Quantum recurrence and matrix Schur functions

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Recurrence and expected return time

A key concept in the study of random processes is the idea of **recurrence**.

A random process is recurrent if it returns to the initial state with probability one. Otherwise it is called transient.

In principle the recurrence of a random process could depend on the initial state, so we should talk about recurrent or transient states for a given random system.

Recurrent states can have different return speeds, which can be measured by the **expected return time**.

Recurrent states can have a finite or infinite expected return time. The last ones are the recurrent states which are closest to the transience.

Random Walks: Pólya recurrence

RW = discrete classical random process $\rightsquigarrow$ discrete-time Markov chain on a countable state space X

- **Transition matrix** $P = (P_{x,y})_{x,y \in X}$ $\quad P_{x,y} \geq 0$ $\quad \sum_{y \in X} P_{x,y} = 1$

  $P_{x,y}$ = probability of transition $x \to y$ in one step

- **Return probability in n steps**

$$p_n = p_n^{(x)} = \sum_{x_1,\dots,x_{n-1}} P_{x,x_1} P_{x_1,x_2} \cdots P_{x_{n-1},x} = (P^n)_{x,x}$$

- **First time return probability in n steps**

$$q_n = q_n^{(x)} = \sum_{x_1,\dots,x_{n-1} \neq x} P_{x,x_1} P_{x_1,x_2} \cdots P_{x_{n-1},x}$$

$$q = \sum_{n=1}^{\infty} q_n$$

Total return probability *(Pólya number)*

x **is recurrent** $\Leftrightarrow$ $q = 1$

$$\tau = \sum_{n=1}^{\infty} n q_n$$

Expected return time

Random Walks: Pólya recurrence

The study of recurrence is greatly aided by the use of **generating functions**

$$p(z) = \sum_{n=0}^{\infty} p_n z^n \qquad\qquad q(z) = \sum_{n=1}^{\infty} q_n z^n$$

A key result relates the first return prob. q_n to the more accesible return prob. p_n

$$q(z) = 1 - \frac{1}{p(z)}$$ **Renewal equation**

This allows us to rewrite the recurrence notions in terms of p_n instead of q_n

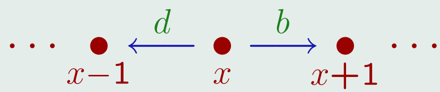
$$q = \sum_{n=1}^{\infty} q_n = q(1) = 1 - \frac{1}{p(1)}$$ *Pólya number*

$$x \textbf{ is recurrent} \quad \Leftrightarrow \quad \sum_{n=0}^{\infty} p_n = \infty$$

$$\tau = \sum_{n=1}^{\infty} n q_n = q'(1) = \lim_{z \to 1} \frac{p'(z)}{p(z)^2}$$ **Expected return time**

Example: Translation invariant birth-death process

$X = \mathbb{Z}$

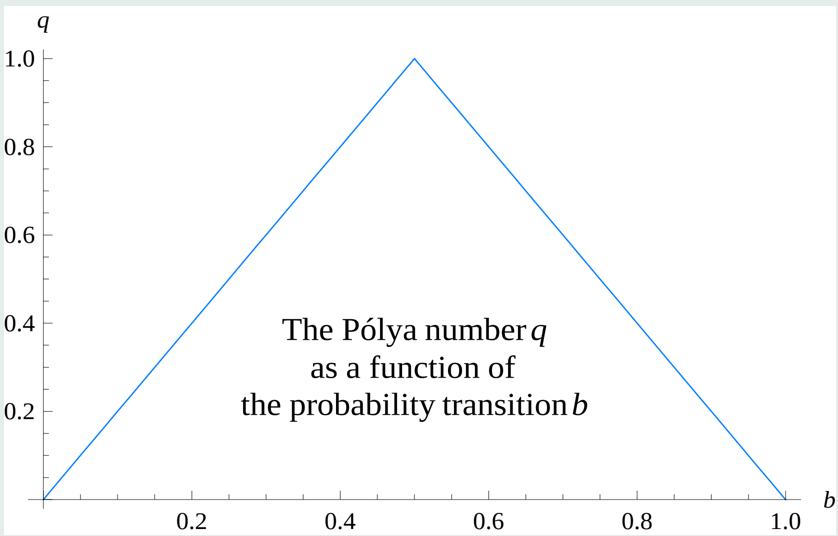


$b, d > 0$

$b + d = 1$

In this case explicit results are available, giving for any state x

$$p(z) = \frac{1}{\sqrt{1 - 4bdz^2}} \qquad q = 1 - \sqrt{1 - 4bd}$$



All the states are recurrent if $b = d = \frac{1}{2}$ and transient otherwise

Random Walks: Spectral characterization of recurrence

For **reversible** Markov chains the transition matrix P is **symmetrizable** $\xrightarrow{\text{spectral theory}}$

For any state $x \in X$ there exists a **spectral measure** m_x on $[-1, 1]$ such that

$$n\text{-th moment} \quad \int_{-1}^{1} t^n \, dm_x(t) \;=\; (P^n)_{x,x} \quad \text{return prob. of } x \text{ in } n \text{ steps}$$

This allows us the use of spectral techniques for RW, but also provides a link to the machinery of orthogonal polynomials on $\mathbb{R}$.

How is the recurrence of a state x codified in its spectral measure $m = m_x$**?**

$$x \textbf{ is recurrent} \;\Leftrightarrow\; \int_{-1}^{1} \frac{dm(t)}{1-t} = \infty$$

$$\tau = \frac{1}{m(\{1\})} \qquad \textbf{Expected return time}$$

Finite expected return time $\Leftrightarrow$ 1 **is a mass point**

Quantum Walks: Why?

- What is a QW? Simplified model of a **quantum system in evolution**
- Why are QW important? Simplest setting to study the quantum behaviour:
  - **Superposition:** quantum systems can be simultaneously in different states
  - **Parallelism:** quantum systems may spread much faster than classical ones
  - **Entanglement:** quantum systems arbitrarily far from each other can be linked

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	RW	**QW**
Randomness	Ignorance	Intrinsic
States	$\nexists$ superposition	$\exists$ superposition
Evolution	Markov process	Unitary process
Measurement	Does not disturb evolution	Projection which alter evolution
Methods	Path counting Fourier analysis Spectral self-adjoint - OP line	Path counting Fourier analysis Spectral unitary - OP circle

Quantum Walks

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- $\|\psi\|^2 = \sum_{x\in X} |c_x|^2 = \text{Prob}(X) = 1 \quad \Rightarrow \quad \psi$ must be unitary**!**

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The non trivial geometry of the state space has measurable consequences!

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- **Evolution = Unitary operator**

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$$\text{Prob} = |\text{amplitude}|^2$$

Quantum Walks: Recurrence

Given a unitary step U and an initial state ψ we search for the return probability to ψ

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- **First time return amplitude in n steps** $\quad a_n^\psi = \langle \psi | U(QU)^{n-1} \psi \rangle \quad \rightsquigarrow \quad \text{Prob}(\psi \xrightarrow[1^{\text{st}} \ \textbf{time}]{n \ \textbf{steps}} \psi) = |a_n^\psi|^2$

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$$R_\psi = \sum_{n=1}^{\infty} |a_n^\psi|^2 \qquad \textbf{Total return probability}$$

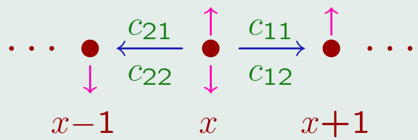
$$\psi \textbf{ is recurrent} \quad \Leftrightarrow \quad R_\psi = 1$$

$$\tau_\psi = \sum_{n=1}^{\infty} n|a_n^\psi|^2 \qquad \textbf{Expected return time}$$

Example: Translation invariant coined walk

Consider a particle with *spin* in an infinite 1D lattice with the one-step amplitudes

$X = \mathbb{Z} \times \{\uparrow, \downarrow\}$



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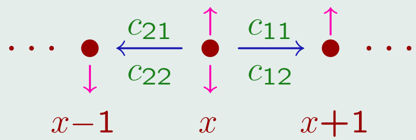

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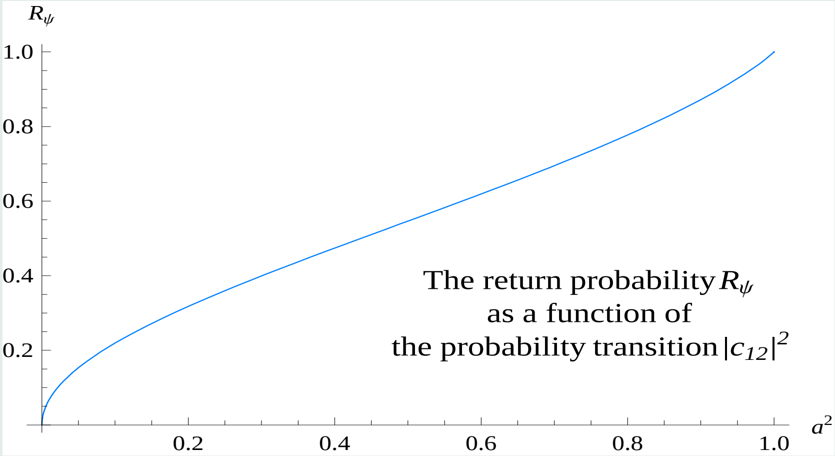
Explicit calculations are possible, giving for any basis state $\psi = |x, \uparrow\rangle,\ |x, \downarrow\rangle$

$$R_\psi = \frac{(1+2\rho^2)\rho a + (1-4\rho^2)\arcsin a}{\frac{\pi}{2} a^4} \qquad \begin{bmatrix} a = |c_{12}| \\ \rho = \sqrt{1-a^2} \end{bmatrix}$$



In contrast to the classical case, no recurrent states appear

Quantum Walks: Spectral characterization of recurrence

In contrast to the classical case the transition matrix U is always unitary $\xrightarrow{\text{spectral theory}}$

For any state $\psi \in \mathcal{H}$ there exists a **spectral measure** μ_ψ on $\mathbb{T} \equiv |z| = 1$ such that

n-th moment $\int_{\mathbb{T}} t^n \, d\mu_\psi(t) = \langle \psi | U^n \psi \rangle = \mu_n^\psi$ return amplitude to ψ in n steps

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$$S_\psi(z) = \sum_{n=0}^{\infty} \mu_n^\psi z^n = \int_{\mathbb{T}} \frac{d\mu_\psi(t)}{1 - tz}$$

Stieltjes function of μ_ψ

$$g_\psi(z) = \sum_{n=1}^{\infty} a_n^\psi z^n$$

???

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$$g_\psi(z) = \sum_{n=1}^{\infty} a_n^\psi z^n = z\overline{f_\psi}(z) \qquad f_\psi(z) = \textbf{Schur function of } \mu_\psi\textbf{!}$$

A Schur function is a function $f\colon \mathbb{D} \longrightarrow \overline{\mathbb{D}}$ analytic on the unit disk $\mathbb{D} \equiv |z| < 1$

Quantum Walks and Schur functions

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They are in one-to-one correspondence with the measures μ on the unit circle $\mathbb{T}$ via

$$f(z) = \frac{1}{z}\frac{F(z)-1}{F(z)+1} \qquad F(z) = \int_{\mathbb{T}} \frac{t+z}{t-z}\, d\mu(t)$$

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Schur Taylor coefficients = First time return amplitudes of QW

The identification of $g_\psi(z) = z\overline{f_\psi}(z)$ as a Schur function is a consequence of

$$g_\psi(z) = 1 - \frac{1}{S_\psi(z)}$$

Quantum renewal equation

Like the classical one!
But for amplitudes instead of probabilities

and is KEY for the spectral analysis of quantum recurrence

Quantum Walks: Spectral characterization of recurrence

Denoting $\langle f,g\rangle = \int_0^{2\pi} \overline{f(e^{i\theta})}\, g(e^{i\theta})\, \frac{d\theta}{2\pi}$ and $\|\cdot\|$ the corresponding norm:

Unitary step U, state ψ $\longrightarrow$ Measure μ_ψ $\longrightarrow$ Schur function f_ψ

$$g_\psi(z) = z\overline{f_\psi}(z) = \sum_{n=1}^{\infty} a_n^\psi z^n$$

Generating function of **first time return amplitudes** a_n^ψ

$$R_\psi = \sum_{n=1}^{\infty} |a_n^\psi|^2 = \|g_\psi\|^2 = \|f_\psi\|^2$$

Total return probability

ψ **is recurrent** $\Leftrightarrow$ $\|f_\psi\| = 1$ $\Leftrightarrow$ $|f_\psi| = 1$ a.e. in $\mathbb{T}$ $\Leftrightarrow$ μ_ψ **is singular**
(f_ψ **is inner**)

$$\tau_\psi = \sum_{n=1}^{\infty} n|a_n^\psi|^2 = \frac{1}{i}\lim_{r\to 1} \langle g_\psi(re^{i\theta}), \partial_\theta g_\psi(re^{i\theta})\rangle = \sharp\, \mathrm{supp}\, \mu_\psi$$

Expected return time

CONSEQUENCES

- The **recurrent states** constitute the **singular subspace** of the unitary step U. Thus, an a.c. spectrum for U is equivalent to the absence of recurrent states.

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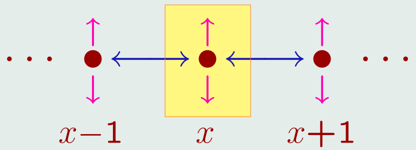
- **Quantum recurrence paradox 1**
  First time return probabilities can be higher than return probabilities **!!!**
  Nothing prevents $|a_n^\psi|^2 > |\mu_n^\psi|^2$. Indeed, there exist QW with a state ψ such that $a_n^\psi \neq 0$ for all n, but $\mu_n^\psi = 0$ for $n \geq 3$.

Quantum Walks: Subspace recurrence

Example Given a state $\psi = \alpha|x,\uparrow\rangle + \beta|x,\downarrow\rangle$ of a coined walk we can be interested in the return probability to the whole site x (instead of to the single state ψ), i.e. the return probability to the subspace span$\{|x,\uparrow\rangle, |x,\downarrow\rangle\}$



These kind of questions, so natural as the previous ones, lead to the notion of *subspace recurrence* as a generalization of the *state recurrence* already analyzed.

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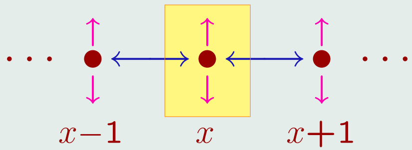

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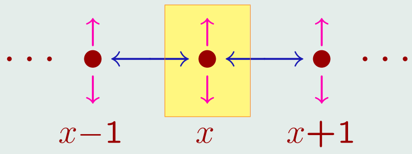

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A precise expression of the **total return probability to** V can be obtained following an approach similar to the case $\dim V = 1$. This simply requires the substitutions

$$\text{Projector onto } \psi \quad \longrightarrow \quad P = \text{Projector onto } V$$

$$\text{Projector onto } \psi^\perp \quad \longrightarrow \quad Q = \text{Projector onto } V^\perp$$

which account for the possible collapses when checking the return to V (instead of ψ).

Quantum Walks: Subspace recurrence

Remind that for state recurrence

- **Return amplitude in n steps** $\quad \mu_n^\psi = \langle\psi|U^n\psi\rangle \quad \rightsquigarrow \quad \text{Prob}(\psi \xrightarrow{n \text{ steps}} \psi) = |\mu_n^\psi|^2$

- **First time return amplitude in n steps** $\quad a_n^\psi = \langle\psi|U(QU)^{n-1}\psi\rangle \quad \rightsquigarrow \quad \text{Prob}(\psi \xrightarrow[1^{\text{st}} \text{ time}]{n \text{ steps}} \psi) = |a_n^\psi|^2$

Quantum Walks: Subspace recurrence

In the case of subspace recurrence

- **Return amplitude in n steps** $\quad \boldsymbol{\mu}_n^V = PU^nP \quad \rightsquigarrow \quad \text{Prob}(\psi \xrightarrow{n \text{ steps}} V) = \|\boldsymbol{\mu}_n^V \psi\|^2$
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$$R_V(\psi) = \sum_{n=1}^{\infty} \|\boldsymbol{a}_n^V \psi\|^2$$ **Total V-return probability**

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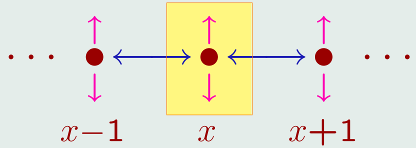
We can rewrite $R_V(\psi) = \langle \psi | \boldsymbol{R}_V \psi \rangle$ as a quadratic form in V giving by

$$\boldsymbol{R}_V = \sum_{n=1}^{\infty} (\boldsymbol{a}_n^V)^\dagger \boldsymbol{a}_n^V$$

Example: Site recurrence in a translation invariant coined walk

Consider the site subspace $V_x = \mathrm{span}\{|x,\uparrow\rangle, |x,\downarrow\rangle\}$ in the previous 1D model

$X = \mathbb{Z} \times \{\uparrow, \downarrow\}$



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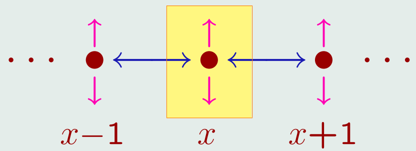
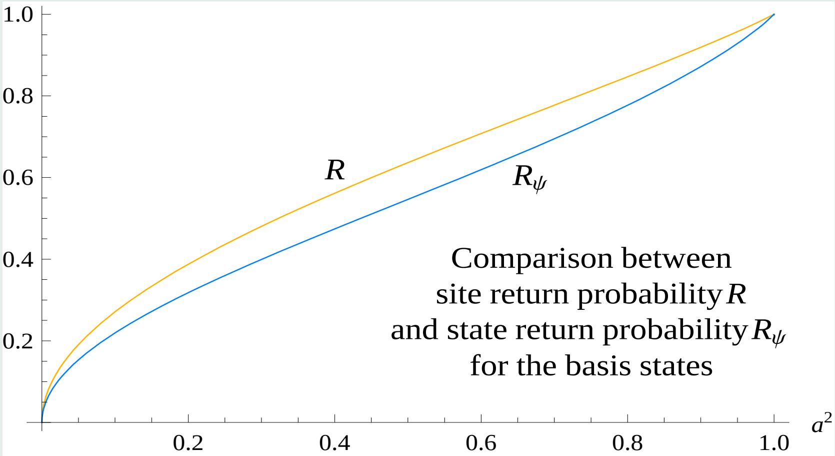


$C = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}$ unitary *coin*

$\boldsymbol{R}_{V_x} = \begin{pmatrix} R & 0 \\ 0 & R \end{pmatrix}$ is a scalar matrix with $R = \dfrac{\rho a + (1-2\rho^2)\arcsin a}{\frac{\pi}{2}a^2}$ $\left[\begin{array}{l} a = |c_{12}| \\ \rho = \sqrt{1-a^2} \end{array}\right]$



Comparison between state and site recurrence for $\psi = |x,\uparrow\rangle, |x,\downarrow\rangle$

Note that $R_\psi \leq R = R_{V_x}(\psi)$ as one should naively expect

The spectral characterization of subspace recurrence requires the association of a matrix measure and a matrix Schur function with each subspace.

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As in the case of a single state, the unitarity of U ensures for any subspace $V \subset \mathcal{H}$ the existence of a **spectral matrix measure** $\boldsymbol{\mu}_V$ on $\mathbb{T}$ such that

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This allows to associate with V a **matrix Schur function** $\boldsymbol{f}_V$

$$\boldsymbol{f}_V(z) = z^{-1}(\boldsymbol{F}_V(z) - I)(\boldsymbol{F}_V(z) + I)^{-1} \qquad \boldsymbol{F}_V(z) = \int_{\mathbb{T}} \frac{t+z}{t-z} \, d\boldsymbol{\mu}_V(t)$$

which is analytic on the unit disk $\mathbb{D}$ and satisfies $\|\boldsymbol{f}_V\| \leq 1$ in $\mathbb{D}$.

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The theory of matrix Schur functions, linked to the matrix version of OP on $\mathbb{T}$, has experienced a strong development influenced by the needs of electrical engineering, signal transmission and processing, prediction theory for stochastic processes, ...

A list to which we should add from now the issue of recurrence in QW:
Matrix Schur functions are the math objects which best codify **subspace** recurrence.

Quantum Walks: Spectral characterization of subspace recurrence

Denoting $\langle\!\langle \boldsymbol{f}, \boldsymbol{g} \rangle\!\rangle = \int_0^{2\pi} \boldsymbol{f}(e^{i\theta})^\dagger \boldsymbol{g}(e^{i\theta}) \frac{d\theta}{2\pi}$ and $|\!|\!| \cdot |\!|\!|$ the corresponding matrix "norm":

Unitary step U, subspace V $\longrightarrow$ Matrix measure $\boldsymbol{\mu}_V$ $\longrightarrow$ Matrix Schur function $\boldsymbol{f}_V$

$$\boldsymbol{g}_V(z) = z\boldsymbol{f}_V^\dagger(z) = \sum_{n=1}^{\infty} \boldsymbol{a}_n^V z^n$$

Generating function of **first time return matrix amplitudes** $\boldsymbol{a}_n^V$

$$\boldsymbol{R}_V = |\!|\!|\boldsymbol{g}_V|\!|\!|^2 = |\!|\!|\boldsymbol{f}_V^\dagger|\!|\!|^2 \quad \rightsquigarrow \quad R_V(\psi) = \langle \psi | \boldsymbol{R}_V \psi \rangle$$

Total V-return probability

Any $\psi \in V$ is V-recurrent $\Leftrightarrow$ $|\!|\!|\boldsymbol{f}_V|\!|\!| = 1$ $\Leftrightarrow$ $\boldsymbol{f}_V$ is unitary a.e. in $\mathbb{T}$ $\Leftrightarrow$ $\boldsymbol{\mu}_V$ **is singular**

($\boldsymbol{f}_\psi$ is inner)

$$\boldsymbol{\tau}_V^r = \frac{1}{i} \langle\!\langle \boldsymbol{g}_V(re^{i\theta}), \partial_\theta \boldsymbol{g}_V(re^{i\theta}) \rangle\!\rangle \quad \rightsquigarrow \quad \tau_V(\psi) = \lim_{r\to1} \langle \psi | \boldsymbol{\tau}_V^r \psi \rangle$$

Expected V-return time

$\tau_V(\psi) < \infty$ **for all** $\psi \in V$ $\Leftrightarrow$ $\boldsymbol{\mu}_V$ **is a finite combination of mass points**

Despite the previous analogies, there are many differences and unexpected relations

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  - The V-AVERAGE of $\tau_V(\psi)$ is linked to a true TOPOLOGICAL INVARIANT

$$\int_V \tau_V(\psi)\, d\psi = \frac{\textbf{winding number of } \det \boldsymbol{g}_V(e^{i\theta})}{\dim V} \qquad \text{(RATIONAL NUMBER)}$$

- **Quantum recurrence paradox 2**
  State return probabilities can be higher than subspace return probabilities **!!!**

The above figure shows an example of this kind of phenomenon in the case of a 1D coined walk.

It represents as a function of t the state and site return probability of the states $\psi(t) = \cos t|x,\uparrow\rangle + \sin t|x,\downarrow\rangle$ lying in the same site x.

We can see that the state return probability (in blue) is occasionally bigger than the site return probability (in red).

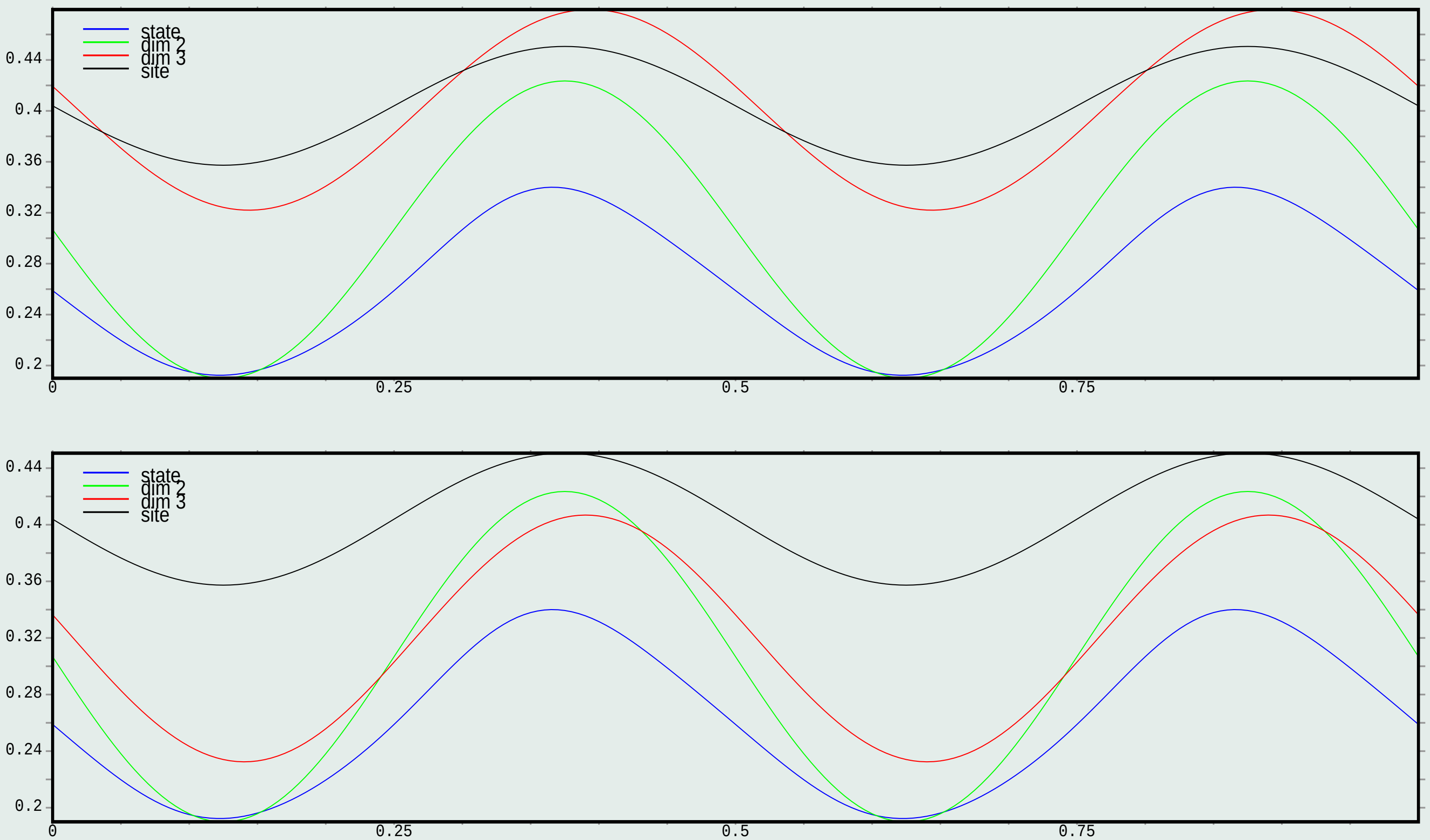

Figure 1: Similar figures for a 2D QW in a square lattice. They compare, for a certain curve of states $\psi(t)$, the return probability to some nested subspaces of dimension 1 (the state), 2, 3, and 4 (the site). The return probability does not necessarily increases when enlarging the subspace.

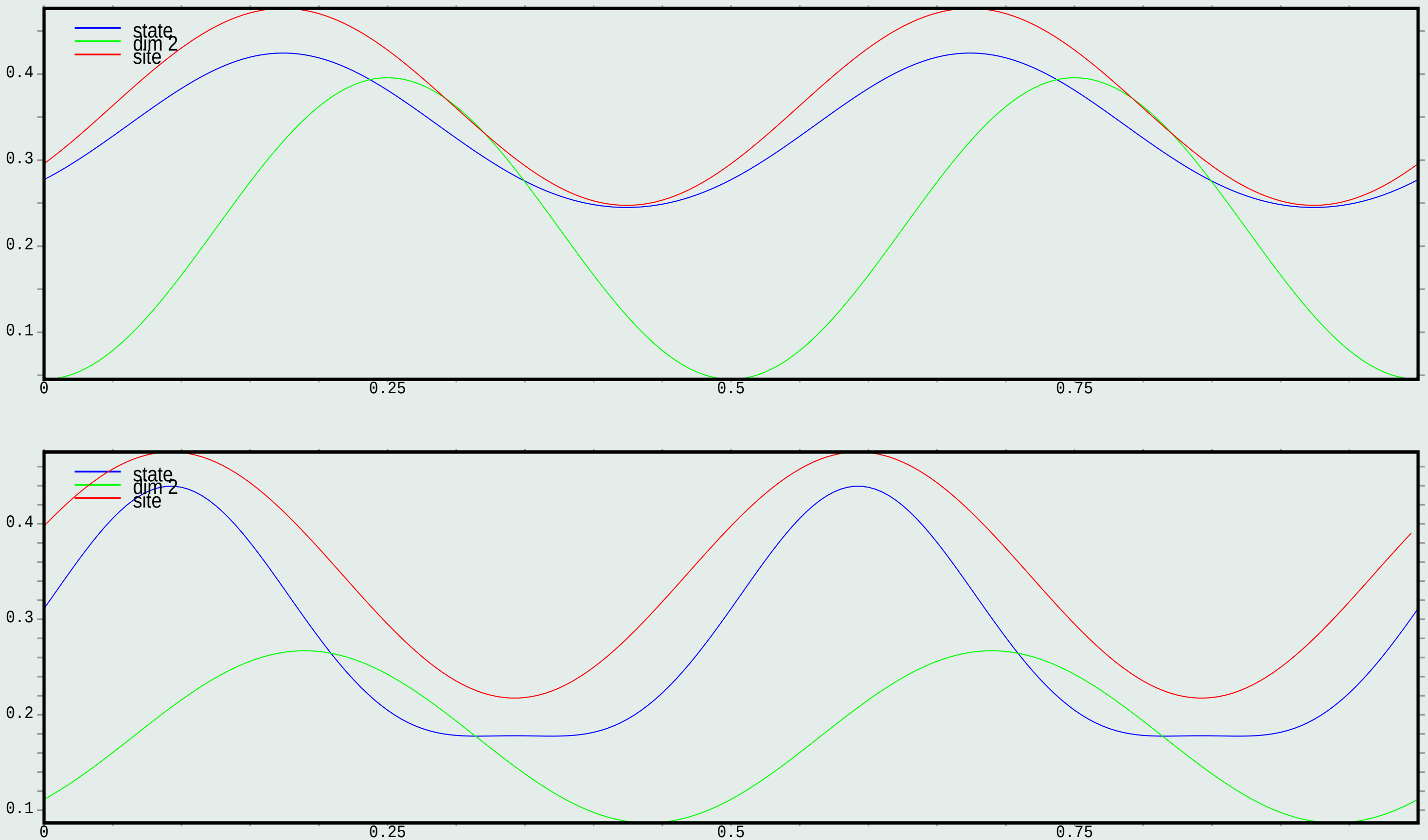

Figure 2: The QW lives now in a 2D hexagonal lattice. The figures compare the return probability of a curve of states to some nested subspaces of dimension 1 (the state), 2 and 3 (the site). The relation between the cases of dimension 1 and 2 is dramatic because it is most of the times the opposite of what one should naively expect.

Quantum Walks: Comments on recurrence

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Quantum recurrence paradoxes

$\rightsquigarrow$ Experimental validation?

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$\int_V \tau_V(\psi)\, d\psi$ RATIONAL or INFINITE is equivalent to

$$\sum_{n=1}^{\infty} n \, \mathrm{Tr}[PU(QU)^{n-1}P] \qquad \text{INTEGER or INFINITE}$$

for any unitary U and orthogonal projectors P, $Q = I - P$

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Dirac equation

$\rightsquigarrow$ Continuous time version?

Schur / OP $\longrightarrow$ **QW**

Schur / OP $\longrightarrow$ **QW**

Schur / OP $\overset{?}{\longleftarrow}$ **QW**

Schur / OP ⟶ **QW**

?

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