Quantum Dynamics on Diamond Fractal Graphs

G. Mograby, M. Derevyagin, G. V. Dunne, R. Balu, K. A. Okoudjou
and L. G. Rogers at al.

Alexander Teplyaev

University of Connecticut

AMS Boston College

1. First Links in the Markov Chain

2. Quantum walk versus random walk

3. Jacobi operators on graphs and perfect quantum state transfer

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Outline

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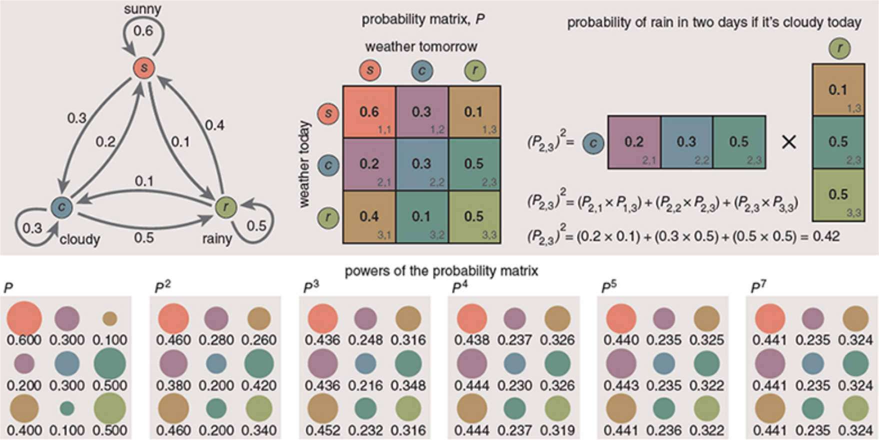
Past, Present and Future



$$\begin{array}{c|ccc} & s & c & r \\ \hline s & 0.6_{1,1} & 0.3_{1,2} & 0.1_{1,3} \\ c & 0.2_{2,1} & 0.3_{2,2} & 0.5_{2,3} \\ r & 0.4_{3,1} & 0.1_{3,2} & 0.5_{3,3} \end{array}$$

$$(P_{2,3})^2 = c\ \begin{bmatrix} 0.2_{2,1} & 0.3_{2,2} & 0.5_{2,3} \end{bmatrix} \times \begin{array}{c} r \\ \begin{bmatrix} 0.1_{1,3} \\ 0.5_{2,3} \\ 0.5_{3,3} \end{bmatrix} \end{array}$$

$$(P_{2,3})^2 = (P_{2,1} \times P_{1,3}) + (P_{2,2} \times P_{2,3}) + (P_{2,3} \times P_{3,3})$$

$$(P_{2,3})^2 = (0.2 \times 0.1) + (0.3 \times 0.5) + (0.5 \times 0.5) = 0.42$$

P

0.600	0.300	0.100
0.200	0.300	0.500
0.400	0.100	0.500

P^2

0.460	0.280	0.260
0.380	0.200	0.420
0.460	0.200	0.340

P^3

0.436	0.248	0.316
0.436	0.216	0.348
0.452	0.232	0.316

P^4

0.438	0.237	0.326
0.444	0.230	0.326
0.444	0.237	0.319

P^5

0.440	0.235	0.325
0.443	0.235	0.322
0.441	0.236	0.322

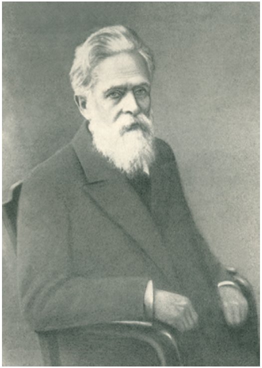
P^7

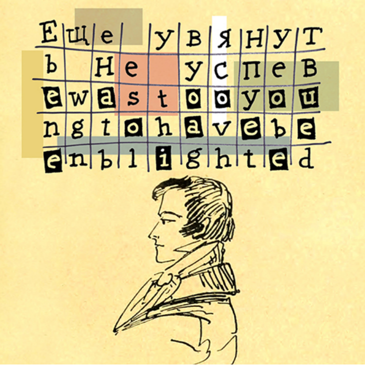
0.441	0.235	0.324
0.441	0.235	0.324
0.441	0.235	0.324

by Hayes, Brian. American Scientist 101.2 (2013): 252.
`https://www.americanscientist.org/article/first-links-in-the-markov-chain`

First Links in the Markov Chain

Probability and poetry were unlikely partners in the creation of a computational tool





When the Russian church excommunicated Leo Tolstoy, Markov asked that he be expelled also. (The request was granted.) In 1902, the leftist writer Maxim Gorky was elected to the Academy, but the election was vetoed by Tsar Nicholas II. In protest, Markov announced that he would refuse all future honors from the tsar.

In 1913, when the tsar called for celebrations of 300 years of Romanov rule, Markov responded by organizing a symposium commemorating a different anniversary: the publication of *Ars Conjectandi* [by Jacob Bernoulli] 200 years before.

In a paper published in 1902 Nekrasov injected the law of large numbers into the centuries-old theological debate about free will versus predestination. His argument went something like this: Voluntary acts – expressions of free will – are like the independent events of probability theory, with no causal links between them. The law of large numbers applies only to such independent events. Data gathered by social scientists, such as crime statistics, conform to the law of large numbers. Therefore the underlying acts of individuals must be independent and voluntary.

Markov first addressed the issue of dependent variables and the law of large numbers in 1906. ... Nekrasov assumed that the law of large numbers requires the principle of independence. Although this notion had been a commonplace of probability theory since the time of Jacob Bernoulli, Markov set out to show that the assumption is unnecessary. The law of large numbers applies perfectly well to systems of dependent variables if they meet certain criteria.

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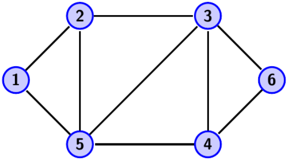
Quantum mechanics on graphs

- Let $G = (V, E)$ be a finite (possibly directed) graph.
- We assume that G has N vertices, i.e. $|V| = N$.
- Equip V with a measure μ.
- Define a Hilbert space

$$\ell^2(G) = \{\psi : V \to \mathbb{C}\} = \mathbb{C}^N,$$

$$\langle \psi, \varphi \rangle = \sum_{x \in V} \psi(x)\overline{\varphi(x)}\mu(x),$$

- The *volume* of the graph G is then given by $vol(G) := \sum_{x \in V} \mu(x)$.



Quantum mechanics on graphs

- A quantum state is represented by a normalized vector $\psi \in \ell^2(G)$.
- A physical quantity (i.e. observable) is represented by a self-adjoint operator A acting on $\ell^2(G)$, i.e.

$$\langle \psi, A\varphi \rangle = \langle A\psi, \varphi \rangle \quad \forall \psi, \varphi \in \ell^2(G)$$

- The energy is represented by a self-adjoint operator called a Hamiltonian H.
- The time dependence of a state is governed by the Schrödinger equation

$$i \frac{\partial}{\partial t} \psi(t) = H \psi(t)$$

Probabilistic interpretation

- Let $\delta_1, \dots, \delta_N$ be the canonical basis of $\mathbb{C}^N$, i.e.

$$\delta_x = \begin{cases} 1 & \text{, on vertex } x, \\ 0 & \text{, on the vertices } V \backslash \{x\} \end{cases}$$

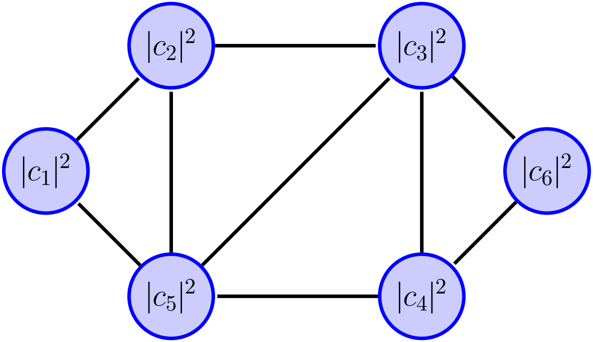
- The normalized vector of δ_x is $e_x := \dfrac{1}{\sqrt{\mu(x)}} \delta_x$.
- Write $\psi \in \ell^2(G)$ as a linear combination

$$\psi = \sum_x c_x e_x$$

where the $c_x \in \mathbb{C}$ satisfy $\sum_x |c_x|^2 = 1$ (because $\langle \psi, \psi \rangle = 1$).

A probability distribution

- Probabilistic interpretation: $\psi = \sum_x c_x e_x$ is in the state e_x with probability $|c_x|^2$.



The time-evolution operator

- H is assumed to be time-independent.
- The Schrödinger equation is solved by

$$\psi(t) = U(t)\psi(0), \quad U(t) := \exp(-itH).$$

- $U(t)$ is unitary.
- $U(t)$ is called a time-evolution operator.

Example: discrete-time quantum walk

- Discrete time $t \in \mathbb{N}$. For $t = n$, we have

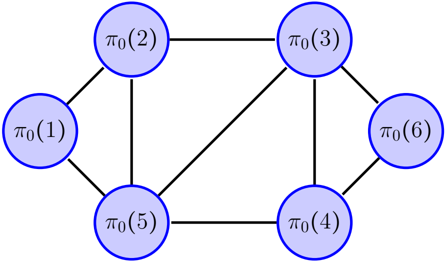
$$\begin{aligned} U(n) &= \exp(-inH) = \exp(-iH)\cdots\exp(-iH) \\ &= U(1)\cdots U(1) = \big(U(1)\big)^n \end{aligned}$$

- We write $U := U(1)$.
- One step of a discrete-time quantum walk is described by U, i.e.

$$\psi(0) \xrightarrow{U} \psi(1) \xrightarrow{U} \psi(2) \xrightarrow{U} \psi(3) \xrightarrow{U} \dots$$

Markov chain comparison

- We start with an initial probability distribution $\pi_0 \in \mathbb{R}^N$.



- Classical random walk: initial probability distribution $\{\pi_0(x)\}_{x\in V}$.
- Quantum walk: probability distribution of initial state $\psi(0)$ via $\{|c_x|^2\}_{x\in V}$.

Markov chain comparison

- Discrete-time classical random walk on N-vertex graph can be represented by a stochastic $N \times N$-matrix P, i.e. $\sum_{j=1}^{N} P_{jk} = 1$.
- The entry P_{jk} represents the probability of making a transition to k from j.
- The initial probability distribution π_0 becomes $P\pi_0$ after one step of the walk, i.e.

$$\pi_0 \to P\pi_0 \to P^2\pi_0 \to P^3\pi_0 \to \dots$$

- Compare to discrete-time quantum walk:

$$\psi(0) \xrightarrow{U} \psi(1) \xrightarrow{U} \psi(2) \xrightarrow{U} \psi(3) \xrightarrow{U} \dots$$

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Motivation

Kempton, Mark, Gabor Lippner, and Shing-Tung Yau. **Perfect state transfer on graphs with a potential**. *Quantum Information and Computation* (2017). **Pretty good quantum state transfer in symmetric spin networks via magnetic field**. *Quantum Information Processing* (2017).

... for paths of length greater than three, there is no potential on the vertices of the path for which perfect state transfer between the endpoints can occur ... this answers a question raised by Godsil ...
... if a graph has two vertices that share a common neighborhood, then there is a potential on the vertex set for which perfect state transfer will occur between those two vertices
... numerous examples where perfect state transfer does not occur without the potential, but adding a potential makes perfect state transfer possible.
... investigate perfect state transfer on graph products, which gives further examples where perfect state transfer can occur.

Jacobi operators on graphs

Definition

A Jacobi operator on a graph $G = (V(G), E(G))$ is a matrix $\mathbf{J} = \big(\mathbf{J}(x,y)\big)_{x,y \in V(G)}$ indexed by the vertices $V(G)$, such that $\mathbf{J}(x,y) = 0$ whenever $(x,y) \notin E(G)$ and $x \neq y$.

- Generalization of graph Laplacians and adjacency matrices.
- Adequate to simulate physical models and define "Hamiltonian operators".

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[0] N. Avni, J. Breuer, and B. Simon. Periodic Jacobi matrices on trees. Adv. Math., 370:107241, 42, 2020.

$\mathbb{Z}$-graded Graphs

We refer to the triple $G = (V(G), E(G), \mathbf{\Pi})$ as a $\mathbb{Z}$-graded graph[1], where

1. $(V(G), E(G))$ is a connected combinatorial graph with a countable set of vertices $V(G)$ and a set of edges $E(G)$.
2. There exists a (rank) function $\mathbf{\Pi} : V(G) \to \mathbb{Z}$, such that for an edge $(x, y) \in E(G)$, we have $\mathbf{\Pi}(y) = \mathbf{\Pi}(x) + 1$
3. For $n \in \mathbb{Z}$, we call $\mathbf{\Pi}^{-1}(n)$ the n-th transversal layer.

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[1] Richard P. Stanley. *Differential Posets*. J. Amer. Math. Soc., 1(4):919–961, 1988. Sergey Fomin. *Duality of graded graphs*. J. Algebraic Combin., 3(4):357–404, 1994.

$\mathbb{Z}$-graded Graphs

The rank function relates a $\mathbb{Z}$-graded graph G to an auxiliary path graph $(V(\mathbb{Z}), E(\mathbb{Z}))$.

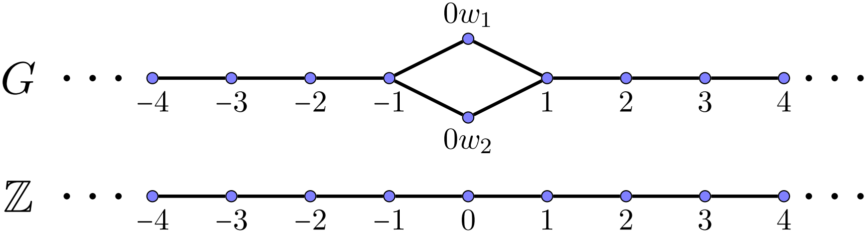

Figure: One of the simplest nontrivial $\mathbb{Z}$-graded graphs G. The rank function provides a transversal decomposition[2], i.e. $V(G) = \bigcup_{n\in\mathbb{Z}} \mathbf{\Pi}^{-1}(n)$.

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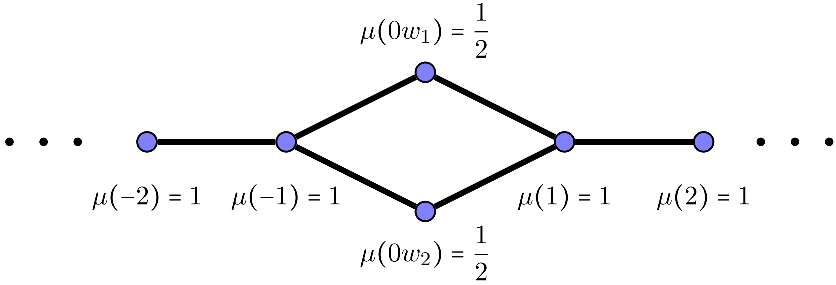
[2] *"stratification of a graph"* in *Quantum probability and spectral analysis of graphs*. Hora, A. and Obata, N., Springer, Berlin, 2007.

Measures on $V(G)$

Given $G = (V(G), E(G), \mathbf{\Pi})$ a $\mathbb{Z}$-graded graph. We equip $V(G)$ with a measure, $\mu_V : V(G) \to [0, \infty]$.

Assumption (1)

We assume $\mu_V(x) > 0$ for all $x \in V(G)$ and that the restriction of μ_V to a transversal layer is a probability measure, i.e , $\mu(\mathbf{\Pi}^{-1}(n)) = 1$, $\forall\ n \in \mathbb{Z}$.

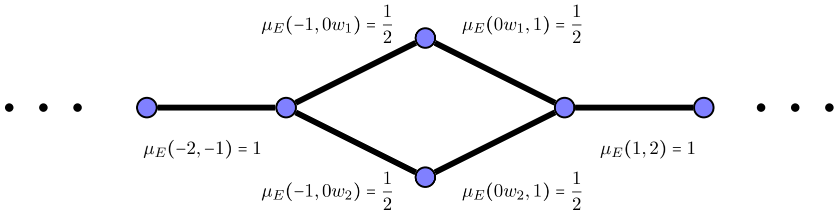


Measures on $E(G)$

We equip the set of edges with a measure $\mu_E : E(G) \to [0, \infty]$, $(x, y) \mapsto \mu_E(x, y)$.

Assumption (2)

We assume $\mu_E(x, y) > 0$ for all $(x, y) \in E(G)$ and that the restriction of μ_E to a transversal layer of edges is a probability measure.

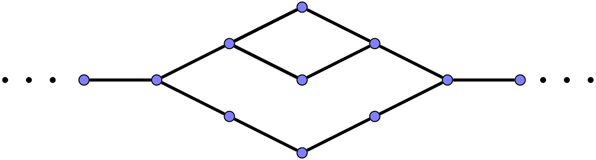


Measure balance assumption

Assumption (3)

Let $x \in V(G)$. *We assume that the following identities hold:*

$$\mu_V(x) = \sum_{(x,y)\in E(G)} \mu_E(x,y), \qquad \mu_V(x) = \sum_{(y,x)\in E(G)} \mu_E(y,x).$$



Hilbert spaces

We introduce the following Hilbert spaces:

$$\begin{aligned}
\ell^2(G) &= \{\psi : V(G) \to \mathbb{C} \mid \langle \psi, \psi \rangle_V < \infty\},\\
\langle \psi, \varphi \rangle_V &= \sum_{x \in V(G)} \psi(x)\overline{\varphi(x)}\mu_V(x),\\
\ell^2(\mathbb{Z}) &= \{\psi : \mathbb{Z} \to \mathbb{C} | \langle \psi, \psi \rangle < \infty\},\\
\langle \psi, \varphi \rangle &= \sum_{n \in \mathbb{Z}} \psi(n)\overline{\varphi(n)}.
\end{aligned}$$

Radial functions and the Averaging Operator $\widetilde{\mathbf{\Pi}}$

Given $G = (V(G), E(G), \mathbf{\Pi})$ a $\mathbb{Z}$-graded graph.

Definition

- The subspace of radial functions is defined as $\ell^2_{rad}(G) = \{\psi \in \ell^2(G) \ \mid \psi(x) = \psi(y)$ if $\mathbf{\Pi}(x) = \mathbf{\Pi}(y)\}$.
- We define the averaging operator as the following mapping

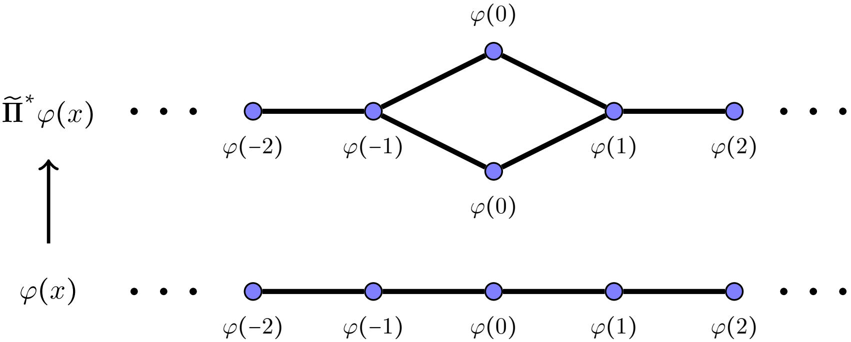
$$\widetilde{\mathbf{\Pi}} : \ell^2(G) \to \ell^2(\mathbb{Z}), \quad \psi \mapsto \widetilde{\mathbf{\Pi}}\psi(n) := \sum_{x \in \mathbf{\Pi}^{-1}(n)} \psi(x)\mu_V(x).$$

We show: $Ker\widetilde{\mathbf{\Pi}} = \ell^2_{rad}(G)^{\perp}$.
Radial-"Angular" decomposition: $\ell^2(G) = \ell^2_{rad}(G) \oplus Ker\widetilde{\mathbf{\Pi}}$.

The adjoint operator of $\widetilde{\Pi}$

Proposition

The averaging operator $\widetilde{\Pi}$ *is bounded with* $\|\widetilde{\Pi}\| = 1$. *Let* $\widetilde{\Pi}^*$ *be the adjoint operator of* $\widetilde{\Pi}$, *then* $\widetilde{\Pi}^*$ *is given by* $\widetilde{\Pi}^* : \ell^2(\mathbb{Z}) \to \ell^2(G)$, $\varphi \mapsto \widetilde{\Pi}^*\varphi(x) = \varphi(\Pi(x))$.



Lifting an Operator

Definition

Let $A : \ell^2(G) \to \ell^2(G)$ be bounded, such that:

- A is a Jacobi operator on a graph G, i.e. it reflects the adjacency relation of the graph G, in the sense that its off-diagonal elements $(A(x,y))_{x \neq y}$ are zero whenever they correspond to non-adjacent vertices.
- We define $B : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ such that $B = \widetilde{\mathbf{\Pi}} A \widetilde{\mathbf{\Pi}}^*$.

We say, the operator A *lifts* B.

$$\begin{tikzcd}
\ell^2(G) \arrow[r, "A"'] & \ell^2(G) \arrow[d, "\widetilde{\mathbf{\Pi}}"] \\
\ell^2(\mathbb{Z}) \arrow[u, "\widetilde{\mathbf{\Pi}}^*"] \arrow[r, "B"'] & \ell^2(\mathbb{Z})
\end{tikzcd}$$

Spectral separation assumption

Definition (Spectral separation assumption)

A bounded linear operator $\mathbf{H} : \ell^2(G) \to \ell^2(G)$ is said to satisfy the spectral separation assumption, if the following hold:

1. $\mathbf{H}(Ker\widetilde{\mathbf{\Pi}}) \subset Ker\widetilde{\mathbf{\Pi}}$, i.e., the subspace $Ker\widetilde{\mathbf{\Pi}}$ is **H**-invariant,
2. $\mathbf{H}(\ell^2_{rad}(G)) \subset \ell^2_{rad}(G)$, i.e., the subspace $\ell^2_{rad}(G)$ is **H**-invariant.

Result: Lifting a tridiagonal Jacobi Matrix

Theorem

Given $G = (V(G), E(G), \mathbf{\Pi})$ *a* $\mathbb{Z}$*-graded graph. Under the Assumptions (1), (2) and (3), for a symmetric tridiagonal Jacobi matrix* **J** *there exists a Jacobi operator* **H** *on* G *that lifts* **J***, i.e.*

$$\mathbf{J} = \widetilde{\mathbf{\Pi}}\mathbf{H}\widetilde{\mathbf{\Pi}}^{*}.$$

H *can be explicitly computed (next two slides), shown to be self-adjoint on* $\ell^2(G)$ *and satisfies the spectral separation assumption, i.e.*

- $\mathbf{H}(Ker\widetilde{\mathbf{\Pi}}) \subset Ker\widetilde{\mathbf{\Pi}}$*, i.e., the subspace* $Ker\widetilde{\mathbf{\Pi}}$ *is* **H***-invariant,*
- $\mathbf{H}(\ell^2_{rad}(G)) \subset \ell^2_{rad}(G)$*, i.e., the subspace* $\ell^2_{rad}(G)$ *is* **H***-invariant.*

Symmetric tridiagonal Jacobi matrix

Let $\mathbf{J} : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$, be the following *symmetric tridiagonal Jacobi matrix*

$$\mathbf{J} = \begin{pmatrix} & \ddots & \vdots & \vdots & \vdots & \iddots \\ \ddots & b(n-1) & a(n-1,n) & 0 & 0 & \dots \\ \dots & a(n-1,n) & b(n) & a(n,n+1) & 0 & \dots \\ \dots & 0 & a(n,n+1) & b(n+1) & a(n+1,n+2) & \dots \\ & \iddots & \vdots & \vdots & \ddots & \end{pmatrix}$$

The Jacobi matrix $\mathbf{J}$ is bounded and self-adjoint on $\ell^2(\mathbb{Z})$.

Jacobi operator on G

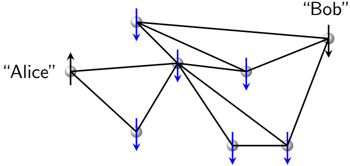
We define $\mathbf{H} = [\mathbf{H}(x,y)]_{x,y\in V(G)}$ with the following matrix elements.

$$\mathbf{H}(x,y) = \begin{cases} b(n) & \text{, if } x = y \text{ and } \Pi(x) = n, \\ \dfrac{\mu_E(x,y)}{\mu_V(x)} a(n,n+1) & \text{, if } (x,y) \in E(G) \text{ and } \Pi(x) = n, \\ \dfrac{\mu_E(y,x)}{\mu_V(x)} a(n-1,n) & \text{, if } (y,x) \in E(G) \text{ and } \Pi(y) = n-1, \\ 0 & \text{, otherwise.} \end{cases}$$

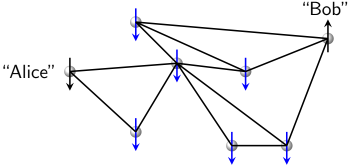
Perfect Quantum State Transfer (PQST)

- PQST on one dimensional Spin Networks[3] is well understood.
- More general Spin Networks? graph properties?
- Transfer of $|A\rangle$ to $|B\rangle$ as PQST? Hamiltonian operator (spin-spin interactions)?

$$|A\rangle$$



$$e^{i\phi}\,|B\rangle = e^{iT\,\mathbf{H}}\,|A\rangle$$



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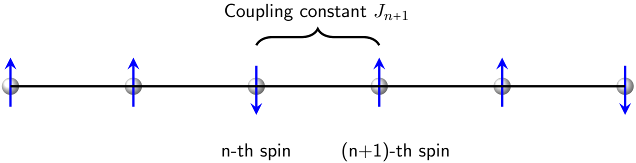
[3] Sougato Bose. *Quantum communication through an unmodulated spin chain*. Physical Review Letters, 91(20):207901, 2003.

1D Spin Chains

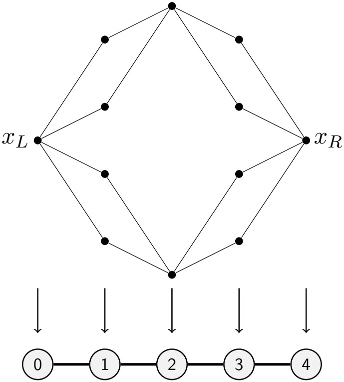
- One dimensional Hamiltonians of the XX-type with nearest-neighbor interactions reduced to the following Jacobi matrix.

$$\mathbf{J} = \begin{pmatrix} B_0 & J_1 & & & \mathbf{0} \\ J_1 & B_1 & J_2 & & \\ & J_2 & B_2 & \ddots & \\ & & \ddots & \ddots & J_N \\ \mathbf{0} & & & J_N & B_N \end{pmatrix}.$$



Example: Berker lattice

- *Transversal decomposition* of finite graphs, then the range of rank function $\mathbf{\Pi}$ is $\mathbb{Z}\bigcap[0,n]$ for some $n \in \mathbb{N}$.
- The left-hand side degree $\deg_- : V(G) \to \mathbb{N}$, $x \in \Pi^{-1}(n)$, then $\deg_-(x)$ assigns the vertex x the number of edges that connect x to vertices in $\Pi^{-1}(n-1)$ (Similarly, we define $\deg_+$).



Special case

Corollary

Let $G = (V(G), E(G), \mathbf{\Pi})$ *be a* $\mathbb{Z}$*-graded graph. For* $x_1, y_1, x_2, y_2 \in V(G)$ *such that both* x_1, y_1 *and* x_2, y_2 *are adjacent, we assume*

$$\mu_E(x_1, y_1) = \mu_E(x_2, y_2), \text{ if } \mathbf{\Pi}(x_1) = \mathbf{\Pi}(x_2) \text{ and } \mathbf{\Pi}(y_1) = \mathbf{\Pi}(y_2).$$

Then the lifted Jacobi matrix takes the form

$$\mathbf{H}(x,y) = \begin{cases} b(n) & \text{if } x = y \text{ and } \mathbf{\Pi}(x) = n, \\ \dfrac{1}{\mathbf{deg}_+(x)} a(n, n+1) & \text{if } (x,y) \in E(G) \text{ and } \mathbf{\Pi}(x) = n, \\ \dfrac{1}{\mathbf{deg}_-(x)} a(n-1, n) & \text{if } (y,x) \in E(G) \text{ and } \mathbf{\Pi}(y) = n-1, \\ 0 & \text{otherwise.} \end{cases}$$

Graph properties

Theorem

Assume that the mappings $\mathbf{deg}_+$ *and* $\mathbf{deg}_-$ *are constant on a transversal layer, i.e., for* $x, y \in \Pi^{-1}(n)$ *we have*

$$\mathbf{deg}_+(x) = \mathbf{deg}_+(y), \quad \mathbf{deg}_-(x) = \mathbf{deg}_-(y).$$

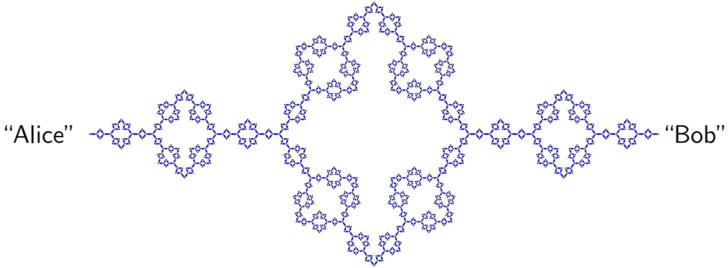
If a PQST on the 1D chain is achieved, i.e. there exists $T > 0$ *such that*

$$e^{iT\mathbf{J}} |0\rangle = e^{i\phi} |N\rangle$$

for some phase ϕ*, then the PQST on* G *is also achieved with the same time* T *and phase* ϕ*, i.e.*

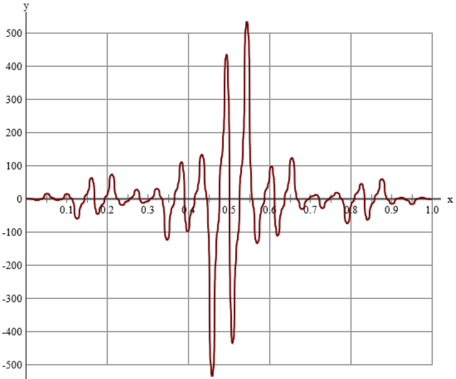
$$e^{iT\,\mathsf{H}} |A\rangle = e^{i\phi} |B\rangle \quad \text{and} \quad e^{iT\,\mathsf{H}} |B\rangle = e^{i\phi} |A\rangle .$$

Diamond fractal-type graphs



Urs Lang and Conrad Plaut. *Bilipschitz embeddings of metric spaces into space forms*. Geom. Dedicata, 87(1-3):285–307, 2001.

E. Akkermans, G. Dunne, and A. Teplyaev, Physical Consequences of Complex Dimensions of Fractals, 2009 EPL 88.



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Thank you for your attention!