# Spectral quantization of discrete random walks on half-line, and orthogonal polynomials on the unit circle

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# Outline

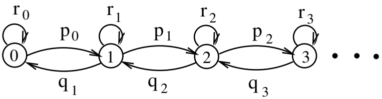
1. OPRL and discrete-time random walks

2. Quantization procedure

3. OPUC and CMV matrices

# Outline

# DISCRETE-TIME RANDOM WALKS




$$\mathcal{P} = \begin{pmatrix} r_0 & p_0 & 0 & 0 & \cdots \\ q_1 & r_1 & p_1 & 0 & \cdots \\ 0 & q_2 & r_2 & p_2 & \cdots \\ 0 & 0 & q_3 & r_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$p_k > 0,\ q_{k+1} > 0,\ r_k \geq 0, \quad p_k + r_k + q_k = 1 \quad \text{for } k \geq 1, \quad p_0 + r_0 = 1$$

Define polynomials $\{Q_k(x)\}_{k=0}^{\infty}$ by the recurrence relations

$$xQ_k(x) = q_k Q_{k-1}(x) + r_k Q_k(x) + p_k Q_{k+1}(x), \qquad k \geq 1,$$
$$Q_0(x) = 1, \qquad p_0 Q_1(x) = x - r_0.$$

The polynomials are orthogonal with respect to a positive measure $\nu$ in the interval $[-1, 1]$ of total mass 1 and infinite support

*[Karlin & McGregor, 1959]*

# The Cauchy–Stieltjes transform

The Cauchy–Stieltjes transform of the measure

$$S(z) = \int_{-1}^{1} \frac{d\nu(x)}{x - z}, \qquad z \in \mathbb{C} \setminus [-1, 1],$$

has the following expansion into continued fractions

$$S(z) = \cfrac{-1}{z - r_0 + \cfrac{p_0 q_1}{z - r_1 + \cfrac{p_1 q_2}{\dots}}}, \qquad \lim_{z\to\infty} S(z) = 0.$$

If the measure is decomposed into absolutely continuous and discrete parts

$$d\nu(x) = u(x)dx + d\nu_s(x),$$

1. The weight is given by $u(x) = \lim_{\varepsilon\to 0^+} \frac{1}{\pi}\mathrm{Im}S(x + i\varepsilon)$.
2. The singular part $\nu_s$ is concentrated on the set $\{x_0 : \lim_{x\to x_0} \mathrm{Im}S(x) = \infty\}$.
3. The mass of any point is given by $\nu(\{x_0\}) = \lim_{\varepsilon\to 0^+} \varepsilon\mathrm{Im}S(x_0 + i\varepsilon)$.

Define constants $\pi_k$, $k \geq 0$, by

$$\pi_0 = 1, \qquad \pi_k = \frac{p_0 p_1 \dots p_{k-1}}{q_1 q_2 \dots q_k}, \quad k \geq 1,$$

The $n$-step transition probabilities $P_{ij}(n)$ from state $i$ to state $j$ may be represented as

$$P_{ij}(n) = \pi_j \int_{-1}^{1} x^n Q_i(x) Q_j(x)\, d\nu(x).$$

The spectral measure originates from the Jacobi symmetric matrix

$$\mathcal{J} = \begin{pmatrix} r_0 & \sqrt{p_0 q_1} & 0 & 0 & \cdots \\ \sqrt{p_0 q_1} & r_1 & \sqrt{p_1 q_2} & 0 & \cdots \\ 0 & \sqrt{p_1 q_2} & r_2 & \sqrt{p_2 q_3} & \cdots \\ 0 & 0 & \sqrt{p_1 q_2} & r_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

which represents the same linear operator but in new basis obtained by suitable scaling of vectors of the starting one.

# Outline

## Szegedy's quantization of Markov chains *[Szegedy, 2004]*

Given a discrete-time classical random walk on a finite set of states $V$, where $|V| = N$, can be represented by an $N \times N$ stochastic matrix $P$, whose entry $P_{jk}$ represents the probability of making a transition from $j$ to $k$, in particular $\sum_{k=1}^{N} P_{jk} = 1$.

Definition of Szegedy's quantum walk starts with tensor doubling $\mathbb{C}^N \otimes \mathbb{C}^N$ of the state space — the state $|j\rangle \otimes |k\rangle = |j,k\rangle$ will be interpreted as PARTICLE IN POSITION $j$ LOOKS AT THE POSITION $k$. The stochastic matrix $P$ allows to define normalized orthogonal vectors

$$|\phi_j\rangle = |j\rangle \otimes \sum_{k=1}^{N} \sqrt{P_{jk}}\, |k\rangle = \sum_{k=1}^{N} \sqrt{P_{jk}}\, |j,k\rangle .$$

$\Pi = \sum_{j=1}^{N} |\phi_j\rangle\langle\phi_j|$ the orthogonal projection on the subspace of the vectors $|\phi_j\rangle$
$R = 2\Pi - \mathbb{I}$ reflection in the subspace spanned by the vectors $|\phi_j\rangle$ (the coin flip operator)
$S = \sum_{j,k=1}^{N} |j,k\rangle\langle k,j|$ the operator that swaps the position and coin registers

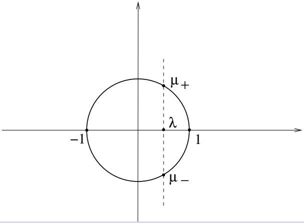
The single step of the quantum walk is defined as the unitary operator $U = SR$ being the composition of coin flip and the position swap

### Proposition

The probability of finding the particle in position $k$ after one step of the quantum walk when starting from the state $|\phi_j\rangle$ is equal to the classical transition probability $P_{jk}$.

$$\langle k,\ell|U\phi_j\rangle = \langle k,\ell|S\phi_j\rangle = \sum_{i=1}^{N} \sqrt{P_{ji}} \langle k,\ell|i,j\rangle = \sqrt{P_{jk}}\delta_{j\ell}, \qquad \sum_{\ell=1}^{N} |\langle k,\ell|U\phi_j\rangle|^2 = P_{jk}$$

# Spectrum of Szegedy's quantum walk operator




**Proposition** *[Szegedy, 2004], [Childs, 2010]*

When $\{|\lambda\rangle\}$ denotes the complete set of eigenvectors of the $N \times N$ symmetric matrix

$$D = \sum_{j,k=1}^{N} \sqrt{P_{jk} P_{kj}} |j\rangle\langle k|,$$

with eigenvalues $\{\lambda\}$, then the evolution operator $U$ has the corresponding eigenvectors

$$|\mu_\pm\rangle = T|\lambda\rangle - \mu_\pm ST|\lambda\rangle, \qquad T = \sum_{j=1}^{N} |\phi_j\rangle\langle j|,$$

with eigenvalues

$$\mu_\pm = \lambda \pm i\sqrt{1-\lambda^2} = e^{\pm i \arccos \lambda},$$

The remaining eigenvalues of $U$ are $\pm 1$ with eigenvectors orthogonal to the subspace spanned by $T|\lambda\rangle$.

The coin space over vertex $k \geq 0$ is spanned by vectors

$$|0,0\rangle,\ |0,1\rangle,\ \text{for } k=0,\ \text{and } |k,k-1\rangle,\ |k,k\rangle,\ |k,k+1\rangle,\ \text{for } k>0,$$

and the corresponding distinguished states read

$$|\phi_0\rangle = \sqrt{r_0}\,|0,0\rangle + \sqrt{p_0}\,|0,1\rangle,\ \text{and} \quad |\phi_k\rangle = \sqrt{q_k}\,|k,k-1\rangle + \sqrt{r_k}\,|k,k\rangle + \sqrt{p_k}\,|k,k+1\rangle, \quad k>0$$

With the lexicographic ordering of the states the quantum evolution operator $U = SR$ has the structure induced by the decompositions

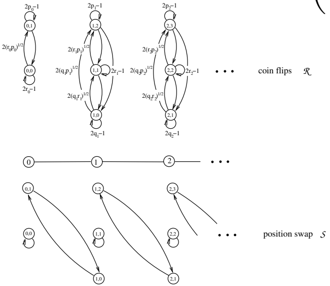
$$R = R_0 \oplus R_1 \oplus R_2 \oplus \dots$$

where

$$R_0 = \begin{pmatrix} 2r_0 - 1 & 2\sqrt{p_0 r_0} \\ 2\sqrt{p_0 r_0} & 2p_0 - 1 \end{pmatrix}, \quad \text{and} \quad R_k = \begin{pmatrix} 2q_k - 1 & 2\sqrt{q_k r_k} & 2\sqrt{p_k q_k} \\ 2\sqrt{q_k r_k} & 2r_k - 1 & 2\sqrt{p_k r_k} \\ 2\sqrt{p_k q_k} & 2\sqrt{p_k r_k} & 2p_k - 1 \end{pmatrix}, \quad k>0,$$

and

$$S = 1 \oplus A \oplus 1 \oplus A \oplus 1 \oplus \dots, \qquad A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$



# Outline

# Orthogonal polynomials on the unit circle (OPUC)

Let $\mathbb{D} = \{z\colon\ |z| < 1\} \subset \mathbb{C}$ be the open unit disk, and let $\mu$ be a measure on the unit circle $\partial\mathbb{D}$ We assume that $\mu$ is nontrivial (i.e., supported on an infinite set) probability measure (i.e., $\mu$ is nonnegative and normalized by $\mu(\partial\mathbb{D}) = 1$)

In the Hilbert space $\mathcal{H} = L^2(\partial\mathbb{D}, d\mu)$ with the inner product antilinear in the left factor, we define the monic polynomials $\Phi_n(z)$, $n = 0, 1, 2, \dots$ by the Gram-Schmidt orthogonalization procedure of the standard basis $1, z, z^2, \dots$. We have then

$$\langle \Phi_n, \Phi_m \rangle = \frac{1}{\kappa_n}\delta_{nm}, \qquad \kappa_n > 0,$$

and the orthonormal polynomials $\varphi_n = \Phi_n/\kappa_n$ satisfy $\langle \varphi_n, \varphi_m \rangle = \delta_{nm}$.

If $P_n$ is a polynomial of degree $n$, define $P_n^*$, the reversed polynomial, by

$$P_n^*(z) = z^n\overline{P_n(1/\bar{z})}, \quad \text{i.e.} \quad P_n(z) = \sum_{j=0}^{n} c_j z^j \;\Rightarrow\; P_n^*(z) = \sum_{j=0}^{n} \bar{c}_{n-j} z^j .$$

The orthogonal polynomials $\Phi_n$ are given by the Szegő recurrence

$$\Phi_0(z) = 1, \qquad \Phi_{n+1}(z) = z\Phi_n(z) - \bar{\alpha}_n\Phi_n^*(z), \qquad \alpha_n = -\overline{\Phi_{n+1}(0)}, \qquad n \geq 0,$$

where the Verblunsky coefficients $\alpha_0, \alpha_1, \alpha_2, \dots$ satisfy $|\alpha_j| < 1$. By Verblunsky's theorem the map $\mu \to \{\alpha_j\}_{j=1}^{\infty}$ sets-up a bijection between the set of nontrivial probability measures on $\partial\mathbb{D}$ and $\times_{j=1}^{\infty}\mathbb{D}$. The Szegő recurrence relations for orthonormal polynomials are

$$\begin{pmatrix} \varphi_{n+1}(z) \\ \varphi_{n+1}^*(z) \end{pmatrix} = \frac{1}{\rho_n}\begin{pmatrix} z & -\bar{\alpha}_n \\ -\alpha_n z & 1 \end{pmatrix}\begin{pmatrix} \varphi_n(z) \\ \varphi_n^*(z) \end{pmatrix} = A(\alpha_n)\begin{pmatrix} \varphi_n(z) \\ \varphi_n^*(z) \end{pmatrix},$$

$$\rho_n = \sqrt{1 - |\alpha_n|^2}, \qquad \varphi_0(z) = \varphi_0^*(z) \equiv 1.$$

The Carathéodory function

$$F(z) = \int_{\partial\mathbb{D}} \frac{e^{i\theta} + z}{e^{i\theta} - z}\, d\mu(\theta)$$

is analytic on $\mathbb{D}$ with non-negative real part, and normalized by $F(0) = 1$. If

$$d\mu(\theta) = w(\theta)\frac{d\theta}{2\pi} + d\mu_s(\theta)$$

is decomposition of the measure into absolutely continuous and singular parts then:

1. The weight is given by $w(\theta) = \lim_{r\to 1^-} \mathrm{Re} F(re^{i\theta})$.
2. The singular part $\mu_s$ is concentrated on the set $\{e^{i\theta} : \lim_{r\to 1^-} \mathrm{Re} F(re^{i\theta}) = \infty\}$.
3. The mass of any point is given by $\mu(\{\theta\}) = \lim_{r\to 1^-} \frac{1-r}{2} F(re^{i\theta})$.

The Schur function

$$f(z) = \frac{1}{z}\frac{F(z) - 1}{F(z) + 1}$$

is analytic on $\mathbb{D}$ with $|f(z)| < 1$ for $z \in \mathbb{D}$. By Geronimus' theorem $f$ has the following continued fraction decomposition

$$f(z) = \alpha_0 + \cfrac{\rho_0^2 z}{\bar{\alpha}_0 z + \cfrac{1}{\alpha_1 + \cfrac{\rho_1^2 z}{\bar{\alpha}_1 z + \cfrac{1}{\dots}}}}.$$

## MOTIVATION

One of the key tools in the case of orthogonal polynomials on the real line is the realization of the measure as the spectral measure of the Jacobi matrix, which comes in as a matrix of multiplication by the real variable $x$. In the case of OPUC the corresponding matrix realization of the measure comes in terms of the CMV martices.

Define the CMV basis $\{\chi_n\}_{n=1}^{\infty}$ by orthonormalizing the sequence $1, z, z^{-1}, z^2, z^{-2}, \ldots$, and define matrix $\mathcal{C}$ by

$$\mathcal{C}_{mn} = \langle \chi_m, z\chi_n \rangle.$$

The matrix is unitary and pentadiagonal

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

and has decomposition $\mathcal{C} = \mathcal{L}\mathcal{M}$, where

$$\mathcal{L} = \Theta_0 \oplus \Theta_2 \oplus \Theta_4 \oplus \ldots, \quad \mathcal{M} = 1 \oplus \Theta_3 \oplus \Theta_5 \oplus \ldots, \qquad \text{and} \quad \Theta_k = \begin{pmatrix} \bar{\alpha}_k & \rho_k \\ \rho_k & -\alpha_k \end{pmatrix}.$$

The monic orthogonal polynomials associated to the measure $\mu$ used to define $\mathcal{C}$ can be found by

$$\Phi_n(z) = \det(z\mathbb{I}_n - \mathcal{C}^{(n)}),$$

where $\mathcal{C}^{(n)}$ is restriction of $\mathcal{C}$ to the upper $n \times n$ block, and the CMV basis can be expressed in terms of $\varphi$ and $\varphi^*$ by

$$\chi_{2k}(z) = z^{-k}\varphi^*_{2k}(z), \qquad \chi_{2k+1}(z) = z^{-k}\varphi_{2k+1}(z),$$

where in order to have formulas consistent it is custom to define $\alpha_{-1} = -1$.

Recall that a cyclic unitary model is a unitary operator $U$ on a separable Hilbert space $\mathcal{H}$ with a distinguished unit vector $v_0$ such that finite linear combinations of $\{U^n v_0\}_{n\in\mathbb{Z}}$ are dense in $\mathcal{H}$. Two cyclic unitary models $(\mathcal{H}, U, v_0)$ and $(\tilde{\mathcal{H}}, \tilde{U}, \tilde{v}_0)$ are called equivalent if there is unitary $W$ from $\mathcal{H}$ onto $\tilde{\mathcal{H}}$ such that

$$WUW^{-1} = \tilde{U}, \qquad Wv_0 = \tilde{v}_0.$$

When all $\alpha_k \in \mathbb{D}$ then the vector $e_0 = (1, 0, 0, 0, \dots)^T$ is cyclic for $\mathcal{C}$ in $\ell^2(\mathbb{N})$. It turns out that each cyclic unitary model is equivalent to a unique CMV model $(\ell^2(\mathbb{N}), \mathcal{C}, e_0)$.

## Szegő projection and Geronimus relations

For OPUC with real Verblunsky coefficients, or equivalently the measure $\mu$ being symmetric with respect to complex conjugation one can define the measure $\nu$ on the segment $[-1,1]$ by

$$\int_{-1}^{1} g(x)\, d\nu(x) = \int_{\partial\mathbb{D}} g(\cos\theta)\, d\mu(\theta).$$

The relation between spectral measures

$$d\mu(\theta) = w(\theta)\frac{d\theta}{2\pi} + d\mu_s, \qquad \text{and} \qquad d\nu(x) = u(x)dx + d\nu_s,$$

has the form

$$u(x) = \frac{w(\arccos x)}{\pi\sqrt{1-x^2}}, \qquad w(\theta) = \pi|\sin\theta| u(\cos\theta).$$

The polynomials orthonormal $p_k(x)$ with respect to the measure $d\nu(x)$ are expressed by the polynomials $\varphi_k(z)$ orthonormal with respect to the measure $d\mu(\theta)$ as follows

$$p_k(x) = \frac{1}{\sqrt{2(1-\alpha_{2k-1})}}\left(z^{-k}\varphi_{2k}(z) + z^k\varphi_{2k}(z^{-1})\right), \qquad x = \frac{1}{2}\left(z + z^{-1}\right).$$

*[Szegő, 1939]*

The coefficients $(r_k, s_k)$, $k = 0, 1, 2, \ldots$, of the corresponding symmetric Jacobi matrix are given in terms of the Verblunsky coefficients by

$$r_k = \frac{1}{2}\Big(\alpha_{2k}(1-\alpha_{2k-1}) - \alpha_{2k-2}(1+\alpha_{2k-1})\Big),$$
$$s_k = \frac{1}{2}\sqrt{(1-\alpha_{2k-1})(1-\alpha_{2k}^2)(1+\alpha_{2k+1})}$$

*[Geronimus, 1958]*

[Cantero, Grünbaum, Moral, Velázquez, 2012]

When $r_k = 0$, $k = 0, 1, 2, \dots$, then in Szegedy's quantization the vectors $|k, k\rangle$ are invariant with respect to the action of $U = SR$ defined above. After removing them, in the restricted space define $U' = S'R'$ where

$$R' = 1 \oplus R'_1 \oplus R'_2 \oplus \dots, \qquad R'_k = \begin{pmatrix} q_k - p_k & 2\sqrt{p_k q_k} \\ 2\sqrt{p_k q_k} & p_k - q_k \end{pmatrix}, \qquad S' = A \oplus A \oplus A \oplus \dots .$$

Then in the CMV picture $S'$ can be identified with the matrix $\mathcal{L}$ for vanishing even Verblunsky coefficients $\alpha_{2k} = 0$, $k = 0, 1, 2, \dots$, while $R'$ plays the role of $\mathcal{M}$ with odd Verblunsky coefficients of the form

$$\alpha_{2k-1} = q_k - p_k, \quad \text{or} \quad p_k = \frac{1}{2}(1 - \alpha_{2k-1}), \; q_k = \frac{1}{2}(1 + \alpha_{2k-1}), \quad k = 0, 1, 2, \dots$$

and the CMV basis is given by the vectors

$$e_{2k} = |k, k+1\rangle, \qquad e_{2k+1} = |k+1, k\rangle, \qquad k = 0, 1, 2, \dots .$$

The final result is equivalent to the CGMV method for quantum walks. Their work contains also relation to the OPUC with vanishing (odd) Verblunsky coefficients

# The discriminant matrix and CMV space

Define

$$|\psi_k\rangle = S|\phi_k\rangle = \sqrt{q_k}\,|k-1,k\rangle + \sqrt{r_k}\,|k,k\rangle + \sqrt{p_k}\,|k+1,k\rangle, \quad k \geq 0,$$

then the elements of the discriminant matrix are given by

$$D_{jk} = \langle \phi_j | U\phi_k\rangle = \langle \phi_j | \psi_k\rangle,$$

and the matrix coincides with the Jacobi matrix $\mathcal{J}$ of Karlin and McGregor

## Lemma

For $k \in \mathbb{N}$

$$U^k|\phi_0\rangle \in \mathrm{span}\{|\phi_0\rangle, |\psi_0\rangle, \dots, |\phi_{k-1}\rangle, |\psi_{k-1}\rangle\},$$

$$U^{-k}|\phi_0\rangle \in \mathrm{span}\{|\phi_0\rangle, |\psi_0\rangle, \dots, |\phi_{k-1}\rangle, |\psi_{k-1}\rangle, |\phi_k\rangle\}$$

## Proposition

The CMV basis of the quantum evolution operator for Szegedy's quantization of the random walk on the half-line with the cyclic vector $e_0 = |\phi_0\rangle$ has the Verblunsky coefficients related with the random walk transition probabilities by the formulas

$$\begin{aligned} q_k &= \frac{1}{2}(1+\alpha_{2k-2})(1+\alpha_{2k-1}), \\ r_k &= \frac{1}{2}\left(\alpha_{2k}(1-\alpha_{2k-1}) - \alpha_{2k-2}(1+\alpha_{2k-1})\right), \qquad k \geq 0, \\ p_k &= \frac{1}{2}(1-\alpha_{2k-1})(1-\alpha_{2k}) \end{aligned}$$

# CMV basis

## Corollary 1

The measures and orthogonal polynomials of the discrete-time random walk and of its quantization are related by the Szegő projection

## Corollary 2

The orthonormal CMV basis $(e_j)_{j\in\mathbb{N}_0}$ and the Verblunsky coefficients $\alpha_j$ of the quantum walks are defined by the recursive application of the operators $S$ and $R$ on the initial vector $e_0 = |\phi_0\rangle$:

$$
\begin{aligned}
S(e_{2k}) &= \alpha_{2k} e_{2k} + \rho_{2k} e_{2k+1}, \qquad k \geq 0, \\
R(e_{2k+1}) &= \alpha_{2k+1} e_{2k+1} + \rho_{2k+1} e_{2k+2},
\end{aligned}
$$

where the sign of $\rho_j = \sqrt{1-\alpha_j^2} > 0$ fixes the orientation of $e_{j+1}$

## Corollary 3

The vectors $(|\phi_k\rangle, |\psi_k\rangle)_{k\in\mathbb{N}_0}$ of the natural quantum walk basis are expressed in terms of the CMV basis as follows

$$
|\phi_k\rangle = \sqrt{\frac{1+\alpha_{2k-1}}{2}}\, e_{2k-1} + \sqrt{\frac{1-\alpha_{2k-1}}{2}}\, e_{2k},
$$

$$
|\psi_k\rangle = \sqrt{\frac{1+\alpha_{2k-1}}{2}}\, (\rho_{2k-2} e_{2k-2} - \alpha_{2k-2} e_{2k-1}) + \sqrt{\frac{1-\alpha_{2k-1}}{2}}\, (\alpha_{2k} e_{2k} + \rho_{2k} e_{2k+1})
$$

# Conclusion

- We define quantization scheme for discrete-time random walks on the half-line consistent with Szegedy's quantization of finite Markov chains
- Motivated by the Karlin and McGregor description of discrete-time random walks in terms of polynomials orthogonal with respect to a measure with support in the segment $[-1, 1]$, we represent the unitary evolution operator of the quantum walk in terms of orthogonal polynomials on the unit circle
- We find the relation between transition probabilities of the random walk with the Verblunsky coefficients of the corresponding polynomials of the quantum walk
- We show that the both polynomial systems and their measures are connected by the classical Szegő projection map
- Our scheme can be applied to arbitrary Karlin and McGregor random walks and generalizes the so called Cantero–Grünbaum–Moral–Velázquez method

## Research in progress

- Connection of quantum walks to integrable equations of the Ablowitz–Ladik hierarchy
- Quantum walks on discrete curves with evolution induced by the shape of the given curve via the discrete Hasimoto transformation
- Quantum walks without classical interpretation

THANK YOU FOR YOUR ATTENTION