Spectral methods for Quantum walks, (aka Discrete time unitary evolutions)

F. Alberto Grünbaum

Math. Dept , UC Berkeley

Rice U. , Oct 27th. , 2013

CLASSICAL RANDOM WALKS have a long history involving modeling in physics (Bernoulli (1769), Laplace (1812) , A. Einstein(1905), P. and T. Ehrenfest (1907), N. Wiener(1922), Courant-Friedrichs-Lewy (1928)........)

Some of these models come from (or are used in) mathematical biology, mathematical finances (Bachelier 1900) , network theory, astronomy, statistical mechanics, solid state physics, polymer chemistry, biology,....etc, etc...for a very long time

The interest in **QUANTUM WALKS** is much more recent. It has been driven in part by the design of quantum search algorithms and the general area known as **QUANTUM COMPUTING**.

QWs "diffuse" faster than CRWs.

In the classical case the expected value of the **SQUARE** of the displacement grows like time, whereas in the case of QWs the typical case is "ballistic behaviour", i.e. the expected value of the **MODULUS** of the displacement grows like time.

In the classical case the fluctuations around this mean behaviour is (typically) given by a Gaussian (THE CENTRAL LIMIT THEOREM). In the case of QWs the results are completely different and largely unexplored. Much more (numerical and laboratory) experimentation is needed.

Are there any "real world" reasons to look into quantum walks??

R. Feynman, Quantum Mechanical Computers, Optics News, 1984.

Y. Aharonov, et. al. , Quantum random walks,
Physical Review A , 1993.

G. Engel, et. al., Evidence for wavelike energy transfer through quantum coherence in photosynthetic systems
Nature, 2007.

A. Peruzzo, et. al. , Quantum walks of correlated photons, Science, 2010.

Kitagawa, Rudner, Berg, Demier, Exploring topological phases with Quantum walks, Phys. Rev. A, 82, 2010.

S. Hoyer, et. al. , Propagating quantum coherence for biological advantage, arXiv June 2011

People working on Quantum walks, starting with Y. Aharonov et.al. (Phys. Rev, A,1993) have used either "path counting" methods or Fourier methods. In the first case it is a good idea to be Dick Feynman, in the second case you are restricted to translation invariant situations.

The idea of using spectral methods was proposed in M.J. Cantero, F. A. Grünbaum, L. Moral, L. Velázquez, *Matrix valued Szegö polynomials and quantum random walks*, quant-ph/0901.2244,

Comm. Pure and Applied Math, vol. LXIII, pp 464–507, 2010.

With the more recent work on recurrence we find that many of the tools of probability, operator theory, complex analysis, OPUC, can be used as tools to discover new phenomena for quantum walks, which apparently had not been noticed so far.

This new method has been applied by us and other people to study localization, etc.

Konno, N. and Segawa, E. , *Localization of discrete time quantum walks on a half line via the CGMV method*, Quantum Information and computation, vol 11, pp 485–495 (2011).

Konno, N. and Segawa, E. ,*One dimensional quantum walks via generating functions and the CGMV method*, arXiv May 2013.

There are also some new results, specially on recurrence by

Recurrence for discrete time unitary evolutons.

F. A. Grünbaum, L. Velázquez, R. Werner and A. Werner (Comm. Math. Physics 2013) as well as in the more recent paper

QUANTUM SUBSPACE RECURRENCE AND SCHUR FUNCTIONS

J. Bourgain, F.A. Grünbaum, L. Velazquez and J. Wilkening, arXiv 2013. to appear in Comm. Math. Physics 2014

I will describe a way of constructing a Quantum walk with discrete time out of a UNITARY OPERATOR and an initial state.

The main tools are the so called CMV matrices and certain pieces of very classical complex and harmonic analysis from the 1910-1920 period.

A quick review of CMV matrices

Let $d\mu(z)$ be a probability measure on the unit circle $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$, and $L^2_\mu(\mathbb{T})$ the Hilbert space of μ-square-integrable functions with inner product

$$(f, g) = \int_{\mathbb{T}} \overline{f(z)}\, g(z)\, d\mu(z).$$

For simplicity we assume that the support of μ contains an infinite number of points.
A very natural **UNITARY** operator to consider in our Hilbert space is given by multiplication by z.
Since the Laurent polynomials are dense in $L^2_\mu(\mathbb{T})$, a natural basis to obtain a matrix representation of U_μ is given by the Laurent polynomials $(\chi_j)_{j=0}^{\infty}$ obtained from the Gram–Schmidt orthonormalization of $\{1, z, z^{-1}, z^2, z^{-2}, \dots\}$ in $L^2_\mu(\mathbb{T})$.

The matrix $\mathcal{C} = (\chi_j, z\chi_k)_{j,k=0}^{\infty}$ of U_μ with respect to $(\chi_j)_{j=0}^{\infty}$ has the form

$$\mathcal{C} = \begin{pmatrix} \overline{\alpha}_0 & \rho_0\overline{\alpha}_1 & \rho_0\rho_1 & 0 & 0 & 0 & 0 & \dots \\ \rho_0 & -\alpha_0\overline{\alpha}_1 & -\alpha_0\rho_1 & 0 & 0 & 0 & 0 & \dots \\ 0 & \rho_1\overline{\alpha}_2 & -\alpha_1\overline{\alpha}_2 & \rho_2\overline{\alpha}_3 & \rho_2\rho_3 & 0 & 0 & \dots \\ 0 & \rho_1\rho_2 & -\alpha_1\rho_2 & -\alpha_2\overline{\alpha}_3 & -\alpha_2\rho_3 & 0 & 0 & \dots \\ 0 & 0 & 0 & \rho_3\overline{\alpha}_4 & -\alpha_3\overline{\alpha}_4 & \rho_4\overline{\alpha}_5 & \rho_4\rho_5 & \dots \\ 0 & 0 & 0 & \rho_3\rho_4 & -\alpha_3\rho_4 & -\alpha_4\overline{\alpha}_5 & -\alpha_4\rho_5 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}, \tag{1}$$

where $\rho_j = \sqrt{1 - |\alpha_j|^2}$ and $(\alpha_j)_{j=0}^{\infty}$ is a sequence of complex numbers such that $|\alpha_j| < 1$. The coefficients α_j are known as the Verblunsky (or Schur, or Szegő, or reflection) parameters of the measure μ, and establish a bijection between the probability measures supported on an infinite set of the unit circle and sequences of points in the open unit disk.

Some pieces of very classical analysis that are useful to study quantum walks (if you want to use the spectral method).

An important tool is the Carathéodory function F of the orthogonality measure μ, defined by

$$F(z) = \int_{\mathbb{T}} \frac{t+z}{t-z}\, d\mu(t), \qquad |z| < 1. \tag{2}$$

F is analytic on the open unit disc with Taylor series

$$F(z) = 1 + 2\sum_{j=1}^{\infty} \overline{\mu}_j z^j, \qquad \mu_j = \int_{\mathbb{T}} z^j\, d\mu(z), \tag{3}$$

whose coefficients provide the moments μ_j of the measure μ.

Another tool in the theory of OP on the unit circle is the so called Schur function related to $F(z)$ and thus to $\boldsymbol{\mu}$, by

$$f(z) = z^{-1}(F(z) - 1)(F(z) + 1)^{-1}, \quad |z| < 1.$$

we have

$$F(z) = (1 + zf(z))(1 - zf(z))^{-1}, \quad |z| < 1.$$

Just as $F(z)$ maps the unit disk to the right half plane, $f(z)$ maps the unit disk to itself.

Both the measure and the Schur function are univocally determined by the Verblunsky coefficients.

A very important fact is that $f(z)$ is INNER, i.e. the limiting values of its modulus on the unit circle are 1, exactly when μ has zero density with respect to Lebesgue measure, i.e. is purely singular. In this case μ can have a singular continuous part and maybe point masses.

Now we construct a large class of QWs, starting in each case with a CMV matrix.

We choose to order the pure states of our system as follows

$|0\rangle \otimes |\uparrow\rangle, |0\rangle \otimes |\downarrow\rangle, |1\rangle \otimes |\uparrow\rangle, |1\rangle \otimes |\downarrow\rangle, \ldots$

and we will describe a way of prescribing a transition mechanism giving rise to a unitary matrix U.

We give a transition mechanism for an arbitrary CMV matrix as above. More explicitly, we allow for the following dynamics with four possible transitions

$$|i\rangle \otimes |\uparrow\rangle \longrightarrow \begin{cases} |i+1\rangle \otimes |\uparrow\rangle & \text{with amplitude } \rho_{i+2}\rho_{i+3} \\ |i-1\rangle \otimes |\downarrow\rangle & \text{with amplitude } \rho_{i+1}\overline{\alpha}_{i+2} \\ |i\rangle \otimes |\uparrow\rangle & \text{with amplitude } -\alpha_{i+1}\overline{\alpha}_{i+2} \\ |i\rangle \otimes |\downarrow\rangle & \text{with amplitude } \rho_{i+2}\overline{\alpha}_{i+3} \end{cases}$$

$$|i\rangle \otimes |\downarrow\rangle \longrightarrow \begin{cases} |i+1\rangle \otimes |\uparrow\rangle & \text{with amplitude } -\alpha_{i+2}\rho_{i+3} \\ |i-1\rangle \otimes |\downarrow\rangle & \text{with amplitude } \rho_{i+1}\rho_{i+2} \\ |i\rangle \otimes |\uparrow\rangle & \text{with amplitude } -\alpha_{i+1}\rho_{i+2} \\ |i\rangle \otimes |\downarrow\rangle & \text{with amplitude } -\alpha_{i+2}\overline{\alpha}_{i+3} \end{cases}$$

The expressions for the amplitudes above are valid for i even. If i is odd then in every amplitude the index i needs to be replaced by $i-1$.

To get a traditional QW's (as those going with a COIN) we need to assume that the **ODD Verblunsky coefficients VANISH**.

In terms of the function $F(z)$ introduced above this means that

$$F(z)F(-z) = 1.$$

In terms of the Schur function $f(z)$ - to be introduced below- this

means that $f(z)$ is EVEN.

For the **traditional** QW on the integers a spin located at site i and pointing up can go to the left and flip orientation with amplitude c_{21}^i or go to the right while keeping its orientation with amplitude c_{11}^i. There are also amplitudes for transitions involving a spin pointing down, so that we have the following allowed transitions

$$|i\rangle \otimes |\uparrow\rangle \longrightarrow \begin{cases} |i+1\rangle \otimes |\uparrow\rangle & \text{with probability amplitude } c_{11}^i \\ |i-1\rangle \otimes |\downarrow\rangle & \text{with probability amplitude } c_{21}^i \end{cases}$$

$$|i\rangle \otimes |\downarrow\rangle \longrightarrow \begin{cases} |i+1\rangle \otimes |\uparrow\rangle & \text{with probability amplitude } c_{12}^i \\ |i-1\rangle \otimes |\downarrow\rangle & \text{with probability amplitude } c_{22}^i \end{cases}$$

where, for each $i \in \mathbb{Z}$,

$$C_i = \begin{pmatrix} c_{11}^i & c_{12}^i \\ c_{21}^i & c_{22}^i \end{pmatrix} \tag{4}$$

is an arbitrary unitary matrix which one calls the i^{th} coin.

People that work with "coined quantum walks" use the special case described above.

A famous important case is described below.

Examples of QWs with a constant coin

The Hadamard QW is an example of the QWs described previously. It corresponds to a constant coin $C_i = H$ given by

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{5}$$

The Hadamard QW is an example of an unbiased QW, i.e., a QW with a constant coin such that all the allowed transitions are equiprobable.

An analog of the Karlin McGregor formula for the quantum case, yielding probability amplitudes, i.e. the main point of CGMV

The KMcG formula looks as follows

$$(\boldsymbol{U}^n)_{j,k} = \int_{\mathbb{T}} z^n \boldsymbol{X}_j(z) d\boldsymbol{\mu}(z) \boldsymbol{X}_k(z)^{\dagger},$$

The quantities $\boldsymbol{X}_j(z)$ are the orthogonal Laurent-Szegö polynomials.

There are scalar as well as block versions of this formula, just as in the classical case. The scalar case appears for walks on the non-negative integers and the block version is needed for the case of walks on the integers.

It is important to notice that we have a way of computing *AMPLITUDES* and that getting probabilities requires recalling the rules of QM.

For example, given a QW on $\mathbb{Z}$ or $\mathbb{Z}_+$, we define $p^{(k)}_{\alpha,\beta}(n)$,i.e. the probability that the walker gets to the site k in n steps having started at the state $|\Psi^{(0)}_{\alpha,\beta}\rangle = \alpha|0\rangle \otimes |\uparrow\rangle + \beta|0\rangle \otimes |\downarrow\rangle$ at the initial time, and this is computed as follows

$$p^{(k)}_{\alpha,\beta}(n) = |\langle \Psi^{(k)}_{1,0}|\mathfrak{U}^n|\Psi^{(0)}_{\alpha,\beta}\rangle|^2 + |\langle \Psi^{(k)}_{0,1}|\mathfrak{U}^n|\Psi^{(0)}_{\alpha,\beta}\rangle|^2.$$

where $\mathfrak{U}$ is the transition operator of the QW.

Assume, for simplicity, that we start at the origin, in a state given by the initial state $\alpha|0\rangle \otimes |\uparrow\rangle + \beta|0\rangle \otimes |\downarrow\rangle$ and we denote with X_n the site k at time n. The possible values of k will go from $-n$ to n in the case of the integers and from 0 to n for the non-negative integers.

A topic of interest is then the study of the quantity

$$Prob\{\gamma \leq X_n/n \leq \delta\}$$

In very few cases the limiting density for this distribution function is known.

The shape of this distribution can depend heavily on the initial state. This analysis is much more elaborate than in the classical case, and some examples will appear later.

In the classical case one would scale X_n not by n, but by its square root.

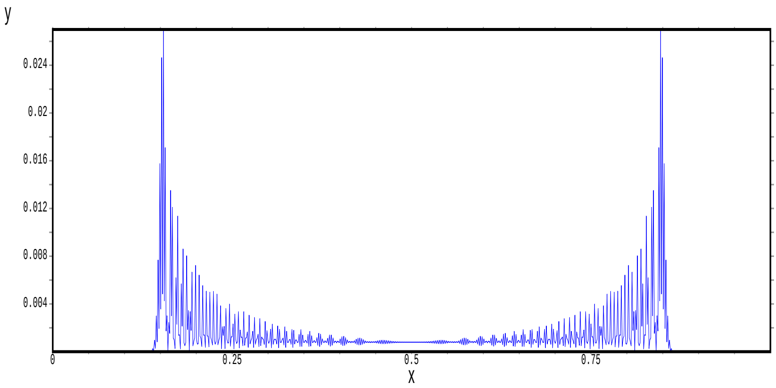
Consider a quantum case, first in the case of all the integers, and ask **what is the analog of the Gaussian?**

We will do this in the case of the Hadamard walk.

I will show the results of a computation using the appropriate CMV matrix. All the plots are obtained by using the relevant CMV matrix and all computations are done in exact arithmetic.

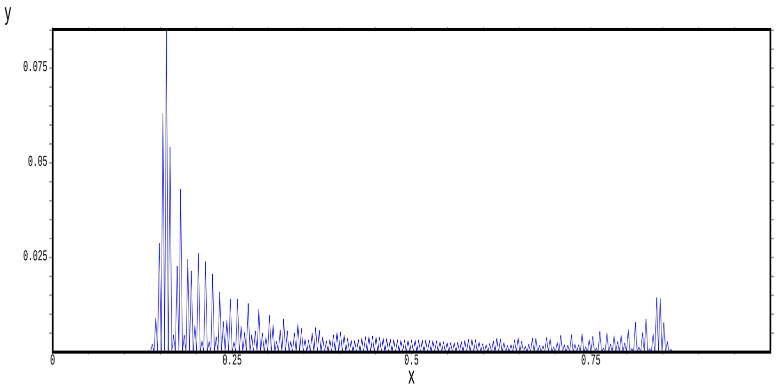
Hadamard QW on the integers, initial state $\alpha|0\rangle \otimes |\uparrow\rangle + \beta|0\rangle \otimes |\downarrow\rangle$, with $\alpha = 1$, $\beta = i$, normalized

800 iterations



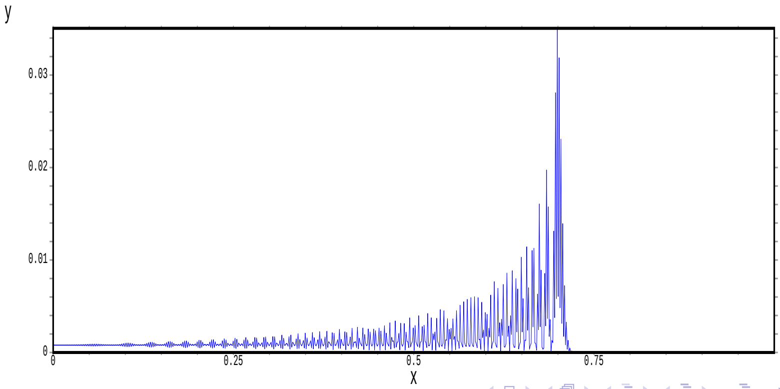
Hadamard QW on the integers initial state $\alpha|0\rangle \otimes |\uparrow\rangle + \beta|0\rangle \otimes |\downarrow\rangle$, with $\alpha = 1$, $\beta = 0$, normalized

200 iterations



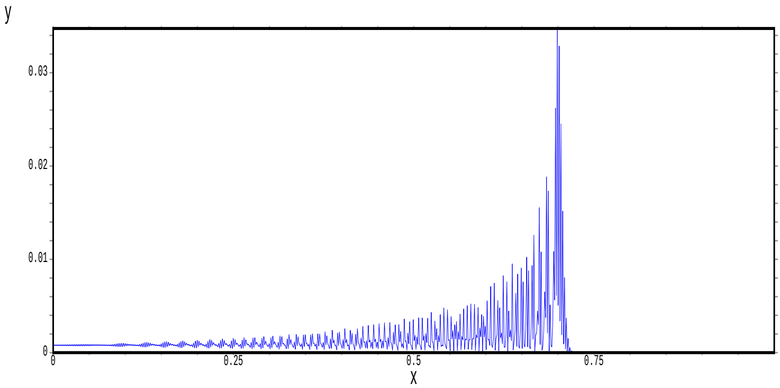
Hadamard QW on the non-negative integers initial state $\alpha|0\rangle \otimes |\uparrow\rangle + \beta|0\rangle \otimes |\downarrow\rangle$, with $\alpha = 1$, $\beta = 0$, i.e. one spin up at the origin

800 iterations



Hadamard QW on the non-negative integers initial state $\alpha|0\rangle \otimes |\uparrow\rangle + \beta|0\rangle \otimes |\downarrow\rangle$, with $\alpha = 1$, $\beta = 1$, normalized

800 iterations



The QW of F. Riesz

The measure on the unit circle that F. Riesz built is formally given by the expression

$$d\mu(z) = \frac{1}{2\pi}\prod_{k=1}^{\infty}(1 + cos(4^k\theta))d\theta = \frac{1}{2\pi}\prod_{k=1}^{\infty}(1 + (z^{4^k} + z^{-4^k})/2)dz/(iz)$$

$$= (\sum_{j=-\infty}^{\infty} \overline{\mu}_j z^j)dz/(iz)$$

Here $z = e^{i\theta}$.

If one truncates this infinite product the corresponding measure has a nice density. These approximations converge weakly to the Riesz measure, with vanishing density and no point masses, a Cantor like measure. We are dealing with a singular continuous measure.

I have started my product from $k = 1$, as in Barry's book, as well as in other references. F. Riesz started with $k = 0$. Each choice has its own advantages.

To do any computations with the Riesz walk we need to have its Schur, or Szegö or Veblunsky coefficients denoted by α_j.

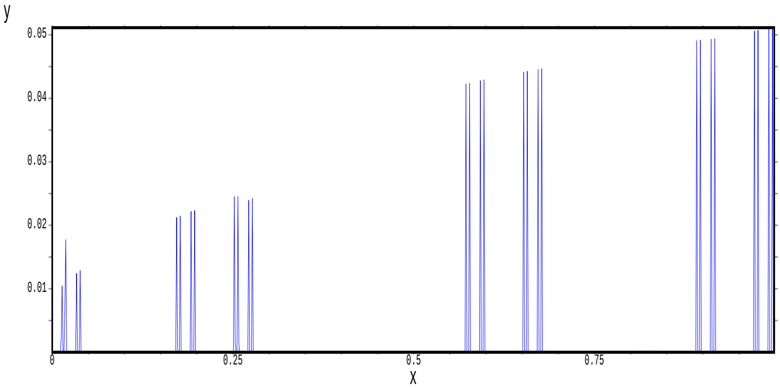
After extensive computation in exact arithmetic I have an ansatz for them (but no complete proof). This is used in all the computations behind the plots that appear later.

The QW of F. Riesz, Grünbaum and Velazquez, arXiv 1111.6630 in Proceedings of FoCAM, Budapest 2011.

How do the previous plots of the distribution of X_n/n look in the case of Riesz?

Riesz' QW, initial state: a spin up at the origin

800 iterations, starting the product with $k = 1$



Before going much further, recall...

ANYONE THAT HAS NOT BEEN SHOCKED BY QUANTUM MECHANICS HAS NOT UNDERSTOOD IT

Niels Bohr

The entire discussion of recurrence properties for a given state ϕ, will depend only on the scalar measure $\mu(du) = \langle \phi | E(du) \phi \rangle$ on the unit circle, which is obtained from the projection valued spectral measure E of U.

The moments of the scalar valued measure μ, i.e. its Fourier coefficients

$$\mu_n = \int \mu(du)\; u^n = \langle \phi | U^n \phi \rangle, \quad n \in \mathbb{Z}. \tag{6}$$

have a nice dynamical interpretation (going all the way to Heisenberg and Born) : they give the **amplitudes** of a return to ϕ in n units of time. The **probabilities** p_n will be the moduli squared of these amplitudes.

Back to the discussion of recurrence in the quantum case.

We consider quantum dynamical systems specified by a unitary operator U

and an initial state vector ϕ.

Any statement we make applies to the pair (U, ϕ)

In each step the unitary is followed by a **PROJECTIVE MEASUREMENT** checking whether the system has returned to the initial state. We call the system recurrent if this eventually happens with probability one.

GVWW recurrence

$$\widetilde{U} = (\mathbb{I} - |\phi\rangle\langle\phi|)U. \tag{7}$$

$$ff_n = \langle\phi|U\widetilde{U}^{n-1}\phi\rangle, \quad n \geq 1. \tag{8}$$

The quantity ff_n is the amplitude for a FIRST return to ϕ in n units of time.

The total probability for events up to and including the n^{th} step, i.e., detection (back at the initial state) at step $k \leq n$ or survival away from the initial state, thus adds up as

$$1 = \sum_{k=1}^{n} |ff_k|^2 + \|\widetilde{U}^n \phi\|^2.$$

The *return probability* is therefore

$$R = \sum_{n=1}^{\infty} |ff_n|^2 = 1 - \lim_{n \to \infty} \|\widetilde{U}^n \phi\|^2. \tag{9}$$

Accordingly, we call the pair (U, ϕ) *recurrent* if $R = 1$, and *transient* otherwise.

We use the *moment generating* or *Stieltjes function*

$$\widehat{\mu}(z) = \sum_{n=0}^{\infty} \mu_n z^n = \int \frac{\mu(dt)}{1 - tz}, \qquad (10)$$

We get

$$\begin{aligned}\widehat{a}(z) &= \sum_{n=1}^{\infty} ff_n z^n = \sum_{n=0}^{\infty} \langle \phi | U \widetilde{U}^n \phi \rangle z^{n+1} \\ &= \frac{\widehat{\mu}(z) - 1}{\widehat{\mu}(z)} \qquad (11) \\ &= z\,\overline{f}(z). \qquad (12)\end{aligned}$$

That is, the **Schur function is essentially the generating function for the first arrival amplitudes.**

The dynamical interpretation of the Taylor coefficients of the Schur function is the source of many nice games.

This is an expression I would love to be able to share with I. Schur and R. Feynman

$$\mu_n = ff_n + ff_{n-1}\mu_1 + \cdots + ff_1\mu_{n-1}$$

This is a quantum analog of the renewal equation that one has in the classical case, but now probabilities have been replaced by amplitudes.

For a recurrent state the expected value for the first return time is always a non-negative integer (or infinity): a topological interpretation in terms of the Schur function

Assume recurrence, i.e. $f(z)$ is inner

$$\tau = \sum_{n=1}^{\infty} |ff_n|^2 \, n. \tag{13}$$

$$g(t) = e^{it}\overline{f}(e^{it}) = \sum_{n=1}^{\infty} ff_n e^{int} \tag{14}$$

has modulus one for all real t. So $g(t)$ winds around the origin an integer number $w(g)$ of times as t goes from 0 to 2π. Integrating over one period $t \in [0, 2\pi]$, we get $2\pi w(g)$, so

$$w(g) = \frac{1}{2\pi} \int_0^{2\pi} dt \; \overline{g(t)} \; \frac{1}{i} \, \partial_t g(t) = \sum_{n=0}^{\infty} \overline{ff_n} \, (n ff_n) = \tau. \tag{15}$$

a first summary

The first return probabilities in our approach are the squared moduli of the Taylor coefficients of the so-called Schur function of the measure, which so far did not seem to have a direct dynamical interpretation.

Our main result is that the process is recurrent iff the Schur function is "inner", i.e., has modulus one on the unit circle.

Furthermore, we show that the winding number of this function has the direct interpretation as the expected time of first arrival, which is hence an integer (or plus infinity).

There are extensions of all the notions above, including the renewal equation, topological interpretations, etc.... in the case when one considers **SITE** to **SITE** recurrence, ignoring the value of the spin.

The notion of monitored recurrence for discrete-time quantum processes taking the initial state as an absorbing state is extended to absorbing subspaces of arbitrary finite dimension.

The generating function approach leads to a connection with the well-known theory of operator-valued Schur functions. This is the cornerstone of a spectral characterization of subspace recurrence.

The spectral decomposition of the unitary step operator driving the evolution yields a spectral measure, which we project onto the subspace to obtain a new spectral measure that is purely singular iff the subspace is recurrent, and consists of a pure point spectrum with a finite number of masses precisely when all states in the subspace have a finite expected return time.

This notion of subspace recurrence also links the concept of expected return time to an Aharonov-Anandan phase that, in contrast to the case of state recurrence, can be non-integer. Even more surprising is the fact that averaging such geometrical phases over the absorbing subspace yields an integer with a topological meaning, so that the averaged expected return time is always a rational number. Moreover, state recurrence can occasionally give higher return probabilities than subspace recurrence, a fact that reveals once more the counterintuitive behavior of quantum systems.

In particular, if V is recurrent and its inner Schur function $\boldsymbol{f}(z)$ has an analytic extension to a neighborhood of the closed unit disk, e.g. if $\boldsymbol{f}(z)$ is a rational inner function, then we can write

$$\tau(\psi) = \int_0^{2\pi} \langle \psi(\theta) | \partial_\theta \psi(\theta) \rangle \, \frac{d\theta}{2\pi i}, \qquad \psi(\theta) = \hat{\boldsymbol{a}}(e^{i\theta})\psi, \tag{16}$$

where $\psi(\theta)$, $\theta \in [0, 2\pi]$, traces out a closed curve on the sphere S_V due to the unitarity of $\hat{\boldsymbol{a}}(e^{i\theta})$. This simple result has a nice interpretation since it relates $\tau(\psi)$ to a kind of **Berry's geometrical phase** . More precisely, *the expected V-return time of a state $\psi \in S_V$ is $-1/2\pi$ times the* **Aharonov-Anandan phase** *associated with the loop $\hat{\boldsymbol{a}}(e^{i\theta})\psi \colon S^1 \to S_V$.*

In the case of state recurrence, one proves that the states ψ with a finite expected return time are characterized by a finitely supported spectral measure $\mu_\psi(d\lambda)$, thus by a rational inner Schur function $f_\psi(z)$. Further, one also finds that $\tau(\psi)$ must be a positive integer whenever it is finite because of its topological meaning: $\tau(\psi)$ is the winding number of $\hat{a}_\psi(e^{i\theta})\colon S^1 \to S^1$, where $\hat{a}_\psi(z) = z\overline{f_\psi}(z)$ is the first return generating function of ψ.

In contrast to a winding number, the Aharonov-Anandan phase is not necessarily an integer because it reflects a geometric rather than a topological property of a closed curve. The expression above for $\tau(\psi)$ is reparametrization invariant, and changes by an integer under closed S^1 gauge transformations $\psi(\theta) \to \tilde{\psi}(\theta) = e^{i\varsigma(\theta)}\psi(\theta)$, $\tilde{\psi}(2\pi) = \tilde{\psi}(0)$. This means that $\tau(\psi)$ is a geometric property of the unparametrized image of $\psi(\theta)$ in S_V, while $e^{i2\pi\tau(\psi)}$ is a geometric property of the corresponding closed curve in the projective space of rays of S_V whose elements are the true physical states of V. In fancier language, S_V is a fiber bundle over such a projective space with structure group S^1, and $e^{-i2\pi\tau(\psi)}$ is the holonomy transformation associated with the usual connection given by the parallel transport defined by $\langle\psi(t)|\partial_t\psi(t)\rangle = 0$.

As a consequence, we cannot expect for $\tau(\psi)$ to be an integer for subspaces V of dimension greater than one.

The following theorem characterizes the subspaces V with a finite averaged expected V-return time and gives a formula for this average.
It can be considered as the extension to subspaces of the results given earlier.
A key ingredient will be the determinant $\det \boldsymbol{T}$ of an operator $\boldsymbol{T}$ on V, that is, the determinant of any matrix representation of $\boldsymbol{T}$.

Consider a unitary step U and a finite-dimensional subspace V with spectral measure $\boldsymbol{\mu}(d\lambda)$, Schur function $\boldsymbol{f}(z)$ and first V-return generating function $\hat{\boldsymbol{a}}(z) = z\boldsymbol{f}^{\dagger}(z)$. Then, the following statements are equivalent:

1. All the states of V are V-recurrent with a finite expected V-return time.
2. All the states of V are recurrent with a finite expected return time.
3. $\boldsymbol{\mu}(d\lambda)$ is a sum of finitely many mass points.
4. $\boldsymbol{f}(z)$ is rational inner.
5. $\det \boldsymbol{f}(z)$ is rational inner.

Under any of these conditions, the average of the expected V-return time is

$$s_V \tau(\psi)\, d\psi = \frac{K}{\dim V}$$

with K a positive integer that can be computed equivalently as

$$K = \sum_k \dim(E_k V) = \sum_k \operatorname{rank} \boldsymbol{\mu}(\{\lambda_k\}) = \deg \det \hat{\boldsymbol{a}}(e^{i\theta}), \quad (17)$$

where λ_k are the mass points of $\boldsymbol{\mu}(d\lambda)$, $E_k = E(\{\lambda_k\})$ are the orthogonal projectors onto the corresponding eigenspaces of $U = \int \lambda\, E(d\lambda)$ and $\deg \det \hat{\boldsymbol{a}}(e^{i\theta})$ is the degree of $\det \hat{\boldsymbol{a}}(e^{i\theta})\colon S^1 \to S^1$, i.e. its **winding number**, which coincides with the number of the zeros of $\det \hat{\boldsymbol{a}}(z)$ inside the unit disk, counting multiplicity.

Let us go back to the statement of Niels Bohr.

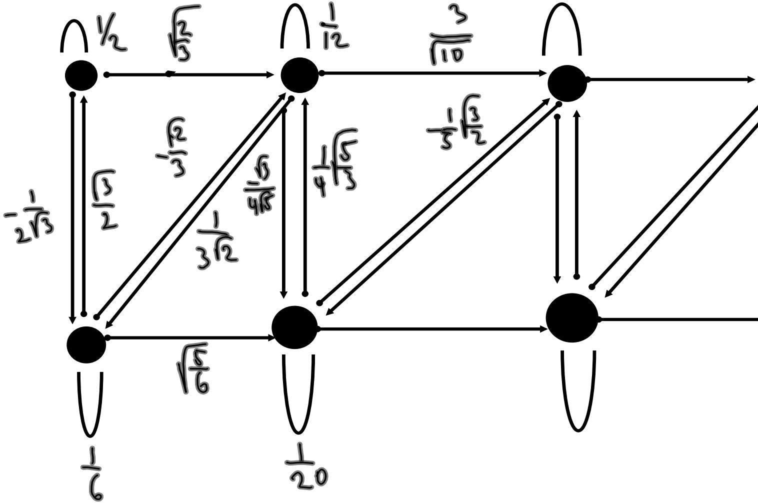
An example of a Quantum walk in the spirit of N. Bohr.

Take for measure on the circle the one with density $1 + cos(\theta)$ (normalized).

Its Verblunsky coefficients are $\alpha_i = (-1)^i/(i+2)$.

The probability (amplitude) of returning to the initial state $|0\rangle \otimes |\uparrow\rangle$ in n steps is 1 for $n = 0$, it is given by $1/2$ for $n = 1$, and equals **ZERO** for all values of $n = 2, 3, 4, ...$

The probability (amplitude) of returning to that same state **FOR THE FIRST TIME** at time n vanishes for $n = 0$ and for $n = 1, 2, 3, ...$ is given by $-(-1/2)^n$.

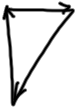


1/2
√(2/3)
1/12
3/√10
-1/(2√3)
√3/2
-√2/3
1/(3√2)
-√3/(4√5)
1/4 √(5/3)
-1/3 √(3/2)
√(5/6)
1/6
1/20

$\mu_0 = 1$

$\mu_1 =$  $= \frac{1}{2}$

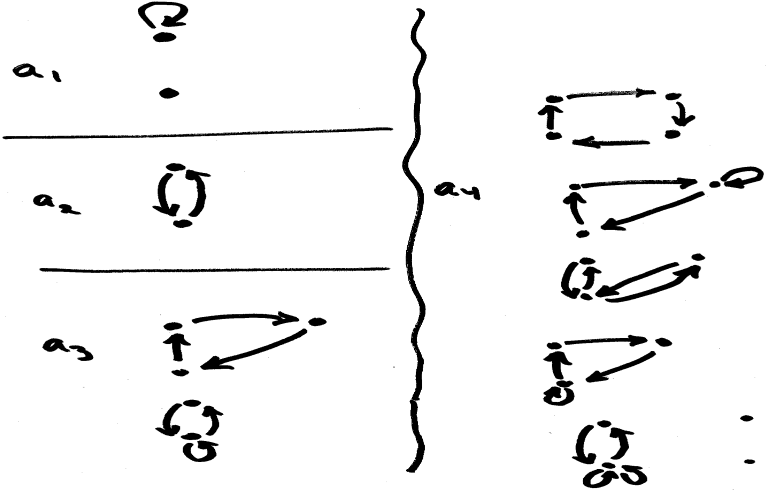
$\mu_2 =$  $+$  $= \frac{1}{4} - \frac{1}{4} = 0$

$\mu_3 =$  $+$  $+$  $+ 2$  $=$

$= \frac{1}{8} - \frac{1}{24} + \frac{1}{6} - \frac{1}{4} = 0$

The probability of eventually returning is $1/3$ and the expected time to return (restricted to the case when the walk returns) is given by $4/9$.

The graphs going with first return amplitudes



with amplitudes given respectively by (the complex conjugates of the expressions)

$$a_1 = \alpha_0,$$

$$a_2 = \rho_0^2 \alpha_1,$$

$$a_3 = \rho_0^2 (\alpha_2 \rho_1^2 - \overline{\alpha}_0 \alpha_1^2),$$

and finally for loops of length 4 we get the amplitude

$$a_4 = \rho_0^2 (\alpha_3 \rho_1^2 \rho_2^2 - \overline{\alpha}_1 \alpha_2^2 \rho_1^2 - 2\alpha_1 \alpha_2 \overline{\alpha}_0 \rho_1^2 + \alpha_1^3 \overline{\alpha}_0^2).$$

One can get another set of examples that might amuse N. Bohr:

one can arrange that the probabilities of a **FIRST RETURN in n STEPS** be non-zero only for $n = 1, 2$ while the probability of a **RETURN in n STEPS** is never zero.

For instance we can have the common value $1/2$ for the first return amplitudes ($n = 1, 2$) and a vanishing value for higher times, and the value $\mu_n = 2/3 + (1/3)(-1/2)^n$ for the return amplitudes ($n = 0, 1, 2, 3, ...$).

The corresponding Verblunsky coefficients are $\alpha_0 = 1/2$ followed by $\alpha_i = 2/(2i + 1)$ for $i = 1, 2, 3, ...$

The measure in question is a delta of strength $2/3$ at $\theta = 0$ plus the density $1/(5 + 4cos(\theta))$.

This example will be SJK recurrent but not GVWW recurrent. The probability of returning to the initial state is $1/4 + 1/4 = 1/2$ and the (restricted) expected time for this return is $3/4$.

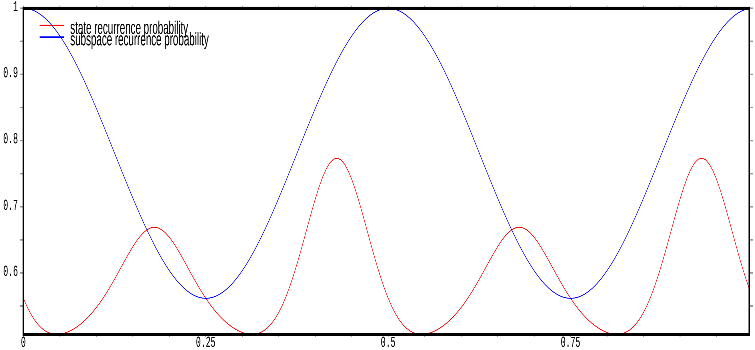
THE RELATION BETWEEN STATE RECURRENCE and SUBSPACE RECURRENCE, in the spirit of N. Bohr

Consider the walk in the non-negative integers with a constant coin given by

$$C = \begin{pmatrix} \sqrt{c} & \sqrt{1-c} \\ \sqrt{1-c} & -\sqrt{c} \end{pmatrix} \tag{18}$$

Comparing two probabilities as a function of the initial state $\cos t\ |0\rangle \otimes |\uparrow\rangle + \sin t\ |0\rangle \otimes |\downarrow\rangle$

Constant coin in the non-negative integers, $c = 6/10$

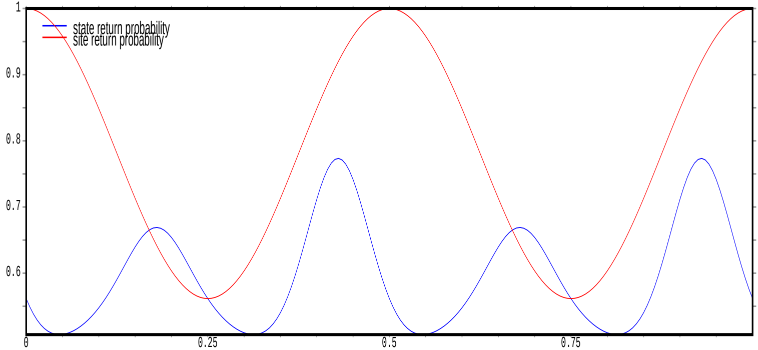


Consider the walk in the non-negative integers with a constant coin given by

$$C = \begin{pmatrix} \sqrt{c} & \sqrt{1-c} \\ \sqrt{1-c} & -\sqrt{c} \end{pmatrix} \tag{19}$$

Comparing two probabilities as a function of the initial state $\cos t\ |0\rangle \otimes |\uparrow\rangle + \sin t\ |0\rangle \otimes |\downarrow\rangle$

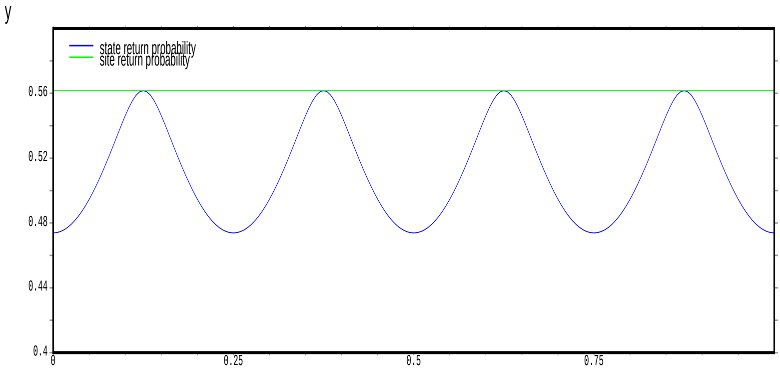
Constant coin in the non-negative integers, $c = 6/10$



Now for the same coin on the integers.

Comparing state and site return probabilities for the one dimensional case as a function of t

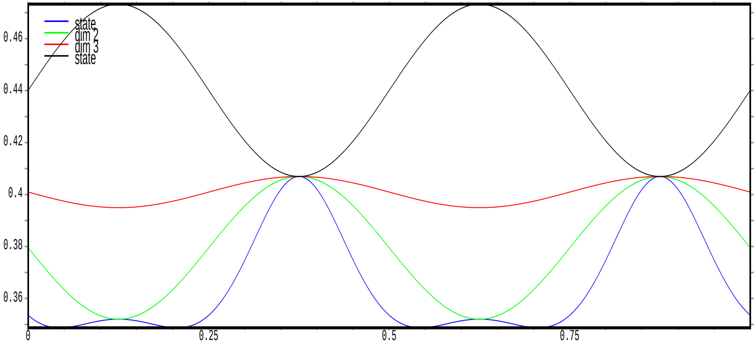
Using complex combinations

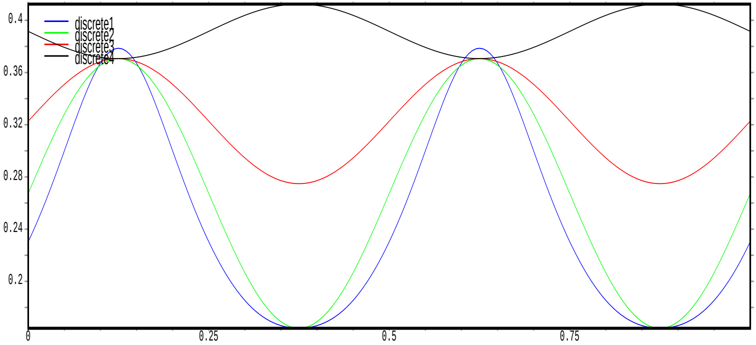


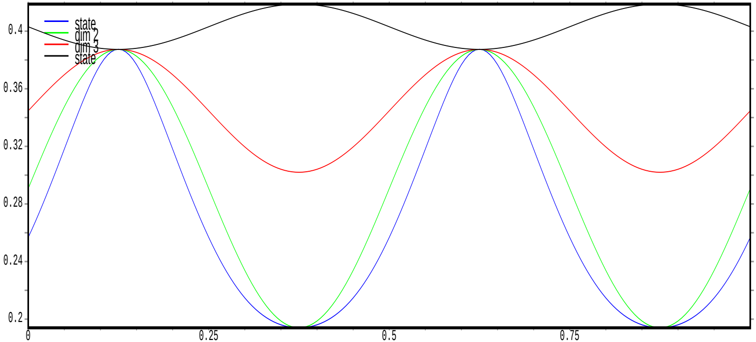
An important point:
One can use the CGMV technology to study (at least some) higher dimensional walks.

This is illustrated below in the case of some well known two dimensional walks.

The next plot involves the 2 dim Grover walk on the square lattice.


state
dim 2
dim 3
state
0.46
0.44
0.42
0.4
0.38
0.36
0
0.25
0.5
0.75


discrete1
discrete2
discrete3
discrete4
0.4
0.36
0.32
0.28
0.24
0.2
0
0.25
0.5
0.75



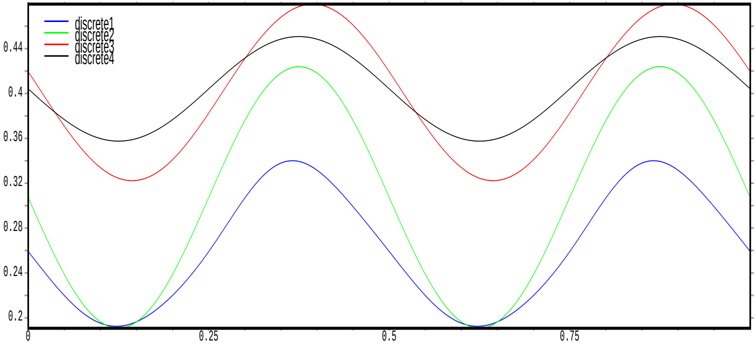
state
dim 2
dim 3
state
0.4
0.36
0.32
0.28
0.24
0.2
0
0.25
0.5
0.75

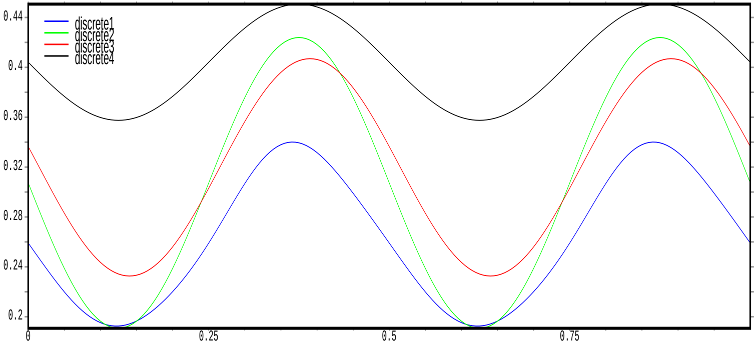
Now the Fourier walk, i.e. the unitary is the DFT for M=4, but the initial state is a combination of spin east, spin north and the third dimension is a combination of spin west and spin south

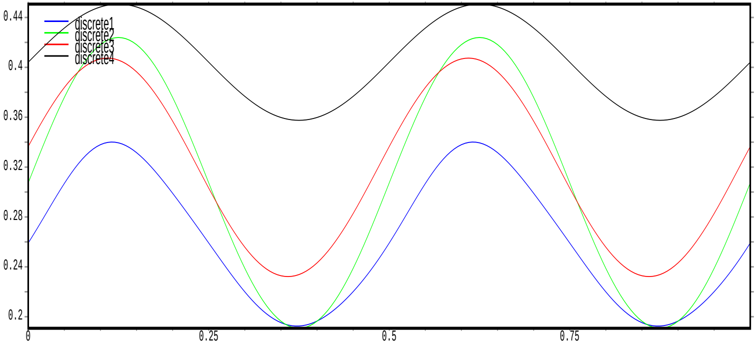
The details of the different four choices are in the next slide.

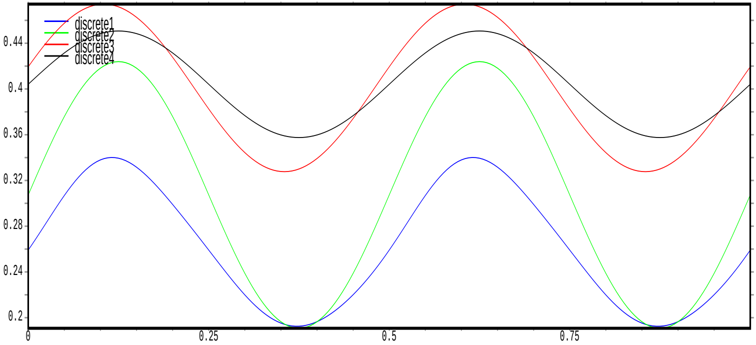
The value of s is (as usual) $s = \pi/4$.

The value of N is $N = 120$.

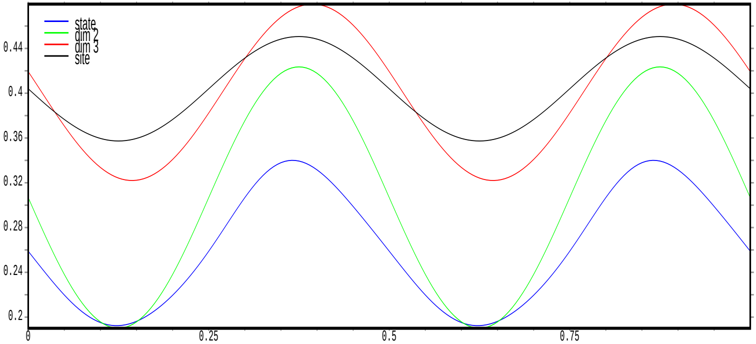

discrete1
discrete2
discrete3
discrete4
0.44
0.4
0.36
0.32
0.28
0.24
0.2
0
0.25
0.5
0.75


discrete1
discrete2
discrete3
discrete4
0.44
0.4
0.36
0.32
0.28
0.24
0.2
0
0.25
0.5
0.75

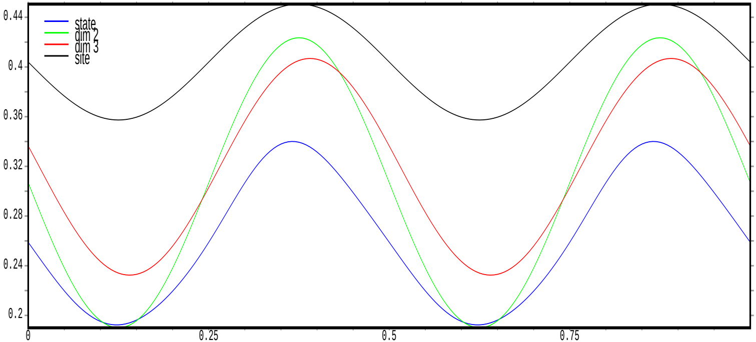

discrete1
discrete2
discrete3
discrete4
0.44
0.4
0.36
0.32
0.28
0.24
0.2
0
0.25
0.5
0.75

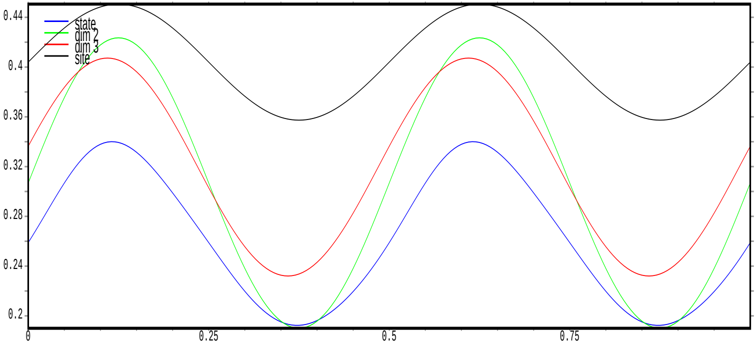

discrete1
discrete2
discrete3
discrete4
0.44
0.4
0.36
0.32
0.28
0.24
0.2
0
0.25
0.5
0.75

The next 4 Fourier two dimensional walks are the same as the ones above, BUT $N = 80$ and the legends are ok.

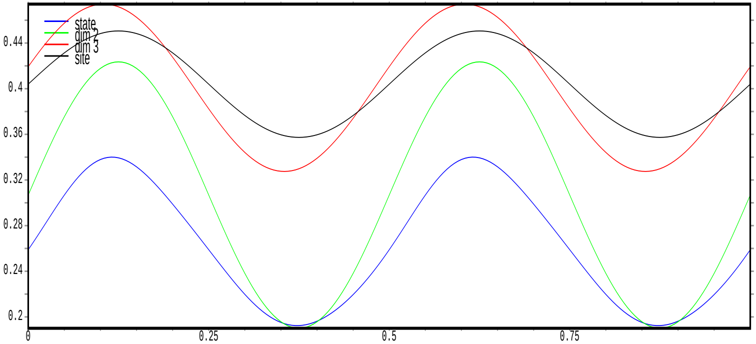


state
dim 2
dim 3
site
0.44
0.4
0.36
0.32
0.28
0.24
0.2
0
0.25
0.5
0.75


0.44
0.4
0.36
0.32
0.28
0.24
0.2
0
0.25
0.5
0.75
state
dim 2
dim 3
site



state
dim 2
dim 3
site
0.44
0.4
0.36
0.32
0.28
0.24
0.2
0
0.25
0.5
0.75

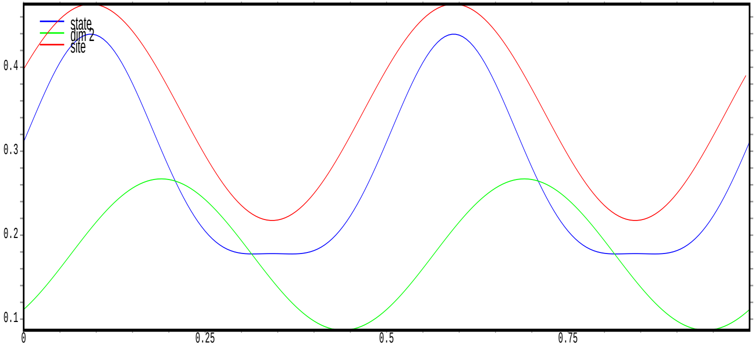


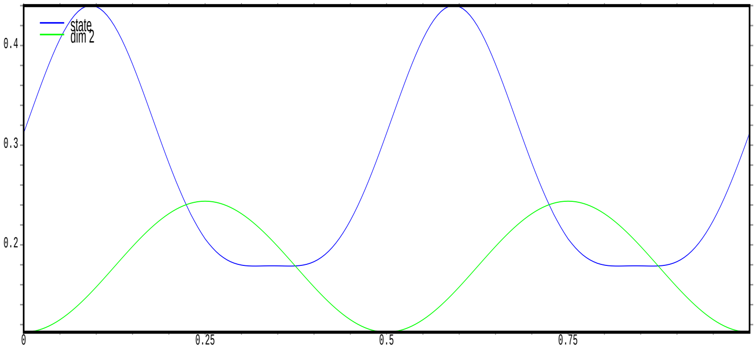
state
dim 2
dim 3
site
0.44
0.4
0.36
0.32
0.28
0.24
0.2
0
0.25
0.5
0.75

Here is one example on an **HEXAGONAL LATTICE**, the coin is the **DFT**$_3$.

The value of N **is** $N = 30$ **and the initial state is given by**

$1/sqrt(2)cost[1, 0, (1 + i)/sqrt(2)] + isint[0, 1, 0]$

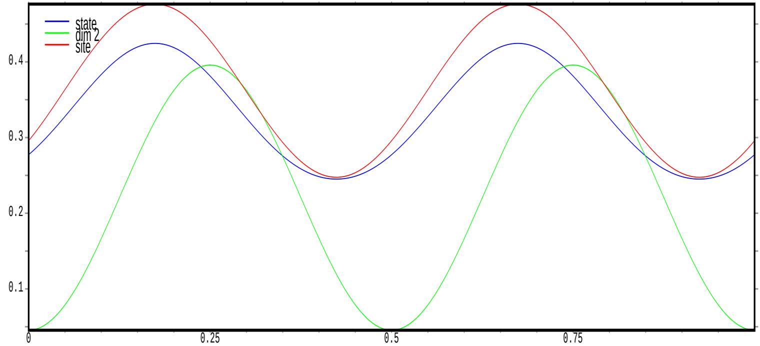

state
dim 2
site
0.4
0.3
0.2
0.1
0
0.25
0.5
0.75



state
dim 2
0.4
0.3
0.2
0
0.25
0.5
0.75

With the same crazy state as in the previous hexagonal case, we do Grover.

We choose $N = 60$.


state
dim 2
site
0.4
0.3
0.2
0.1
0
0.25
0.5
0.75