Recurrence of Unitary and Stochastic Quantum Walks

Martin Štefaňák

Department of Physics, Faculty of Nuclear Sciences and Physical Engineering
Czech Technical University in Prague

Algebraic Graph Theory Seminar, 3. 11. 2025

Outline

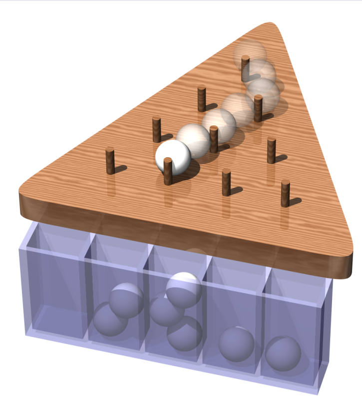
Random Walk

- Walker hops randomly between vertices of a graph
- Prescribed rules for jumps
- Discrete-time steps

Probability distribution $p(x, t)$

- Starts the walk at the vertex 0
- Trajectories connecting vertices 0 and x in t steps
- Each trajectory has a probability
- Sum all probabilities — $p(x, t)$

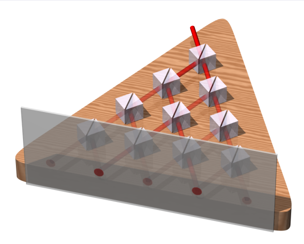
Galton board
Random walk on a line



Quantum Walk

- Walker is a quantum particle
- Discrete-time unitary evolution
- Coherent spreading instead of random jumps
- Quantum walker evolves into a state of superposition of being on different vertices (until measurement)

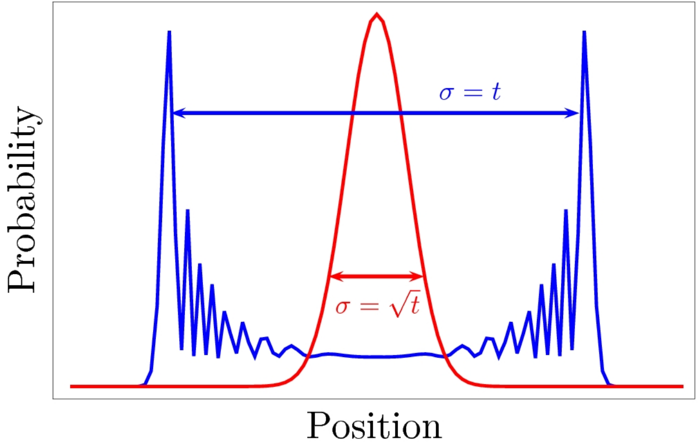
Optical Galton board
Quantum walk on a line



Probability distribution after t steps $p(x,t)$?

- Each trajectory from 0 to x has a probability amplitude
- Sum all amplitudes — wave function $\psi(x,t)$ — interference
- Probability distribution — $p(x,t) = |\psi(x,t)|^2$

Comparison of Random and Quantum Walk on a Line



- Classical walk — diffusion
- Quantum walk — wave propagation

Two-state Quantum Walk on a Line

- Quantum walk on 1D lattice, walker moves left/right in every step
- Position space — $|x\rangle$, $x \in \mathbb{Z}$, coin space — $|L\rangle$, $|R\rangle$
- Unitary operator for a single step — $U = S \cdot (I \otimes C)$
- Conditional shift S — moves walker according to the coin state

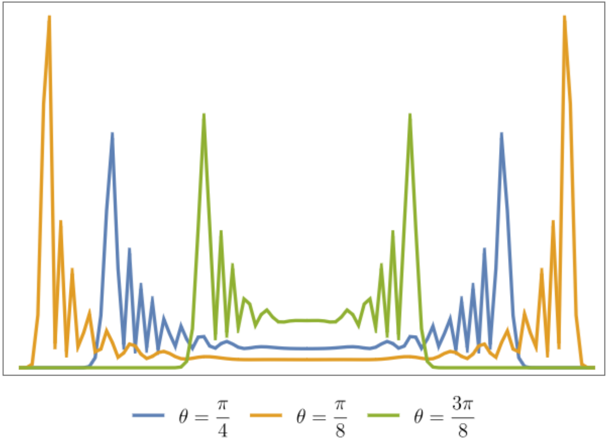
$$S|x, L\rangle = |x-1, L\rangle, \quad S|x, R\rangle = |x+1, R\rangle$$

- Coin operator — unitary transformation on the coin space

$$C(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}, \quad C(\pi/4) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \; - \; \text{Hadamard coin}$$

- QW is analogy of correlated RW — keep direction with $\cos^2\theta$, change with $\sin^2\theta$
- For $\theta = \pi/4$ correlated RW reduces to simple RW

Role of Coin Parameter θ



- θ determines the speed of propagation
- After t steps wavefronts are at positions $\approx \pm t \cos\theta$

Outline

Recurrence in classical random walks

- Consider probabilities of first return after n steps q_n
- Mutually exclusive events — recurrence probability is given by a sum

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

- Relation between q_n and probability to be at origin after n steps p_n

$$\begin{aligned} p_0 &= 1, \quad p_1 = q_1, \quad p_2 = q_2 + q_1 p_1 \\ p_n &= q_n + q_{n-1} p_1 + \ldots + q_1 p_{n-1} \end{aligned}$$

- Introduce generating functions for probabilities

$$\mu(z) = \sum_{n=0}^{\infty} p_n z^n, \quad a(z) = \sum_{n=1}^{\infty} q_n z^n, \quad z < 1$$

- We find the relation between generating functions

$$\mu(z) = 1 + \mu(z) a(z) \Longrightarrow a(z) = 1 - \mu(z)^{-1}$$

Recurrence in classical random walks

- Recurrence probability obtained by limit $z \to 1^-$

$$P = \lim_{z \to 1^-} a(z) = 1 - \frac{1}{\sum\limits_{n=0}^{+\infty} p_n} = 1 - \frac{1}{\Sigma}, \quad \Sigma = \sum_{n=0}^{+\infty} p_n$$

- $P = 1 \iff \Sigma$ diverges
- For unbiased random walk on $\mathbb{Z}^d$ — $p_n \sim n^{-\frac{d}{2}}$
- Classical random walks are recurrent $(P = 1)$ for $d = 1, 2$,
- Transient $(P < 1)$ for $d \geq 3$ (Polya, 1921)
- Relation between q_n and p_n will not hold in the quantum case
- However, there will be a similar relation between amplitudes (or their generating functions)

Monitored evolution of quantum walk

- Unitary step U followed by a measurement at the origin $\Pi_0 = |0\rangle\langle 0| \otimes I_c$
- Stop if we find the walker, continue otherwise — complementary projection $\Pi_0^\perp$
- State of the quantum walker after n steps — conditional wave function

$$|\psi^{(c)}(n)\rangle = \frac{1}{\sqrt{s_{n-1}}} U\, \tilde{U}^{n-1} |\psi(0)\rangle, \quad \tilde{U} = \Pi_0^\perp\, U$$

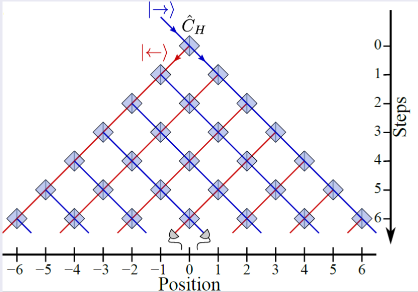
- Survival probability — prob. of not being absorbed at the origin in first $n-1$ steps

$$s_{n-1} = \left\| \tilde{U}^{n-1} |\psi(0)\rangle \right\|^2$$

- Conditional probability to be at the origin — $p_n^{(c)} = |\langle 0|\psi^{(c)}(n)\rangle|^2$
- First return probability — $q_n = s_{n-1}\; p_n^{(c)}$

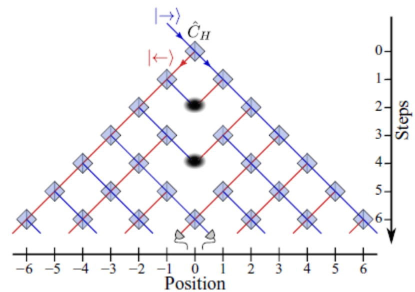
Recurrence in Quantum Walks

QW without measurements



- Provides p_n

QW with measurements



- Provides $p_n^{(c)}$ and q_n

No simple relation between first return probability q_n and prob. of being at origin p_n

Recurrence in Quantum Walks

- Fundamental difference between measurement in classical and quantum case
- Random walker has a position, measurement merely reveals it
- Position of a quantum walker is not defined until we make a measurement

Recurrence probability of a quantum walk

$$P = \sum_{n=1}^{\infty} q_n \neq 1 - \frac{1}{\sum\limits_{n=0}^{\infty} p_n}$$

- First return probabilities q_n

$$q_n = \|a_n \psi\|^2$$

- First return amplitude operator (note that $\Pi_0 \psi = \psi$)

$$a_n = \Pi_0 U \tilde{U}^{n-1} \Pi_0$$

Generating functions

- n-th step return amplitude operators (without prior monitoring)

$$\mu_n = \Pi_0 U^n \Pi_0$$

- Operator valued generating functions ($z \in \mathbb{C}$, $|z| < 1$)

$$\mu(z) = \sum_{n=0}^{\infty} \mu_n z^n, \quad a(z) = \sum_{n=1}^{\infty} a_n z^n$$

- Resolvents for U and $\tilde{U}$

$$G(z) = \sum_{n=0}^{\infty} U^n z^n = (I - zU)^{-1}, \quad \tilde{G}(z) = \sum_{n=0}^{\infty} \tilde{U}^n z^n = (I - z\tilde{U})^{-1}$$

Renewal equations for generating functions

- Relations between generating functions and resolvents

$$\mu(z) = \Pi_0 G(z) \Pi_0, \quad a(z) = z \Pi_0 U \tilde{G}(z) \Pi_0$$

- Additional properties

$$\tilde{G}(z) - I = z \tilde{U} \tilde{G}(z), \quad \Pi_0 \tilde{G}(z) \Pi_0 = \Pi_0$$

- Resolvent identities

$$G(z) - \tilde{G}(z) = z G(z) \Pi_0 U \tilde{G}(z) = z \tilde{G}(z) \Pi_0 U G(z)$$

- Leads to relations

$$\mu(z) - \Pi_0 = \mu(z) a(z) = a(z) \mu(z)$$

Renewal equation

- Renewal equations

$$\mu(z) - \Pi_0 = \mu(z)a(z) = a(z)\mu(z)$$

- All operators act on the origin subspace

$$\mu(z) = |0\rangle\langle 0| \otimes \mu_c(z), \quad a(z) = |0\rangle\langle 0| \otimes a_c(z), \quad \Pi_0 = |0\rangle\langle 0| \otimes I_c$$

- Relation for operators acting on the coin space (amplitude generating functions)

$$a_c(z) = I_c - \mu_c(z)^{-1}$$

- Reminder — relation for classical generating functions for probabilities

$$a(z) = 1 - \mu(z)^{-1}$$

Recurrence probability

- Recurrence probability can be evaluated with

$$P = \int_0^{2\pi} \|a_c(e^{it})\psi_c\|^2 \frac{dt}{2\pi} = \langle\psi_c|R|\psi_c\rangle$$

- Recurrence probability operator

$$R = \int_0^{2\pi} a_c^\dagger(e^{it})a_c(e^{it})\frac{dt}{2\pi}$$

Grünbaum et al., Commun. Math. Phys. **320**, 543 (2013)

Outline

Generating functions and resolvent for homogeneous case

- Evolution operator in the momentum representation

$$U = \int_0^{2\pi} \frac{dk}{2\pi} |k\rangle\langle k| \otimes U(k), \quad U(k) = S(k)\cdot C, \quad S(k) = \mathrm{diag}(e^{ik}, e^{-ik})$$

- Resolvent

$$G(z) = \int_0^{2\pi} \frac{dk}{2\pi} |k\rangle\langle k| \otimes (I_c - zU(k))^{-1}$$

- Generating function — Stieltjes operator

$$\begin{aligned} \mu(z) &= \Pi_0 G(z) \Pi_0 = |0\rangle\langle 0| \otimes \mu_c(z) \\ \mu_c(z) &= \int_0^{2\pi} \frac{dk}{2\pi} (I_c - zU(k))^{-1} \end{aligned}$$

Resolvent in momentum picture

- Evolution operator in the momentum picture

$$U(k) = \begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix} \cdot \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix} = \begin{pmatrix} e^{ik}\cos\theta & \sin\theta e^{ik} \\ \sin\theta e^{-ik} & -e^{-ik}\cos\theta \end{pmatrix}$$

- Resolvent in the Fourier space

$$(I_c - zU(k))^{-1} = \frac{1}{f(z,k)} \begin{pmatrix} 1 + ze^{-ik}\cos\theta & z\sin\theta e^{ik} \\ z\sin\theta e^{-ik} & 1 - ze^{ik}\cos\theta \end{pmatrix}$$

$$f(z,k) = 1 - 2iz\cos\theta\sin k - z^2$$

- Stieltjes operator

$$\mu_c(z) = \int_0^{2\pi} \frac{dk}{2\pi}(I_c - zU(k))^{-1}$$

Evaluation of Stieltjes operator

- Stieltjes operator — involves integrals of the form ($n = 0, \pm 1$)

$$\mathcal{I}(n) = \int_0^{2\pi} \frac{dk}{2\pi} \frac{e^{ink}}{f(z,k)} = \frac{1}{2\pi i} \oint \frac{x^n dx}{b(x)}, \quad x = e^{ik}$$

$$b(x) = x(1-z^2) - z(1-x^2)\cos\theta$$

- Can be evaluated with residues

$$\mu_c(z) = \frac{1}{2g(z)} \begin{pmatrix} 1 - z^2 + g(z) & (1 - z^2 - g(z))\tan\theta \\ -(1 - z^2 - g(z))\tan\theta & 1 + z^2 + g(z) \end{pmatrix}$$

$$g(z) = \sqrt{1 + 2z^2\cos(2\theta) + z^4}$$

First return generating function and Recurrence probability operator

- Renewal equation

$$a_c(z) = I_c - \mu_c(z)^{-1}$$

- First return generating operator

$$a_c(z) = \frac{1 + z^2 - g(z)}{2} \begin{pmatrix} 1 & -\cot\theta \\ \cot\theta & 1 \end{pmatrix}$$

- Recurrence probability operator

$$R = \int_0^{2\pi} a_c^\dagger(e^{it}) a_c(e^{it}) \frac{dt}{2\pi}$$

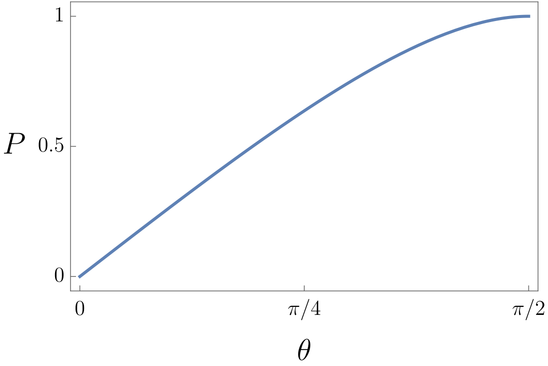
- It is a multiple of identity

$$a_c^\dagger(z) a_c(z) = \frac{|1 + z^2 - g(z)|^2}{4\sin^2\theta} I_c$$

Recurrence of a Quantum Walk on a Line

- Recurrence probability independent of the initial coin state

$$P = \frac{1}{8\pi \sin^2\theta} \int_0^{2\pi} |1 + e^{2it} - g(e^{it})|^2 dt = \frac{2}{\pi}\left[\theta(1-\cot^2\theta) + \cot\theta\right] < 1$$



- Faster spreading due to interference — transience already for $d = 1$
- For Hadamard walk

$$P(\pi/4) = \frac{2}{\pi} \approx 0.636$$

Outline

Discrete-time Quantum Stochastic Walk

What happens when we interpolate between Quantum Walk and Random Walk?

- Evolution where choose between RW/QW in each step
  - With probability p we make a balanced random walk
  - With probability $1-p$ we make a quantum walk
- Model can be formulated as a Discrete-time Quantum Stochastic Walk (DTQSW)

$$\rho(t+1) = \mathcal{T}\rho(t) = (1-p)\underbrace{U\rho(t)U^\dagger}_{\text{QW}} + p\underbrace{\left(\frac{1}{2}S_L\rho(t)S_L^\dagger + \frac{1}{2}S_R\rho(t)S_R^\dagger\right)}_{\text{RW}}$$

- $S_{L/R}$ shifts the whole quantum state one lattice site to the left/right

Recurrence of DTQSW — Grünbaum and Velázquez, Adv. Math. (2018)

- Recurrence of DTQSW — recurrence of a CPTP map $\mathcal{T}$
- We know the values for the endpoints $p = 0$ (unitary QW) and $p = 1$ (RW)

$$P(p=0) = \frac{2}{\pi}\left[\theta(1-\cot^2\theta) + \cot\theta\right], \quad P(p=1) = 1 \text{ independent of } \theta$$

What happens in between?

- Direct numerical simulation allows to study recurrence for $t \sim 500$ steps
- Convergence is much slower than for the unitary quantum walk
- Alternative approach with generating functions allows to effectively consider 10^5 steps

Recurrence of DTQSW

- Recurrence probability

$$P = \sum_{n=1}^{\infty} q_n = \lim_{z \to 1^-} \mathrm{Tr}\left[\mathcal{F}(z)\rho(0)\right]$$

- (Reduced) first-return functions (FR)

$$\mathcal{F}(z) = \mathcal{P} f(z) \mathcal{P}, \quad f(z) = (I - \mathcal{Q})\mathcal{T}(I - z\mathcal{Q}\mathcal{T})^{-1}(I - \mathcal{Q})$$

- Projections acting on density matrices

$$\mathcal{P}\,\rho = \Pi_0\,\rho\,\Pi_0, \quad \mathcal{Q}\,\rho = \Pi_0^{\perp}\,\rho\,\Pi_0^{\perp}$$

- Renewal equation - relates FR function and Stieltjes operator

$$f(z) = I - \mu(z)^{-1}$$

Recurrence of DTQSW

- CPTP map in the momentum picture

$$\mathcal{T} = \int_0^{2\pi} \frac{dk_1}{2\pi} \int_0^{2\pi} \frac{dk_2}{2\pi} \, |k_1, k_2\rangle\langle k_1, k_2| \otimes V(k_1, k_2)$$

$$V(k_1, k_2) = (1-p)U(k_1) \otimes U(k_2) + p\cos(k_1 + k_2) I_c \otimes I_c$$

- Resolvent

$$(I - z\hat{\mathcal{T}})^{-1} = \int_0^{2\pi} \frac{dk_1}{2\pi} \int_0^{2\pi} \frac{dk_2}{2\pi} |k_1, k_2\rangle\langle k_1, k_2| \otimes A(z, k_1, k_2)$$

$$A(z, k_1, k_2) = [I_c \otimes I_c - zV(k_1, k_2)]^{-1}$$

Recurrence of DTQSW

- Stieltjes operator

$$\mu(z) = (I - \mathcal{Q})(I - z\mathcal{T})^{-1}(I - \mathcal{Q})$$

- Stieljes operator can be expressed as a sum

$$\mu(z) = \sum_{\substack{x,y,m,n \\ xm=yn=0}} |x, m\rangle\langle y, n| \otimes A_{xm,yn}(z)$$

- $A_{xm,yn}(z)$ have to be evaluated numerically

$$A_{xm,yn}(z) = \int_0^{2\pi} \frac{dk_1}{2\pi} \int_0^{2\pi} \frac{dk_2}{2\pi} A(z, k_1, k_2) e^{ik_1(x-y)+ik_2(m-n)}$$

- FR functions

$$f(z) = I - \mu(z)^{-1}, \qquad \mathcal{F}(z) = \mathcal{P} f(z) \mathcal{P}$$

Recurrence of DTQSW

- FR functions can be numerically evaluated for z close to 1
- Approximation of the recurrence probability

$$\tilde{P}_z = \mathrm{Tr}\left[\mathcal{F}(z)\rho(0)\right] = \sum_{n=1}^{\infty} q_n z^n$$

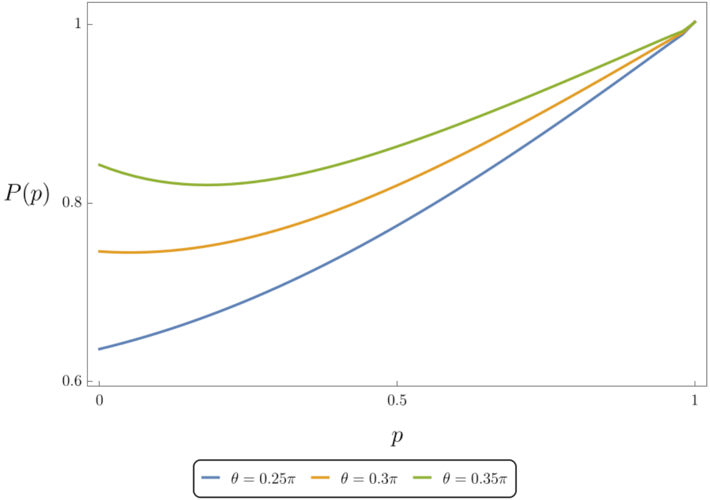
- Summing the exact first return probabilities

$$P_t = \sum_{n=1}^{t} q_n$$

- Choosing z corresponds to effective number of steps $t_{\mathrm{eff}} = 1/(1-z)$

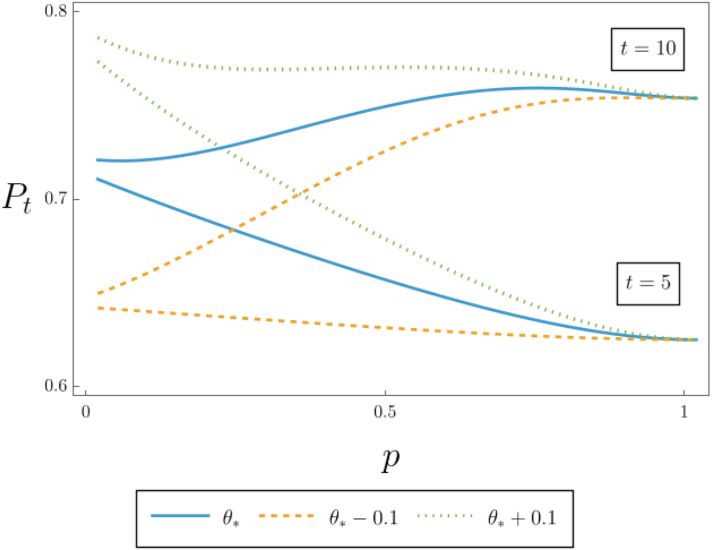
$$z = 0.99999 \implies t_{\mathrm{eff}} = 10^5$$

Recurrence of DTQSW — Stefanak et al., arXiv:2501.08674



- For small θ recurrence probability is purely increasing function of p
- With increasing θ $P(p)$ become non-monotonic
- Classical randomness can help the quantum walker to escape, despite the fact that classical random walk is recurrent

Recurrence of DTQSW — Stefanak et al., arXiv:2501.08674



- Minima at $p \neq 0$ for $\theta > \theta_* \approx 0.2892\pi$ develop in the first few steps
- The fact that they persist in the limit $t \to \infty$ is due to quantum interference
- Non-monotonicity of $P(p)$ arises from interplay of quantum and classical dynamics

References

- G. Pólya, Math. Ann. **84**, 149 (1921)
- F. A. Grünbaum, et al., Commun. Math. Phys. **320**, 543 (2013)
- F. A. Grünbaum and L. Velázquez, Advances Math. **326**, 352 (2018)
- M. Štefaňák, V. Potoček, I. Yalcinkaya, A. Gabris and I. Jex, arXiv:2501.08674




Thank you for your attention