Quantum Walks: Localization and Recurrences

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Trento, 2010

Outline

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Motivation

- Random walks are one of the cornerstones of theoretical computer science — database search, graph connectivity, 3-SAT, permanent of a matrix,...
- Quantum walks could solve the same problems on a quantum computer, with a speed-up

Random Walks

- Probabilities
- Different paths adds up
- Diffusion
- Spread slowly

$$\sigma \sim \sqrt{t}$$

Quantum Walks

- Probability amplitudes
- Different paths interfere
- Wave propagation
- Spread fast

$$\sigma \sim t$$

Continuous-time Quantum Walks

- Schrödinger equation, hamiltonian $\Longleftrightarrow$ adjacency matrix
- Suitable for description of coherent energy transfer
- Efficient energy transfer in photosynthetic systems

G. S. Engel et al., Nature **446**, 782 (2007)
M. Mohseni et al., J. Chem. Phys. **129**, 174106 (2008)
F. Caruso et al., J. Chem. Phys. **131**, 105106 (2009)

- Universal computational with a continuous-time quantum walk

A. M. Childs, Phys. Rev. Lett. 102, 180501 (2009)

Discrete-time (Coined) Quantum Walks

- Discrete-time evolution by a unitary propagator
- Require an additional degree of freedom — coin
- Suitable algorithmic tool
- Database search by quantum walk — SKW algorithm

N. Shenvi et al., Phys. Rev. A **67**, 052307 (2003)

- Discrete-time quantum walk is a universal computational primitive

N. B. Lovett et al., *pre-print* arXiv:0910.1024

Experiments

- Atom in an optical trap

M. Karski et al., Science **325**, 174 (2009)

- Ion in a linear trap

H. Schmitz et al., Phys. Rev. Lett. **103**, 090504 (2009)

- Single photon in an optical loop

A. Schreiber et al., Phys. Rev. Lett. **104**, 050502 (2010)

Quantum Walk on a Line

- Particle lives on 1-D lattice — position space

$$\mathcal{H}_P = \ell^2(\mathbb{Z}) = \mathrm{Span}\left\{|m\rangle | m \in \mathbb{Z}\right\}$$

- Moves in a discrete time steps on a lattice

$$\text{RW: } m \longrightarrow m-1, m+1 \Longrightarrow \text{QW: } |m\rangle \longrightarrow |m-1\rangle + |m+1\rangle$$

- Does not preserve orthogonality

$$\text{orthogonal} \left\{ \begin{array}{ccc} |0\rangle & \longrightarrow & |1\rangle + |-1\rangle \\ |2\rangle & \longrightarrow & |1\rangle + |3\rangle \end{array} \right\} \text{non-orthogonal}$$

- To make the time evolution unitary we need an additional degree of freedom — coin space

$$\mathcal{H}_C = \mathrm{Span}\left\{|L\rangle, |R\rangle\right\}$$

Quantum Walk on a Line

- Time evolution equation

$$|\psi(t)\rangle = U^t|\psi(0)\rangle, \quad U = S\cdot(I_P\otimes C)$$

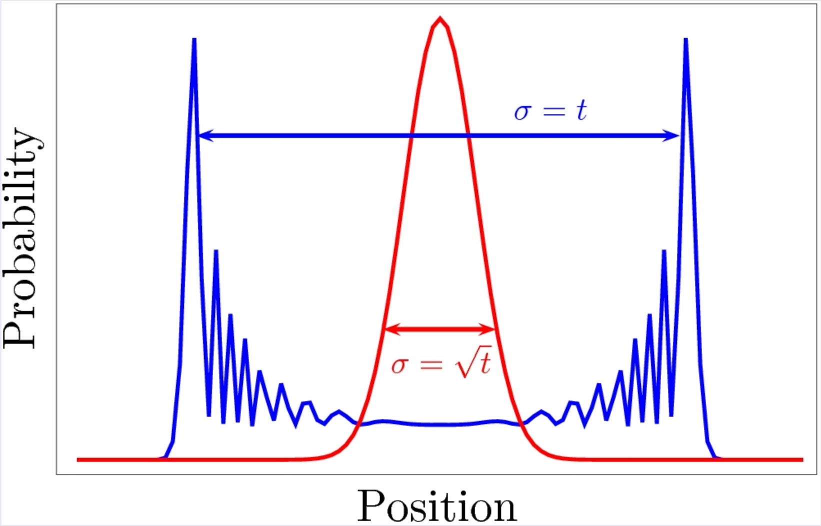
- Initial state $|\psi(0)\rangle$ — initial position + orientation of the coin
- Displacement operator

$$S = \sum_m \left(|m+1\rangle\langle m|\otimes|R\rangle\langle R| + |m-1\rangle\langle m|\otimes|L\rangle\langle L|\right)$$

- Coin flip C - rotates the coin state before the step itself
- e.g. Hadamard matrix

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

Quantum Walk on a line



Outline

Pólya Number of a Random Walk

G. Pólya, Math. Ann. **84**, 149 (1921)

- Probability that a random walk (RW) on $\mathbb{Z}^d$ starting at the origin **0** ever returns to the origin
- If $p_0(t)$ is the probability that the walker is at the origin after t steps then the Pólya number is given by

$$P = 1 - \frac{1}{\sum\limits_{t=0}^{\infty} p_0(t)}$$

- Random walk is recurrent if $P = 1$
- Random walk is transient if $P < 1$ - non-zero escape probability
- Unbiased random walks are recurrent for the dimensions $d = 1, 2$, transient for $d \geq 3$
- Biased random walks are transient for any dimension d

Recurrence of Random Walks

Criterion of recurrence

- Random Walk is recurrent if and only if

$$\sum_{t=0}^{+\infty} p_0(t) = +\infty \quad \Longleftrightarrow \quad p_0(t) \sim t^{-1} \quad \text{or slower}$$

- Recurrence is fully determined by the asymptotics of $p_0(t)$

- For a unbiased RW on $\mathbb{Z}^d$ the probability $p_0(t)$ scales like

$$p_0(t) \sim t^{-\frac{d}{2}}$$

- For $d = 1, 2$ the walks are recurrent $\Longrightarrow P = 1$
- For $d \geq 3$ the walks are transient $\Longrightarrow P < 1$
- For a biased RW $p_0(t)$ decays exponentially $\Longrightarrow P < 1$

Outline

Pólya Number of a Quantum Walk

MŠ, I. Jex, T. Kiss, Phys. Rev. Lett. **100**, 020501 (2008)

Problem

Measurement change the state of the particle

Our definition

- Prepare an ensemble of particles in the same initial state
- Take *n*-th particle, make *n* steps, measure at the origin
- In the *n*-th trial — click with $p_0(n)$, no click with $1 - p_0(n)$
- No click at all — occurs with $\overline{P} = \prod_{t=1}^{+\infty}(1 - p_0(t))$
- Complementary event — at least one click — recurrence
- Pólya number of a QW — $P = 1 - \prod_{t=1}^{+\infty}(1 - p_0(t))$

Recurrence of Quantum Walks

Criterion of recurrence

- Quantum Walk is recurrent if and only if

$$\prod_{t=1}^{+\infty}\Big(1-p_0(t)\Big)=0 \quad\Longleftrightarrow\quad \sum_{t=0}^{+\infty}p_0(t)=+\infty$$

- As for classical Random Walks, recurrence of Quantum Walks is fully determined by the asymptotics of $p_0(t)$

- Quantum Walk is recurrent if $p_0(t)\sim t^{-1}$ or slower
- Quantum Walk is transient if $p_0(t)$ decays faster than t^{-1}
- Probability at the origin is influenced by the additional degrees of freedom - coin operator C and the initial state $|\psi\rangle$

Outline

Hilbert Space of Quantum Walks

- Given by the tensor product

$$\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_C$$

- Position space

$$\mathcal{H}_P = \ell^2(\mathbb{Z}^d) = \mathrm{Span}\left\{|\mathbf{m}\rangle | \mathbf{m} \in \mathbb{Z}^d\right\}$$

- Coin space - determined by the set of displacements which the walker can make in a single step

$$\mathbf{m} \longrightarrow \mathbf{m} + \mathbf{e}_j$$

$$\mathcal{H}_C = \mathrm{Span}\left\{|\mathbf{e}_j\rangle | \mathbf{e}_j \in \mathbb{Z}^d, j = 1, \ldots, n\right\}$$

Time Evolution of Quantum Walks

- Time evolution is determined by

$$|\psi(t)\rangle \equiv \sum_{\mathbf{m},j} \psi_j(\mathbf{m}, t)|\mathbf{m}\rangle \otimes |\mathbf{e}_j\rangle = U^t|\psi(0)\rangle$$

$$U = S \cdot (I_P \otimes C)$$

- Displacement operator

$$S = \sum_{\mathbf{m},j} |\mathbf{m} + \mathbf{e}_j\rangle\langle\mathbf{m}| \otimes |\mathbf{e}_j\rangle\langle\mathbf{e}_j|$$

- Coin flip C — unitary operator on $\mathcal{H}_C$

Time Evolution of Quantum Walks

- Vectors of probability amplitudes

$$\psi(\mathbf{m}, t) \equiv (\psi_1(\mathbf{m}, t), ..., \psi_n(\mathbf{m}, t))^T$$

- Time evolution of amplitudes — set of difference equations

$$\psi(\mathbf{m}, t) = \sum_l C_l \psi(\mathbf{m} - \mathbf{e}_l, t - 1), \quad C = \sum_l C_l$$

- Translational invariance — the matrices C_l are independent of $\mathbf{m}$
- Fourier transformation

$$\widetilde{\psi}(\mathbf{k}, t) \equiv \sum_{\mathbf{m}} \psi(\mathbf{m}, t) e^{i\mathbf{m}\cdot\mathbf{k}}, \quad \mathbf{k} \in (-\pi, \pi]^d$$

simplifies the time evolution equation

Time Evolution in the Fourier Picture

- Time evolution equation in the Fourier picture

$$\widetilde{\psi}(\mathbf{k},t) = \widetilde{U}(\mathbf{k})\widetilde{\psi}(\mathbf{k},t-1) = \widetilde{U}^t(\mathbf{k})\widetilde{\psi}(\mathbf{k},0)$$

- Propagator in the Fourier picture

$$\widetilde{U}(\mathbf{k}) \equiv D(\mathbf{k}) \cdot C$$

$$D(\mathbf{k}) \equiv \mathcal{D}\left(e^{i\mathbf{e}_1\cdot\mathbf{k}}, \ldots, e^{i\mathbf{e}_n\cdot\mathbf{k}}\right)$$

- Walk starts localized at the origin - Fourier transformation of the initial state is identical to the initial coin state

$$\psi(\mathbf{m},0) = 0 \quad \text{for} \quad \mathbf{m} \neq \mathbf{0} \Longrightarrow \widetilde{\psi}(\mathbf{k},0) = \psi(\mathbf{0},0) \equiv \psi$$

Solution of the Time Evolution Equations

Solution in the momentum picture

Matrix $\widetilde{U}(\mathbf{k})$ is unitary — eigenvalues $\lambda_j(\mathbf{k}) = \exp\left(i\omega_j(\mathbf{k})\right)$
corresponding eigenvectors $v_j(\mathbf{k})$

$$\widetilde{\psi}(\mathbf{k}, t) = \sum_j e^{i\omega_j(\mathbf{k})t} \left(v_j(\mathbf{k}), \psi\right) v_j(\mathbf{k})$$

Solution in the position representation

$$\psi(\mathbf{m}, t) = \sum_j \left[\int\limits_{(-\pi,\pi]^d} \frac{d\mathbf{k}}{(2\pi)^d} e^{i(\omega_j(\mathbf{k})t - \mathbf{m}\cdot\mathbf{k})} \left(v_j(\mathbf{k}), \psi\right) v_j(\mathbf{k}) \right]$$

Amplitude at the origin

$$\psi(\mathbf{0},t) = \sum_j \left[\int\limits_{[-\pi,\pi]^d} \frac{d\mathbf{k}}{(2\pi)^d} \quad e^{i\omega_j(\mathbf{k})t} \cdot \left(v_j(\mathbf{k}),\psi\right) \cdot v_j(\mathbf{k}) \right]$$

- Asymptotics of $\psi(\mathbf{0},t)$ can be analyzed e.g. by the method of stationary phase
- Stationary points of the phases $\omega_j(\mathbf{k})$

$$\mathbf{k}_0 \quad \text{such that} \quad \nabla\omega_j(\mathbf{k}_0) \equiv \mathbf{0}$$

  determines the asymptotic behaviour
- Overlap between the initial state ψ and the eigenvector $v_j(\mathbf{k})$ can effectively cancel a stationary point

$$\left(v_j(\mathbf{k}_0),\psi\right) \equiv 0$$

Outline

Grover Walk on a Plane

MŠ, T. Kiss and I. Jex, Phys. Rev. A **78**, 032306 (2008)

- Coin $\Longleftrightarrow$ 4x4 Grover matrix
- Eigenvalues of the propagator

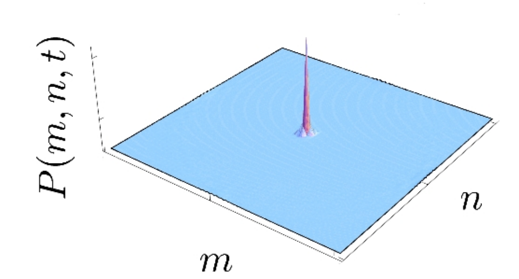
$$\lambda_{1,2} = \pm 1, \quad \lambda_{3,4}(k_1,k_2) = e^{\pm i\omega(k_1,k_2)}, \quad \cos\left(\omega(k_1,k_2)\right) = \cos k_1 \cos k_2$$

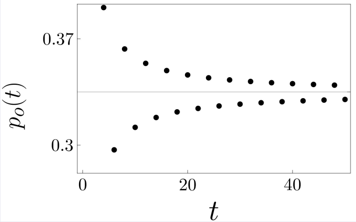
- Contribution from $\lambda_{1,2}$ is constant $\times$ from $\lambda_{3,4}$ decays like t^{-2}
- Probability at the origin $p_0(t)$ behaves like a constant except for

$$\psi_G = \frac{1}{2}\left(1,-1,-1,1\right)^T$$

which is orthogonal to $v_{1,2}(\mathbf{k})$ for any **k**

Probability Distribution for the Grover Walk



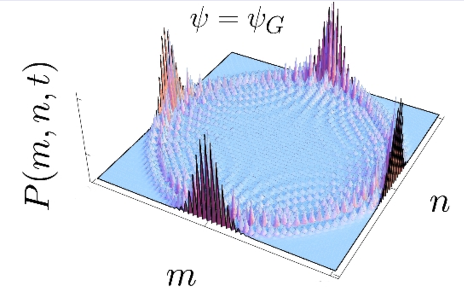


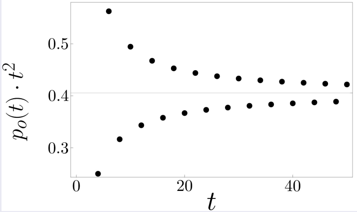
- For any initial state $\psi \neq \psi_G$ the probability at the origin behaves like a constant

$$p_0(t) \sim \mathrm{const}$$

- Exponential localization
- The walk is recurrent

Probability Distribution for the Grover Walk





- For the initial state $\psi = \psi_G$ the probability at the origin decays fast

$$p_0(t) \sim t^{-2}$$

- Localization disappears
- The walk is transient

Fourier Walk on a Plane

MŠ, T. Kiss and I. Jex, Phys. Rev. A **78**, 032306 (2008)

- Coin $\Longleftrightarrow$ 4x4 Fourier matrix
- Stationary points follow from the implicit equation

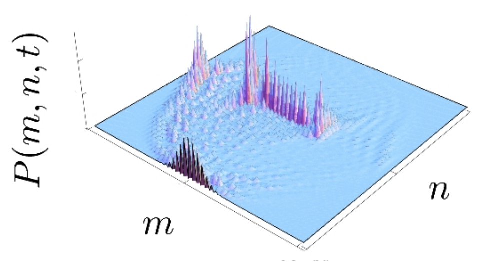
$$\Phi(\mathbf{k},\omega) \equiv \det\left(\widetilde{U}_F(\mathbf{k}) - e^{i\omega} I\right) = 0$$

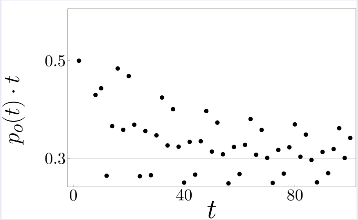
- 1st order stationary points $\Longrightarrow$ contribution $\sim t^{-2}$
- Two phases have saddle lines $\Longrightarrow$ contribution $\sim t^{-1}$
- Probability at the origin $p_0(t)$ decays like t^{-1} except for

$$\psi \in \psi_F(a,b) = (a,b,a,-b)^T$$

which are orthogonal to $v_{1,2}(\mathbf{k})$ for $\mathbf{k}$ lying at the saddle lines

Probability Distribution for the Fourier Walk



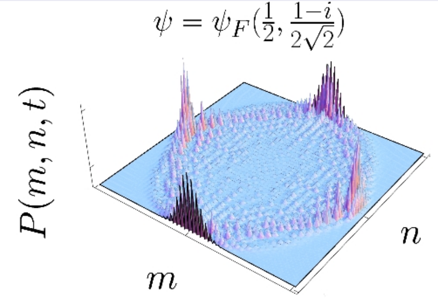


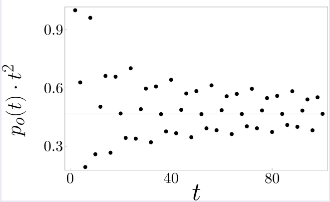
- For any initial state which is not a member of the family ψ_F the probability at the origin decays slowly

$$p_0(t) \sim t^{-1}$$

- The walk is recurrent

Probability Distribution for the Fourier Walk





- For the initial states belonging to the family ψ_F the probability at the origin decays fast

$$p_0(t) \sim t^{-2}$$

- The walk is transient

Outline

Classical Biased Walk on a Line

- Step to the right by r units with probability p
- Spreading is diffusive

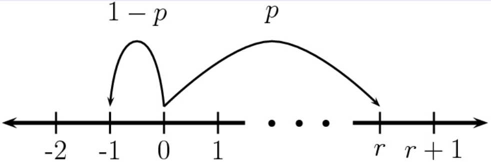
$$\sigma \sim \sqrt{t}$$

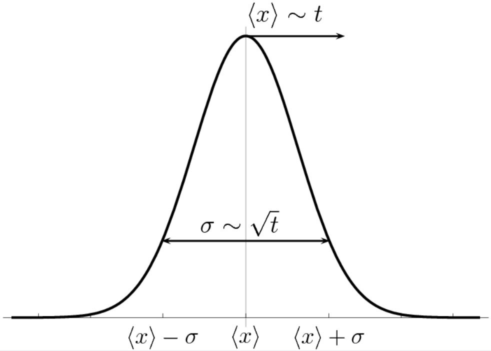
- Mean varies linearly

$$\langle x \rangle = [p(r+1) - 1]\, t$$

- Recurrence $\iff$ vanishing mean

$$p = \frac{1}{r+1}$$



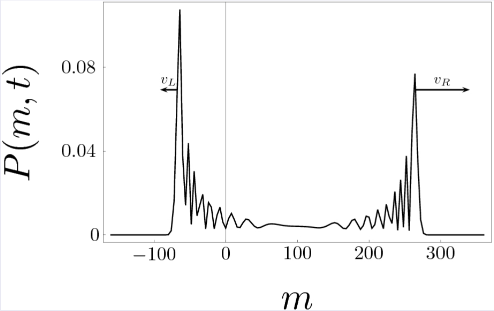


Biased Quantum Walk on a Line

MŠ, T. Kiss and I. Jex, New J. Phys. **11**, 043027 (2009)

- Step to the right by r units
- Coin operator

$$C = \begin{pmatrix} \sqrt{\rho} & \sqrt{1-\rho} \\ \sqrt{1-\rho} & -\sqrt{\rho} \end{pmatrix}$$



- Both mean and variance grows linearly
- Two peaks propagating with constant velocities v_L and v_R
- Probability in between the two peaks behave like $P(m,t) \sim t^{-1}$
- Recurrence $\Longleftrightarrow$ $v_L \leq 0$ and $v_R \geq 0$

Recurrence and Velocities of the Peaks

- Velocities can be found by the method of stationary phase

$$\psi(m,t) = \sum_{j=1}^{2} \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{i(\omega_j(k)-\alpha k)t} \left(v_j(k),\psi\right) v_j(k), \quad \alpha = \frac{m}{t}$$

- Peaks $\Longleftrightarrow$ slower decay of the probability $\Longleftrightarrow$ modified phase has higher order stationary point

$$\omega_j''(k_0) = 0, \qquad \omega_j'(k_0) = v_{L,R}$$

$$v_L = \frac{r-1}{2} - \frac{r+1}{2}\sqrt{\rho}, \quad v_R = \frac{r-1}{2} + \frac{r+1}{2}\sqrt{\rho}$$

Condition of Recurrence

$$\rho_R \geq \left(\frac{r-1}{r+1}\right)^2$$

Outline

Stationary and Oscillating States

- Recurrence $\Longleftrightarrow$ partial revival of the probability at the origin
- Some eigenvalues of $\tilde{U}(\mathbf{k})$ may be independent of the momenta $\mathbf{k}$ (typically single $\lambda_1 = +1$ or two $\lambda_{1,2} = \pm 1$)

The propagator U has a point spectrum

- Corresponding eigenvectors — stationary states
- Linear combinations — oscillating states
- The eigenvectors of $\tilde{U}(\mathbf{k})$ corresponding to constant eigenvalues depend on the momenta $\mathbf{k}$

Stationary and oscillating states are not localized

- Localized initial states has to spread

Grover Walk on a Plane

- Propagator in the momentum picture

$$\tilde{U}(\mathbf{k}) = \mathrm{Diag}\left(e^{ik_1}, e^{-ik_1}, e^{ik_2}, e^{-ik_2}\right) \cdot \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{pmatrix}$$

- Two eigenvalues are constant - $\lambda_{1,2} = \pm 1$
- Corresponding eigenvectors

$$\begin{aligned} v_1(\mathbf{k}) &= \left(e^{ik_1}(1+e^{ik_2}), 1+e^{ik_2}, e^{ik_2}(1+e^{ik_1}), 1+e^{ik_1}\right) \\ v_2(\mathbf{k}) &= \left(e^{ik_1}(1-e^{ik_2}), -1+e^{ik_2}, e^{ik_2}(1-e^{ik_1}), -1+e^{ik_1}\right) \end{aligned}$$

Grover Walk on a Plane

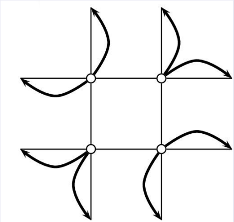
- Position representation — inverse Fourier transformation

$$
\begin{aligned}
|\psi_1\rangle &= \frac{1}{\sqrt{8}}\Big(|0,0\rangle(|L\rangle + |D\rangle) + |1,0\rangle(|R\rangle + |D\rangle) + \\
&\quad + |0,1\rangle(|L\rangle + |U\rangle) + |1,1\rangle(|R\rangle + |U\rangle)\Big) \\
|\psi_2\rangle &= \frac{1}{\sqrt{8}}\Big(-|0,0\rangle(|L\rangle + |D\rangle) + |1,0\rangle(|R\rangle + |D\rangle) + \\
&\quad + |0,1\rangle(|L\rangle + |U\rangle) - |1,1\rangle(|R\rangle + |U\rangle)\Big)
\end{aligned}
$$

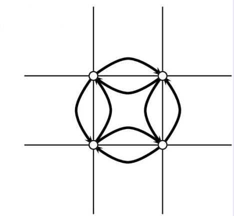
- $|\psi_{1,2}\rangle$ are stationary states
- Linear combinations are oscillating states

Stationary State $|\psi_1\rangle$

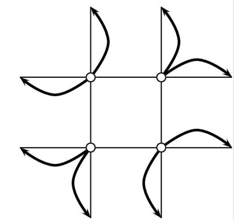
$t = 0$



$t = 0$, coin flip

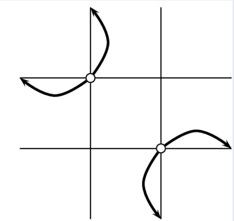


$t = 1$

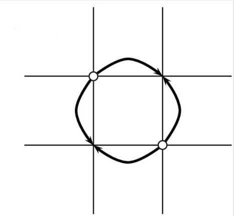


Oscillating State $|\psi_1\rangle + |\psi_2\rangle$

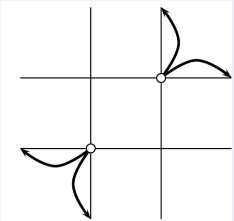
$t = 0$



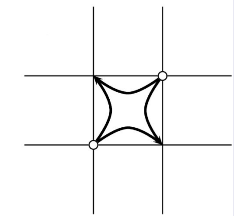
$t = 0$, coin flip



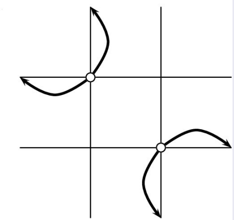
$t = 1$



$t = 1$, coin flip



$t = 2$



Outline

Summary

Main Results

- Extension of the concept of recurrence and Pólya number to quantum walks
- Recurrence of a quantum walk is determined by the coin operator C and the initial state ψ
- Recurrence is more stable against bias
- Full-revivals of a quantum state are possible

References

MŠ, I. Jex and T. Kiss, Phys. Rev. Lett. **100**, 020501 (2008)
MŠ, T. Kiss and I. Jex, Phys. Rev. A **78**, 032306 (2008)
MŠ, T. Kiss and I. Jex, New J. Phys. **11**, 043027 (2009)

Thank you for your attention