pi\epsilon txyz^2}\frac{\sqrt{A}}{B}|^2 \tag{5.44}$$

For the purpose of the following discussion we refer to the four $\mathbf{z}\in\mathbf{W}$ as $\mathbf{z}_1 = \mathbf{z}$, $\mathbf{z}_2 = -\mathbf{z}$, $\mathbf{z}_3 = \overline{\mathbf{z}}$, and $\mathbf{z}_4 = -\overline{\mathbf{z}}$. As G and xyz^2 are each homogeneous of even degree (we will see this for G shortly), then as a result of the conjugacy of the critical points, if we ignore the $\mathbf{z}^{-\mathbf{r}}$ terms, the first two summands have equal contribution to the sum (we denote this $c(\mathbf{r})$) while the second two summands each have complex conjugate contribution $\overline{c(\mathbf{r})}$. When $\lambda t + \mu t + t \in 2\mathbb{Z}$, $c(\mathbf{r})\mathbf{z}_1^{-\mathbf{r}} = c(\mathbf{r})\mathbf{z}_2^{-\mathbf{r}}$ and $\overline{c(\mathbf{r})}\mathbf{z}_3^{-\mathbf{r}} = \overline{c(\mathbf{r})}\mathbf{z}_4^{-\mathbf{r}} = \overline{c(\mathbf{r})\mathbf{z}_1^{-\mathbf{r}}}$. Thus the sum is $|2c(\mathbf{r})\mathbf{z}_1^{-\mathbf{r}} + 2\overline{c(\mathbf{r})\mathbf{z}_1^{-\mathbf{r}}}|^2 = |4\Re(c(\mathbf{r})\mathbf{z}_1^{-\mathbf{r}})|^2 = 16|c(\mathbf{r})|^2\cos^2(\text{Arg}(c(\mathbf{r})\mathbf{z}_1^{-\mathbf{r}})) = 16|\mathbf{z}_1^{-\mathbf{r}} \cdot \frac{G}{-8\pi\epsilon t x_1 y_1 z_1^2} \cdot \frac{\sqrt{A}}{B}|^2\cos^2(\rho) = |\frac{A}{4\pi^2 t^2 B^2}| \cdot |G|^2\cos^2(\rho)$. The definition of ρ is then

$$\rho_{\xi_0,\xi} = \text{Arg}\left(\mathbf{z}_1^{-\mathbf{r}} \frac{G_{\xi_0,\xi}(\mathbf{z}_1)}{8\pi\epsilon t x_1 y_1 z_1^2} \frac{\sqrt{A}}{B}\right). \tag{5.45}$$

When $\lambda t + \mu t + t \notin 2\mathbb{Z}$, the contributions from $\mathbf{z}_1$ and $\mathbf{z}_2$ will sum to 0, as will the contributions from $\mathbf{z}_3$ and $\mathbf{z}_4$. This is as we expect for any nearest neighbor walk on $\mathbb{Z}^2$, so we assume that $\lambda t + \mu t + t \in 2\mathbb{Z}$ going forward. Then if we let $\psi = p/\cos^2(\rho)$ represent the upper envelope of the probability distribution, we now have the formula

$$\psi_{\xi_0,\xi} \sim \frac{(\lambda+\mu+1)(\lambda+\mu-1)(\lambda-\mu+1)(\lambda-\mu-1)}{4\pi^2 t^2[1-2(\lambda^2+\mu^2)]^2} \cdot |G_{\xi_0,\xi}|^2 \tag{5.46}$$

It only remains to determine each value of $|G_{\xi_0,\xi}|$. Multiplying by $\hat{H}$ to clear denominators in the matrix $I - zMU_{\text{Had}}$ we get the matrix

$$\mathbf{G}(\mathbf{z}) = \begin{bmatrix} G_{R,R} & G_{R,L} & G_{R,U} & G_{R,D} \\ G_{L,R} & G_{L,L} & G_{L,U} & G_{L,D} \\ G_{U,R} & G_{U,L} & G_{U,U} & G_{U,D} \\ G_{D,R} & G_{D,L} & G_{D,U} & G_{D,D} \end{bmatrix}$$

where $G_{R,R} = 2yx - zx - xzy^2 - zy + z^3y$, $G_{R,L} = -z(y - z - zy^2 + z^2y)$, $G_{R,U} = (-z^2 + zx + zy - yx)zy$, $G_{R,D} = z(yzx - x - z^2y + z)$, $G_{L,R} = -x^2z(y - z - zy^2 + z^2y)$, $G_{L,L} = (z^3yx - yzx - zy^2 - z + 2y)x$, $G_{L,U} = -(z - y)(-1 + zx)yzx$, $G_{L,D} = -(zy - 1)(-1 + zx)zx$, $G_{U,R} = (z - y)(-z + x)zx$, $G_{U,L} = -(z - y)(-1 + zx)z$, $G_{U,U} = -zx^2y + z^3x - zx + 2yx - zy$, $G_{U,D} = (-z + x)z(-1 + zx)$, $G_{D,R} = xz(yzx - x - z^2y + z)y$, $G_{D,L} = -(zy - 1)z(-1 + zx)y$, $G_{D,U} = (-z + x)zy^2(-1 + zx)$, and $G_{D,D} = -(zx^2 - z^3yx + yzx - 2x + z)y$.

We observe that each entry of $\mathbf{G}(\mathbf{z})$ is homogeneous of even degree as promised. Now simplifying $|\mathbf{G}(\mathbf{z}_1)|^2$ by first writing each entry in terms of trigonometric functions of α, β and γ, we obtain

$$|G_{R,R}|^2 = 4|(\cos(\gamma) - \cos(\beta) - \sin^2(\gamma)\cos(\alpha) + \sin(\alpha)\sin(\gamma)\cos(\gamma))^2 + \tag{5.47}$$

$$(-\sin(\gamma) + \cos(\alpha)\sin(\gamma)\cos(\gamma) + \sin(\alpha)\sin^2(\gamma))^2| \tag{5.48}$$

$$|G_{R,L}|^2 = 4(\cos(\gamma) - \cos(\beta))^2 \tag{5.49}$$

$$|G_{R,U}|^2 = 4|(1 - \cos(\alpha)\cos(\gamma) - \sin(\alpha)\sin(\gamma))(1 - \cos(\beta)\cos(\gamma) - \sin(\beta)\sin(\gamma)) \tag{5.50}$$

$$|G_{R,D}|^2 = 4|(1 - \cos(\alpha)\cos(\gamma) - \sin(\alpha)\sin(\gamma))(1 - \cos(\beta)\cos(\gamma) + \sin(\beta)\sin(\gamma)) \tag{5.51}$$

$$|G_{L,R}|^2 = |G_{R,L}|^2 \tag{5.52}$$

$$|G_{L,L}|^2 = 4|(\cos(\gamma) - \cos(\beta) - \sin^2(\gamma)\cos(\alpha) - \sin(\alpha)\sin(\gamma)\cos(\gamma))^2 + \tag{5.53}$$

$$(-\sin(\gamma) + \cos(\alpha)\sin(\gamma)\cos(\gamma) - \sin(\alpha)\sin^2(\gamma))^2| \tag{5.54}$$

$$|G_{L,U}|^2 = 4|(1 - \cos(\alpha)\cos(\gamma) + \sin(\alpha)\sin(\gamma))(1 - \cos(\beta)\cos(\gamma) - \sin(\beta)\sin(\gamma)) \tag{5.55}$$

$$|G_{L,D}|^2 = 4|(1 - \cos(\alpha)\cos(\gamma) + \sin(\alpha)\sin(\gamma))(1 - \cos(\beta)\cos(\gamma) + \sin(\beta)\sin(\gamma)) \tag{5.56}$$

$$|G_{U,R}|^2 = |G_{R,U}|^2 \tag{5.57}$$

$$|G_{U,L}|^2 = |G_{L,U}|^2 \tag{5.58}$$

$$|G_{U,U}|^2 = 4|(\cos(\gamma) - \cos(\alpha) - \sin^2(\gamma)\cos(\beta) + \sin(\beta)\sin(\gamma)\cos(\gamma))^2 + \tag{5.59}$$

$$(-\sin(\gamma) + \cos(\beta)\sin(\gamma)\cos(\gamma) + \sin(\beta)\sin^2(\gamma))^2| \tag{5.60}$$

$$|G_{U,D}|^2 = 4(\cos(\gamma) - \cos(\alpha))^2 \tag{5.61}$$

$$|G_{D,R}|^2 = |G_{R,D}|^2 \tag{5.62}$$

$$|G_{D,L}|^2 = |G_{L,D}|^2 \tag{5.63}$$

$$|G_{D,U}|^2 = |G_{U,D}|^2 \tag{5.64}$$

$$|G_{D,D}|^2 = 4|(\cos(\gamma) - \cos(\alpha) - \sin^2(\gamma)\cos(\beta) - \sin(\beta)\sin(\gamma)\cos(\gamma))^2 + \tag{5.65}$$

$$(-\sin(\gamma) + \cos(\beta)\sin(\gamma)\cos(\gamma) - \sin(\beta)\sin^2(\gamma))^2| \tag{5.66}$$

and taking the coordinatewise squared norm:

$$|\mathbf{G}(\mathbf{z}_1)|^2 = 4\frac{B^2}{A}\begin{bmatrix} \frac{(\lambda+\mu+1)(\lambda-\mu+1)}{(\lambda+\mu-1)(\lambda-\mu-1)} & 1 & \frac{\lambda+\mu+1}{\lambda+\mu-1} & \frac{\lambda-\mu+1}{\lambda-\mu-1} \\ 1 & \frac{(\lambda+\mu-1)(\lambda-\mu-1)}{(\lambda+\mu+1)(\lambda-\mu+1)} & \frac{\lambda-\mu-1}{\lambda-\mu+1} & \frac{\lambda+\mu-1}{\lambda+\mu+1} \\ \frac{\lambda+\mu+1}{\lambda+\mu-1} & \frac{\lambda-\mu-1}{\lambda-\mu+1} & \frac{(\lambda+\mu+1)(\lambda-\mu-1)}{(\lambda+\mu-1)(\lambda-\mu+1)} & 1 \\ \frac{\lambda-\mu+1}{\lambda-\mu-1} & \frac{\lambda+\mu-1}{\lambda+\mu+1} & 1 & \frac{(\lambda+\mu-1)(\lambda-\mu+1)}{(\lambda+\mu+1)(\lambda-\mu-1)} \end{bmatrix}$$

Substituting the values of above $G_{\xi_0,\xi}(\mathbf{z}_1)$ into Equation (5.46) completes the proof of Theorem 5.24. $\square$

5.6 QRWs on $\mathbb{Z}^d$ for $d > 2$

In this final section we begin to confront the questions: "How much can the work above be generalized?", "Can the unitary coinflip alone tell us whether $\mathcal{V}_1$ will be smooth?" and "What will happen when we consider walks in higher dimensions?" Even walks on $\mathbb{Z}^3$ are in uncharted territory.

5.6.1 Smooth Walks on $\mathbb{Z}^d$

We begin with a simple observation, stated below as a proposition:

Proposition 5.27. *If U has an eigenvalue ζ with multiplicity greater than 1, then $\mathcal{V}_1 := \{\mathbf{z} : |z_1| = \ldots |z_{d+1}| = 1$ and $H(\mathbf{z}) = 0\}$ with $H := \det(I - z_{d+1}MU)$ is not smooth.*

PROOF: Given units $z_1, \ldots z_d$, $H(\mathbf{z}) = 0$ if and only if $1/z_{d+1}$ is an eigenvalue of the matrix MU. With $z_1 = \ldots = z_d = 1$, MU has the multiple eigenvalue ζ, and thus the equation $H = 0$ has the repeated root $(1, \ldots, 1, 1/\zeta)$. Hence ∇H vanishes at $(1, \ldots, 1, 1/\zeta)$ so $\mathcal{V}_1$ is not smooth. In a nearest neighbor walk ∇H vanishes at $(-1, \ldots, -1, -1/\zeta)$ as well. $\square$.

We now observe that the family $B(p)$ of Section 5.3 lies within the three parameter family

$$B(a,b,c) = \begin{pmatrix} a & b & c & d \\ -b & a & -d & c \\ -c & d & a & -b \\ -d & -c & b & a \end{pmatrix}$$

of special orthogonal matrices (with $d = \sqrt{1 - a^2 - b^2 - c^2}$), each of which has two nonsimple eigenvalues, $a \pm i\sqrt{1 - a^2}$. As $a = \sqrt{p/2}$ for the $B(p)$ matrices, it is immediate that ∇H vanishes for these walks at the points $\pm(1, 1, \sqrt{p/2} \pm i\sqrt{1 - p/2})$.

The result above is not an if and only if statement, so there is no guarantee $\mathcal{V}_1$ is smooth for every walk based on a matrix within the three parameter family

$$S(a,b,c) = \begin{pmatrix} a & b & c & d \\ -b & a & -d & c \\ c & -d & -a & b \\ -d & -c & b & a \end{pmatrix}$$

of orthogonal matrices (with $d = \sqrt{1-a^2-b^2-c^2}$), each of which has the four simple eigenvalues $a \pm i\sqrt{1-a^2}, 1$ and -1. This family includes the families $S(p)$ and $A(p)$ of Section 5.3 for which we showed that $\mathcal{V}_1$ is smooth.

All the data to this point, however, does point to the possibility that an if and only if version of Proposition 5.27 could be true. If so, then the following conjecture is true.

Conjecture 5.28. *For any nondegenerate $U = S(a,b,c)$, the variety $\mathcal{V}_1$ is smooth.*

By nondegenerate, we mean nondeterministic (the walk would be deterministic if $a = 1$) and irreducible. If $c = d = 0$ we would call the walk reducible as it would be equivalent to two walks on the line. While this statement is only a conjecture, we can prove the following proposition, giving us two two parameter families of matrices associated with smooth walks:

Proposition 5.29. *For any nondegenerate $U = S(a,b,c)$ with $c^2 = d^2$, the variety $\mathcal{V}_1$ is smooth.*

Proof: For a generic member of the family $S(a,b,c)$,

$\mathbf{z} \in \mathcal{V}_1 \iff H(e^{i\alpha}, e^{i\beta}, e^{i\gamma}) = 0$ with

$$H = 2\sin(\gamma)\left[\cos(\gamma) - a\cos(\alpha)\right] - 2a\sin(\beta)\cos(\gamma) + (a^2+c^2)\sin(\alpha+\beta) + (b^2+c^2-1)\sin(\alpha-\beta) \quad (5.67)$$

If $\mathcal{V}_1$ is not smooth, then H, H_α, H_β and H_γ vanish together. Differentiating Equation (5.67) with respect to each variable we obtain

$$H_\alpha = 0 \iff \sin(\gamma) = \left[(a^2+c^2)\cos(\alpha+\beta) + (1-b^2-c^2)\cos(\alpha-\beta)\right]/2a\sin(\alpha)$$

$$H_\beta = 0 \iff \cos(\gamma) = \left[(a^2+c^2)\cos(\alpha+\beta) + (1-b^2-c^2)\cos(\alpha-\beta)\right]/2a\cos(\beta)$$

$$H_\gamma = \cos(\gamma)\left[\cos(\gamma) - a\cos(\alpha)\right] - \sin(\gamma)\left[\sin(\gamma) - a\sin(\beta)\right]$$

By the hypothesis $c^2 = d^2$, we have $1-b^2-c^2 = a^2+c^2$, and using the appropriate trigonometric identities we find that

$$H_\alpha = 0 \iff \sin(\gamma) = \frac{a^2-b^2+1}{2a}\sin(\beta)$$
$$H_\beta = 0 \iff \cos(\gamma) = \frac{a^2-b^2+1}{2a}\cos(\alpha)$$

In addition to obtaining formulas for $\cos(\gamma)$ and $\sin(\gamma)$, we see that $\cos^2(\alpha)+\sin^2(\beta) = \left(\frac{2a}{a^2-b^2+1}\right)^2$. Then substituting into the equation $H_\gamma = 0$ and solving we get

$$\cos^2(\alpha) = \frac{2a^2}{(1-b^2+a^2)^2} = \sin^2(\beta).$$

Thus $\cos(\alpha) = \frac{a}{1-b^2+a^2}\sigma_\alpha\sqrt{2}$, $\sin(\beta) = \frac{a}{1-b^2+a^2}\sigma_\beta\sqrt{2}$, $\cos(\gamma) = \sigma_\alpha/\sqrt{2}$ and $\sin(\gamma) = \sigma_\beta/\sqrt{2}$ for appropriate second roots of unity σ_α and σ_β. Finally, substituting these values into Equation (5.67) we get that H vanishes as well if and only if $(a^2+c^2)c^2 = 0$. Now if $c^2 = 0$ then the matrix $S(a,b,c)$ is block diagonal, and therefore degenerate. If $a^2+c^2 = 0$ for $a, c \in \mathbb{R}$, then $a = c = 0$ and the walk is again degenerate. Thus for a nondegenerate choice of a, b and c, $\mathcal{V}_1$ is smooth. $\square$.

While a walk on $\mathbb{Z}^d$ for d greater than 2 with smooth $\mathcal{V}_1$ has yet to be discovered, more work concerning the inverse of Proposition 5.27 could lead to such a walk. Meanwhile, we demonstrate a seven parameter family of walks on $\mathbb{Z}^4$ that will each have $\mathcal{V}_1$ smooth if the inverse is true. Just as the families of orthogonal matrices $B(a,b,c)$ and $S(a,b,c)$ reflect the symmetries of $(\mathbb{Z}/(2\mathbb{Z}))^2$, we present the family $S(a,b,c,d,e,f,g)$ of orthogonal matrices reflecting the symmetries of $(\mathbb{Z}/(2\mathbb{Z}))^3$:

$$S(a,b,c,d,e,f,g) = \begin{pmatrix} a & b & c & d & e & f & g & h \\ b & -a & d & -c & f & -e & h & -g \\ c & -d & -a & b & g & -h & -e & f \\ d & c & -b & -a & -h & -g & f & e \\ e & -f & -g & h & -a & b & c & -d \\ f & e & h & g & -b & -a & -d & -c \\ -g & h & -e & f & c & -d & a & -b \\ -h & -g & f & e & -d & -c & b & a \end{pmatrix}$$

with $h = \sqrt{1-a^2-b^2-c^2-d^2-e^2-f^2-g^2}$. If we let $A = a^2+c^2+d^2+e^2+f^2$ and $B = 1-A$, then $S(a,b,c,d,e,f,g)$ has distinct eigenvalues: $-a \pm i\sqrt{1-a^2}, \pm\sqrt{A-B\pm 2i\sqrt{AB}}, 1$ and -1.

5.6.2 The Hadamard Walk on $\mathbb{Z}^d$

Much of the previous work on QRWs has been concerned with Hadamard walks. For some reason, the accepted generalization U^n_{Had} of the Hadamard matrix to dimension n is the matrix with all diagonal entries equal to $a_n > 0$ and all other entries equal to b_n. For U^n_{Had} to be unitary, we need $a_n^2 + (n-1)b_n^2 = 1$ and $2a_nb_n + (n-2)b_n^2 = 0$. Solving we find $a_n = 1-2/n$ and $b_n = -2/n$. Thus we can write $U^n_{\text{Had}} := I - \frac{2}{n}\mathbf{1}$ where $\mathbf{1}$ is the matrix of all 1's. As we saw in Section 5.5, for the walk on $\mathbb{Z}^2$ based on U^4_{Had}, $\mathcal{V}_1$ is not smooth, though we can still deliver asymptotics as $|E| < \infty$. We show that for a walk on $\mathbb{Z}^d$ based on U^{2d}_{Had}, with d greater than 2, $|E| = \infty$, so we cannot recover asymptotics with a theorem like 5.9. In particular, $H(\mathbf{z}) = \det(I - z_{d+1}MU^{2d}_{\text{Had}})$ (with M the nearest neighbor matrix) vanishes to order $2d-1$ at the point $\mathbf{z} = (1,\ldots,1,1)$, to order $2d-3$ at the point $\mathbf{z} = (z_1, 1, \ldots, 1)$ and to order $d-1$ at the point $\mathbf{z} = (z_1,\ldots,z_1)$ for each unit z_1. It is likely that this carries over to hindrances to analyzing the walk with methods different than our own, leading to the skepticism that exists regarding QRWs on $\mathbb{Z}^d$ for d greater than 2.

The facts mentioned above about the vanishing of H are apparent once we prove the following proposition.

Proposition 5.30. *For the nearest neighbor Hadamard walk on* $\mathbb{Z}^d$

$$H(\mathbf{z}) = \left[\Pi_{j=1}^{d}(1 - z_j z_{d+1})(z_j - z_{d+1})\right]\left[1 + \frac{1}{d}\sum_{j=1}^{d}\frac{z_j z_{d+1}}{1 - z_j z_{d+1}} + \frac{z_{d+1}}{z_j - z_{d+1}}\right] \tag{5.68}$$

Proof: As described above $H(\mathbf{z}) = \det(I - MU_{\text{Had}}^{2d} z_{d+1})$ with $U_{\text{Had}}^{2d} := I - \frac{1}{d}\mathbf{1}$ and M the matrix with diagonal entries $z_1, z_1^{-1}, \dots, z_d, z_d^{-1}$. If we replace row k of the matrix $A = I - MU_{\text{Had}}^{2d} z_{d+1}$ with row k minus row 1 for each $2 \le k \le 2d$, we get the matrix with equivalent determinant

$$A' = \begin{pmatrix} 1 - z_1 z_{d+1} + \frac{1}{d} z_1 z_{j+1} & \frac{1}{d} z_1^{-1} z_{d+1} & \frac{1}{d} z_2 z_{d+1} & \dots & \frac{1}{d} z_d z_{d+1} & \frac{1}{d} z_d^{-1} z_{d+1} \\ -(1 - z_1 z_{d+1}) & 1 - z_1^{-1} z_{d+1} & 0 & \dots & \dots & 0 \\ -(1 - z_1 z_{d+1}) & 0 & 1 - z_2 z_{d+1} & 0 & \dots & 0 \\ \vdots & \vdots & 0 & \ddots & 0 & \dots \\ -(1 - z_1 z_{d+1}) & 0 & \dots & 0 & 1 - z_d z_{d+1} & 0 \\ -(1 - z_1 z_{d+1}) & 0 & \dots & \dots & 0 & 1 - z_d^{-1} z_{d+1} \end{pmatrix}$$

The determinant of A' is easy to calculate as only d elements of the symmetric group $\mathcal{S}_d$ make nonzero contributions. The contributors are the identity (meaning the product of the diagonal entries) and the single transpositions $(1, j)$ (in cycle notation). Thus

$$\det(A) = \det(A') = \left[\Pi_{j=1}^{d}(1 - z_j z_{d+1})(1 - z_j^{-1} z_{d+1})\right]\left[1 + \frac{1}{d}\sum_{j=1}^{d}\frac{z_j z_{d+1}}{1 - z_j z_{d+1}} + \frac{z_j^{-1} z_{d+1}}{1 - z_j^{-1} z_{d+1}}\right].$$

Simplifying the fractions within fractions completes the proof. $\square$.

If we now let $P(\mathbf{z}) = \Pi_{j=1}^{d}(1 - z_j z_{d+1})(z_j - z_{d+1})$, then as $P(\mathbf{z})$ vanishes to degrees $2d$, $2d - 2$ and d at the points $\pm(1, \dots, 1)$, $(z_1, 1, \dots, 1)$ and $(z_1, \dots, z_1)$, respectively, H vanishes to degrees $2d - 1$, $2d - 3$ and $d - 1$ at these points. This proves the assertions related to the difficulty in deriving asymptotics for this walk.

In order to determine the Gauss map for these walks, we prove the following proposition in which $z_j = e^{iZ_j}$ for each $1 \le j \le d + 1$.

Proposition 5.31. *For the nearest neighbor Hadamard walk on* $\mathbb{Z}^d$

$$\mathbf{z} \in \mathcal{V}_1 \iff \tilde{P}(\mathbf{z}) \cdot \sin(Z_{d+1}) \sum_{j=1}^{d} \frac{1}{\cos(Z_{d+1}) - \cos(Z_j)} = 0 \tag{5.69}$$

where

$$\tilde{P}(\mathbf{z}) = \prod_{j=1}^{d} \left[\cos(Z_{d+1}) - \cos(Z_j)\right].$$

Proof: Beginning with the result of Proposition 5.30, we observe that $(1 - z_j z_{d+1})(z_j - z_{d+1}) = 2z_j z_{d+1}\left[\cos(Z_{d+1}) - \cos(Z_j)\right]$. Thus $P = (2z_{d+1})^d \left[\prod_{j=1}^{d} z_j\right] \tilde{P}$. Then

$$H = P\left[1 + \frac{1}{d}\sum_{j=1}^{d} -1 + \frac{\cos(Z_{d+1}) - z_{d+1}}{\cos(Z_{d+1}) - \cos(Z_j)}\right] = P\sum_{j=1}^{d} \frac{-i\sin(Z_{d+1})}{\cos(Z_{d+1}) - \cos(Z_j)}$$

Observing that $-iP = 0 \iff \tilde{P} = 0$ on $\mathcal{V}_1$ completes the proof. □

When $d = 3$ we denote (Z_1, Z_2, Z_3, Z_4) as (X_1, X_2, X_3, Z) and simplify the above expression as follows: $z \in \mathcal{V}_1 \iff \sin(Z) = 0$ or

$$3\cos^2(Z) - 2\left[\sum_{j=1}^{3} \cos(X_j)\right]\cos(Z) + \cos(X_1)\cos(X_2) + \cos(X_1)\cos(X_3) + \cos(X_2)\cos(X_3) = 0. \tag{5.70}$$

Thus for given X_1, X_2 and X_3, the values of Z are given explicitly by $0, \pi, \pm\arccos(\alpha_+)$ and $\pm\arccos(\alpha_-)$ where α_+ and α_- are the two solutions to the quadratic equation in $\cos(Z)$ above. As with the Hadamard walk on $\mathbb{Z}^2$, $\mathcal{V}_1$ decomposes into components $C_1 \cup C_2$. For any X_1, X_2 and X_3, Z is dictated by Equation (5.70) on C_1 while $\sin(Z) = 0$ on C_2. As with the walk on $\mathbb{Z}^2$, the image of the Gauss map of C_2 is the origin. To determine the image of the Gauss map of C_1 we differentiate Equation (5.70) with respect to X_1, and obtain the partial derivative:

$$\frac{\partial Z}{\partial X_1} = \frac{\sin(X_1)}{\sin(Z)} \Big/ \left(3 + \left[\frac{\cos(X_2) - \cos(X_3)}{\cos(Z) - \cos(X_2) + \cos(Z) - \cos(X_3)}\right]^2\right)$$

By the symmetry of Equation (5.70), we obtain $\frac{\partial Z}{\partial X_2}$ and $\frac{\partial Z}{\partial X_3}$ by permutations of the indices. Varying X_1, X_2, and X_3 and plotting $\mathbf{dir}\,(\mathbf{z}) = (-\frac{\partial Z}{\partial X_1}, -\frac{\partial Z}{\partial X_2}, -\frac{\partial Z}{\partial X_3})$ we obtain the image of the Gauss map below. (Note: As the image is symmetric with respect to each axis, we only include half the picture.)

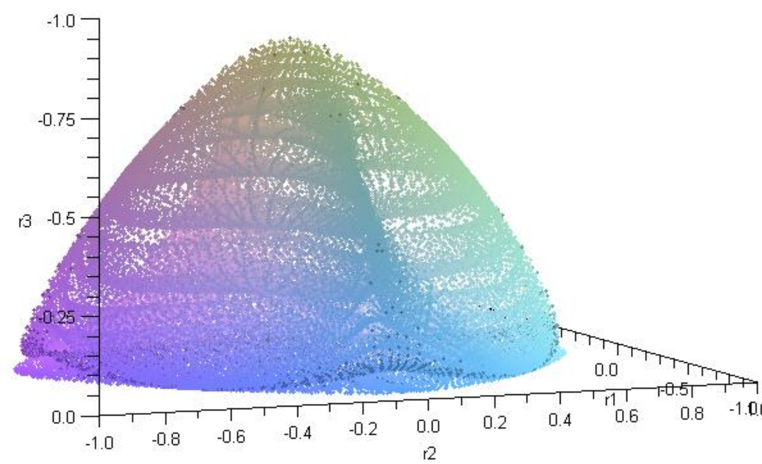

Figure 20: Half the image of the Gauss map for the Hadamard walk on $\mathbb{Z}^3$

6 Conclusions and Further Areas of Study

In this thesis we have reviewed and developed several methods to better understand Quantum Random Walks via generating functions. For each walk we studied on $\mathbb{Z}^d$ we found a region growing linearly in time t in which the probability of finding the particle was inversely proportion to t^d, and showed that the constant of proportionality was a function of Gaussian curvature. We demonstrated that probability decays exponentially outside this region, and for two chirality walks on the line we showed that between the two regions lies one of Airy-like behavior. In the simplest cases of nearest neighbor walks on $\mathbb{Z}$, a three-chirality walk on $\mathbb{Z}$ and the Hadamard walk on $\mathbb{Z}^2$, we determined exact asymptotics as well.

Quantum Random Walks on $\mathbb{Z}^d$ for d greater than 2 are still relatively uncharted territory. Variations of the methods in this thesis, tailored to higher dimensional problems with the aid of more sophisticated computer algebra systems, could prove productive. For walks on $\mathbb{Z}^4$, analysis of the class $S(a, b, c, d, e, f, g)$ of orthogonal matrices with distinct eigenvalues would be a good place to begin.

In addition, it would be exciting to see more work on a general approach to the study of Quantum Random Walks. Theorems concerning what behavior is and is not generic in QRWs could cut to the chase in a way that the study of further individual walks does not. That being said, the results for families of walks contained in this thesis should prove helpful in this endeavor.

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