Recurrence properties of Quantum Walks

F. Alberto Grünbaum

Math. Dept , UC Berkeley

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Thanks!!! and apologies...

A plan for the talk

Recurrence for discrete time unitary evolutions CMP **320** 2013 pp-543-569. F.A. Grünbaum, L. Velazquez, A. Werner and R. Werner.

Quantum recurrence of a subspace and operator valued Schur functions CMP (published online Mar 19 2014) J. Bourgain, F.A. Grünbaum, L. Velazquez and J. Wilkening

Ask the audience for help with a few questions about the literature.

In the case of classical random walks the notion of recurrence goes back at least to Polya (1921).

In the case of Quantum walks a definition has been proposed by M. Stefanak, T. Kiss and I. Jex in 2008. This definition has been used by several workers in the area of Quantum walks.

We introduce a **different** notion of recurrence which brings lots of classical analysis into use.

We consider discrete time quantum dynamical systems specified by a unitary operator U and an initial state vector 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.

In the presence of recurrence we study the distribution of the "first arrival time" , showing that (rather surprinsingly) its **EXPECTED VALUE** is always an **INTEGER** (or infinite) for which we give a topological interpretation.

A key role in our theory is played by the first arrival amplitudes, which turn out to be the (complex conjugated) Taylor coefficients of the Schur function of the spectral measure. This provides a dynamical interpretation for these quantities, which appears to be new.

These terms will be defined below.

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.

Equally important is the fact that natural questions from the point of view of quantum walks lead to apparently open problems in the beautiful line of work started a long time ago by people like I. Schur and earlier workers.

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)

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

$$\mu_n = \int \mu(du)\ u^n = \langle \phi | U^n \phi \rangle, \quad n \in \mathbb{Z}. \tag{1}$$

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.

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.

We will see later that there are ways of writing down the Schur function that connects it with notions that have appeared in other fields with names such as "characteristic function" or "transfer function" going back to work of people like Livsic, Brodskii, Sz-Nagy, Foias, Lax-Phillips, etc. etc.

A very important fact is that $f(z)$ is INNER, i.e. the limiting values of its modulus on the unit circe 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.

I will be asking later for extensions of this result in the case of operator valued Schur functions associated to a subspace, in particular in the case of infinite dimensional subspaces.

Now we concentrate on our definition of recurrence for a general Quantum walk , i.e. the recent work with Velazquez, Werner and Werner. GVWW

We consider quantum dynamical systems specified by a unitary operator U and an initial state vector 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.

Immediately, this presents us with a problem, which is typical for many generalizations of classical concepts to the quantum world: The definition as given for Markov chains clearly requires some **MONITORING** of the process: we have to check after every step whether the particle has returned. But this monitoring, if it is to give any non-trivial information about the system, necessarily changes the dynamics. Therefore, there are two options: We can either try to reformulate the problem in such a way that the monitoring is not needed, or else we include the monitoring into the description.

The main difference between the approach of Stefanak, T. Kiss and I. Jex (SJK,2008) and the one of Grünbaum, Velazquez, Werner and Werner (GVWW,2012) is that the first one avoids monitoring while ours take monitoring into account explicitly.

GVWW recurrence

$$\widetilde{U} = (\mathbb{I} - |\phi\rangle\langle\phi|)U. \tag{4}$$

$$a_n = \langle\phi|U\widetilde{U}^{n-1}\phi\rangle, \quad n \geq 1. \tag{5}$$

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

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

The *return probability* is therefore

$$R = \sum_{n=1}^{\infty} |a_n|^2 = 1 - \lim_{n \to \infty} \|\widetilde{U}^n \phi\|^2. \tag{6}$$

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

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

$$\widehat{\mu}(z) = \sum_{n=0}^{\infty} \mu_n z^n = \int \frac{\mu(dt)}{1 - tz}, \tag{7}$$

We get

$$\begin{aligned}
\widehat{a}(z) &= \sum_{n=1}^{\infty} ff_n z^n = \sum_{n=0}^{\infty} \langle \phi | U \widetilde{U}^n \phi \rangle z^{n+1} \\
&= \frac{\widehat{\mu}(z) - 1}{\widehat{\mu}(z)} && (8) \\
&= z \, \overline{f}(z). && (9)
\end{aligned}$$

We use the convention that, for an analytic function g, the analytic function with the conjugated Taylor coefficients is denoted by $\overline{g}$, i.e., $\overline{g}(z) = \overline{g(\overline{z})}$.

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

The expected value for the first return time: a topological interpretation in terms of the Schur function

$$\tau = \sum_{n=1}^{\infty} |a_n|^2 \, n. \tag{10}$$

$$g(t) = e^{it}\overline{f}(e^{it}) = \sum_{n=1}^{\infty} a_n e^{int} \tag{11}$$

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. Locally we can write $g(t) = \exp(i\gamma(t))$, so the angular velocity is

$$\partial_t \gamma(t) = \frac{\partial_t g(t)}{ig(t)} = \overline{g(t)} \, \frac{1}{i} \, \partial_t g(t). \tag{12}$$

Integrating this over one period $t \in [0, 2\pi]$, we get $2\pi w(g)$, so

$$w(g) = \frac{1}{2\pi} \int_0^{2\pi} dt \, \overline{g(t)} \, \frac{1}{i} \, \partial_t g(t) = \sum_{n=0}^{\infty} \overline{a_n} \, (n a_n) = \tau. \tag{13}$$

When is the pair (U, ϕ) recurrent according to the GVWW definition?

Decompose the scalar valued orthogonality measure into its singular and its absolutely continuous parts.

If the second one is missing, and only then, the process is GVWW recurrent.

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

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

$$\mu_n = \bar{a}_n + \bar{a}_{n-1}\mu_1 + \cdots + \bar{a}_1\mu_{n-1}$$

Here a_n denote the Taylor coefficients of $zf(z)$ and μ_n are the moments of the measure.

This is a quantum analog of the renewal equation that one has in the classical case.

A challenge:

Does the factorization into inner-outer functions have any probabilistic interpretation?

Before going much further, recall...

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

Niels Bohr

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.

We emphasize the difference between the **first** V-return probabilities and the quantities $\|PU^n\psi\|^2$, which also represent the probability of finding the system in the subspace V, but performing the projective measurement only in the n-th step, i.e. without any intermediate monitoring of the process. To distinguish both kind of probabilities we will refer to $\|PU^n\psi\|^2$ as the *n-step V-return probability* of ψ.

First V-return probabilities and V-return probabilities can be written as $\|\boldsymbol{a}_n\psi\|^2$ and $\|\boldsymbol{\mu}_n\psi\|^2$ respectively, where $\boldsymbol{a}_n$ and $\boldsymbol{\mu}_n$ are the operators on V given by

$$\begin{aligned} \boldsymbol{a}_n &= PU\tilde{U}^{n-1}P && \textit{n-step first } V\textit{-return amplitude operator},\\ \boldsymbol{\mu}_n &= PU^nP && \textit{n-step } V\textit{-return amplitude operator}. \end{aligned} \tag{14}$$

Connections with transfer functions, characteristic functions, etc.

The values of μ_V, F_V and f_V must be considered as operators on V so that, for instance, $F_V(0)$ is the identity operator on V. From the spectral decomposition of U we find that the the moments of a spectral measure provide the power expansion of the corresponding U-Carathéodory function,

$$F_V(z) = P(U + z\mathbf{1}_H)(U - z\mathbf{1}_H)^{-1}P.$$

The analog of this result for the power expansion of U-Schur functions is not so trivial and was obtained recently. It states that

$$f_V(z) = P(U - z\tilde{P})^{-1}P = \sum_{n \geq 1} a^{\dagger}_{V,n} z^{n-1}, \qquad a_{V,n} = PU(\tilde{P}U)^{n-1}P, \tag{15}$$

This expression reveals a connection with the "transfer or characteristic function" of Livsic and other authors.

Following the quantum terminology, we will refer to the operator coefficients $a_{V,n}$ as the first return amplitudes of V. The generating function of these amplitudes

$$a_V(z) = \sum_{n\geq 1} a_{V,n} z^n = zUP(\mathbf{1}_V - z\tilde{P}U)^{-1}P = zf_V^\dagger(z), \qquad g^\dagger(z) = g(\overline{z})^\dagger, \tag{16}$$

will be called the first return generating function of V.

A very important quantum mechanical role is played by a certain type of factorization of unitaries, of which I show an example below.

$$\begin{pmatrix} \frac{-1}{3} & \frac{2}{3} & \frac{-1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{2}{3} & \frac{-1}{3} & \frac{-1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{2}{3} & \frac{2}{3} & \frac{1}{6} & \frac{-1}{6} & \frac{-1}{6} & \frac{-1}{6} \\ 0 & 0 & \frac{1}{2} & \frac{-1}{2} & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{-1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{-1}{2} \end{pmatrix} = \begin{pmatrix} \frac{-1}{3} & \frac{2}{3} & \frac{2}{3} & 0 & 0 & 0 \\ \frac{2}{3} & \frac{-1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ \frac{2}{3} & \frac{2}{3} & \frac{-1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{-1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{-1}{2} & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{-1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{-1}{2} \end{pmatrix},$$

show "overlapping factorizations".

A question for the audience:

Does this kind of overlapping factorization show up in other areas?

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

$$\tau(\psi) = \int_0^{2\pi} \langle \psi(\theta) | \partial_\theta \psi(\theta) \rangle \, \frac{d\theta}{2\pi i}, \qquad \psi(\theta) = \hat{\boldsymbol{a}}(e^{i\theta})\psi, \tag{17}$$

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 $\hat{a}_\psi(e^{i\theta})$: $S^1 \to S^1$, 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

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

with K a positive integer that can be computed equivalently as

$$K = \sum_k \dim(E_k V) = \sum_k rank\, \boldsymbol{\mu}(\{\lambda_k\}) = \deg \det \hat{\mathbf{a}}(e^{i\theta}), \qquad (18)$$

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 $\deg \det \hat{\mathbf{a}}(e^{i\theta})$ is the degree of $\det \hat{\mathbf{a}}(e^{i\theta})\colon S^1 \to S^1$, i.e. its **winding number**, which coincides with the number of the zeros of $\det \hat{\mathbf{a}}(z)$ inside the unit disk, counting multiplicity.

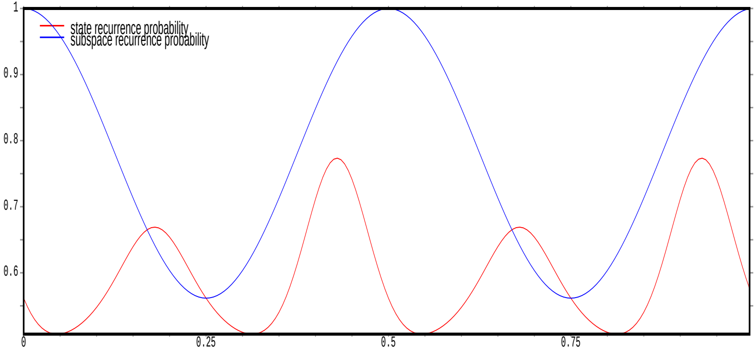
THE RELATION BETWEEN STATE RECURRENCE and SUBSPACE RECURRENCE, in the spirit of N. Bohr

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

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

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

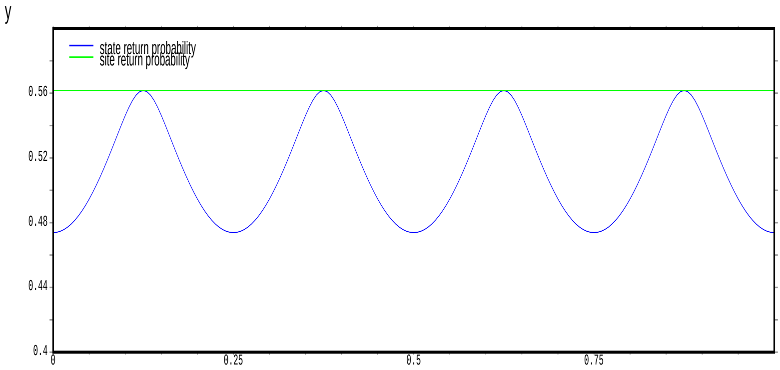
Constant coin in the non-negative integers, $c = 6/10$



Now for the same coin on the integers.

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

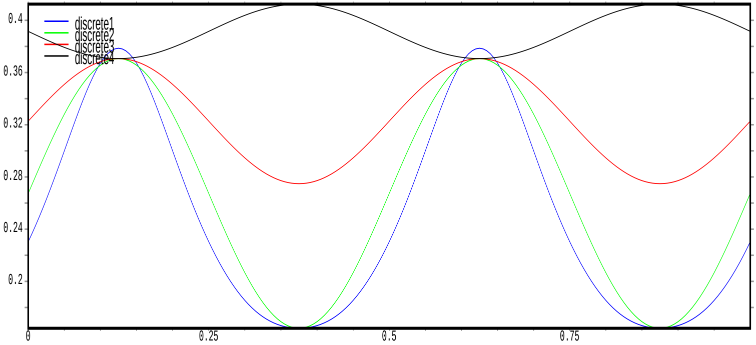
Using complex combinations



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.

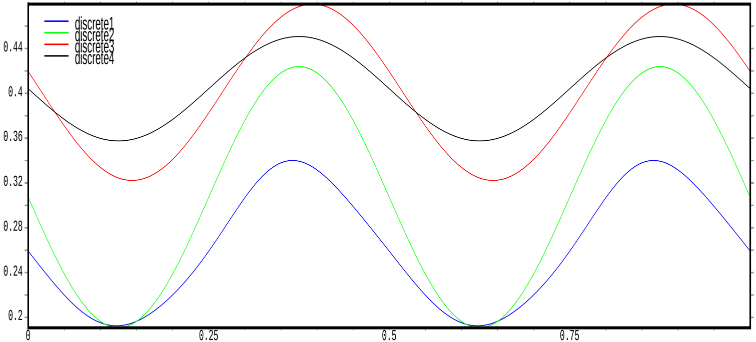

discrete1
discrete2
discrete3
discrete4
0.4
0.36
0.32
0.28
0.24
0.2
0
0.25
0.5
0.75

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
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discrete4
0.44
0.4
0.36
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0.28
0.24
0.2
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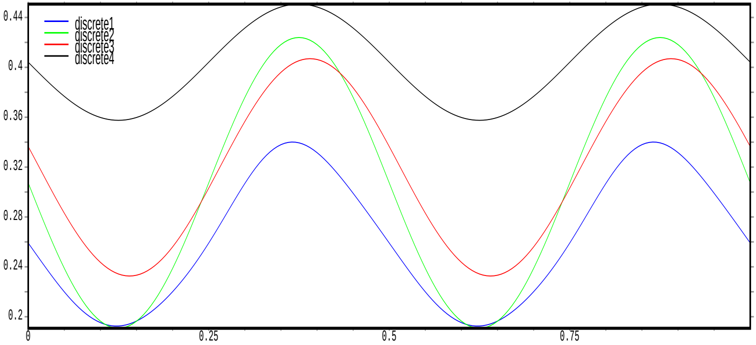
0.25
0.5
0.75

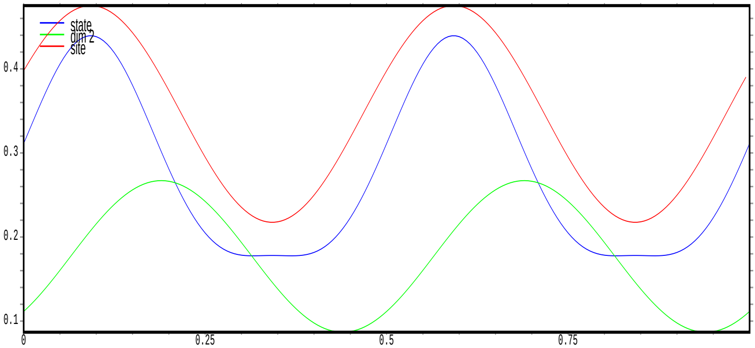


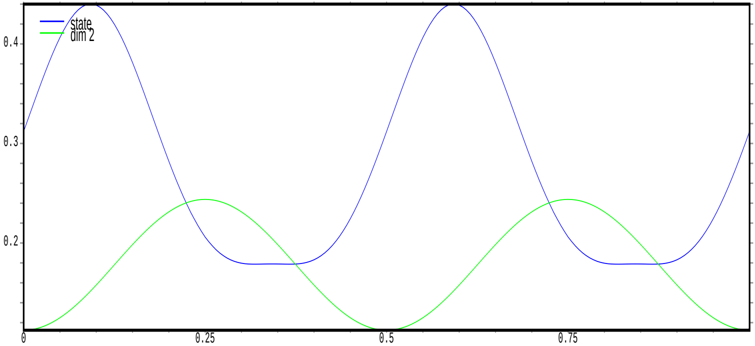
0.44
0.4
0.36
0.32
0.28
0.24
0.2
0
0.25
0.5
0.75
discrete1
discrete2
discrete3
discrete4

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

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

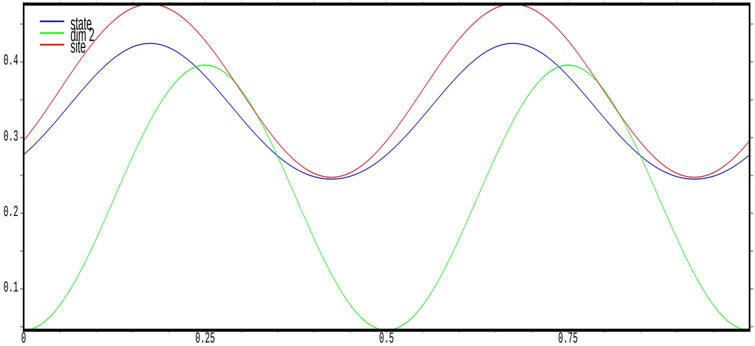
$1/sqrt(2)cost[1, 0, (1 + i)/sqrt(2)] + isint[0, 1, 0]$


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