Quantum random walks and Szegö orthogonal polynomials.
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Quantum discrete integrable systems
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Thanks for the chance to talk here.

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I will assume that you are not familiar with QRWs....
I think our work fits with the theme of this workshop since it has something to do with Quantum systems, one can get exact formulas for the evolution, and it is certainly discrete, both in time and physical space.
What is my objective with this talk?

We have found a phenomenon that seems to be quite different when you compare quantum random walks (QRWs) and classical random walks. I would like to get some feedback and learn from you if this has appeared (maybe in a different form) in the study of quantum systems.
Plan for the talk

Classical random walks.
Some integrable (solvable) examples.
The role of orthogonal polynomials and their orthogonality measure
(Spectral theory for the corresponding transition probability matrix)

Some important probabilistic questions that can be answered in
terms of spectral quantities.

Szegő polynomials, a revised version.
A canonical pentadiagonal representation for any unitary operator
with a cyclic vector.
i.e. an analog of the very classical (Stone) story for selfadjoint
operators with a cyclic vector: tridiagonal matrices or more
precisely Jacobi matrices.
Quantum random walks, some examples.
Using scalar and matrix valued Szegő polynomials to do the spectral analysis of QRWs.

Questions:

Are there any important differences between classical and quantum random walks?

QRWs "diffuse" faster (pointed out by earlier workers specially in computer science interested in "quantum computing")

Some basic differences in terms of recurrence and transience (the main result in our work)
What are some of the usual tools to study simple random walks such as processes with nearest neighbours transitions?

Path counting

Fourier methods (applicable only when you have translation invariance)
Starting with work by S. Karlin and J. McGregor (and others) one knows that several probabilistic issues involving birth-and-death processes, i.e. random walks on the nonnegative integers with nearest neighbour transitions can be studied in terms of the orthogonal polynomials and the orthogonality measure going along with the corresponding tridiagonal transition probability matrix.

I will review this in a few examples below, but here are the general facts.
If $\mathbb{P}$ denotes the one-step transition probability matrix for a birth and death process on the non-negative integers,

$$
\mathbb{P} = \begin{pmatrix}
  r_0 & p_0 & 0 & 0 \\
  q_1 & r_1 & p_1 & 0 \\
  0 & q_2 & r_2 & p_2 \\
  \vdots & \vdots & \vdots & \ddots
\end{pmatrix}
$$

there is a powerful tool to analyze the random walk in question.
If one introduces the polynomials $Q_j(x)$ by the conditions $Q_{-1}(0) = 0$, $Q_0(x) = 1$ and using the notation

$$Q(x) = \left( \begin{array}{c} Q_0(x) \\ Q_1(x) \\ \vdots \end{array} \right)$$

one insist on the recursion relation

$$FQ(x) = xQ(x)$$

one proves the existence of a unique measure $\psi(dx)$ supported in $[-1,1]$ such that

$$\pi_j \int_{-1}^1 Q_i(x)Q_j(x)\psi(dx) = \delta_{ij}$$
and one gets the Karlin-McGregor representation formula

$$(P^n)_{ij} = \pi_j \int_{-1}^{1} x^n Q_i(x) Q_j(x) \psi(dx).$$

This expression (nothing but the spectral theorem) will be the main tool in our analysis, both in the classical as well as in the quantum case.

When dealing with a random walk on the integers, instead of the non-negative integers one can consider matrix valued orthogonal polynomials, as M.G. Krein did back in 1949, and give a formula very similar to the one above. The same story will reappear in the quantum case.
For a general Markov chain a state is called recurrent if, having started there, one returns to it (eventually) with probability one. A recurrent state is called positive recurrent if the expected value for the time of (first) return to it is finite. When dealing with a birth-and-death process on the non-negative integers the corresponding orthogonality measure $\psi(dx)$ has support in the interval $[-1,1]$ and plays an important role in studying these notions.
For instance the process is recurrent exactly when the integral
\[ \int_{-1}^{1} \frac{d\psi(\lambda)}{1 - \lambda} \]
diverges. (Notice some abuse of language....to be fixed later)
The process returns to the origin in a finite expected time when the measure has a mass at \( x = 1 \). The existence of
\[ \lim_{n \to \infty} (P^n)_{ij} \]
is equivalent to \( \psi(dx) \) having no mass at \( x = -1 \).
In some cases all the ingredients that go into this formula can be computed explicitly.

As an example suppose that we have $r_1 = r_2 = \ldots = 0$, $q_1 = q_2 = \ldots = q$ and $p_1 = p_2 = \ldots = p$, with $0 \leq p \leq 1$ and $q = 1 - p$.

One can show that

$$Q_j(x) = \left(\frac{q}{p}\right)^{j/2} \left[2(p_0 - p)/p_0 T_j(x^*) + (2p - p_0)/p_0 U_j(x^*) - r_0/p_0(p/q)^{1/2}U_{j-1}(x^*)\right]$$

where $T_j$ and $U_j$ are the Chebyshev polynomials of the first and second kind, and $x^* = x/(2\sqrt{pq})$. The polynomials $Q_j(x)$ are orthogonal with respect to a spectral measure in the interval $[-1, 1]$ which can also be determined explicitly.
An important result: in a Markov chain where all states communicate, then we have a nice dichotomy: either all states are recurrent or none is recurrent.

Recall that our birth-and-death process is recurrent exactly when

$$\int_{-1}^{1} \psi(dx) \frac{1}{1-x} = \infty.$$  \hspace{1cm} (1)

Notice that this integral is the sum of all moments of the measure $\psi(dx)$ and that the $n^{th}$ moment is the probability of going from the state 0 to itself in $n$ steps.
Note that the expression

\[ S(z) = \int_{-1}^{1} \frac{\psi(dx)}{z - x} \tag{2} \]

is essentially the generating function for the moments of the measure.
I look now at three examples, where the last two have physical relevance.
A Chebyshev type example

The example below illustrates nicely how certain recurrence properties of the process are related to the presence of point masses in the orthogonality measure. This is seen by comparing the two integrals at the end of the section.

Consider the matrix

\[
P = \begin{pmatrix}
0 & 1 & 0 \\
q & 0 & p \\
0 & q & 0 & p \\
& & \ddots & \ddots & \ddots \\
\end{pmatrix}
\]

with \(0 \leq p \leq 1\) and \(q = 1 - p\).
We have

\[ Q_j(x) = \left( \frac{q}{p} \right)^{j/2} \left[ (2 - 2p)T_j \left( \frac{x}{2 \sqrt{pq}} \right) + (2p - 1)U_j \left( \frac{x}{2 \sqrt{pq}} \right) \right] \]

where \( T_j \) and \( U_j \) are the Chebyshev polynomials of the first and second kind.
If $p \geq 1/2$ we have

$$\left( \frac{p}{1-p} \right)^n \int_{-\sqrt{4pq}}^{\sqrt{4pq}} Q_n(x)Q_m(x) \frac{\sqrt{4p1-x^2}}{1-x^2} dx = \delta_{nm} \begin{cases} 2(1-p)\pi, & n = 0 \\ 2p(1-p)\pi, & n \geq 1 \end{cases}$$
while if \( p \leq 1/2 \) we get a new phenomenon, namely the presence of point masses in the spectral measure

\[
\left( \frac{p}{1-p} \right)^n \left[ \int_{-\sqrt{4pq}}^{\sqrt{4pq}} Q_n(x)Q_m(x) \frac{\sqrt{4pq - x^2}}{1-x^2} dx \\
+ (2 - 4p)\pi(Q_n(1)Q_m(1) + Q_n(-1)Q_m(-1)) \right] \\
= \delta_{nm} \begin{cases} 
2(1-p)\pi, & n = 0 \\
2p(1-p)\pi, & n \geq 1 
\end{cases}
\]
The integers vs the non-negative integers.

Consider the example of random walk on the integers, when the probabilities of going right or left are \( p \) and \( q \) respectively.

If we “fold” the integers, by relabelling the natural sequence

\[
\cdots -3, -2, -1, 0, 1, 2, 3, \ldots
\]

in the fashion

\[
\ldots 5, 3, 1, 0, 2, 4, 6, \ldots
\]

then the transition probability matrix goes from being a scalar tridiagonal doubly infinite one with \( p \) in the \( i, i+1 \) diagonal and \( q \) in the \( i+1, i \) diagonal.
to the following semi-infinite block tridiagonal matrix (with $2 \times 2$ blocks)

\[
P = \begin{pmatrix}
0 & q & p & 0 & 0 & 0 & 0 & 0 & 0 & \ldots \\
p & 0 & 0 & q & 0 & 0 & 0 & 0 & 0 & \ldots \\
q & 0 & 0 & 0 & p & 0 & 0 & 0 & 0 & \ldots \\
0 & p & 0 & 0 & 0 & q & 0 & 0 & 0 & \ldots \\
0 & 0 & q & 0 & 0 & 0 & p & 0 & 0 & \ldots \\
0 & 0 & 0 & p & 0 & 0 & 0 & q & 0 & \ldots \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots
\end{pmatrix}, \quad p+q = 1.
\]
For this first example the appropriate matrix measure is already found in the original paper by S. Karlin and J. McGregor. It is given by

\[
dM(x) = \frac{1}{\sqrt{4pq - x^2}} \begin{pmatrix} 1 & x/2q \\ x/2q & p/q \end{pmatrix} dx, \quad |x| \leq \sqrt{4pq}.
\]

The matrix valued orthogonal polynomials are given by

\[
P_k(x) = \begin{pmatrix} (q/p)^{\frac{k}{2}} & 0 \\ 0 & (p/q)^{\frac{k}{2}} \end{pmatrix}\left\{1U_k(x^*) - \begin{pmatrix} 0 & (q/p)^{\frac{1}{2}} \\ (p/q)^{\frac{1}{2}} & 0 \end{pmatrix} U_{k-1}(x^*)\right\}
\]

where \(x^* = x/2\sqrt{pq}\).
The Ehrenfest urn model

Consider the case of a Markov chain in the finite state space
0, 1, 2, ..., 2N where the matrix $P$ given by

$$
\begin{pmatrix}
0 & 1 & 0 & 0 & \cdots \\
\frac{1}{2N} & 0 & \frac{2N-1}{2N} & 0 & \cdots \\
\frac{2}{2N} & 0 & \frac{2N-2}{2N} & 0 & \cdots \\
\frac{3}{2N} & 0 & \frac{2N-3}{2N} & 0 & \cdots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
\frac{N-1}{2N} & 0 & \frac{2N-(N-1)}{2N} & 0 & \frac{1}{2N} \\
\frac{N}{2N} & \frac{2N-N}{2N} & 0 & \frac{2N-(N+1)}{2N} & 0
\end{pmatrix}
$$

This situation arises in a model introduced by P. and T. Ehrenfest, in an effort to illustrate the issue that irreversibility and recurrence can coexist.
In deals with two urns and balls of one color, each one has a label $1, \ldots, 2N$. 
The background here is, of course, the famous $H$-theorem of L. Boltzmann, and its ensuing controversy. Lorentz, Poincaré, ... This model has also been considered in dealing with a quantum mechanical version of a discrete harmonic oscillator by Schrödinger himself.

In this case the corresponding orthogonal polynomials (on a finite set) can be given explicitly. Consider the so called Krawtchouk polynomials, given by means of the (truncated) Gauss series

$$
_{2}F_{1}\left(\begin{array}{c}
 a, b \\
 c
\end{array}; z \right) = \sum_{0}^{2N} \frac{(a)_{n}(b)_{n}}{n!(c)_{n}} z^{n}
$$

with

$$(a)_{n} \equiv a(a + 1) \ldots (a + n - 1), \quad (a)_{0} = 1$$
The polynomials are given by

\[ K_i(x) = \tilde{\text{F}}_1 \left( \frac{-i, -x}{-2N}; 2 \right) \]

\[ x = 0, 1, \ldots, 2N; \quad i = 0, 1, \ldots, 2N \]

Observe that

\[ K_0(x) \equiv 1, K_i(2N) = (-1)^i. \]

The orthogonality measure is read off from

\[ \sum_{x=0}^{2N} K_i(x) K_j(x) \frac{\binom{2N}{x}}{2^{2N}} = \frac{(-1)^i!}{(-2N)_i} \delta_{ij} \equiv \pi_i^{-1} \delta_{ij} \quad 0 \leq i, j \leq 2N. \]
These polynomials satisfy the second order difference equation

\[
\frac{1}{2}(2N - i)K_{i+1}(x) - \frac{1}{2}2NK_i(x) + \frac{i}{2}K_{i-1}(x) = -xK_i(x)
\]

and this has the consequence that

\[
\begin{pmatrix}
0 & 1 \\
\frac{1}{2N} & 0 & \frac{2N-1}{2N} \\
\frac{2}{2N} & 0 & \frac{2N-2}{2N} \\
\vdots & \ddots & \ddots \\
\frac{2N}{2N} & \frac{2N}{2N} & \frac{1}{2N} \\
0 & \frac{1}{2N} & 0 \\
\frac{2N}{2N} & 0 & 0 \\
\end{pmatrix}
\begin{pmatrix}
K_0(x) \\
K_1(x) \\
\vdots \\
K_{2N}(x)
\end{pmatrix}
= \left(1 - \frac{x}{N}\right)
\begin{pmatrix}
K_0(x) \\
K_1(x) \\
\vdots \\
K_{2N}(x)
\end{pmatrix}
\]

any time that \(x\) is one of the values \(x = 0, 1, \ldots, 2N\).
This means that the eigenvalues of the matrix $P$ above are given by the values of $1 - \frac{x}{N}$ at these values of $x$, i.e.,

$$1, 1 - \frac{1}{N}, \ldots, -1$$

and that the corresponding eigenvectors are the values of $[K_0(x), K_1(x), \ldots, K_{2N}(x)]^T$ at these values of $x$. 
Since the matrix $P$ above is the one step transition probability matrix for our urn model the Karlin-McGregor formula takes the form

$$(P^n)_{ij} = \pi_j \sum_{x=0}^{2N} \left( 1 - \frac{x}{N} \right)^n K_i(x) K_j(x) \frac{\binom{2N}{x}}{2^{2N}}.$$

We can use these expressions to rederive some results given by Mark Kac a long time ago.
Every state $i = 0, \ldots, 2N$ is recurrent and that the expected time to return to it is given by

\[
\frac{2^{2N}}{\binom{2N}{i}}.
\]


The moral of this is clear: if $i = 0$ or $2N$, or close to these values, i.e., we start from a state where most balls are in one urn it will take on average a huge amount of time to get back to this state.

For $N = 10000$ and a repetition rate of 1 second M. Kac gives about $10^{6000}$ years as the expected time.

If on the other hand $i = N$, i.e., we are starting from a very balanced state, then we will (on average) return to this state fairly soon.

Again, for $N = 10000$ and a repetition rate of 1 second M. Kac gives about 175 seconds as the expected time.

Thus we see how the issues of irreversibility and recurrence are rather subtle and that certain models show how they can coexist.
In a very precise sense these polynomials are discrete analogs of those of Hermite in the case of the real line.
The Hahn polynomials, Laplace and Bernoulli

The Bernoulli–Laplace model for the exchange of heat between two bodies consists of two urns, labeled 1 and 2. Initially there are $W$ white balls in urn 1 and $B$ black balls in urn 2. The transition mechanism is as follows: a ball is picked from each urn and these two balls are switched. It is natural to expect that eventually both urns will have a nice mixture of white and black balls.

The state of the system at any time is described by $w$, defined to be the number of white balls in urn 1. It is clear that we have, for $w = 0, 1, \ldots, W$

\[
\begin{align*}
P_{w, w+1} & = \frac{W - w}{W} \frac{W - w}{B} \\
P_{w, w-1} & = \frac{w}{W} \frac{B - W + w}{B} \\
P_{w, w} & = \frac{w}{W} \frac{W - w}{B} + \frac{W - w}{W} \frac{B - W + w}{B}.
\end{align*}
\]
A challenge:
the polynomials seen above, Krawtchouk and Hahn, are at the two lower levels of a table containing a hierarchy of polynomials with remarkable mathematical properties.

The next level up is given by the Racah, or Wilson or Askey-Wilson polynomials.

Where is the elementary physical model, urns and balls, whose solution is given in terms of these polynomials????
It is time to move on to QRWs after a final look at classical random walks.
We give now a different description of classical random walks. This is not the only way to describe these simple processes, but this facilitates the transition to the quantum case.

Consider, for simplicity, a discrete time random walk in a denumerable state space which we take to be the non-negative integers \( i = 0, 1, 2, \ldots \).

The state of the system at time \( n \) is given by a row vector \( \pi_{i,n} \).

This is also called the probability distribution at time \( n \). The \( i^{th} \) component is interpreted as the probability that a particle can be found at site \( i \) at time \( n \).

These non-negative quantities \( \pi_{i,n} \) are assumed to add up to one, for any \( n \), when summed over \( i \) in the set of non-negative integers.
The evolution of the system is given by some transition probability matrix $P = (P_{i,j})$. This means that for each state $i$ we have a collection of “transition probabilities” $P_{i,j}$ with the condition that these non-negative numbers add up to one when summed over the index $j$. $P_{i,j}$ is interpreted as the probability of a transition from site $i$ to site $j$ in one unit of time.
The Markov nature of our process is given by the fact that at time $t = 1$ the new probability distribution gives weight
\[ \sum_{j=0}^{\infty} \pi_{j,0} P_{j,i} \]
to the $i^{th}$ site. In other words the state at time $t = 1$ is the vector obtained by multiplying the probability distribution at time 0, namely $\pi_{j,0}$, by $P$. The Markov property says that the process starts from scratch at any integer time, so that the probability distribution (i.e., the state of the system) at time $t = n$ is obtained by taking the product of the row vector $\pi_{j,0}$ and the matrix $P^n$. 

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Moving on to quantum random walks.
A system has a (denumerable) set \{\{i\}\}_{i \in I} of measurable states called “pure states”. The state \lvert \Psi_n \rangle of the system at time n is a (complex) superposition \lvert \Psi_n \rangle = \sum_{i \in I} \psi_{i,n} \lvert i \rangle of pure states, so it is described by a “wave function” \psi_{i,n} with \textit{i} running over the pure states. Therefore, a state can be identified with its wave function. The complex number \psi_{i,n} is no longer a probability but a probability amplitude, so that the actual probability to be in the state \lvert i \rangle at time n is \lvert \psi_{i,n} \rvert^2. The total probability of finding the system at time n must be 1, thus the wave function must satisfy the condition
\[ \sum_{i \in I} \lvert \psi_{i,n} \rvert^2 = 1. \] (3)
In the time invariant case the time evolution of the system is characterized by a single unitary operator $U$ on the Hilbert state space: $|\Psi_n\rangle = U^n |\Psi_0\rangle$. If $U = (U_{i,j})_{i,j \in I}$ is the unitary matrix such that $U|i\rangle = \sum_{j \in I} U_{i,j} |j\rangle$, the evolution of the wave function is governed by

$$\psi_n = \psi_0 U^n, \quad \psi_n = (\psi_{i,n})_{i \in I}. \quad (4)$$
Following the analogy with a quantum physical system, the simplest way to get a QRW is to consider that every site \( i \in I \) has an internal degree of freedom of spin 1/2 type, i.e., taking values \( s \in S = \{\uparrow, \downarrow\} \). The space state is a tensor product spanned by \( \{|i\rangle \otimes |\uparrow\rangle, |i\rangle \otimes |\downarrow\rangle\}_{i \in I} \).

We will be considering mostly the cases when \( I \) is either the set of non-negative integers or the set of all integers. The evolution of the wave function \( \psi_{i,s,n} \) satisfies (??) when summing in \( i \in I \) and \( s \in S \), so its evolution is given similarly to (??) by a unitary operator \( U \) on \( L^2(I \times S) \).
Although the choice $\mathcal{I} = \mathbb{Z} \geq 0$ would be as natural as $\mathcal{I} = \mathbb{Z}$, the first one has not received too much attention in the quantum case, maybe due to the difficulties to work with a non translation invariant system. However, just as in the classical case, QRWs on the non-negative integers are more natural for an orthogonal polynomial approach. Indeed, from this point of view, QRWs on the non-negative integers will be the cornerstone for the analysis of QRWs on the integers.
Schematically, the allowed transitions are

\[ |i⟩ ⊗ |↑⟩ \rightarrow \begin{cases} |i + 1⟩ ⊗ |↑⟩ & \text{with probability amplitude } c_{i1}^1 \\ |i - 1⟩ ⊗ |↑⟩ & \text{with probability amplitude } c_{i2}^1 \end{cases} \]

\[ |i⟩ ⊗ |↓⟩ \rightarrow \begin{cases} |i + 1⟩ ⊗ |↑⟩ & \text{with probability amplitude } c_{i1}^2 \\ |i - 1⟩ ⊗ |↓⟩ & \text{with probability amplitude } c_{i2}^2 \end{cases} \]

where, for each \( i \in \mathbb{Z} \),

\[ C_i = \begin{pmatrix} c_{i1}^1 & c_{i2}^1 \\ c_{i1}^2 & c_{i2}^2 \end{pmatrix} \] \hspace{1cm} (5)

is an arbitrary unitary matrix which we will call the \( i^{th} \) coin.

Notice that this is already more general than the Hadamard example usually discussed in the literature.
The transition matrix $U$ is the unitary doubly infinite matrix

$$
\begin{array}{cccccc}
0 & c_{21}^{-2} & 0 & 0 & c_{11}^{-2} & \\
\vdots & \ddots & \ddots & \ddots & \ddots & \\
c_{22}^{-2} & 0 & 0 & c_{12}^{-2} & 0 & \\
\vdots & \ddots & \ddots & \ddots & \ddots & \\
0 & c_{21}^{-1} & 0 & 0 & c_{11}^{-1} & \\
c_{22}^{-1} & 0 & 0 & c_{12}^{-1} & 0 & \\
\end{array}
$$

$$
\begin{array}{cccccc}
0 & 0 & 0 & c_{11}^{0} & \\
\vdots & \ddots & \ddots & \ddots & \ddots & \\
c_{21}^{0} & 0 & 0 & c_{12}^{0} & 0 & \\
\vdots & \ddots & \ddots & \ddots & \ddots & \\
0 & c_{21}^{1} & 0 & 0 & c_{11}^{1} & \\
c_{22}^{1} & 0 & 0 & c_{12}^{1} & 0 & \\
\end{array}
$$
which has the structure of a doubly infinite CMV matrix with null odd Verblunsky parameters
\[
\begin{array}{cccc}
0 & \sigma_0 & 0 & 0 \\
0 & \sigma_0 & 0 & 0 \\
0 & \sigma_0 & 0 & 0 \\
0 & \sigma_0 & 0 & 0 \\
0 & \sigma_0 & 0 & 0 \\
0 & \sigma_0 & 0 & 0 \\
\end{array}
\]
QRWs with a constant coin
The Hadamard QRW is an example of the QRWs described previously. It corresponds to a constant coin $C_i = H$ given by

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{6}$$

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

Here is another example

$$C = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix}. \tag{7}$$
Punch line

In the case of a large class of quantum random walks on the integers there is a natural tool that takes the place of the matrix valued orthogonal polynomials on the real line.

This will be the theory of Laurent $2 \times 2$ matrix valued orthogonal polynomials associated with a certain kind of unitary matrices, namely CMV matrices. This is a ready made tool that combines the necessary features for a quantum mechanical description of the phenomenon of nearest neighbours transitions: unitarity and a block tridiagonal shape.
1 Szegő polynomials and CMV matrices

All the information about a QRW is encoded in the unitary operator $U$ governing the evolution of the system. Therefore, it is not strange that the theory of canonical matrix representations of unitary operators on Hilbert spaces should play an important role in the study of QRWs.

Surprisingly, such a theory has been developed only recently giving rise to the so-called CMV matrices, related to the Szegő polynomials.
The basic idea is that, as a consequence of the spectral theorem, any unitary operator is unitarily equivalent to a direct sum of unitary multiplication operators, i.e., operators of the type

\[ U_\mu : L^2_\mu(T) \to L^2_\mu(T) \]

\[ f(z) \mapsto zf(z) \quad (8) \]

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

\[ (f, g) = \int_T f(z) \overline{g(z)} \, d\mu(z). \]

Thus, it is enough to discuss the canonical representations of unitary multiplication operators. Moreover, we can suppose that \( \mu \) has an infinite support, otherwise \( L^2_\mu(T) \) is finite-dimensional, so \( U_\mu \) is unitarily diagonalizable.
Since the Laurent polynomials are dense in $L^2_{\mu}(\mathbb{T})$, a natural basis to obtain a matrix representation of $U_{\mu}$ is given by the Laurent polynomials $(\chi_j)_{j=0}^{\infty}$ obtained from the Gram-Schmidt orthonormalization of $\{1, z, z^{-1}, z^2, z^{-2}, \ldots\}$ in $L^2_{\mu}(\mathbb{T})$.

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

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

(9)
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 $\alpha_j$ are known as the Verblunsky parameters of the measure $\mu$, and establish a bijection between the probability measures supported on an infinite set of the unit circle and the sequences in the open unit disk.
Another equally natural basis would be the Laurent polynomials \((x_j)_{j=0}^\infty\) obtained from the orthonormalization of \(\{1, z^{-1}, z, z^{-2}, z^2, \ldots\}\). They are given by

\[ x_j(z) = \chi_j(1/z) \]

and, consequently, the matrix of \(U_\mu\) with respect to \((x_j)_{j=0}^\infty\) is the transpose \(C^T\) of \(C\).

As a consequence, we have the identities

\[ \chi(z)C = z\chi(z), \quad \chi = (\chi_0, \chi_1, \chi_2, \ldots), \quad \chi_0 = 1, \]

\[ Cx(z) = zx(z), \quad x = (x_0, x_1, x_2, \ldots)^T, \quad x_0 = 1, \]  

which can be viewed as recurrences which determine the orthonormal Laurent polynomials. This is the analog of the starting point in the tridiagonal case.
The Verblunsky parameters have a special meaning in terms of the Szegő polynomials \((\varphi_j)_{j=0}^{\infty}\), which come from orthonormalizing \(\{z^j\}_{j=0}^{\infty}\).

These polynomials are not so useful as a basis because the polynomials are not always dense in \(L_2^2(\mathbb{T})\). Nevertheless, they are related to the orthonormal Laurent polynomials by

\[
\begin{align*}
\chi_{2j}(z) &= z^{-j} \varphi_{2j}^*(z), \\
\chi_{2j+1}(z) &= z^{-j} \varphi_{2j+1}(z), \\
x_{2j}(z) &= z^{-j} \varphi_{2j}(z), \\
x_{2j+1}(z) &= z^{-j-1} \varphi_{2j+1}^*(z),
\end{align*}
\]

where \(\varphi_j^*(z) = z^j \varphi_j(1/z)\).
The key result is that the Szegő polynomials are determined by the recurrence relation

\[ \rho_j \varphi_{j+1}(z) = z \varphi_j(z) - \overline{\alpha}_j \varphi_j^*(z), \quad \varphi_0 = 1, \tag{12} \]

so the recurrence for the monic orthogonal polynomials \((\phi_j)_{j=0}^\infty\) is

\[ \phi_{j+1}(z) = z \phi_j(z) - \overline{\alpha}_j \phi_j^*(z), \quad \phi_0 = 1, \tag{13} \]

which shows that \(\alpha_j = -\phi_{j+1}(0)\).
Another tool for the study of Szegő polynomials is the Carathéodory function $F$ of the orthogonality measure $\mu$, defined by

$$F(z) = \int_T \frac{t+z}{t-z} \, d\mu(t), \quad |z| < 1.$$  \hspace{1cm} (14)

$F$ is analytic on the open unit disc with McLaurin series

$$F(z) = 1 + 2 \sum_{j=1}^{\infty} \mu_j z^j, \quad \mu_j = \int_T z^j \, d\mu(z),$$  \hspace{1cm} (15)

whose coefficients provide the moments $\mu_j$ of the measure $\mu$.

$F$ can be obtained as

$$F(z) = \lim_{j \to \infty} \frac{\tilde{\varphi}_j(z)}{\varphi_j^*(z)}, \quad |z| < 1,$$  \hspace{1cm} (16)

where $\tilde{\varphi}_j$ are the Szegő polynomials whose Verblunsky parameters are given by $-\alpha_j$ if the original ones were $\alpha_j$. 

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The Carathéodory function is a shortcut that allows one to recover the measure from the Szegő polynomials. If
\[
d\mu(e^{i\theta}) = w(\theta) \frac{d\theta}{2\pi} + d\mu_s(e^{i\theta}), \quad \theta \in (-\pi, \pi], \quad \mu_s \text{ singular},
\]
the weight \( w(\theta) \) is given by
\[
w(\theta) = \lim_{r \to 1} F(re^{i\theta}), \tag{18}
\]
and the support of \( \mu_s \) lies on \( \{e^{i\theta} : \lim_{r \to 1} F(re^{i\theta}) = \infty\} \). In particular, \( e^{i\theta_0} \) is a mass point of \( \mu \) with mass \( \mu(\{e^{i\theta_0}\}) \) if and only if
\[
\mu(\{e^{i\theta_0}\}) = \lim_{r \to 1} \frac{1 - r}{2} F(re^{i\theta_0}) \neq 0. \tag{19}
\]
Two natural extensions of CMV matrices are of interest to us: doubly infinite CMV matrices and block CMV matrices.
We finally take up the issue of recurrence of a QRW. By using our method we see some marked differences between the classical and the quantum case. This exhibits the benefits of using the notions introduced here to analyze QRWs.
2 Recurrence properties of QRWs

The notion of quantum recurrence can be described nicely in terms of the Carathéodory function introduced earlier, which will play in the quantum case a similar role to the generating function of the moments for a classical random walk. Nevertheless, the condition for the characterization of quantum recurrence will be somewhat different from (??).

The study of the recurrence properties in the quantum case raises special issues because a quantum measurement destroys the initial evolution since the system collapses into a pure state when a measurement is performed. Therefore, the notion of a return to a given state for the first time in a certain number of steps has to be interpreted with care in the quantum case. Such an analysis in terms of a specific measurement scheme, involving an ensemble of identically prepared QRWs, has been proposed recently.
The bottom line of this analysis is that, in the quantum case, the recurrence of a state is characterized by the divergence of the series of probabilities to return to such a state in $n$ steps. After the modifications which are necessary to make sense of the notion of recurrence in the quantum case, this result is completely analogous to the classical one.
More precisely, following the interpretation of the quantum recurrence given by SKJ, a state $\psi$ of a QRW with transition matrix $U$ is recurrent exactly when

$$\sum_{n=1}^{\infty} p_n(\psi) = \infty, \quad p_n(\psi) = |\psi U^n \psi^\dagger|^2,$$

(20)

where $p_n(\psi)$ stands for the probability to return to the state $\psi$ in $n$ steps.
Consider a QRW on the non-negative integers with non-trivial distinct coins. The recurrence of the state numbered as 0, i.e., the spin up at site 0, is characterized by the divergence of 
\[ \sum_{n=1}^{\infty} |(U^n)_{0,0}|^2 = \sum_{n=1}^{\infty} |\mu_n|^2. \]
From the McLaurin series (??) of the related Carathéodory function \( F(z) \) we obtain
\[
\int_0^{2\pi} |F(e^{i\theta})|^2 \frac{d\theta}{2\pi} = 1 + 2 \sum_{n=1}^{\infty} |\mu_n|^2,
\]
where \( F(e^{i\theta}) = \lim_{r \to 1} F(re^{i\theta}) \), which exists for Lebesgue almost every \( \theta \in [0, 2\pi) \).

Therefore, \( |0\rangle \otimes |\uparrow\rangle \) is recurrent exactly when the radial limit of \( F(z) \) does not lie on \( L^2_{2\pi}(\mathbb{T}) \).
The condition (??) for the classical recurrence at the origin depends only on the behaviour of generating function \( S(z) \) of the moments at \( z = 1 \). In contrast, the characterization of the quantum recurrence in terms of Carathéodory functions has to do with their global behaviour on the whole unit circle.
We get results about the recurrence of a local state, i.e., a state which is a superposition of a finite number of pure states.

Here is one such result.

The local states of a QRW on the non-negative integers with non trivial distinct coins are all transient if and only if the state $|0\rangle \otimes |\uparrow\rangle$ is transient.
Here are some more results.
Consider first the Hadamard coin on the non-negative integers. The corresponding Carathéodory function can be written as

\[ F(z) = \sqrt{\frac{(z + z_0)(z + \bar{z}_0)}{(z - z_0)(\bar{z} - z_0)}}, \quad z_0 = \frac{1}{\sqrt{2}}(1 + i), \]

for some choice of the square root. \(|F|^2\) has two singularities on \(\mathbb{T}\): \(z_0\) and \(\bar{z}_0\).

Neither is Lebesgue integrable, so the state given by a spin up at the origin is recurrent.
Any superposition of up and down states at site 0 has an associated function lying in span\{X_0, X_1\} = span\{1, z^{-1}\} = z^{-1}span\{1, z\}. Such a function cannot cancel both singularities of \( F \), thus any mixed spin state at the origin is recurrent.
However, transient states can appear if we consider a mixing of spin states at sites 0 and 1. The Laurent polynomial associated with a state $a |0⟩⊗|↑⟩ + b |0⟩⊗|↓⟩ + c |1⟩⊗|↑⟩$ is in 
$\text{span}\{X_0, X_1, X_2\} = \text{span}\{1, z^{-1}, z^2\} = z^{-1}\text{span}\{1, z, z^2\}$, so it can vanish at both, $z_0$ and $\overline{z}_0$. The Laurent polynomial related to such a state is $a + bX_1 + cX_2$, so it is transient exactly when

$$a + bX_1(z_0) + cX_2(z_0) = 0, \quad a + bX_1(\overline{z}_0) + cX_2(\overline{z}_0) = 0.$$ 

Since $X_1(z) = 1 - \sqrt{2}z^{-1}$ and $X_2(z) = -X_1(1/z)$ we find that the solutions of the above equations are $a = 0$ and $c = -b$. This means that the transient states with the desired form are spanned by 

$$|0⟩⊗|↓⟩ - |1⟩⊗|↑⟩.$$
Following a similar reasoning, and using the form of the third orthonormal Laurent polynomial
\[ X_3(z) = 1 + \sqrt{2}(z - z^{-1})(1 - \sqrt{2}z^{-1}), \]
it is easy to obtain the transient states mixing all the up and down states at sites 0 and 1.
The result is that such transient states are those lying in the span of
\[ |0\rangle \otimes |\downarrow\rangle - |1\rangle \otimes |\uparrow\rangle, \quad |0\rangle \otimes |\uparrow\rangle + |1\rangle \otimes |\downarrow\rangle. \]
Let us see what happens if we change the Hadamard coin by another equiprobable coin like (??). Then, the Carathéodory function
\[ F(z) = \frac{\sqrt{1 + z^4} - i\sqrt{2}z}{z^2 + 1} \]
has a single non integrable singularity at \( i \) because \( -i \) is a removable one. Thus the spin up at the origin is recurrent once again.
However, in contrast with the Hadamard coin, this QRW has transient states at the origin. Such transient states $a \ket{0} \otimes \ket{\uparrow} + b \ket{0} \otimes \ket{\downarrow}$ have an associated Laurent polynomial $a + bX_1$ which must vanish at $i$. Since $X_1(z) = - (\sqrt{2}z^{-1} + i)$ we find that $a + bX_1(i) = 0$ is solved by $b = i(1 + \sqrt{2})a$, which shows that the states spanned by

$$\ket{0} \otimes \ket{\uparrow} + i(1 + \sqrt{2}) \ket{0} \otimes \ket{\downarrow}$$

are transient.
We can also look for the transient states mixing the spin states at sites 0 and 1. Using the fact that $X_2(z) = -\overline{X_1(1/z)}$ and $X_3(z) = 1 + i\sqrt{2}(z - z^{-1})(i\sqrt{2}z^{-1} - 1)$ we obtain a 3-dimensional subspace of transient states

$$a |0\rangle \otimes |\uparrow\rangle + b |0\rangle \otimes |\downarrow\rangle + c |1\rangle \otimes |\uparrow\rangle + d |1\rangle \otimes |\downarrow\rangle$$

given by the equation

$$a + i(\sqrt{2} - 1)(b + c) + (i(\sqrt{2} - 1))^2d = 0.$$ 

The QRWs analyzed above are archetypal examples of QRWs on the non-negative integers with a non trivial constant coin. They show the two possible recurrence behaviours, if one leaves aside the singular case of a diagonal coin, which is related to null Verblunsky parameters.

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Finally, consider the Hadamard coin on the integers. Just as in the case of the Hadamard coin on the non-negative integers, the Carathéodory function

\[ F(z) = \frac{1}{\sqrt{1 + z^4}} F_0(z), \quad F_0(z) = \begin{pmatrix} 1 + z^2 & \sqrt{2}z \\ \sqrt{2}z & 1 + z^2 \end{pmatrix}, \]

has singularities at \( z_0 = (1 + i)/\sqrt{2} \) and \( z_0 \), but also at \(-z_0\) and \(-z_0\). Any of them can cause the non integrability of \( |f F f|^2 \) for a 2-dimensional vector valued Laurent polynomial \( f \).
The local transient states are those whose associated vector Laurent polynomial $f$ is such that the scalar Laurent polynomial $f F_0 f^\dagger$ vanishes at $\pm z_0$ and $\pm \bar{z}_0$. On these singularities $F_0$ is proportional to a semidefinite matrix,

$$F_0(\pm z_0) = (1 + i) \begin{pmatrix} 1 & \pm 1 \\ \pm 1 & 1 \end{pmatrix}, \quad F_0(\pm \bar{z}_0) = (1 - i) \begin{pmatrix} 1 & \pm 1 \\ \pm 1 & 1 \end{pmatrix},$$

hence $f F_0 f^\dagger$ vanishes on such points if and only if $f F_0$ does so. Any vector Laurent polynomial $f = (a_1, a_2) X_0 + (b_1, b_2) X_1$ has the form $f(z) = z^{-1} p(z)$ where $p$ is a vector polynomial with $\deg p \leq 1$. Therefore, $\deg p F_0 \leq 3$ and $f F_0$ can not vanish on four different points. This means that any superposition of spin states at sites $-1$ and $0$ is recurrent. Taking into account the translation invariance of the QRW, we find that any superposition of spin states which mixes only two contiguous sites is recurrent.
Thus, a transient state must involve sites which are not contiguous. The simplest way to do that is to consider a vector Laurent polynomial \( f = (a_1, a_2)X_0 + (b_1, b_2)X_1 + (c_1, c_2)X_2 \) which corresponds to a state
\[
c_2 |−2⟩⊗|⟩ + b_1 |−1⟩⊗|⟩ + a_2 |−1⟩⊗|⟩ + a_1 |0⟩⊗|⟩ + b_2 |0⟩⊗|⟩ + c_1 |1⟩⊗|⟩.
\]
Using the expressions
\[
X_1(z) = \begin{pmatrix} \sqrt{2}z^{-1} & -1 \\ 1 & -\sqrt{2}z^{-1} \end{pmatrix}, \quad X_2(z) = X_1(1/z),
\]
the conditions \( f(\pm z_0)F_0(\pm z_0) = f(\pm z_0)F_0(\pm z_0) = 0 \) become
\[
(a_1, a_2) \begin{pmatrix} 1 \\ \pm1 \end{pmatrix} + i(b_1, b_2) \begin{pmatrix} \mp1 \\ 1 \end{pmatrix} + i(c_1, c_2) \begin{pmatrix} \pm1 \\ -1 \end{pmatrix} = 0,
\]
\[
(a_1, a_2) \begin{pmatrix} 1 \\ \pm1 \end{pmatrix} + i(b_1, b_2) \begin{pmatrix} \mp1 \\ -1 \end{pmatrix} + i(c_1, c_2) \begin{pmatrix} \pm1 \\ 1 \end{pmatrix} = 0.
\]
which have the solutions $a_1 = a_2 = 0$, $b_1 = c_1$ and $b_2 = c_2$. That is, the transient states obtained are spanned by

$$| -2 \rangle \otimes | \downarrow \rangle + |0 \rangle \otimes | \downarrow \rangle, \quad | -1 \rangle \otimes | \uparrow \rangle + |1 \rangle \otimes | \uparrow \rangle.$$  

Then, the translation invariance permits us to identify as transient subspaces all those spanned by states with the form

$$|k \rangle \otimes | \downarrow \rangle + |k + 2 \rangle \otimes | \downarrow \rangle, \quad |k + 1 \rangle \otimes | \uparrow \rangle + |k + 3 \rangle \otimes | \uparrow \rangle.$$  

These kinds of results are not specific of the Hadamard QRW, but similar recurrence properties hold for any non trivial and non diagonal constant coin on the integers. Such recurrence properties are a consequence of the general expression for the Carathéodory function $F$, which shows that $F$ has four singularities on the unit circle, with the only exception being the case of null Verblunsky parameters, which corresponds to a diagonal coin. More precisely, for an arbitrary non trivial and non diagonal coin, $F = (1/\sqrt{q})F_0$ with $q$ a scalar polynomial of degree 4 with 4 different roots on $T$ and $F_0$ a matrix polynomial of degree 2 which is proportional to a semidefinite non null matrix on the roots of $q$. These general results are the only ingredients necessary to deduce recurrence properties qualitatively similar to those ones obtained above for the Hadamard QRW on the integers.
The fact that any state at a given site is recurrent for an unbiased QRW on the integers was proved in SKJ. However, the fact that the states mixing only two consecutive sites are recurrent too, as well as the existence of transient states involving non-contiguous sites is new. Moreover, the comments of the previous paragraph show that these recurrence properties also hold for any QRW with a non trivial and non diagonal constant coin. These general results, together with the analysis of the recurrence for QRWs on the non-negative integers, illustrate some of the possibilities of this new approach to QRWs.
Conclusions

Classical random walks have been traditionally studied using three different methods. Two of these have already been used in the quantum case. We propose an approach to the study of QRWs that is inspired by the third of these methods.

Our approach reproduces known results, but also provides new ones and new methods of analysis, like the use of the orthonormal Laurent polynomials to study the asymptotics or the analysis of quantum recurrence using Carathéodory functions.
This approach can handle non translation invariant QRWs, as well as situations where the structure of the one step transitions is richer than the ones considered so far. This approach can also be adapted in a natural way to deal with cases when the walk can go to infinity in rather complicated networks as well as in the case of regular networks in various dimensions.
Whereas in the classical case when dealing with an irreducible random walk we have a simple dichotomy: either all states are recurrent or all states are transient, we have seen here examples where the situation in the quantum case is much more involved. This remains as an important area for further investigation.

It is also important to note that this approach can be easily adapted to the case when the number of degrees of freedom in our spins is arbitrary. One should consider some examples such as the Grover or the Fourier ones.