Integrable discrete systems, orthogonal polynomials, and quantum walks

Adam Doliwa
doliwa@matman.uwm.edu.pl

University of Warmia and Mazury, Olsztyn, Poland

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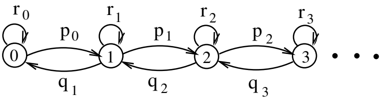
Outline

1. OPRL and discrete-time random walks
2. Quantization procedure
3. OPUC and CMV matrices

OUTLINE



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

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

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 ν in the interval $[-1, 1]$ of total mass 1 and infinite support

[Karlin & McGregor, 1959]

Define constants π_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.

Orthogonal polynomials and Toda equations

The monic versions $\tilde{Q}_k(x) = x^k + \ldots$ of the orthogonal polynomials $Q_k(x)$ satisfy the following three-term recurrence relations

$$x\tilde{Q}_k(x) = \tilde{Q}_{k+1}(x) + b_k\tilde{Q}_k(x) + a_k\tilde{Q}_{k-1}(x),$$

where

$$a_k = \frac{\int [\tilde{Q}_k(x)]^2 d\nu(x)}{\int [\tilde{Q}_{k-1}(x)]^2 d\nu(x)}, \qquad b_k = \frac{\int x[\tilde{Q}_k(x)]^2 d\nu(x)}{\int [\tilde{Q}_k(x)]^2 d\nu(x)}.$$

Assume that measure undergoes evolution of the form

$$d\nu(x,t) = e^{-xt} d\nu(x), \qquad t \in \mathbb{R}_+,$$

well known in the theory of continuous-time birth and death processes, then the coefficients of the three-term relation satisfy the Toda lattice equations in the form given by Flaschka

$$\dot{a}_k(t) = a_k(t)(b_{k-1}(t) - b_k(t)),$$
$$\dot{b}_k(t) = a_k(t) - a_{k+1}(t).$$

To obtain the discrete-time Toda lattice equations one considers the following variation of the measure

$$d\nu_t(x) = x^t d\nu(x), \qquad t \in \mathbb{N}_0.$$

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

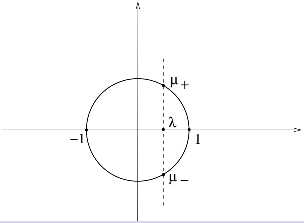
The single step of the quantum walk is defined as the unitary operator $U = SR$ being the composition of coin flip and the position swap

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 ± 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

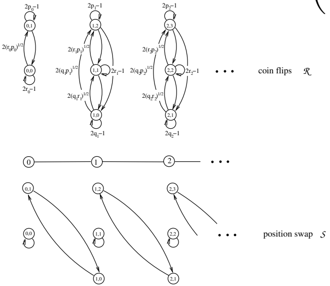
$$R = R_0 \oplus R_1 \oplus R_2 \oplus \dots$$

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 μ be a measure on the unit circle $\partial\mathbb{D}$ We assume that μ is nontrivial (i.e., supported on an infinite set) probability measure (i.e., μ 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 $\Phi_n(z)$, $n = 0, 1, 2, \ldots$ by the Gram-Schmidt orthogonalization procedure of the standard basis $1, z, z^2, \ldots$. We have then

$$\langle \Phi_n, \Phi_m \rangle = \frac{1}{\kappa_n^2}\delta_{nm}, \qquad \kappa_n > 0,$$

and the orthonormal polynomials $\varphi_n = \kappa_n \Phi_n$ 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 Φ_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 $\alpha_0, \alpha_1, \alpha_2, \ldots$ 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

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

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

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 μ 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 φ and φ^* 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 μ being symmetric with respect to complex conjugation one can define the measure ν 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]

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

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

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

Corollary

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

$$P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{n!2^n}(1-x)^{-\alpha}(1+x)^{-\beta}\frac{d^n}{dx^n}\left((1-x)^{\alpha+n}(1+x)^{\beta+n}\right), \qquad n \geq 0,$$

are orthogonal with respect to the measure on $[-1,1]$

$$d\nu(x) = (1-x)^{\alpha}(1+x)^{\beta}dx, \qquad \alpha,\beta > -1.$$

They reduce to the Gegenbauer ($\alpha=\beta$), Legendre ($\alpha=\beta=0$), Chebyshev polynomials of the first ($\alpha=\beta=-\frac{1}{2}$) or the second ($\alpha=\beta=\frac{1}{2}$) kind. Also the Laguerre and Hermite polynomials can be derived as certain limiting cases of the Jacobi polynomials.

The corresponding polynomials defined by

$$Q_n^{(\alpha,\beta)}(x) = \frac{P_n^{(\alpha,\beta)}(x)}{P_n^{(\alpha,\beta)}(1)},$$

satisfy three term recurrence

$$xQ_n^{(\alpha,\beta)}(x) = p_n^{(\alpha,\beta)}Q_{n+1}^{(\alpha,\beta)}(x) + r_n^{(\alpha,\beta)}Q_n^{(\alpha,\beta)}(x) + q_n^{(\alpha,\beta)}Q_{n-1}^{(\alpha,\beta)}(x),$$

with the coefficients

$$p_n^{(\alpha,\beta)} = \frac{2(n+\alpha+1)(n+\alpha+\beta+1)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)},$$

$$r_n^{(\alpha,\beta)} = \frac{\beta^2-\alpha^2}{(2n+\alpha+\beta)(2n+\alpha+\beta+2)},$$

$$q_n^{(\alpha,\beta)} = \frac{2n(n+\beta)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)},$$

In the above

$$p_n^{(\alpha,\beta)} + r_n^{(\alpha,\beta)} + q_n^{(\alpha,\beta)} = 1, \qquad p_0^{(\alpha,\beta)} > 0, \quad q_0^{(\alpha,\beta)} = 0, \qquad p_n^{(\alpha,\beta)} > 0, \qquad q_n > 0 \quad \text{for} \quad n > 0.$$

In order to be random walk polynomials they have to satisfy the recurrence with $r_n^{(\alpha,\beta)} \geq 0$, which needs $\alpha = \beta$ or $\beta \geq |\alpha|$.

The corresponding quantum walks are governed by circular analogs of the Jacobi polynomials, obtained by Szegő, are given by the weight

$$w(\theta) = (1 - \cos\theta)^{\alpha + 1/2}(1 + \cos\theta)^{\beta + 1/2}, \qquad \alpha, \beta > -1, \qquad \theta \in [0, 2\pi].$$

The Verblunsky coefficients for the measure have been found by Golinskii and Badkov and read

$$\alpha_n = -\frac{\alpha + \frac{1}{2} + (-1)^{n+1}(\beta + \frac{1}{2})}{n + \alpha + \beta + 2}.$$

THEOREM *[Golinskii, 2006]*

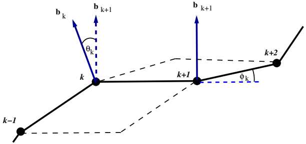
Assume that measure on $\partial\mathbb{D}$ undergoes evolution of the form

$$d\mu(\zeta,t) = C(t)e^{t(\zeta+\zeta^{-1})}d\mu(\zeta,0), \qquad C^{-1}(t) = \int_{\partial\mathbb{D}} e^{t(\zeta+\zeta^{-1})}d\mu(\zeta,0), \qquad t \in \mathbb{R}_+,$$

then the Verblunsky coefficients satisfy the first equation of the Ablowitz–Ladik hierarchy (known as the Schur flow in OPUC community)

$$\dot{\alpha}_k(t) = (1 - |\alpha_k(t)|^2)(\alpha_{k+1}(t) - \alpha_{k-1}(t))$$

[Ablowitz & Ladik, 1976]



ABLOWITZ–LADIK HIERARCHY AND DISCRETE CURVES *[AD & Santini, 1995]*

When φ_k is the angle of curvature of a discrete curve in $\mathbb{E}^3$, and θ_k is the angle of torsion then in the $SU(2)$ representation of the Frenet frame we have

$$\alpha_k = \sin(\varphi_k/2)\mathrm{e}^{i\sigma_k},$$

where $\sigma_k = \sum_j^k \theta_j$ is the discrete analogue of the Hasimoto transformation

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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 improves the so called Cantero–Grünbaum–Moral–Velázquez method

Research in progress

- Quantum walks on discrete curves with evolution operators induced by their shapes
- Quantum walks without classical interpretation

THANK YOU FOR YOUR ATTENTION