Short time behavior of continuous time quantum walks on graphs

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Work done in collaboration with
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Motivation

Continuous time quantum walks (CTQW)

- give physically realizable implementations of quantum algorithms

  E. Farhi and S. Gutmann, *Phys. Rev. A* **58**, *915 (1998).*

  A. M. Childs and J. Goldstone, *Phys. Rev. A* **70**, *042312 (2004).*

  R. Portugal, *Quantum walks and search algorithms, Springer-Verlag (2013).*

  D. A. Meyer and T. G. Wong, *Phys. Rev. Lett.* **114**, *110503 (2015).*

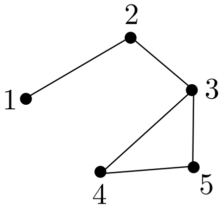
- model successfully coherent transport phenomena

  FMO complex - M. Mohseni, P. Rebentrost, S. Lloyd, and A. Aspuru-Guzik, *J. Chem. Phys.* **129**, *11B603 (2008).*

  F. Caruso, A. W. Chin, A. Datta, S. F. Huelga, and M. B. Plenio, *J. Chem. Phys.* **131**, *09B612 (2009).*

Both in case of closed and open systems there are plenty of examples where the efficiency and advantage of CTQW over CTRW has been demonstrated.

What kind of quantum quantum walks do we want to study?



$$A = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{pmatrix}$$

- Pure CTQW:
$$H = A\,.$$
- One-particle tight-binding models with potentials:
$$H = A + V\,.$$
- Time-reversal-symmetry breaking (chiral) quantum walks:
$$H_{ch} = \sum_{\{n,m\}\in\mathcal{E}} e^{i\theta_{nm}}|n\rangle\langle m| + e^{-i\theta_{nm}}|m\rangle\langle n|.$$
- Time-dependent CTQWs.
- Open/stochastic quantum walks:
$$\dot{\rho}(t) = \mathfrak{L}_\omega \rho(t)\,.$$

The question to be studied

If t is small, what can we say about the transition matrix entry $\langle y|e^{-iHt}|x\rangle$?

Possible applications:

- Understanding the dynamics of CTQW in open and closed quantum systems
- It can be interpreted as a distance oracle

  C. Mathieu and H. Zhou *Lec. Not. Comp. Sci.* **7965**, *733 (2013).*

Previous results concerned classical random walks:

$$p(y,t|x) = c(x,y)t^{d(x,y)} + \mathcal{O}(t^{d(x,y)+1})$$

M. Keller, D. Lenz, F. Mnch, M. Schmidt, and A. Telcs, *Bull. Lon. Mat. Soc.* **48**, *935 (2016).*

Prerequisites for the mathematical result

- We consider a Hilbert space whose orthonormal basis $\{|v\rangle\}_{v\in\mathcal{V}}$ are labeled by the vertices of the graph $\mathcal{G}$.
- The graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is simple but can be directed.
- We consider a time-dependent operator $M(t)$ satisfying the property $\langle m|M(t)|n\rangle \not\equiv 0$ if and only if the directed edge $(n, m) \in \mathcal{E}$.
- We would like to solve the $\frac{d}{dt}X(t) = M(t)X(t)$ matrix differential equation.
- We denote the path amplitude (in the Dyson series/Magnus expansion/Picard iteration) corresponding to a path $p \in \mathcal{P}(n, m)$ by

$$\Phi_p[M(t)] = \int_0^t \mathrm{d}s_d \cdots \int_0^{s_2} \mathrm{d}s_1 \, \langle p_d|M(s_d)|p_{d-1}\rangle \cdots \langle p_1|M(s_1)|p_0\rangle.$$

Main mathematical results I.

The solution of the matrix differential equation

$$\frac{d}{dt}X(t) = M(t)X(t), \qquad X(0) = \mathbb{1},$$

satisfies the inequality

$$\left| \langle m|X(t)|n\rangle - \sum_{p\in\mathcal{P}(n,m)} \Phi_p[M(t)] \right| \leq \mathrm{e}^{t/\tau_T} \frac{(t/\tau_T)^{d(n,m)+1}}{(d(n,m)+1)!} .$$

for all vertices n and m of distance $d(n,m)$.

- The sum goes over the shortest paths $\mathcal{P}(n,m)$ running from n to m.
- The $\Phi_p[M(t)]$ is the path amplitude of p.
- $M(t)$ is not necessarily hermitian, it can be anything
- τ_T is a constant depending on $M(t)$:

$$\tau_T^{-1} = \max_{0\leq t\leq T} \|M(t)\|.$$

Main mathematical result II.

What does that mean?

- τ_T defines the timescale.
- If $t \lesssim \tau_T$, then

$$\langle m|X(t)|n\rangle = \sum_{p\in\mathcal{P}(n,m)} \Phi_p[M(t)] + \mathcal{O}\big((t/\tau_T)^{d(n,m)+1}\big)\,.$$

Examples:

- Comparison of CTRW and CTQW
- Tight-binding models with potentials
- Chiral quantum walks
- Open CTQW systems

Comparison of CTRW and CTQW

We have a simple, undirected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ containing no self-loops. The CTRW dynamics is generated by the Laplacian of the graph: $L = D - A$,

$$p_{\mathrm{R}}(u, t|v) = \langle u| \exp(-Lt)|v\rangle \,.$$

The unitary walk on the same graph is generated by $-\mathrm{i}L$ (or $-iH = -iA$) with transition probabilities

$$p_{\mathrm{Q}}(u, t|v) = |\langle u| \exp(-\mathrm{i}Lt)|v\rangle|^2.$$

It turns out that the timescales are equal:

$$\sum_p \Phi_p^{CTRW}(t) = \frac{\ell(u,v)}{d(u,v)!}\,, \qquad \sum_p \Phi_p^{CTQW}(t) = (-\mathrm{i})^{d(u,v)} \sum_p \Phi_p^{CTRW}(t).$$

Comparison of CTRW and CTQW

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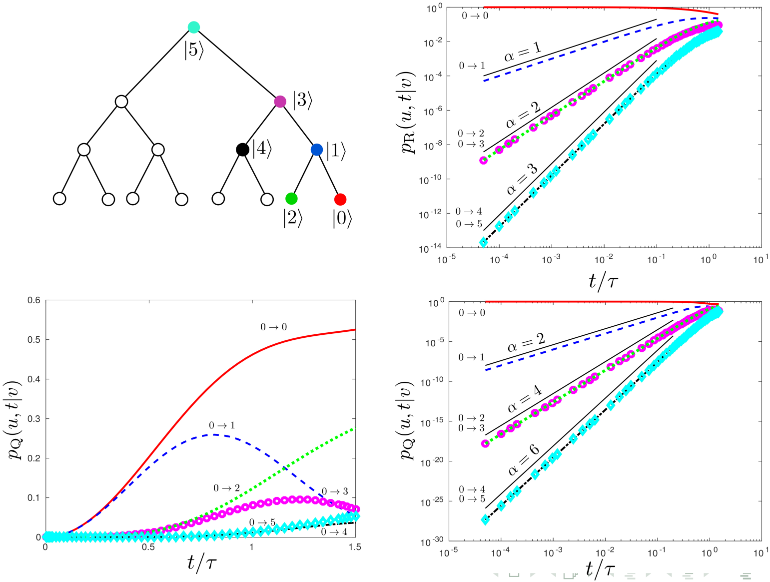


Tight-binding models with potentials

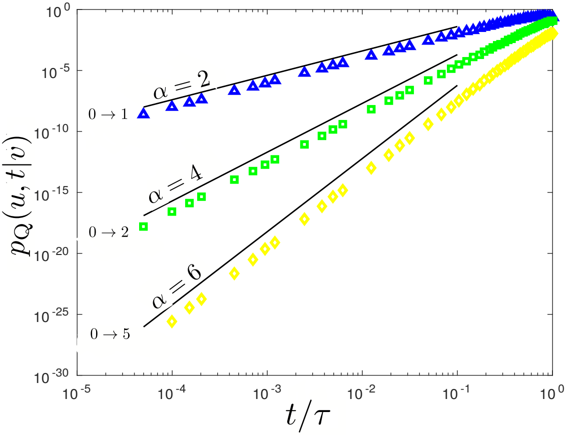
Consider a one-particle tight-binding model with onsite potentials $H = A + V$. The hitting probabilities are

$$p_{\mathrm{TB}}(u, t|v) = |\langle u| \exp(-\mathrm{i}(A + V)t)|v\rangle|^2.$$

We choose the on-site potentials from an ensemble of independent, identically distributed Gaussian random variables with mean zero and unit variance:

$$\sum_p \Phi_p^{TB}(t) = \ell(u, v)(-\mathrm{i}t)^{d(u,v)}/d(u, v)!\,.$$

Tight-binding models with potentials



Tight-binding models with potentials

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$$\hat{H}(t) = \exp(-Vt)\hat{H} \exp(Vt).$$

$$\tau^{-1} = \mathrm{d}_{\max}(\mathcal{G}) \max_{n \neq m} |\langle n|\hat{H}|m\rangle|.$$

Chiral quantum walks

The Hamiltonian of a chiral quantum walk is

$$H_{ch} = \sum_{n \sim_{\mathcal{G}} m} \mathrm{e}^{i\theta_{nm}} |n\rangle\langle m| + \mathrm{e}^{-i\theta_{nm}} |m\rangle\langle n|.$$

Z. Zimborás et al, *Scientific Reports* **3**, *2361 (2013)*; DaWei Lu et al, *Phys. Rev. A 93, 042302 (2016).*

Complex phases assigned to the edges can give rise to destructive interference:

$$\sum_{p \in \mathcal{P}(u,v)} \Phi_p(t) = \sum_{p \in \mathcal{P}(u,v)} e^{i \sum_k \theta_{p_k, p_{k+1}}} \frac{t^{d(u,v)}}{d(u,v)!}$$

Chiral quantum walks

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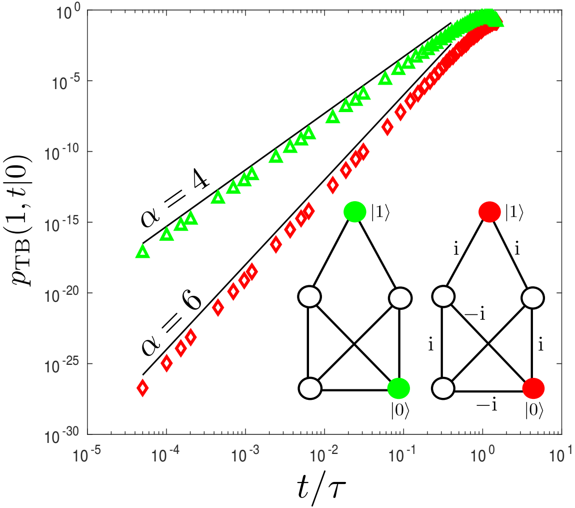


Time-dependent Hamiltonian

Let us consider the following Hamiltonian:

$$H(t) = \Lambda^{+}(t) A \Lambda(t)$$

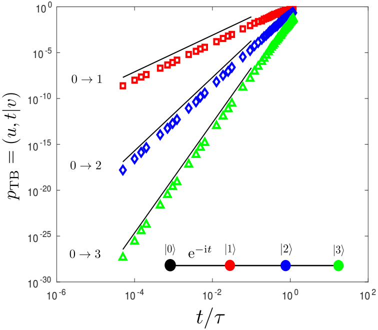
where the $\Lambda(t)$ is a diagonal unitary and A is the adjacency matrix.
Note that the timescales in this special case

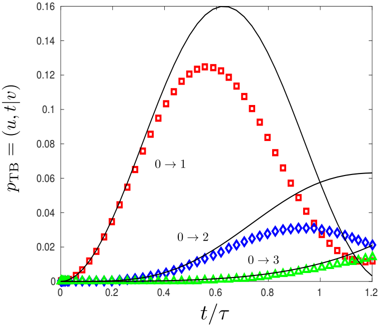
- the time-dependent chiral quantum walk encoded by $H(t)$ is never trivial even in the case when A corresponds to a tree;
- unitary transformation keeps the timescales.

The transition matrix:

$$\langle v|U(t)|0\rangle = \frac{1}{\Omega^d}\left(-\sum_{u=0}^{v-1}(-\mathrm{i}\Omega)^u \frac{t^u}{u!} + e^{-\mathrm{i}\Omega t}\right) + \mathcal{O}(t^{d+1}).$$

Time-dependent Hamiltonian





Open CTQW

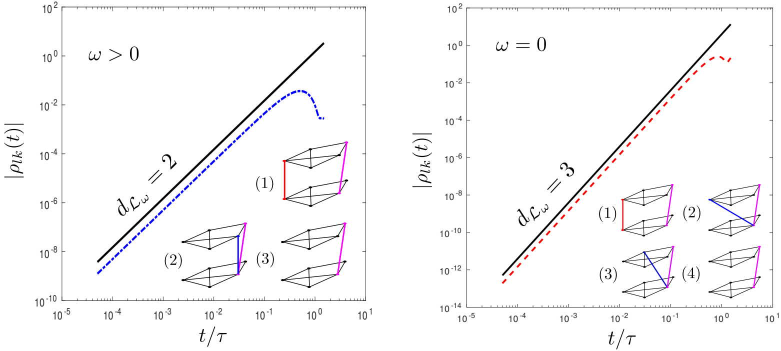
Let us consider an open system dynamics in the Markovian regime. The time evolution described by the usual Lindblad equation. We restrict our attention to the so called STQW: $\dot{\rho}(t) = \mathfrak{L}_\omega \rho(t)$,

$$\begin{aligned} \mathfrak{L}_\omega \rho &= -\mathrm{i} \sum_{v \in \mathcal{V}} V_v [\hat{v}, \rho] - \mathrm{i} \sum_{e \in \mathcal{E}} [\hat{e}, \rho] \\ &\quad + \omega \sum_{e \in \mathcal{E}} \left(\hat{e}^+ \rho \hat{e} - \frac{1}{2} \{ \hat{e}\hat{e}^+, \rho \} \right), \end{aligned}$$

where $\hat{v} = |v\rangle\langle v|$ and if $e \equiv n \to m$ is and edge of the graph, then $\hat{e} = |m\rangle\langle n|$. The relative strength of the CTRW part is measured by the $\omega \geq 0$ parameter.

There is a natural way to view this process taking place on a graph $\mathcal{L}$ obtained from the complete, directed graph $\mathcal{K}_{d^2}$ of d^2 nodes, whose vertices are labeled by the matrix units E_{nm} and whose edges $E_{kl} \to E_{nm}$ are deleted when the corresponding matrix entry $\mathrm{Tr}[E^*_{nm} \mathfrak{L} E_{kl})]$ vanishes.

Open CTQW


$\omega > 0$
$d_{\mathcal{L}_\omega} = 2$
$|\rho_{lk}(t)|$
t/τ
(1)
(2)
(3)
$\omega = 0$
$d_{\mathcal{L}_\omega} = 3$
(4)

Publication:

- Phys. Rev. A **100**, 062320 (2019).

Thank you for the Attention!