

Algebraic Graph Theory and Quantum Walks

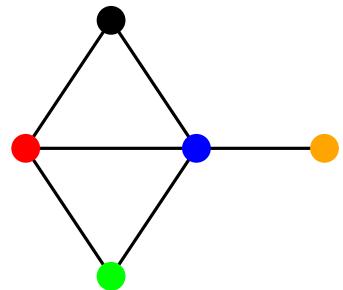
Krystal Guo



UNIVERSITY OF AMSTERDAM
Korteweg de Vries Institute for Mathematics

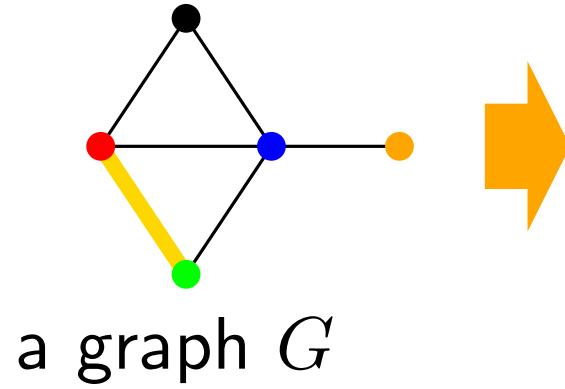
45ACC, University of Western Australia, Perth, Dec 12, 2023.

Algebraic Graph Theory



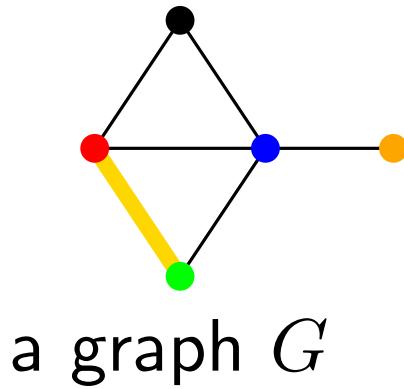
a graph G

Algebraic Graph Theory



$$\begin{array}{c} \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \\ \bullet \quad \left[\begin{array}{ccccc} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{array} \right] \\ \bullet \quad \text{adjacency matrix} \\ A := A(G) \end{array}$$

Algebraic Graph Theory

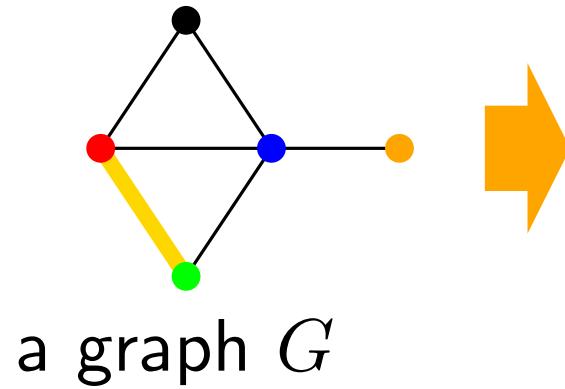


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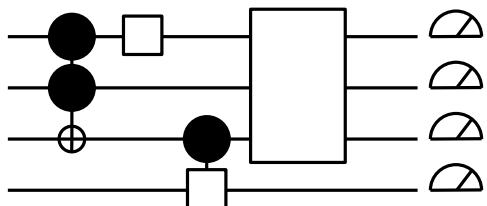
spectral bounds
cospectrality
matrix algebras
etc.

Algebraic Graph Theory

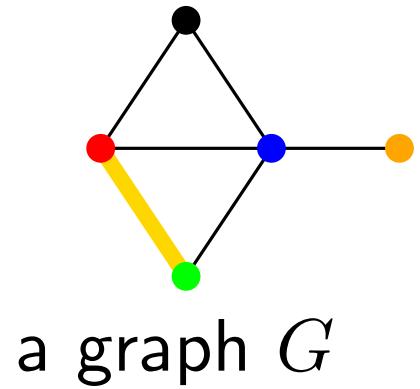


$$\begin{array}{c} \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \\ \bullet \quad \left[\begin{array}{ccccc} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{array} \right] \\ \text{adjacency matrix} \\ A := A(G) \end{array}$$

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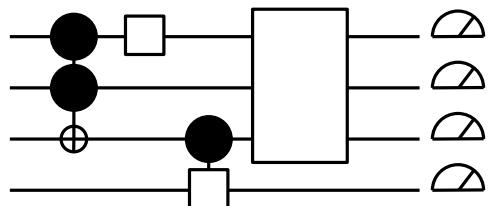
Algebraic Graph Theory



adjacency matrix
 $A := A(G)$

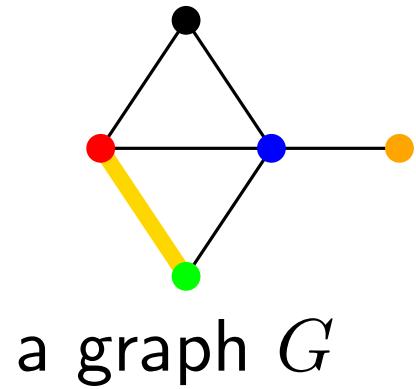
$$\begin{matrix} & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \left[\begin{array}{ccccc} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{array} \right] \\ \bullet & & & & \end{matrix}$$

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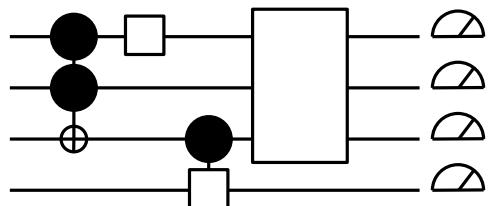


transition
matrix

Algebraic Graph Theory



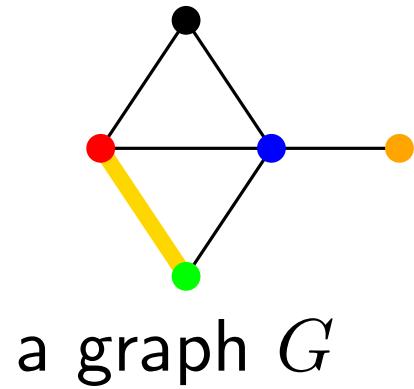
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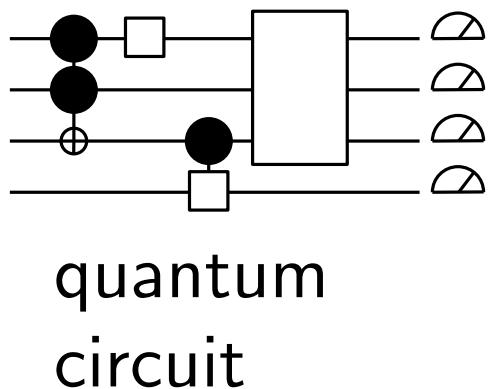
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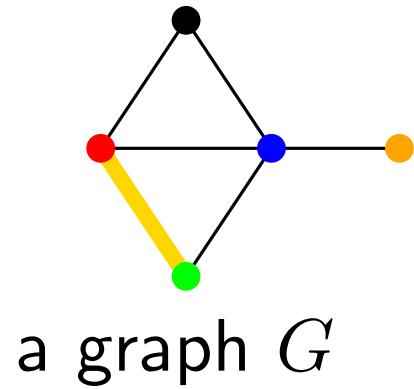


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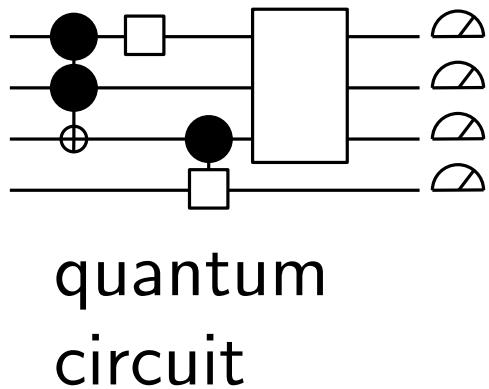
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properties of the
quantum walk

Algebraic Graph Theory

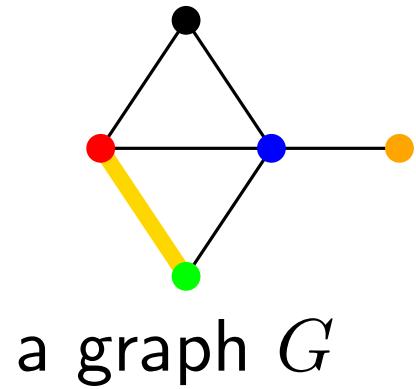


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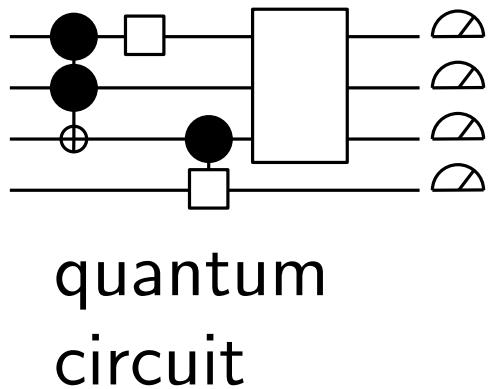
$$\begin{array}{c} \downarrow \\ \text{transition} \\ \text{matrix} \\ \rightarrow \\ \text{properties of the} \\ \text{quantum walk} \end{array}$$

Algebraic Graph Theory



adjacency matrix
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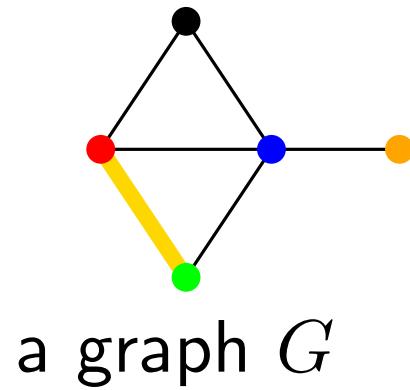


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Algebraic Graph Theory

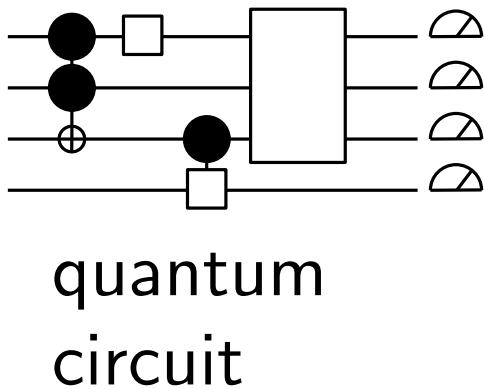


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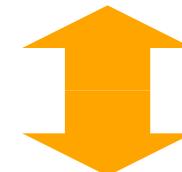
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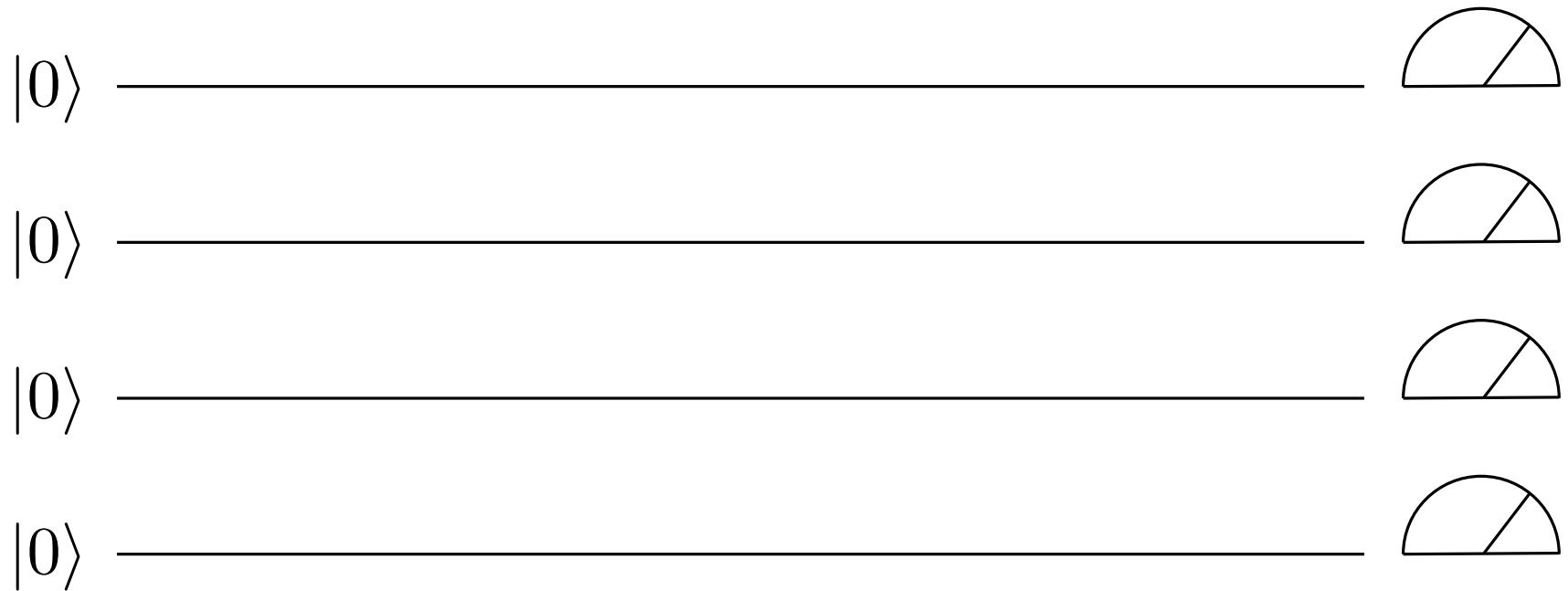
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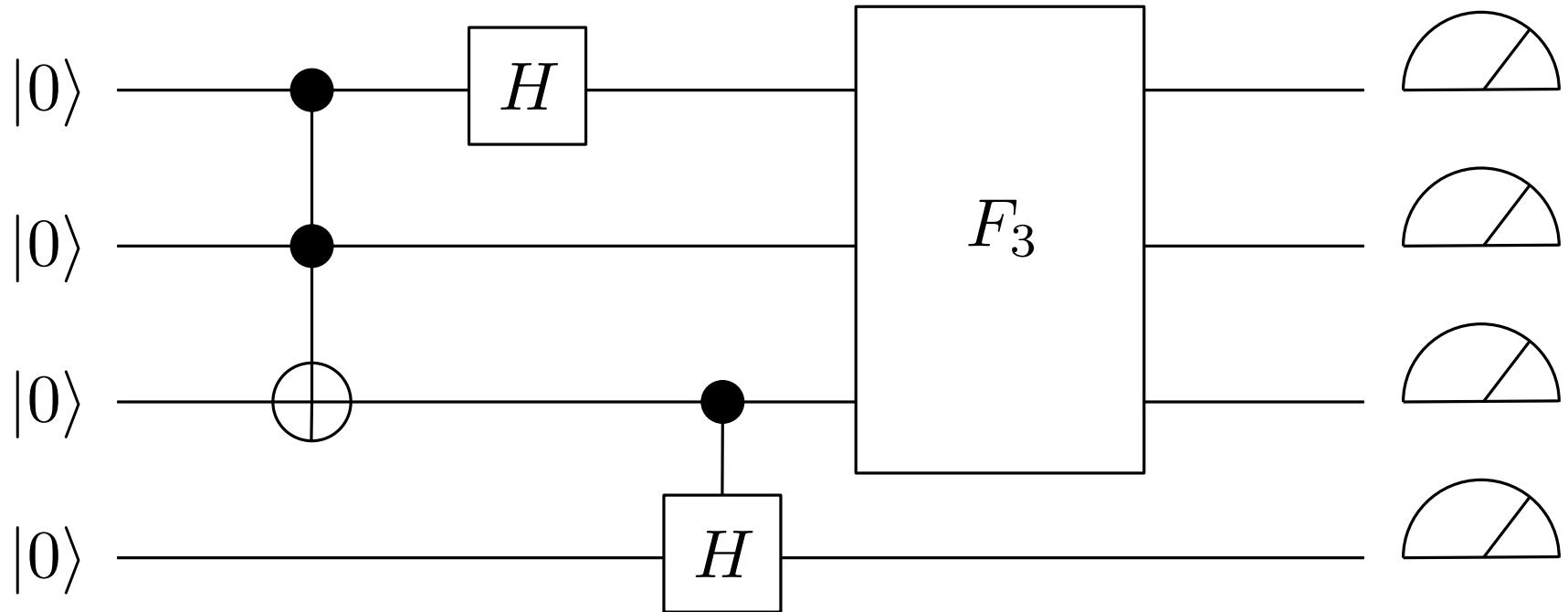
Continuous-time Quantum Walks

Quantum computing

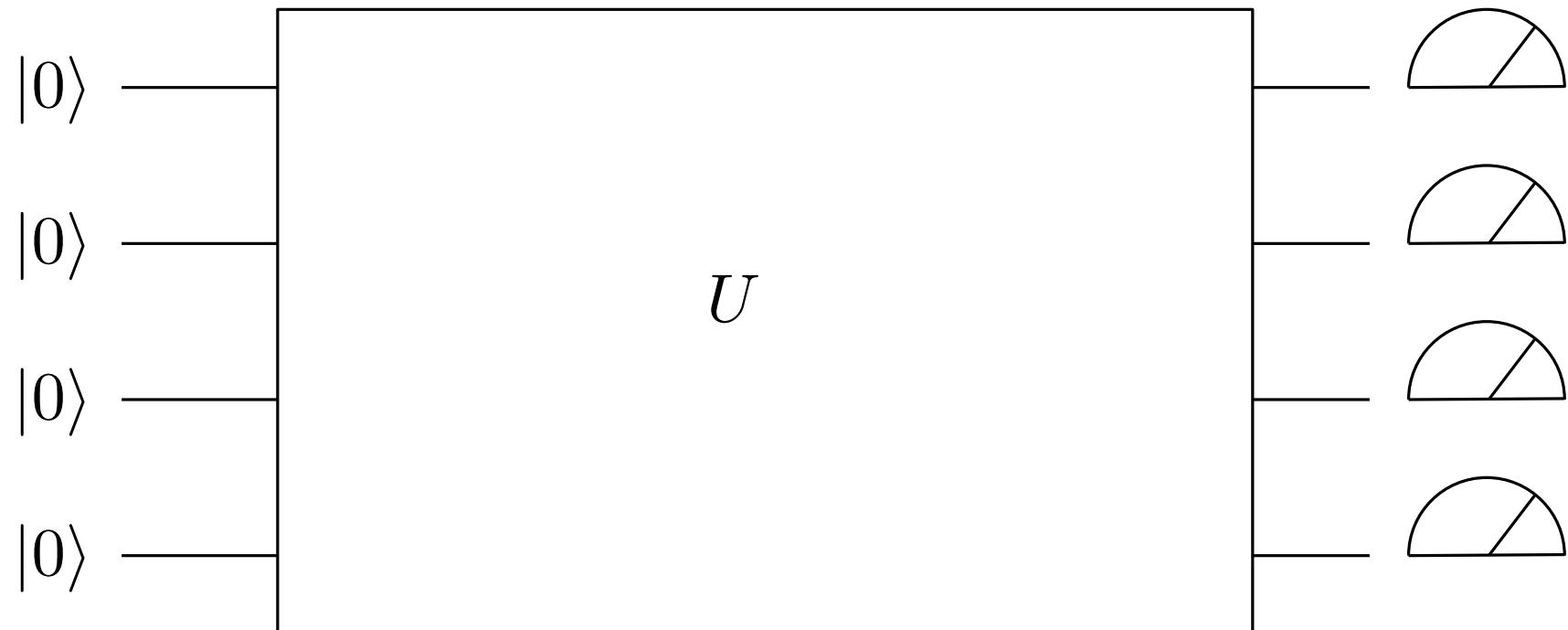
UvA



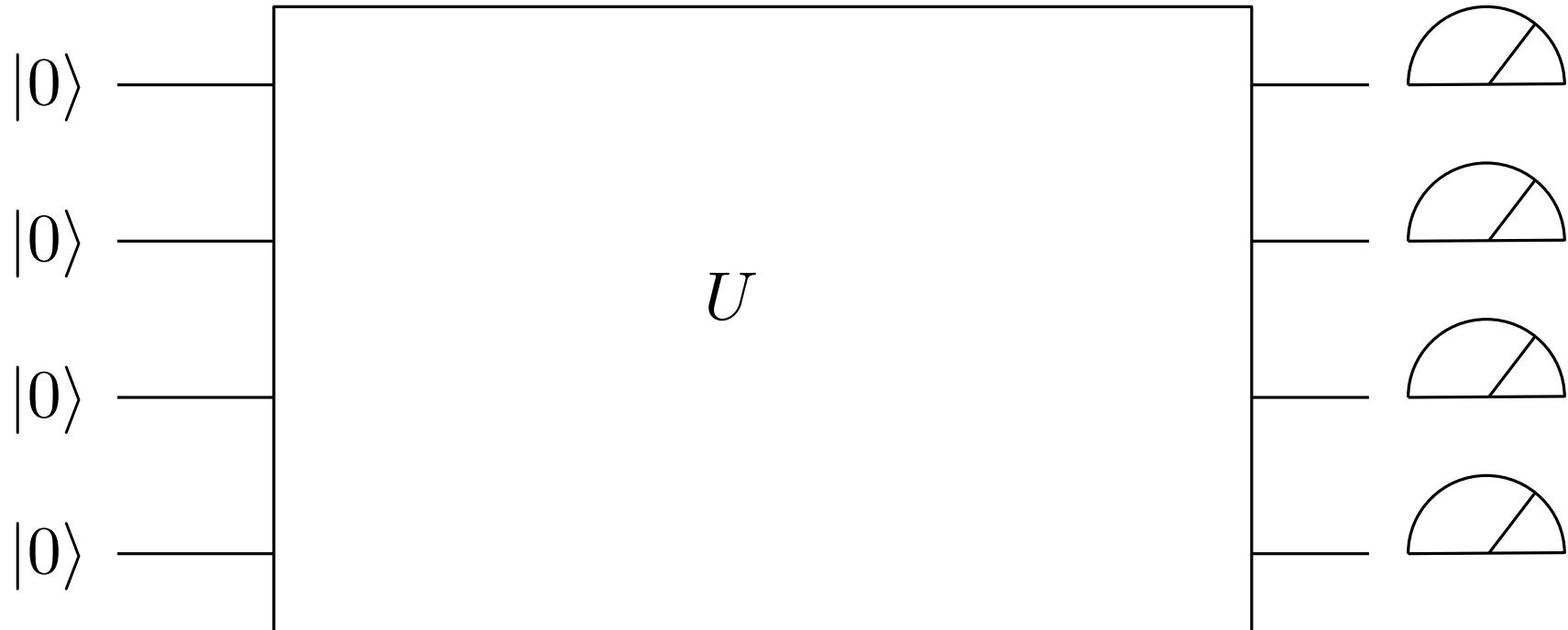
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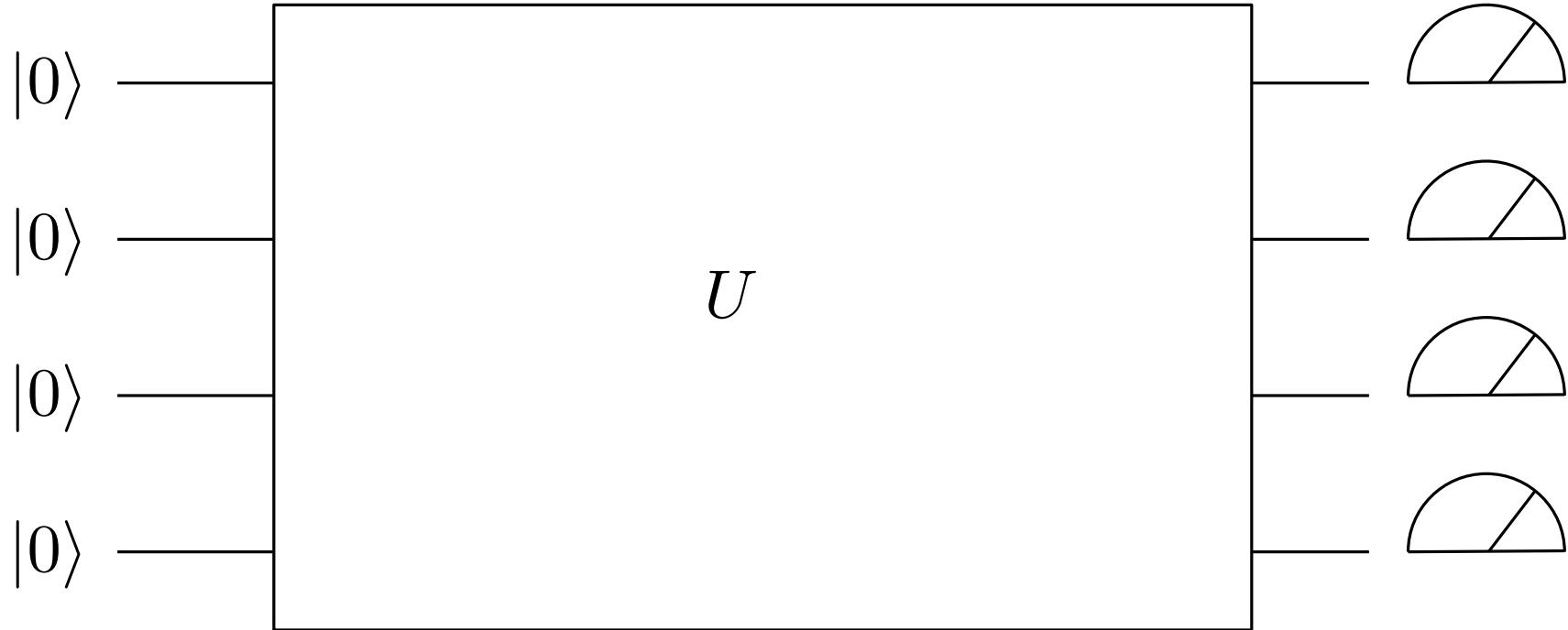


Quantum computing



With some assumptions about the system, we can model it by a $n \times n$ matrix, $U(t) = e^{itA}$ where A is the adjacency matrix of an underlying graph.

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XY-Hamiltonian

Pauli
matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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$$\sigma_x^u = I_2 \otimes I_2 \otimes \cdots \otimes \sigma_x \otimes I_2 \otimes \cdots \otimes I_2$$

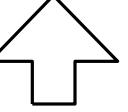

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Hamiltonian of graph G :

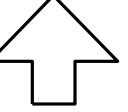
$$H_{xy} = \frac{1}{2} \sum_{uv \in E} (\sigma_x^u \sigma_x^v + \sigma_y^u \sigma_y^v)$$

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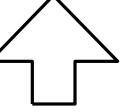
time t : state is $\phi(t) = e^{-itH\frac{2\pi}{h}} \phi_0$

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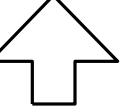
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$$e^{itA}$$

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Continuous-time quantum walk

"... quantum walk can be regarded as a universal computational primitive, with any desired quantum computation encoded entirely in some underlying graph." Andrew Childs [arXiv:0806.1972](https://arxiv.org/abs/0806.1972)

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Transition matrix

$$U(t) = \exp(itA)$$

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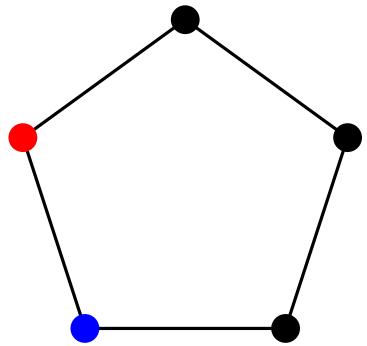
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$$\begin{aligned} U(t) &= \exp(itA) \\ &= I + itA - \frac{1}{2!}t^2A^2 - \frac{i}{3!}t^3A^3 + \dots \end{aligned}$$

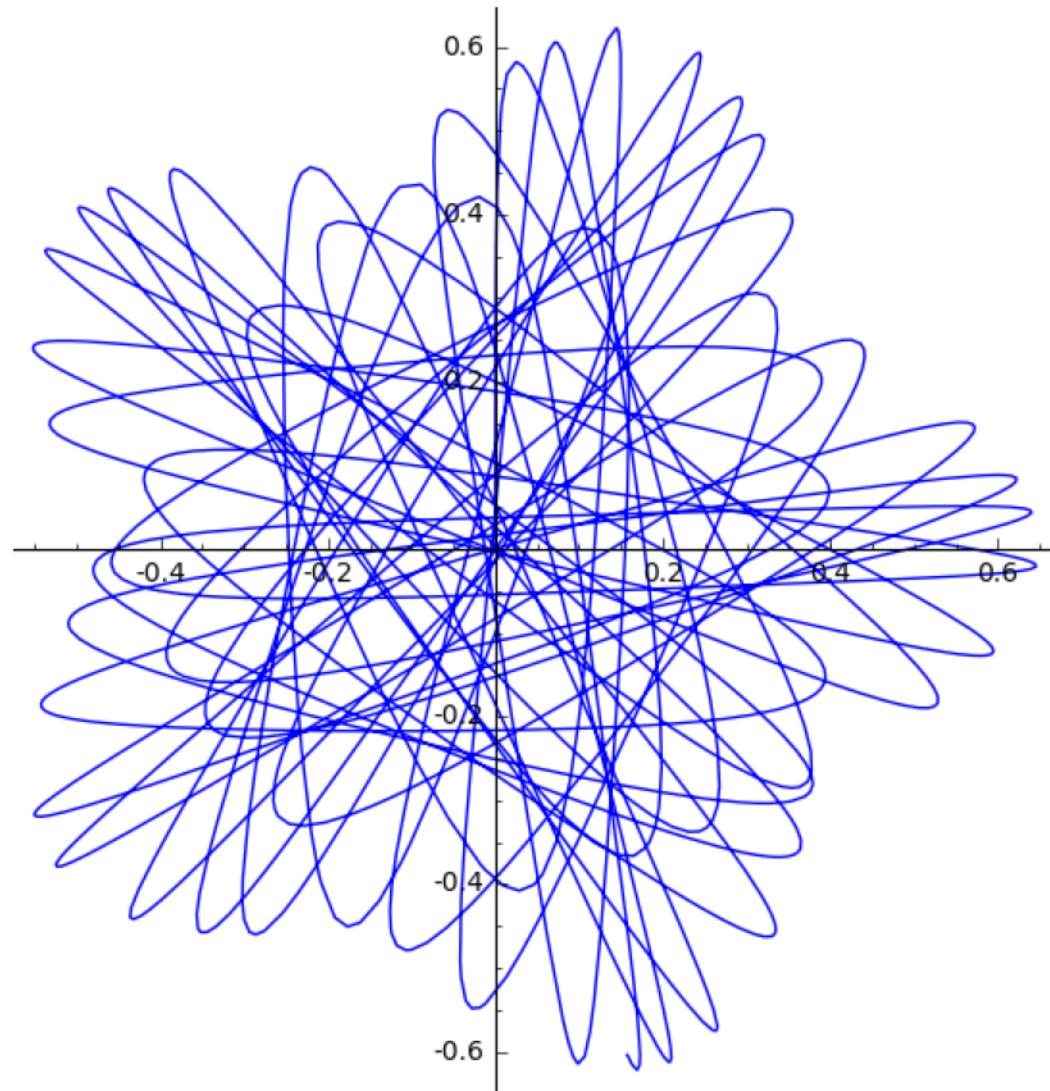
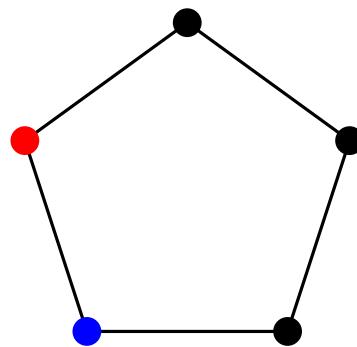
Example

$U(t)_{\color{red}a,\color{blue}b}$ for $t \in [0, 100]$.



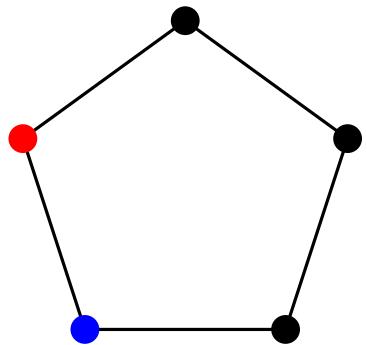
Example

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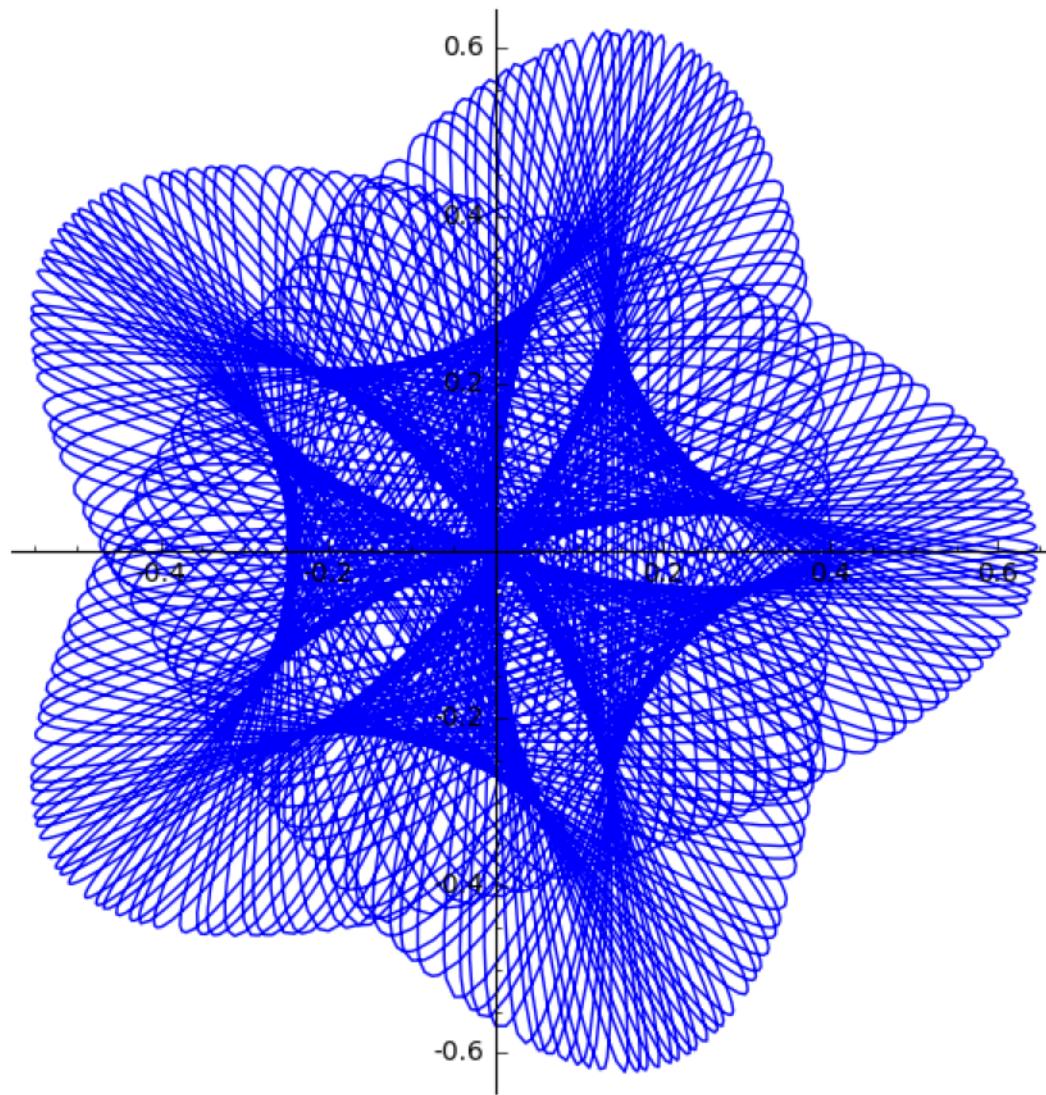
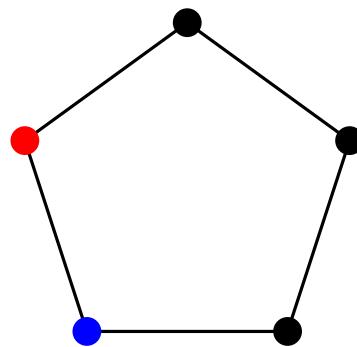
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More context: quantum search

Problem: given a “marked” value, search N locations to find the location whose content is the given value.

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Classically, one cannot do better than checking $O(N)$ locations.

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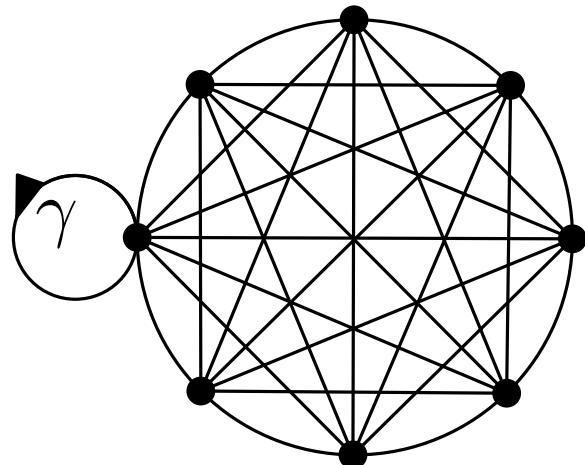
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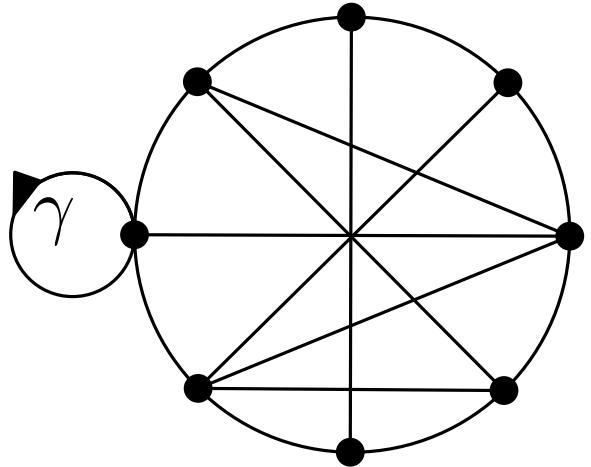
Grover’s search is equivalent to running a quantum walk on K_N with a marked vertex, with the Laplacian matrix, and doing a measurement after \sqrt{N} time.

More context: quantum search

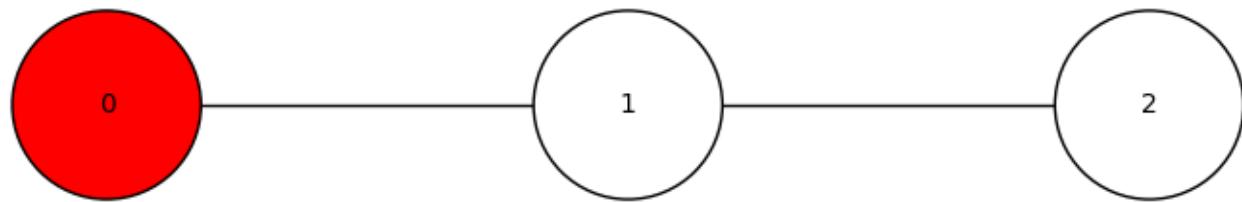
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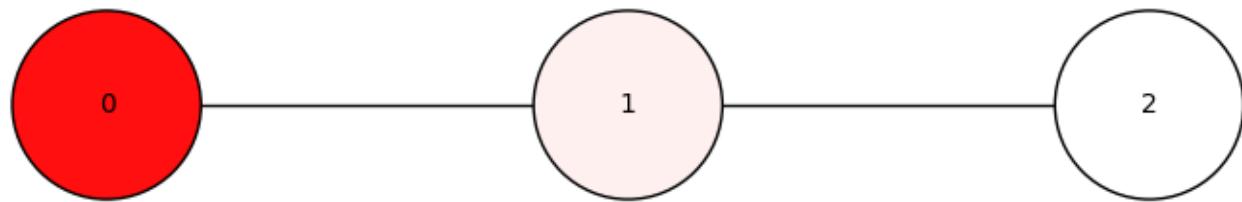


Spatial quantum search is when we run the analogous search on a marked graph. It is not known for which graphs, spatial search has a quadratic speedup.



$$M(t) = U(t) \circ \bar{U}(t) = \begin{pmatrix} 1.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 1.0 \end{pmatrix}$$

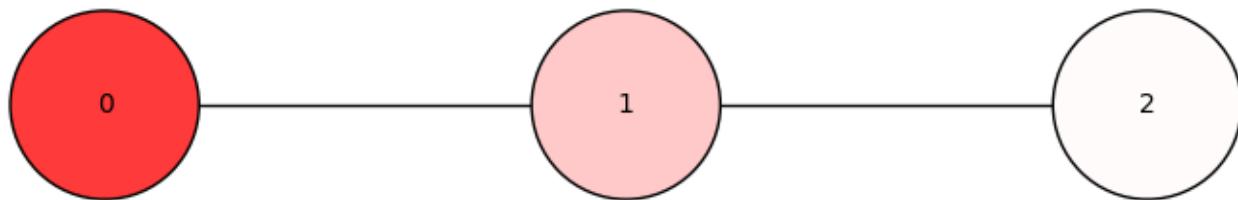
$$t = 0$$



$$\begin{pmatrix} 0.939105 & 0.059939 & 0.000956 \\ 0.059939 & 0.880122 & 0.059939 \\ 0.000956 & 0.059939 & 0.939105 \end{pmatrix}$$

$t = 0$

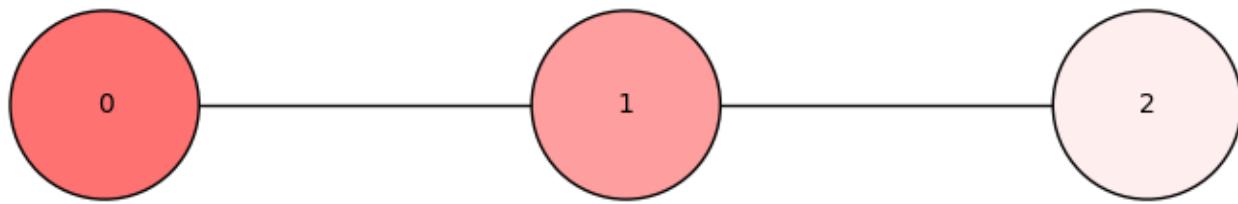
Time incrementing by 0.25.



$$\begin{pmatrix} 0.774615 & 0.211014 & 0.014371 \\ 0.211014 & 0.577972 & 0.211014 \\ 0.014371 & 0.211014 & 0.774615 \end{pmatrix}$$

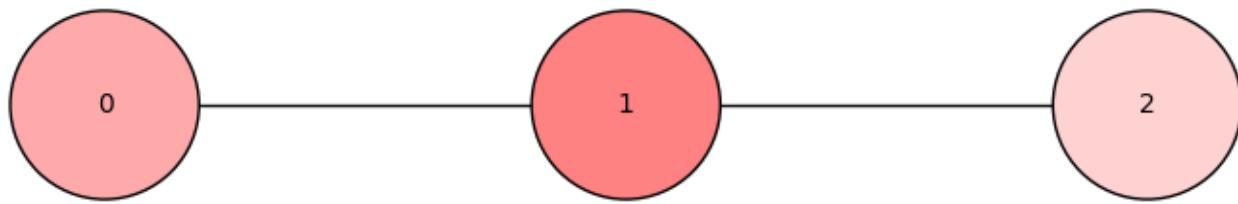
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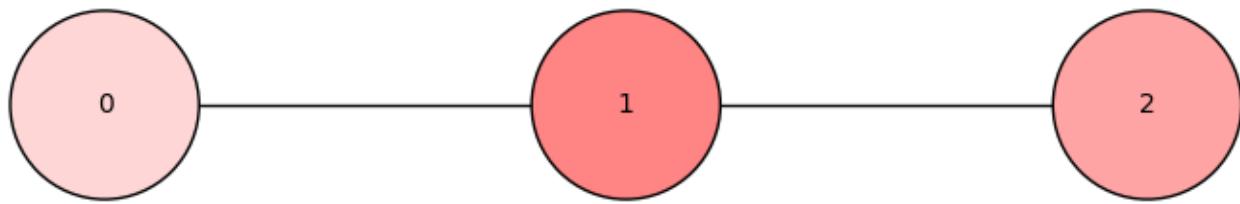
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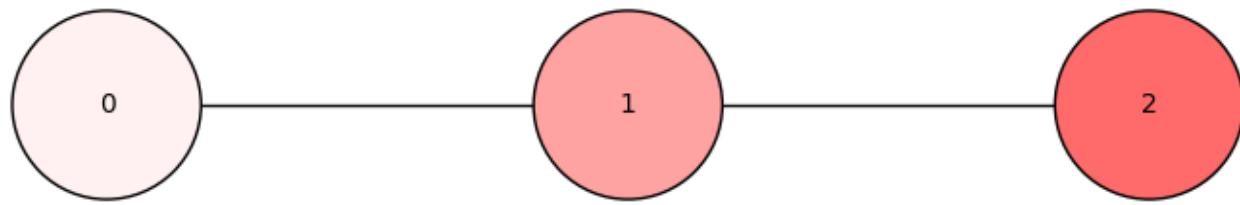
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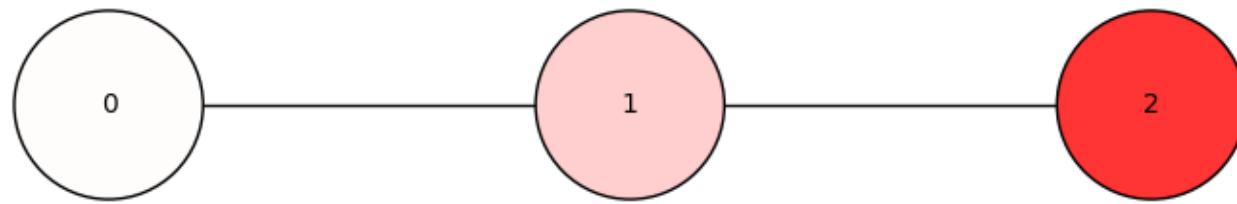
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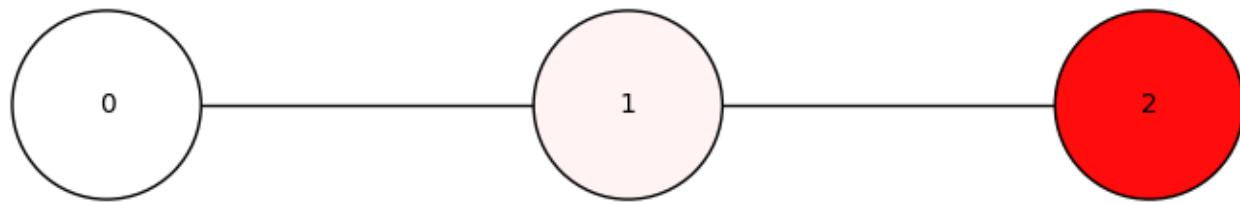
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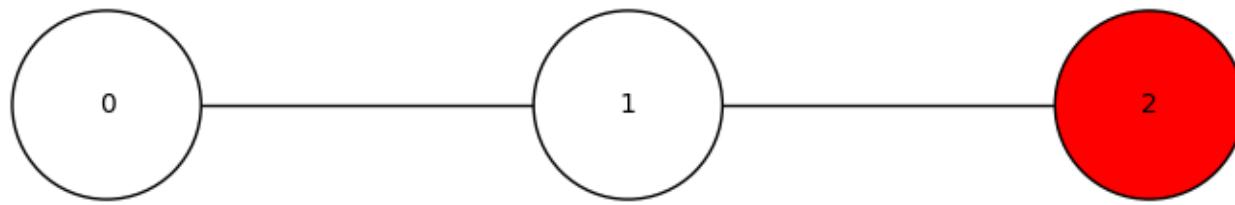
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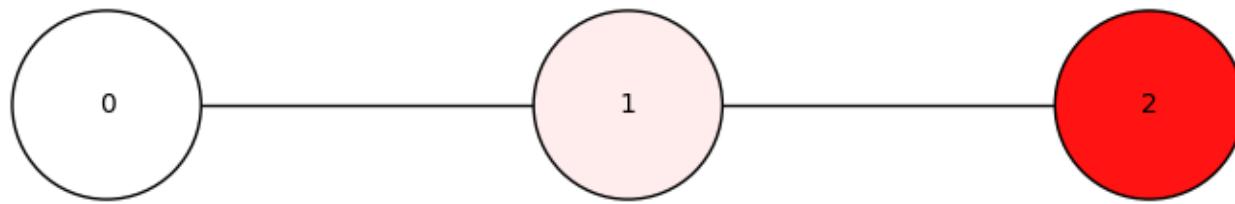
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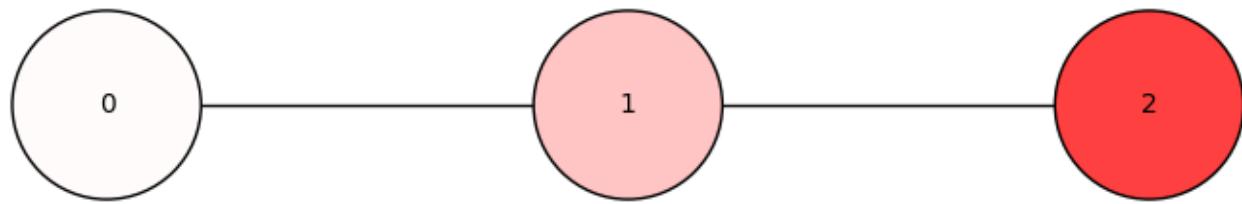
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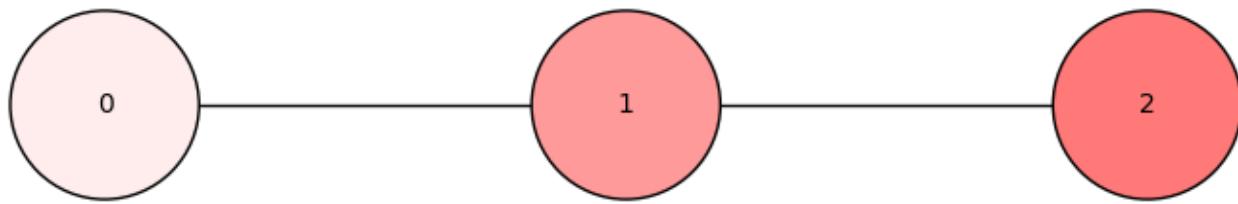
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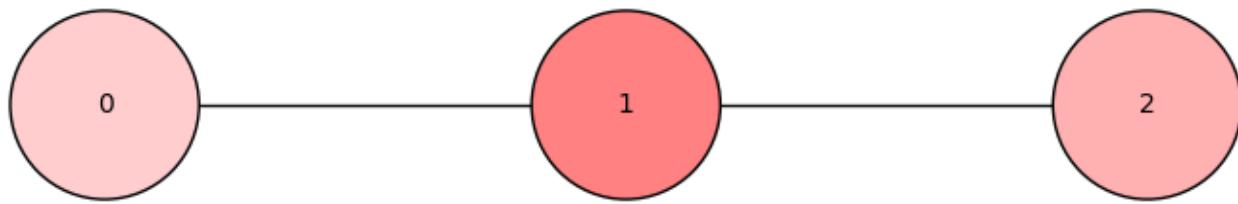
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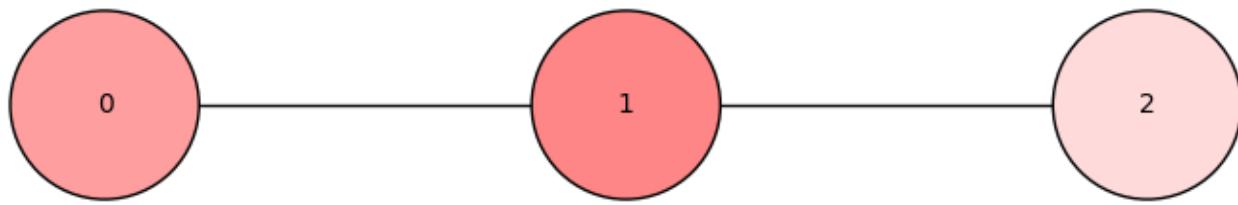
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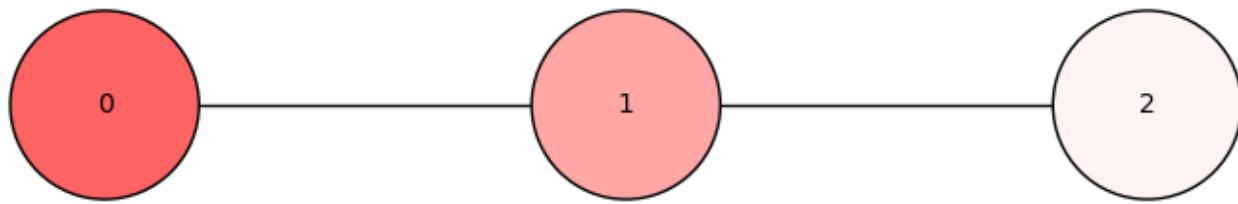
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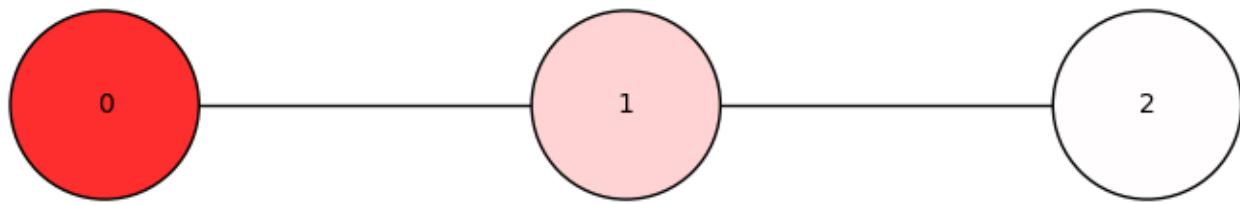
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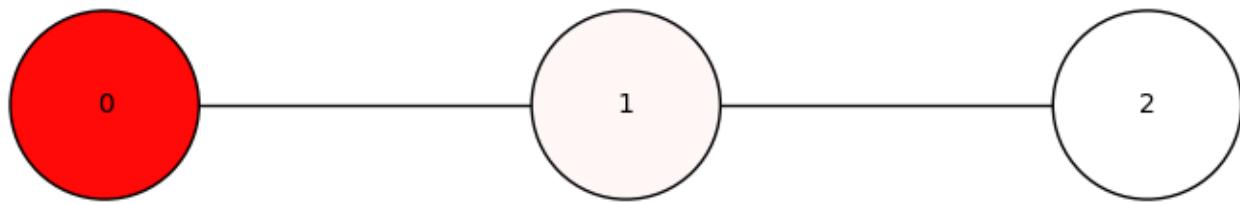
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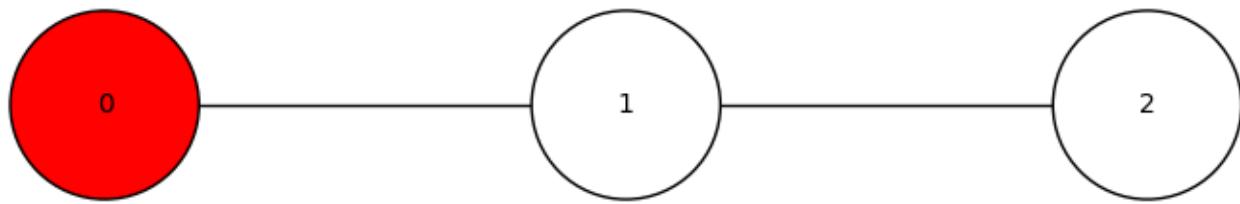
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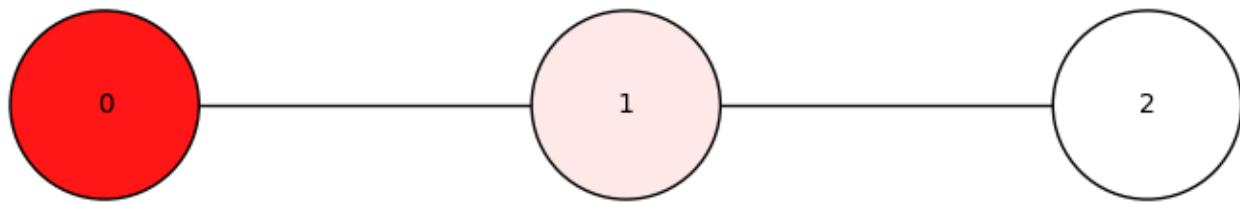
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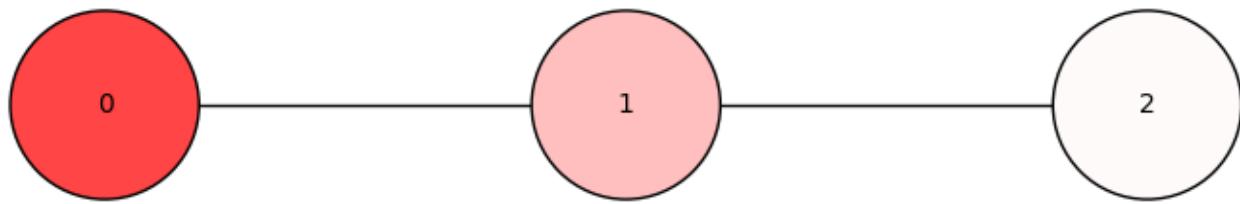
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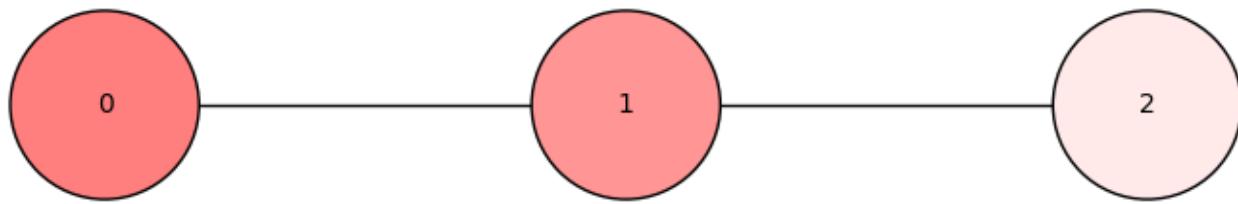
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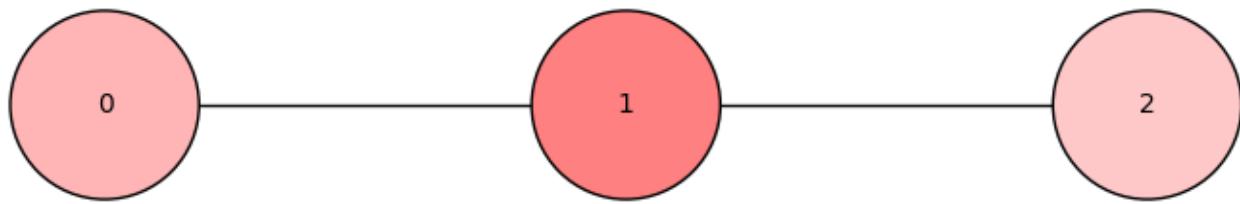
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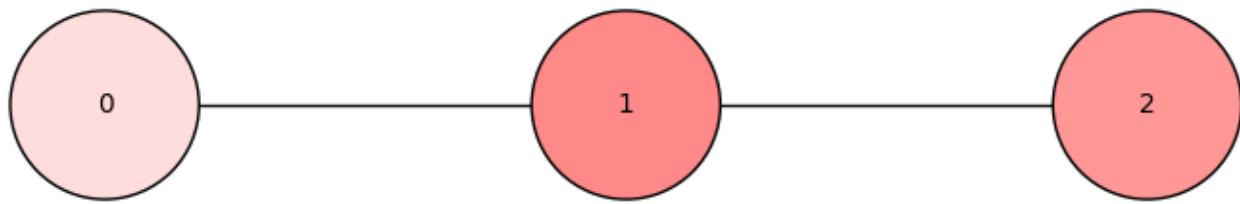
$t = 0$

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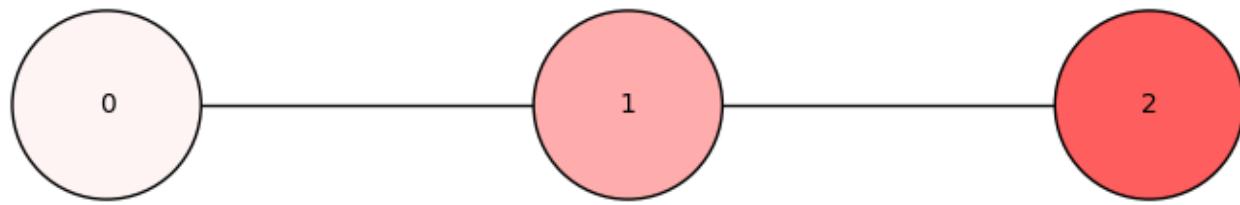
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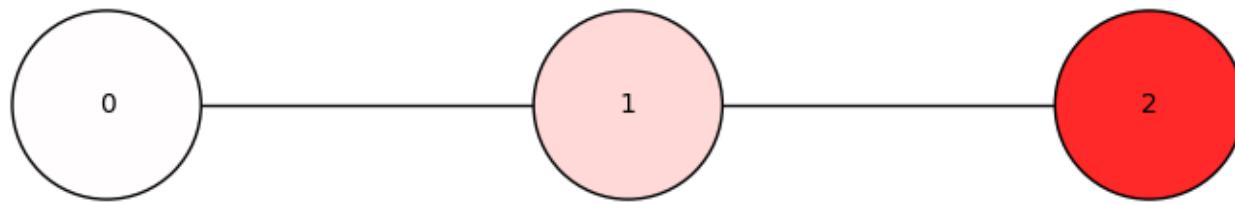
$t = 0$

Time incrementing by 0.25.



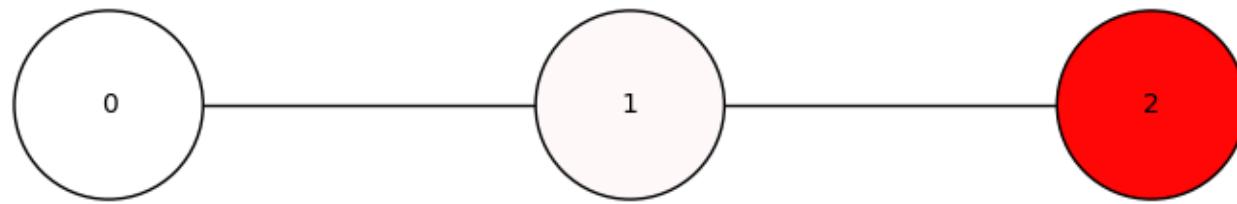
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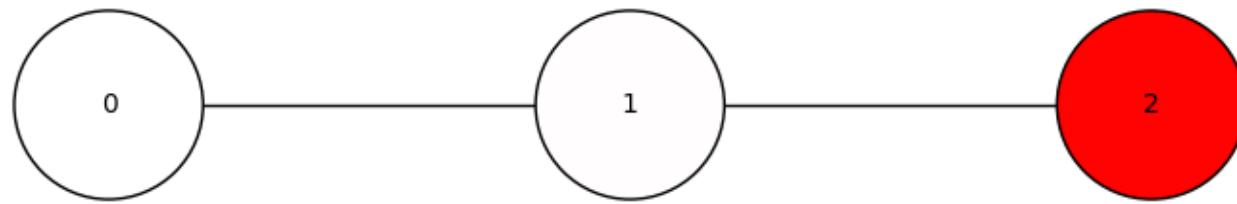
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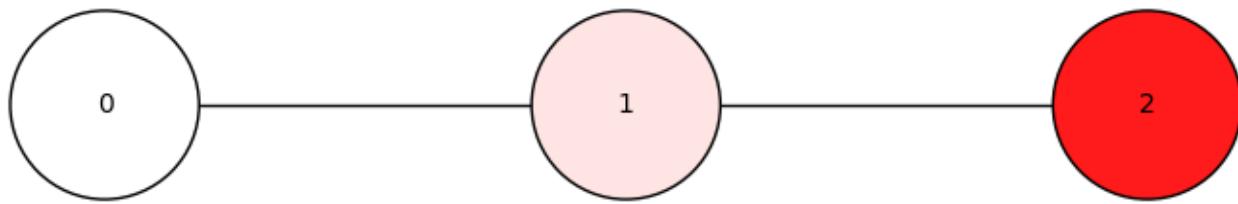
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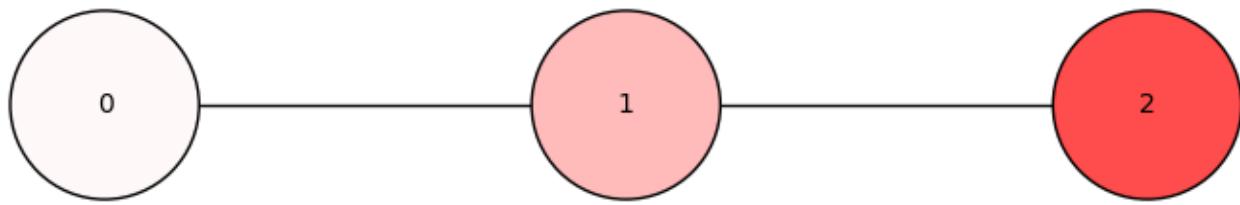
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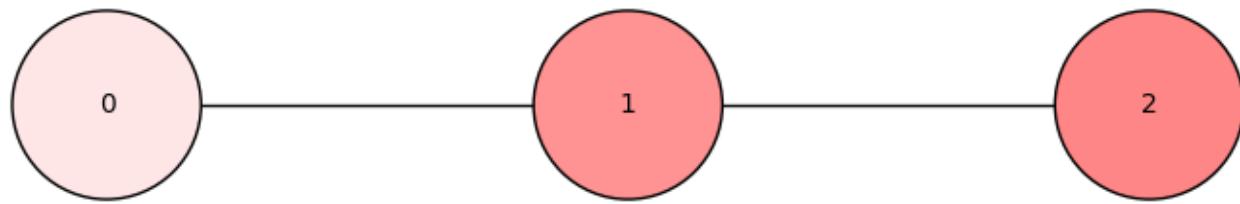
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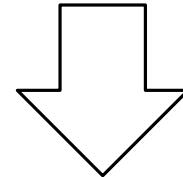
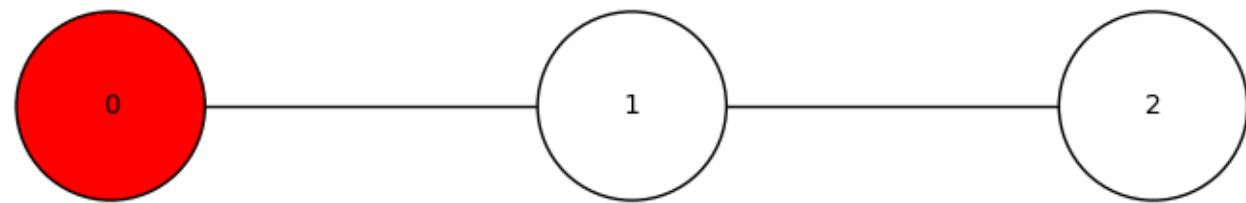


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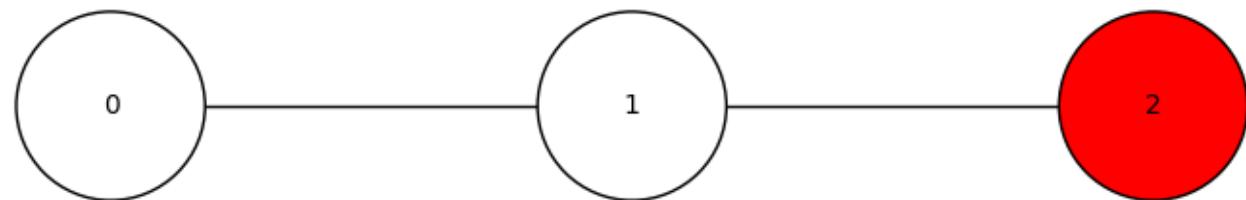
Perfect state transfer:

start



time τ

$t = 0$



Perfect state transfer: paths

Perfect state transfer from a to b :

there exists a time τ , such that probability of measuring at b , having started at a , is 100%.

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Theorem (Godsil 2012)

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The only paths which admit perfect state transfer are P_2 and P_3 .

Pretty good state transfer from a to b :

for every $\epsilon > 0$, there exists τ such that there exists a time τ , such that probability of measuring at b , having started at a , is at least $100 - \epsilon\%$.

Pretty good state transfer

Theorem (Godsil, Kirkland, Severini, and Smith 2012)

P_n has pretty good state transfer
if and only if $n + 1$ is a prime, twice a prime or a
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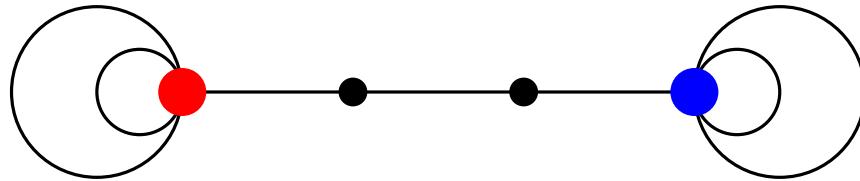
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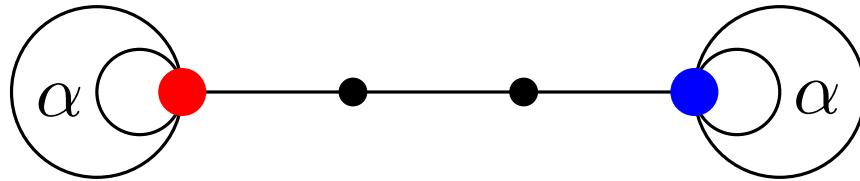
Theorem (Coutinho, Guo and van Bommel² 2017)

P_n has pretty good state transfer between internal vxs if and only if $n + 1 = 2^r p$ where p is a prime.

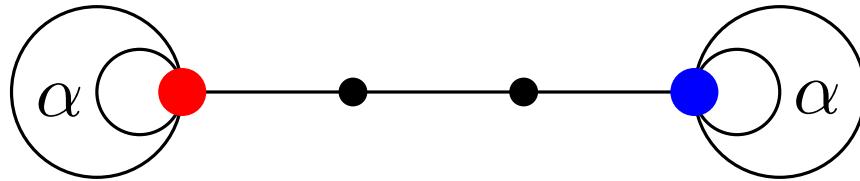
Perfect state transfer on paths revisited



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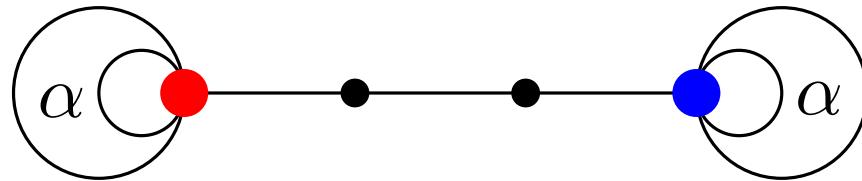
Perfect state transfer on paths revisited



Conjecture (Casaccino, Lloyd, Mancini, and Severini '09)

For any n , one can find α so that there is perfect state transfer from to in P_n .

Perfect state transfer on paths revisited



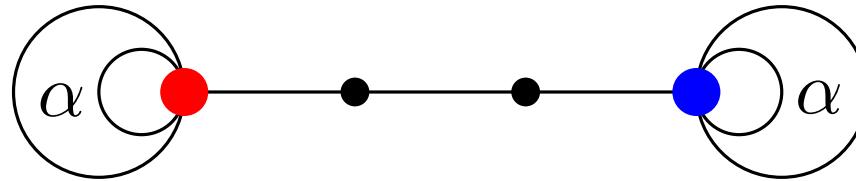
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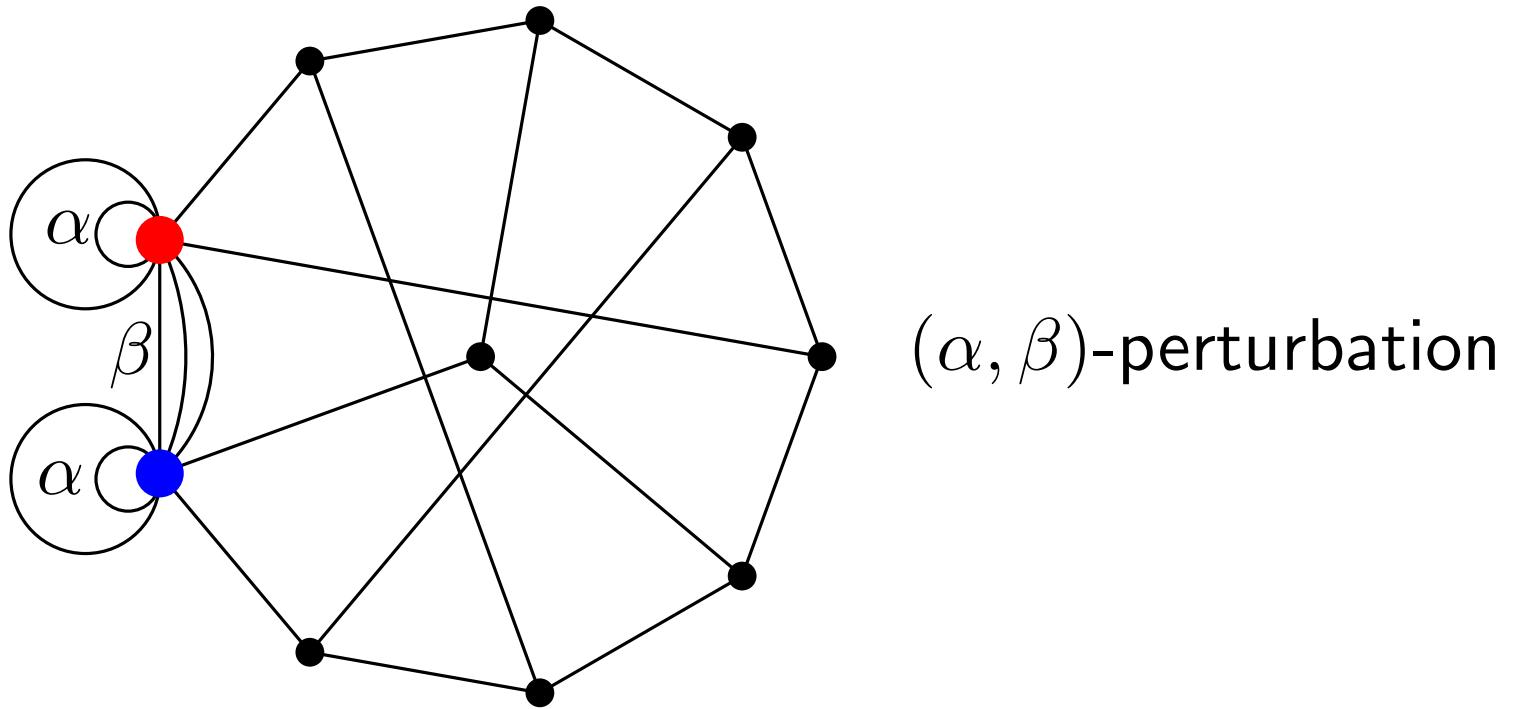
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Perfect state transfer in strongly regular graphs



Theorem (Godsil, Guo, Kempton and Lippner 2019)

For any strongly regular graph coming from an orthogonal array, there exists α and β such that the (α, β) -perturbation admits perfect state transfer.

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In fact, the "good" values of α, β are dense in the reals.

Discrete-time Quantum Walks

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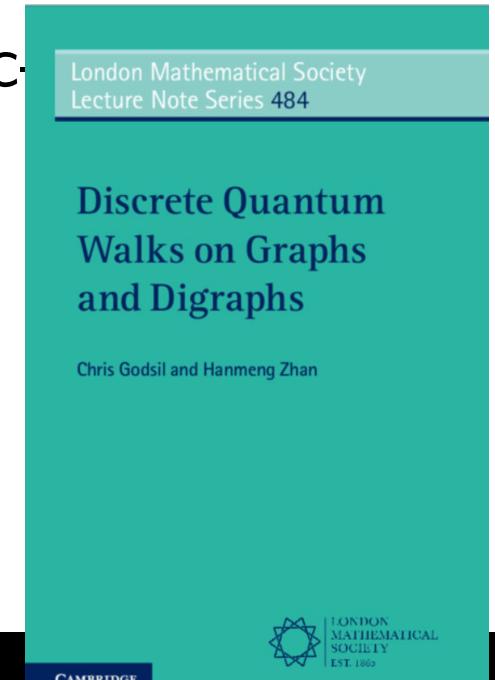
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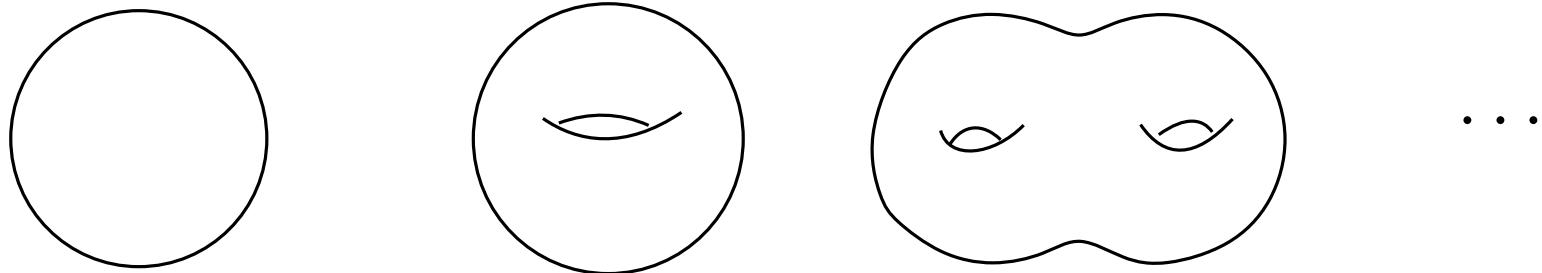
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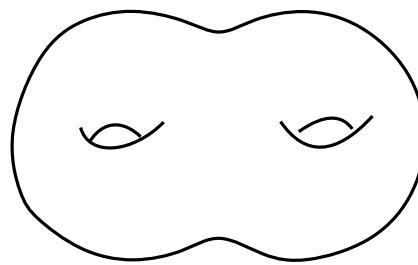
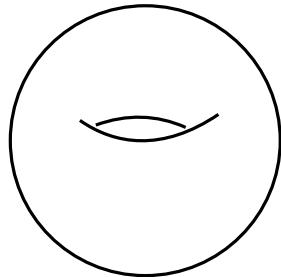
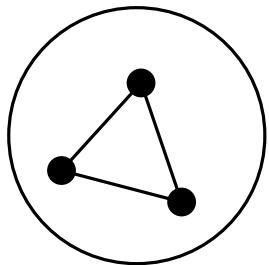
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Graph embeddings

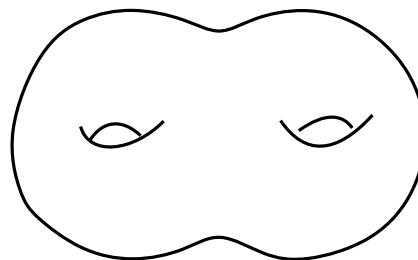
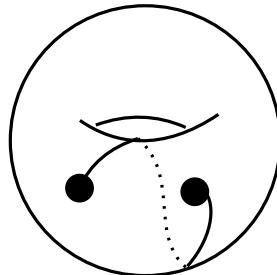
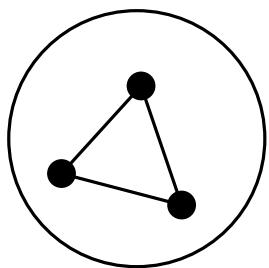


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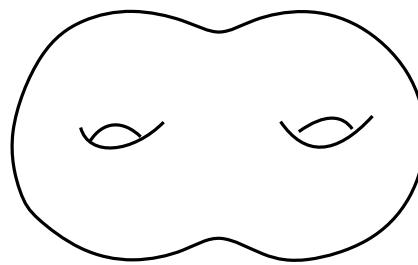
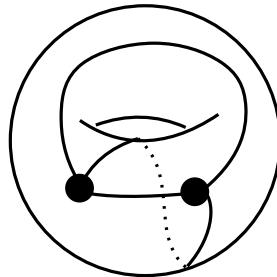
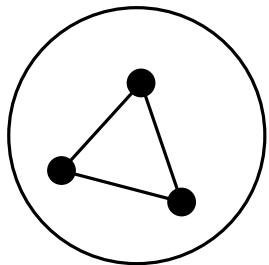
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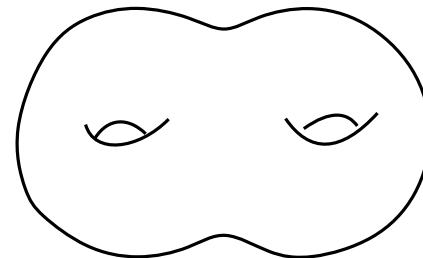
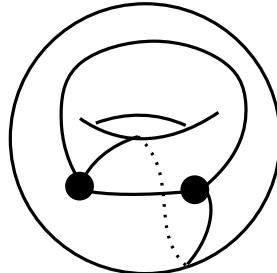
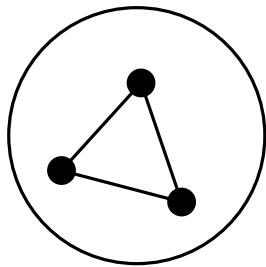
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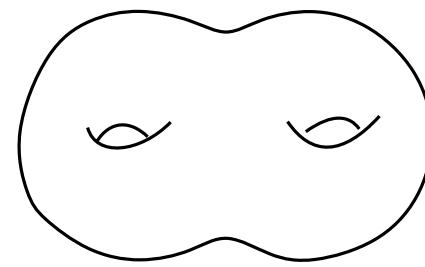
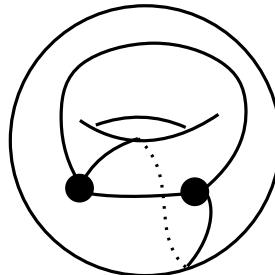
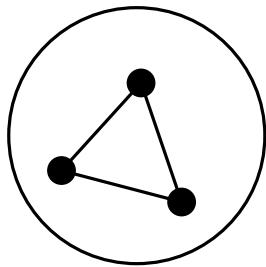
Graph embeddings



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Intuitively, we draw graphs on (orientable) surfaces such that the edges do not cross and “uses” the handles.

Graph embeddings

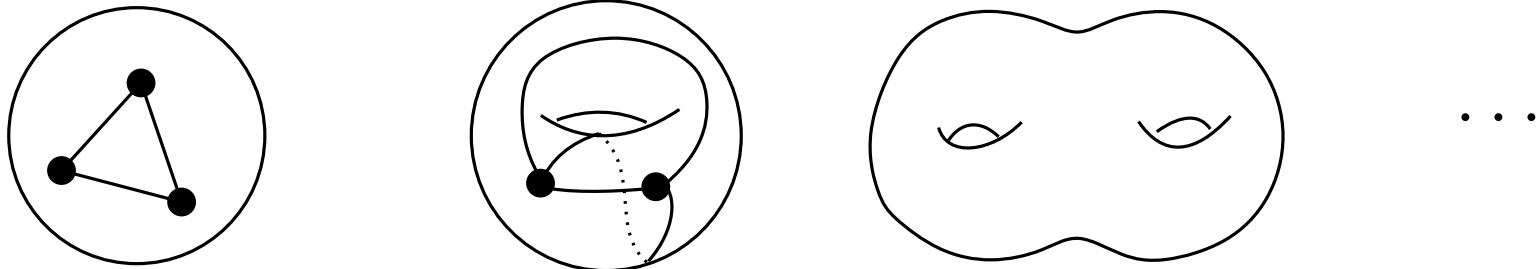


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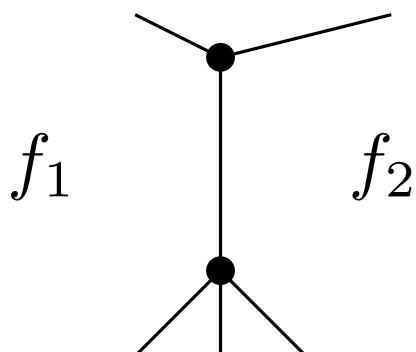
This divides the surface in to regions called *faces*, such that each edge is on two faces.

Graph embeddings

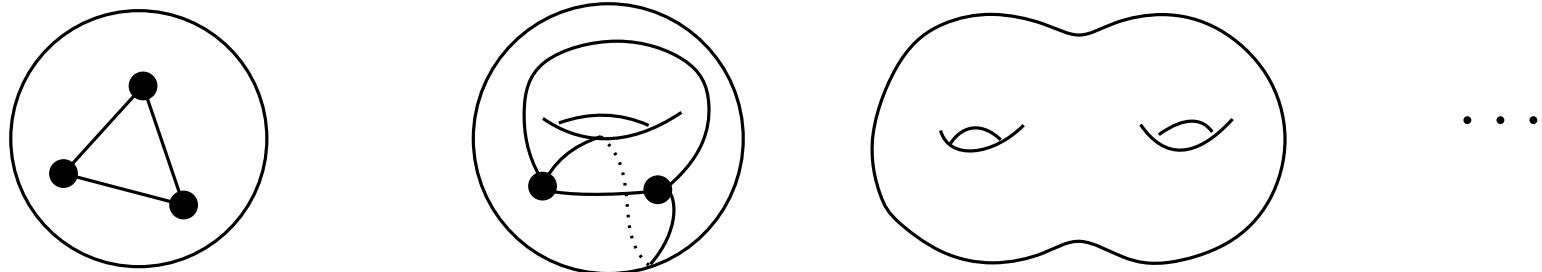


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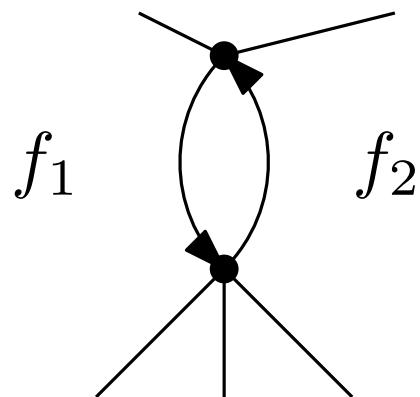


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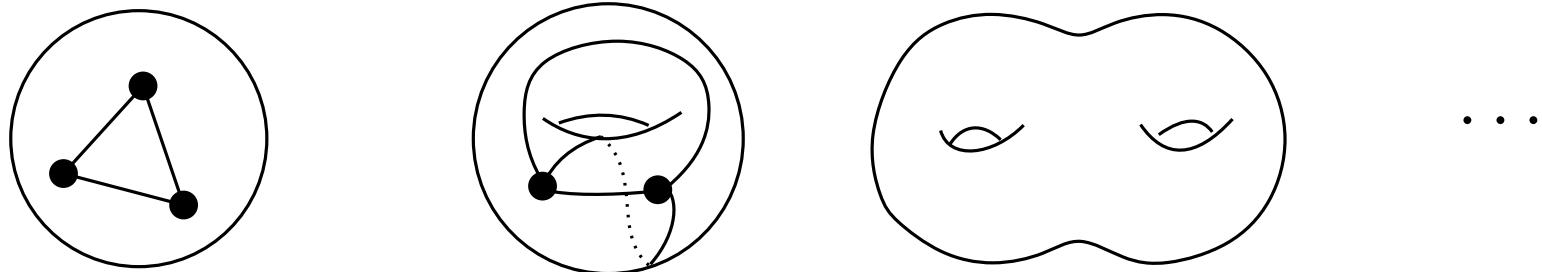


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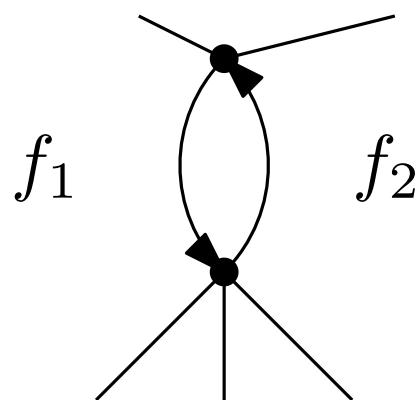


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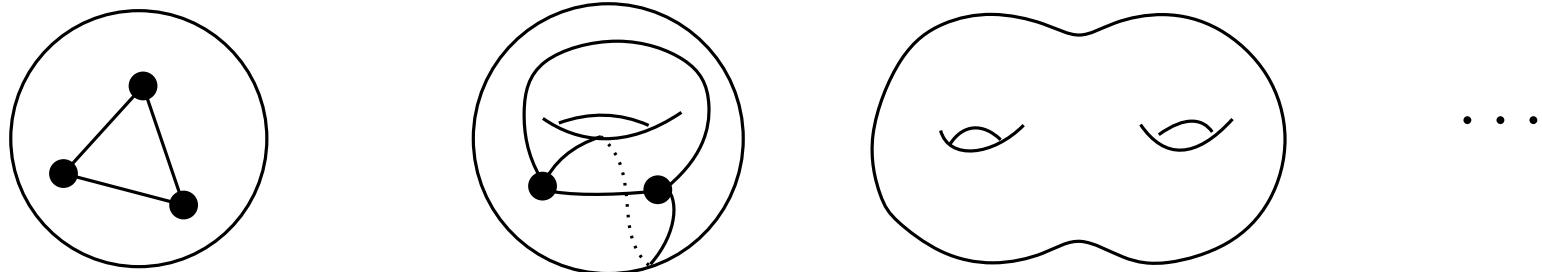
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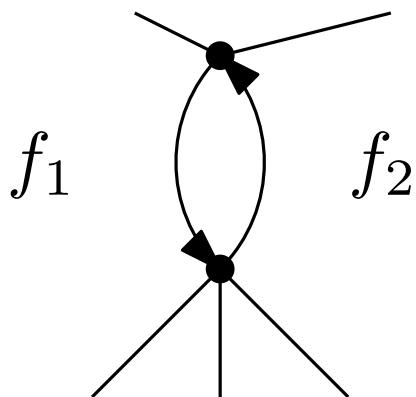
M is the arc-face incidence matrix and we take $P = MM^T$.

Graph embeddings



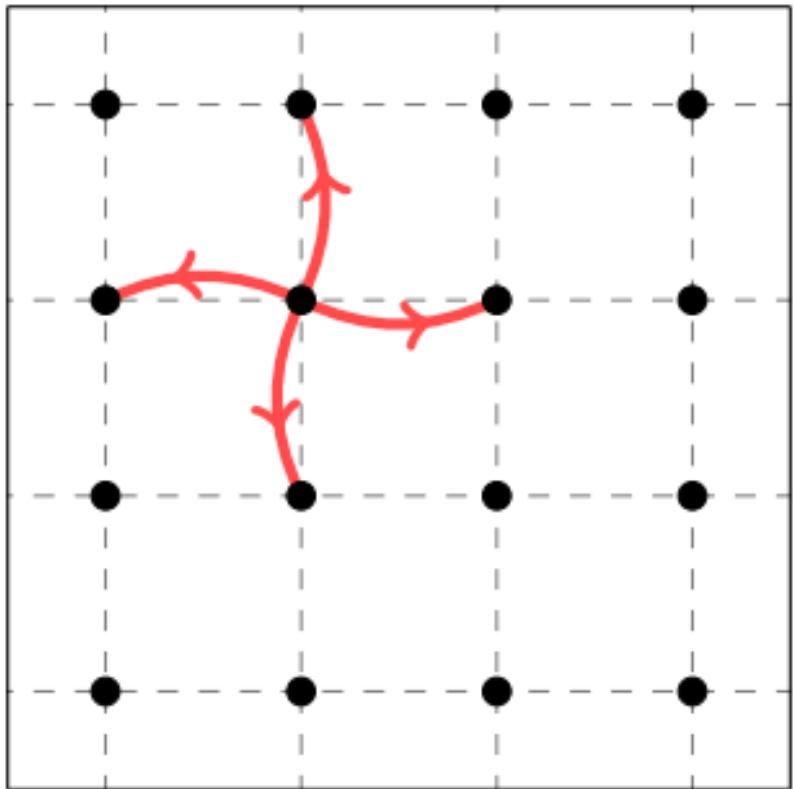
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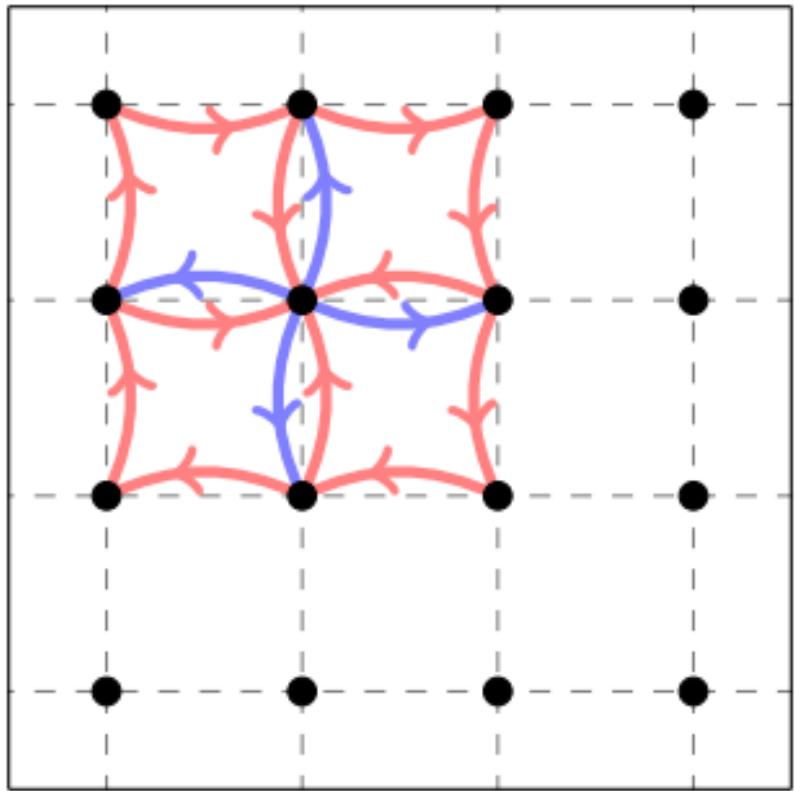
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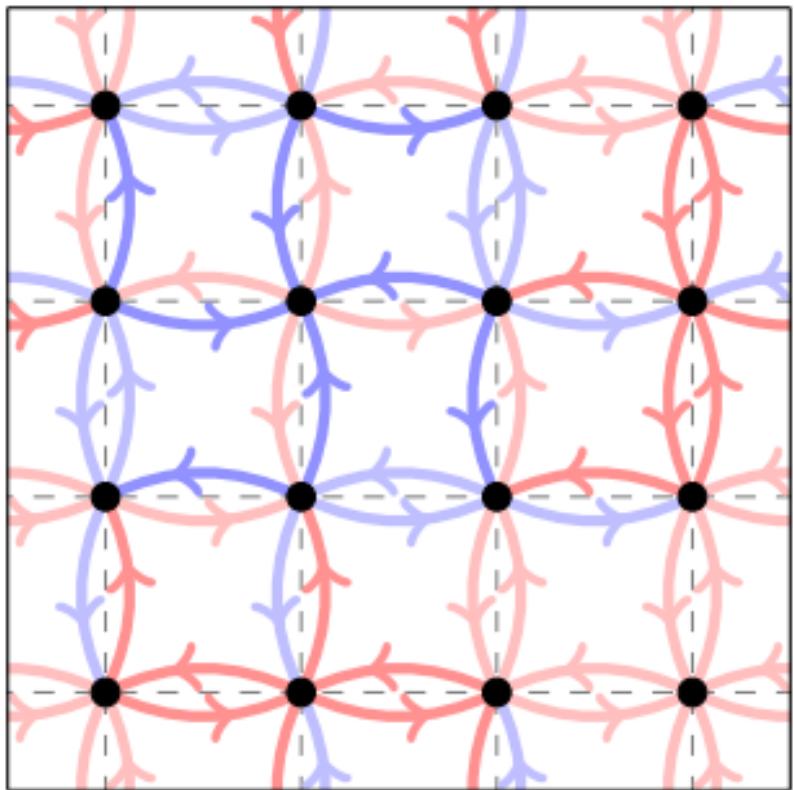


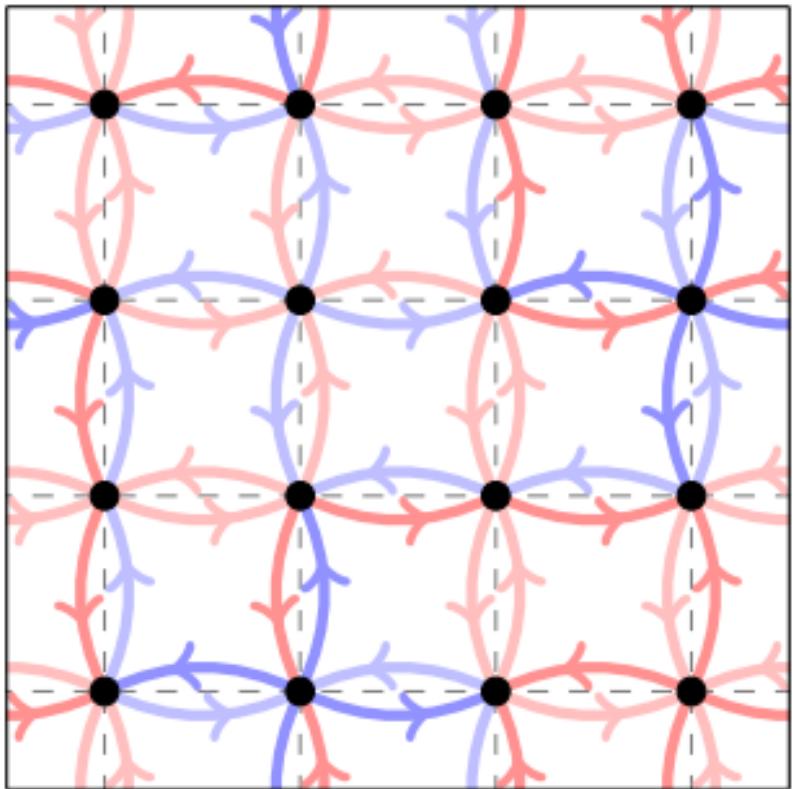
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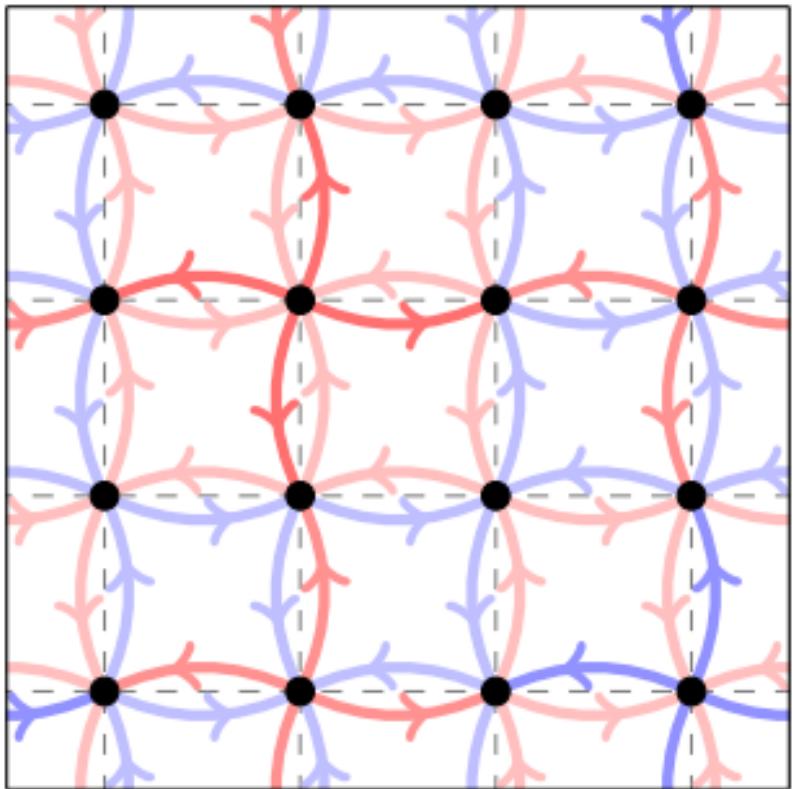
First considered by Zhan in 2020, generalizing various walks on the toroidal grid.

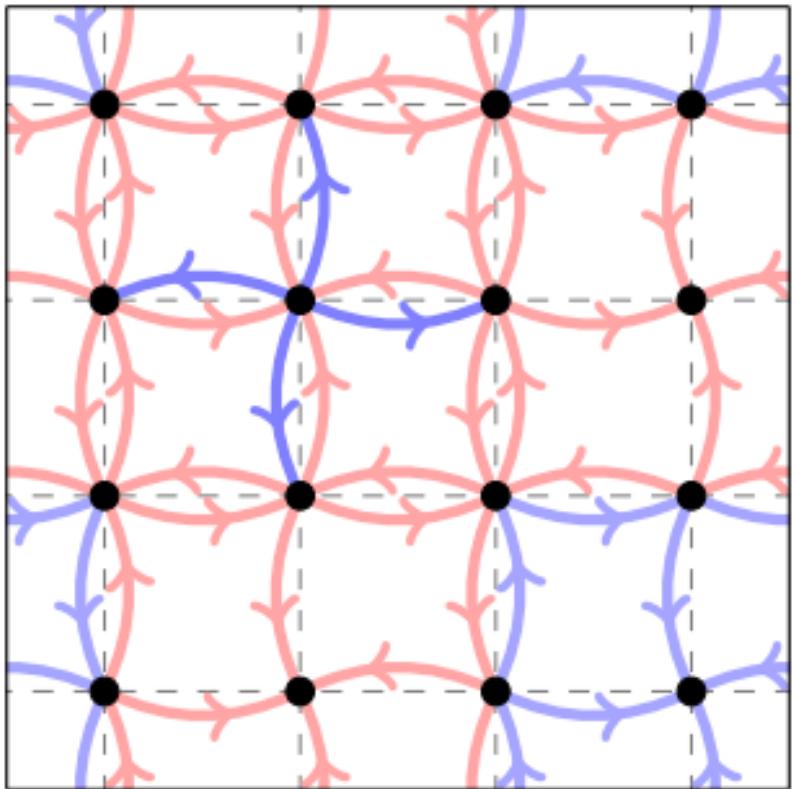
 $t = 0$

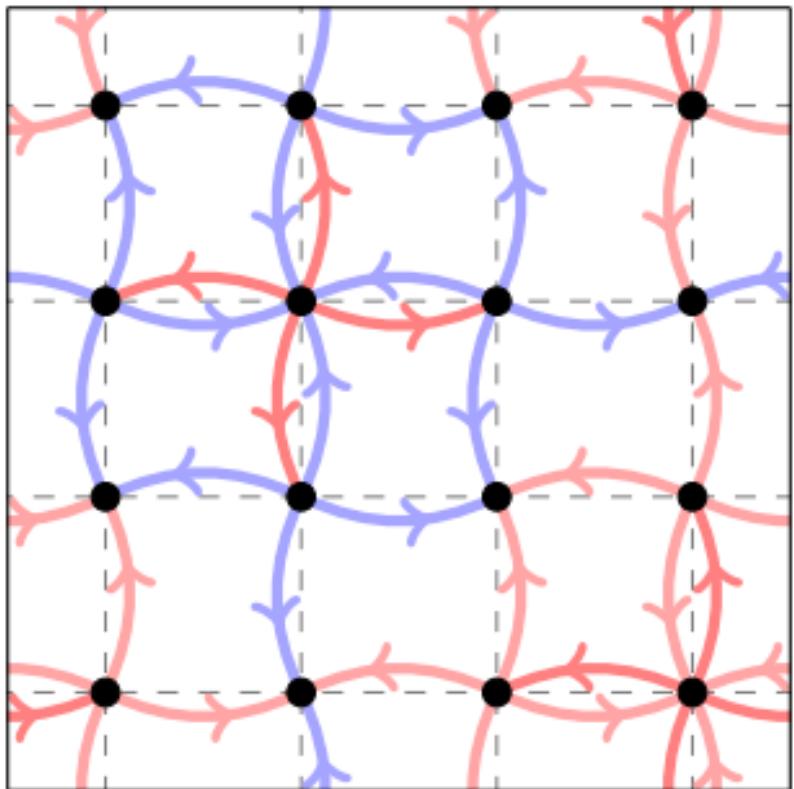

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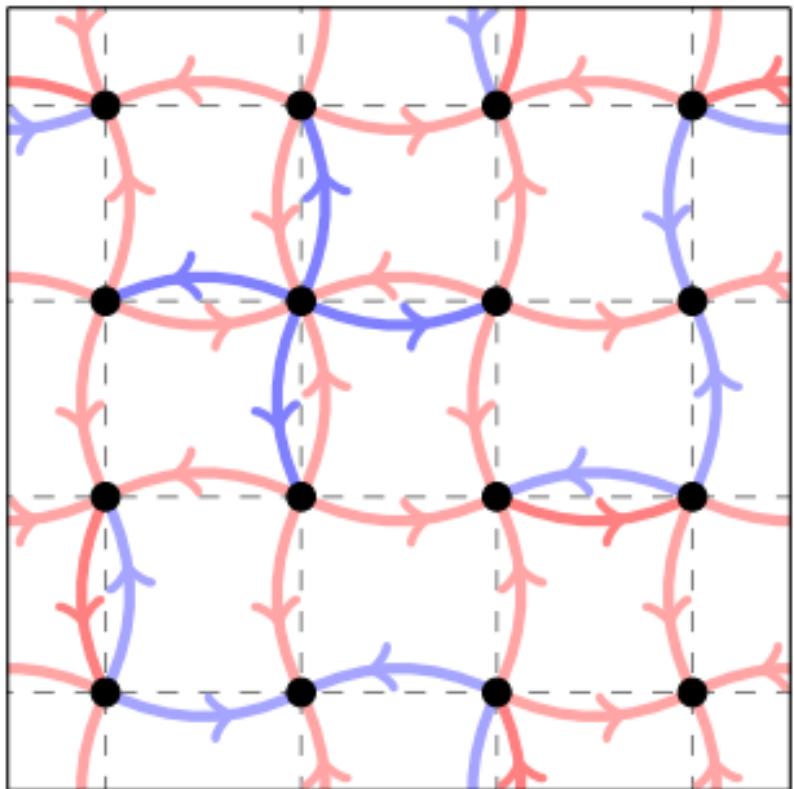
 $t = 2$

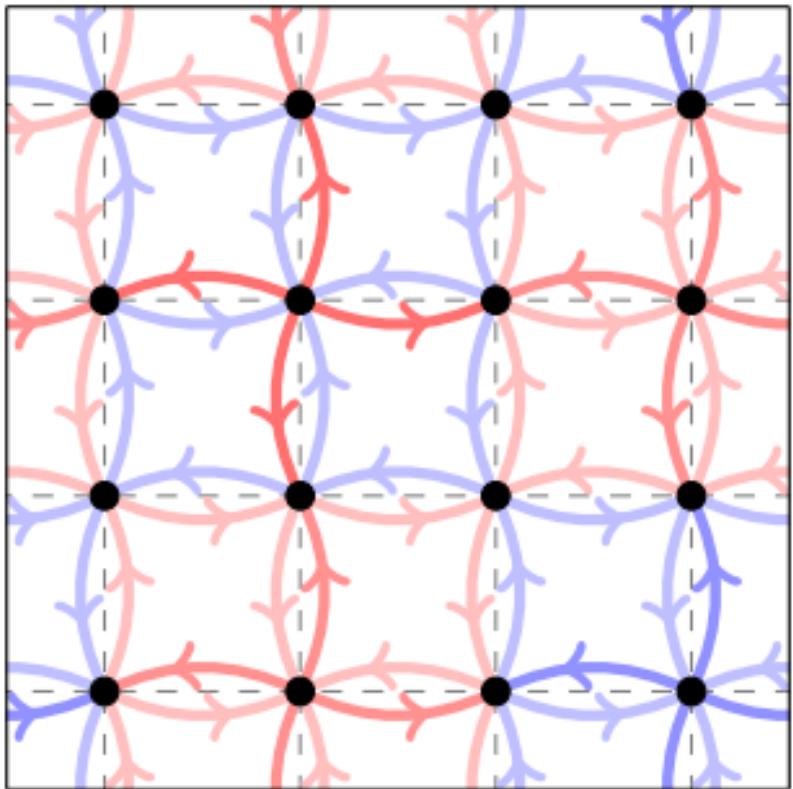
 $t = 3$

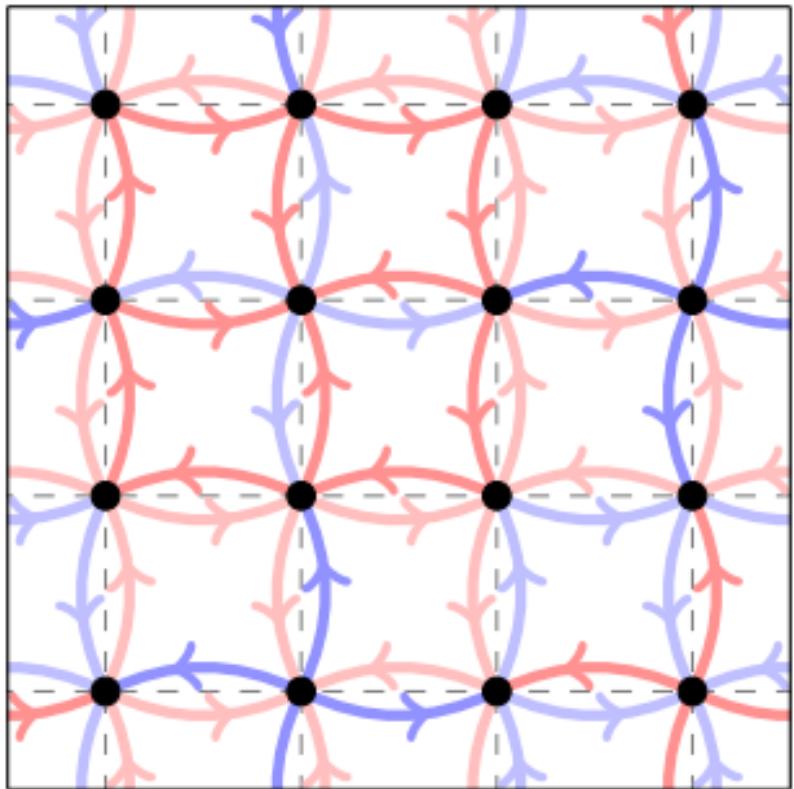

$$t = 4$$

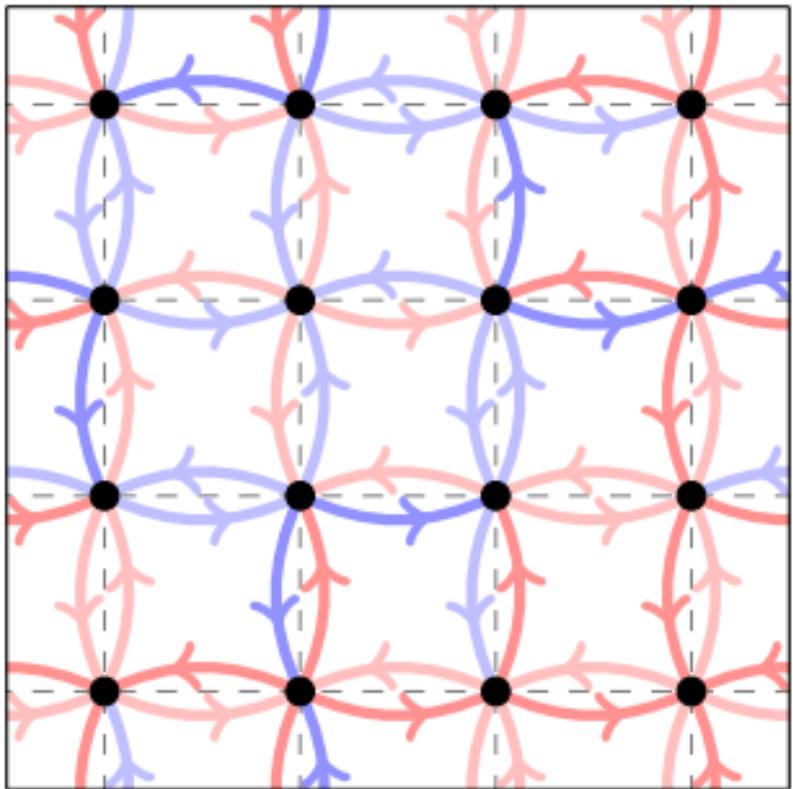
 $t = 5$

 $t = 6$

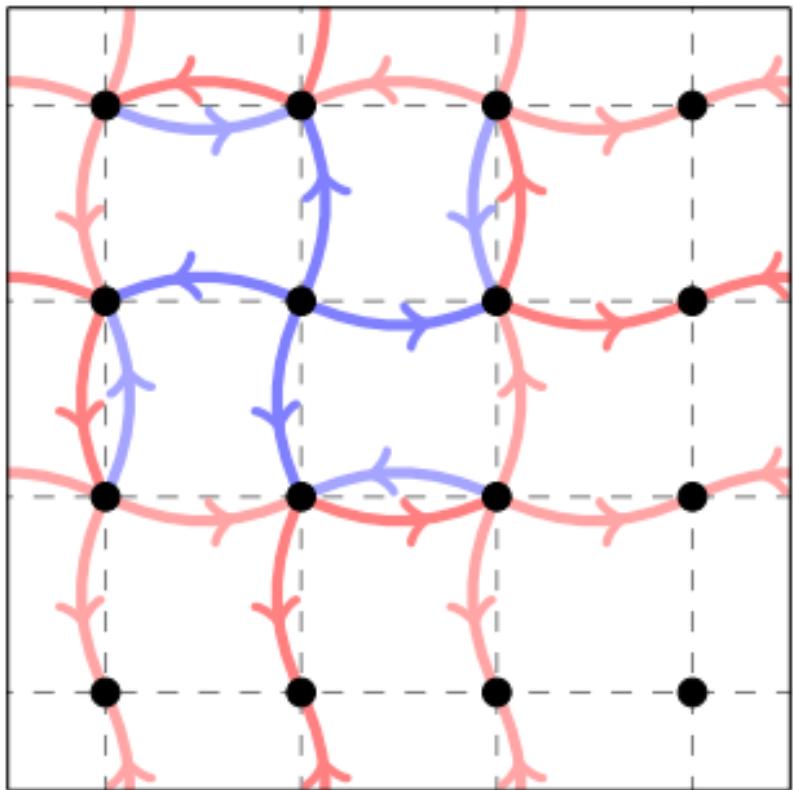
 $t = 7$

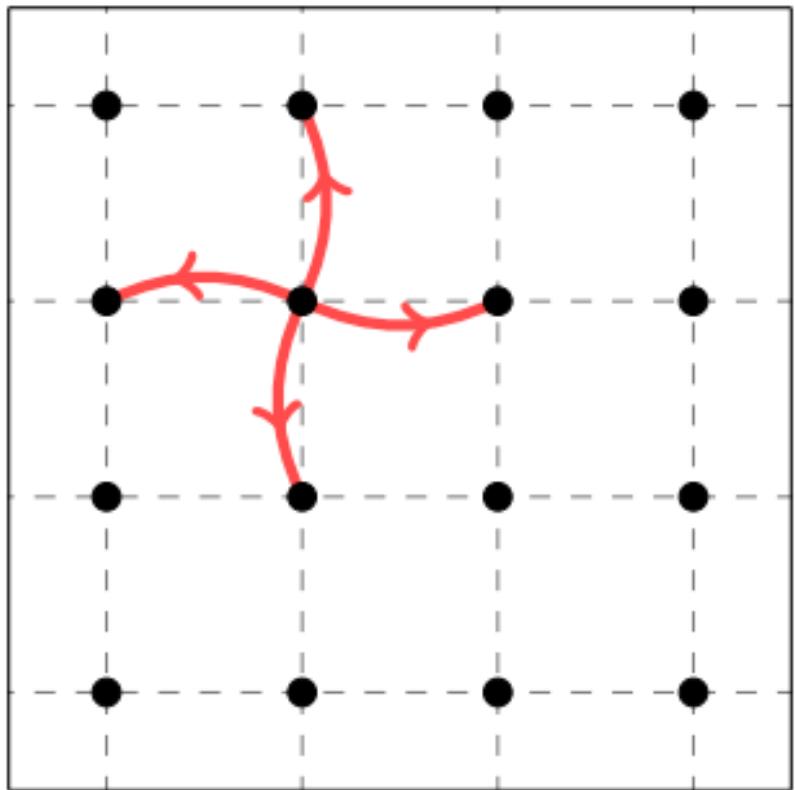
 $t = 8$

 $t = 9$

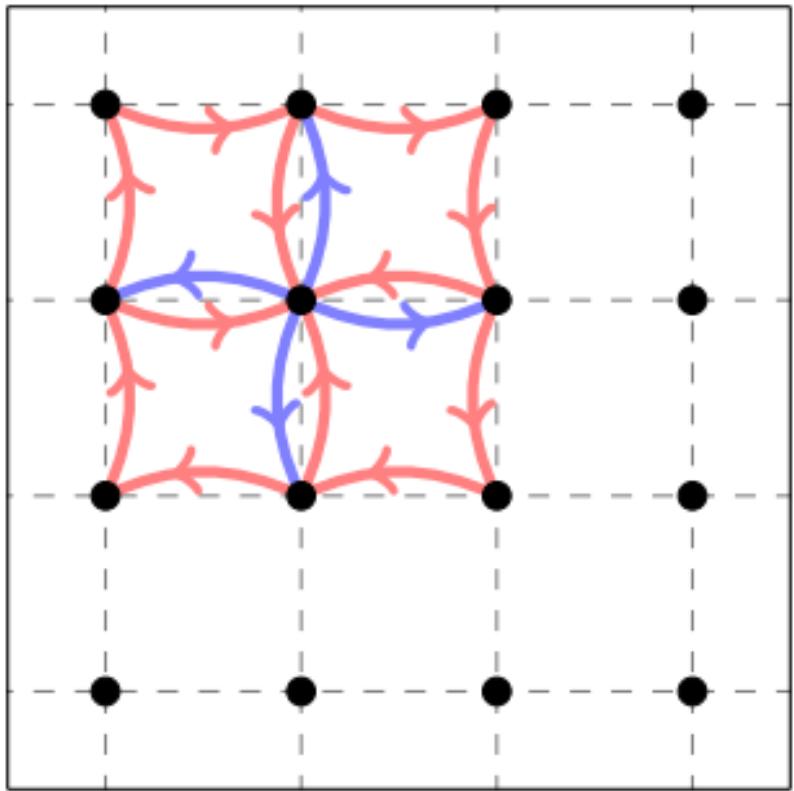


$t = 10$

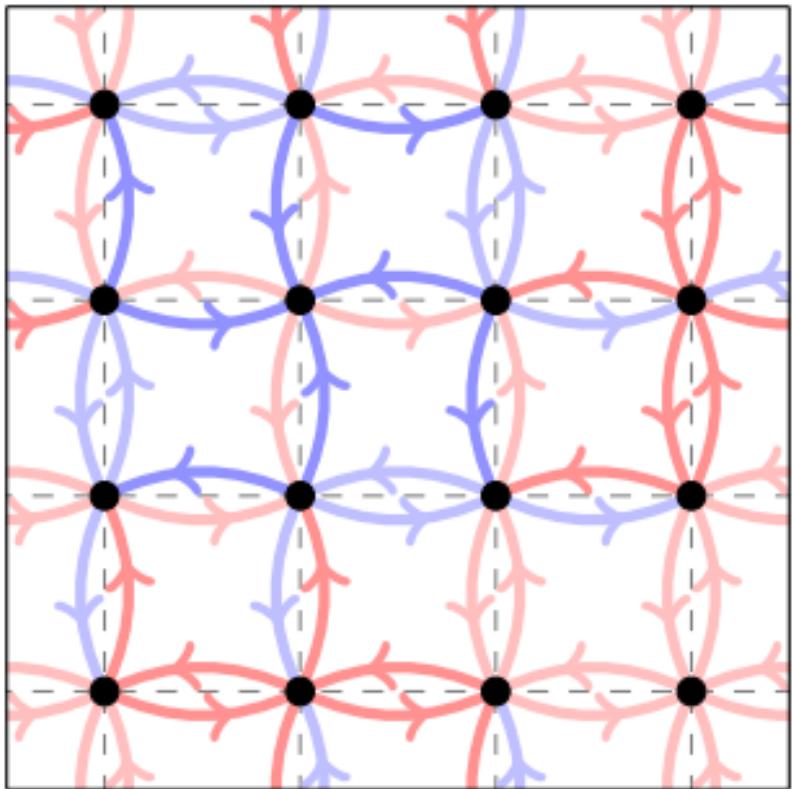
 $t = 11$



$t = 12$



$t = 13$



$t = 14$

State transfer

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Define $B_t = N^T U^t N$.

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State transfer

Perfect state transfer

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Theorem (Guo & Schmeits 2022+)

For any two reflection walk, $B_t = T_t(B_1)$, where T_t is the t th Chebyshev polynomial of the first kind.

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Only the values $s = 1, 2, 6, 12$ appeared in these computations.

Conjecture

Let X be an orientably-regular map, and let U be its transition matrix. If $s > 0$ is such that $U^s = I$ and $U^r \neq I$ for all $r < s$, then $s \in \{1, 2, 6, 12\}$.

Lemma (Guo & Schmeits 2022+)

Let X be a map for which an associated matrix has rational eigenvalues. Assume that $U^\tau = I$ for some $\tau > 1$ and $U^s \neq I$ for all $s < \tau$, then $\tau \in \{2, 3, 4, 6, 12\}$.

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Open problem

What are some topological properties (genus, etc.). which affect the quantum walk?

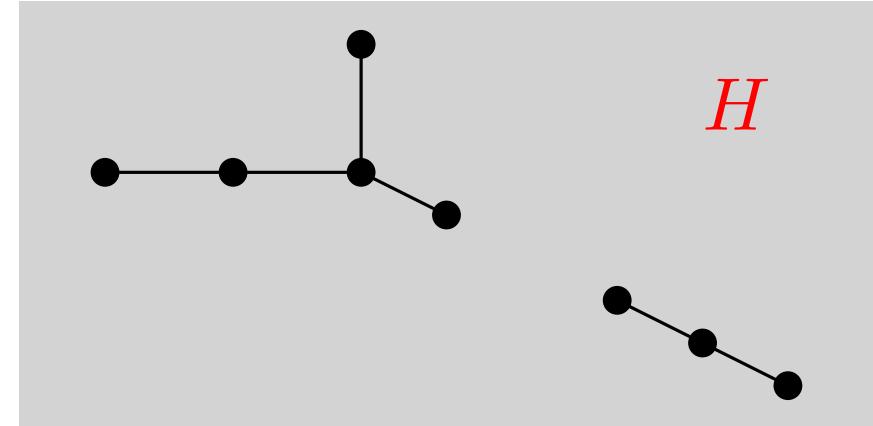
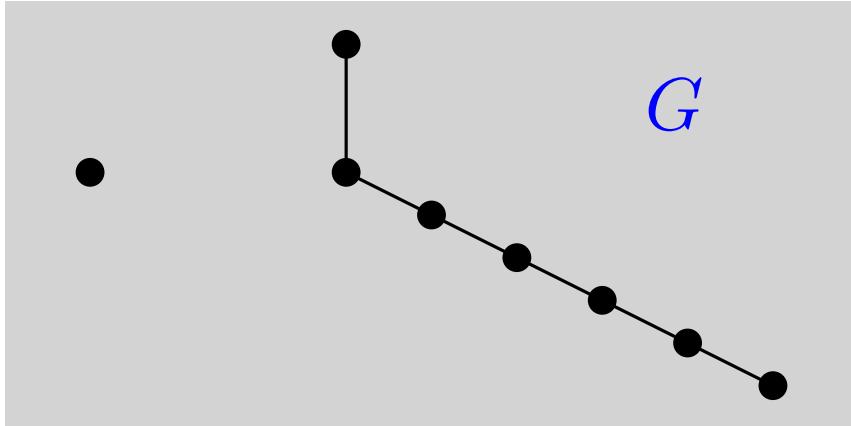
Extensions of cospectrality

Cospectral things

Cospectral graphs: graphs cospectral with respect to the adjacency matrix

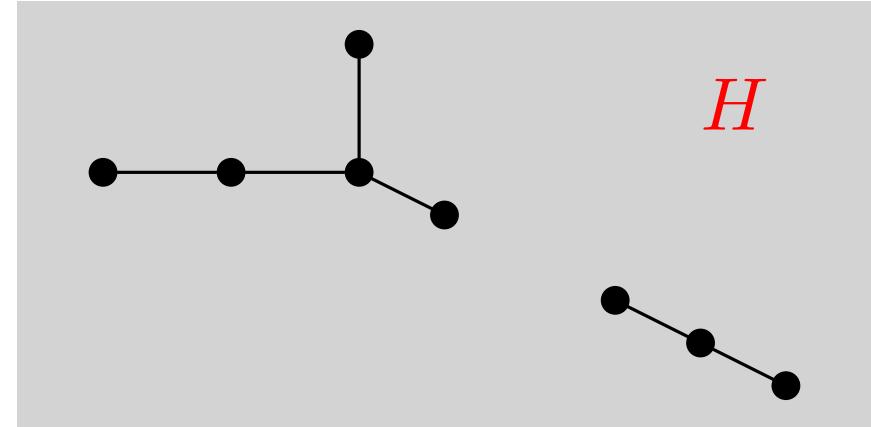
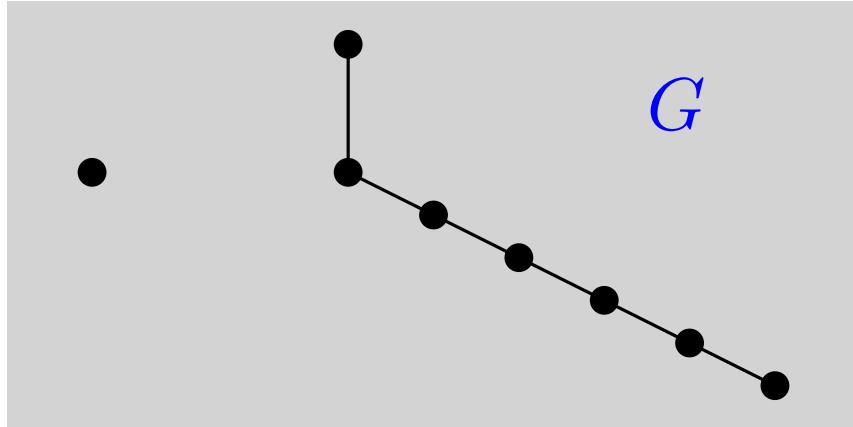
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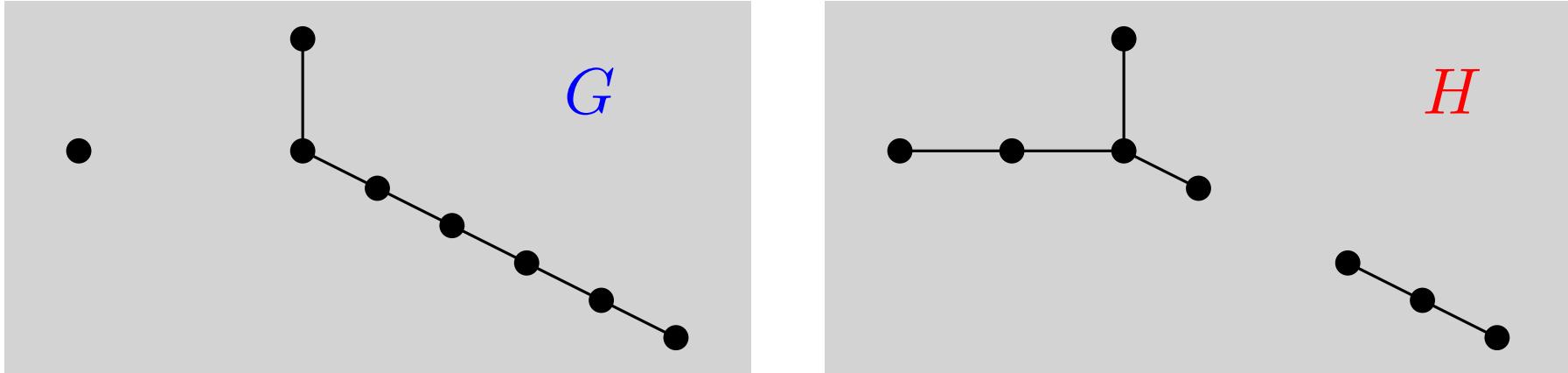
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$$\phi(A(G), x) = \phi(A(H), x)$$

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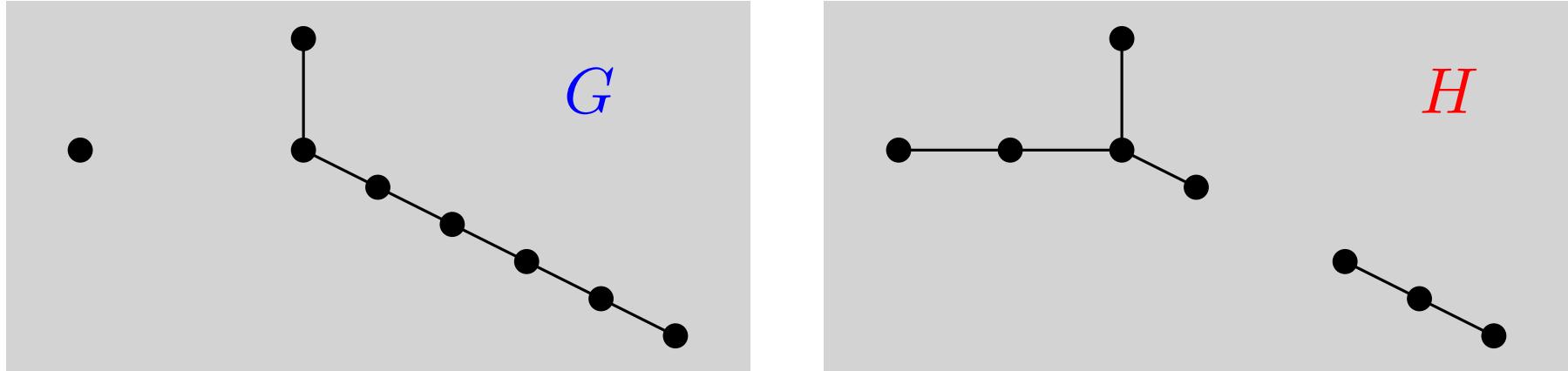
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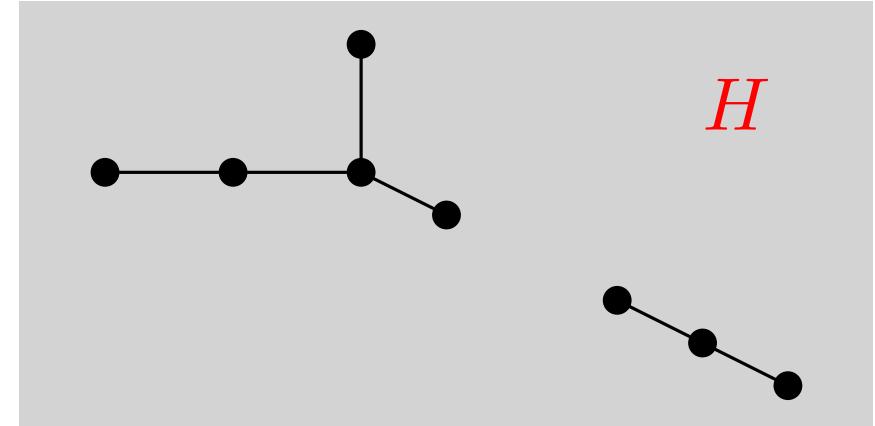
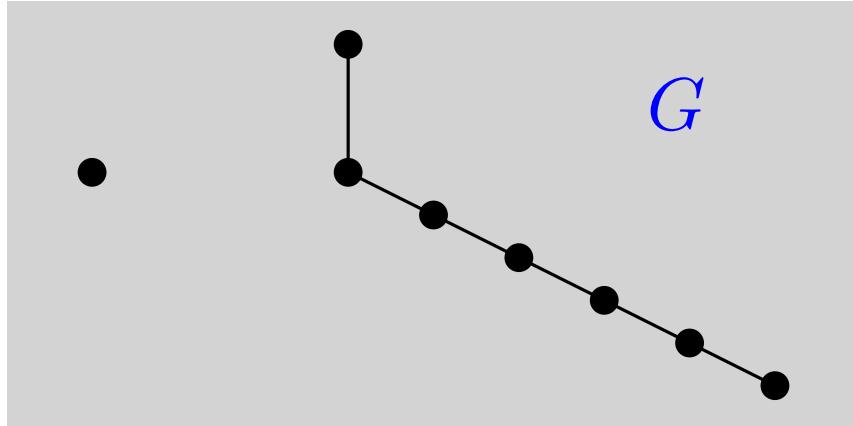


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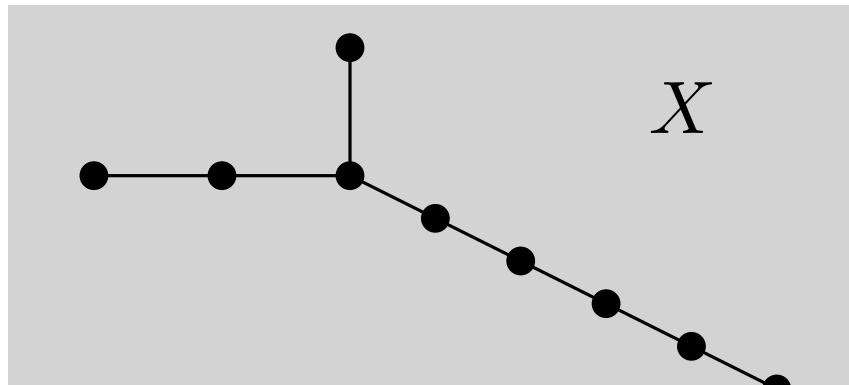
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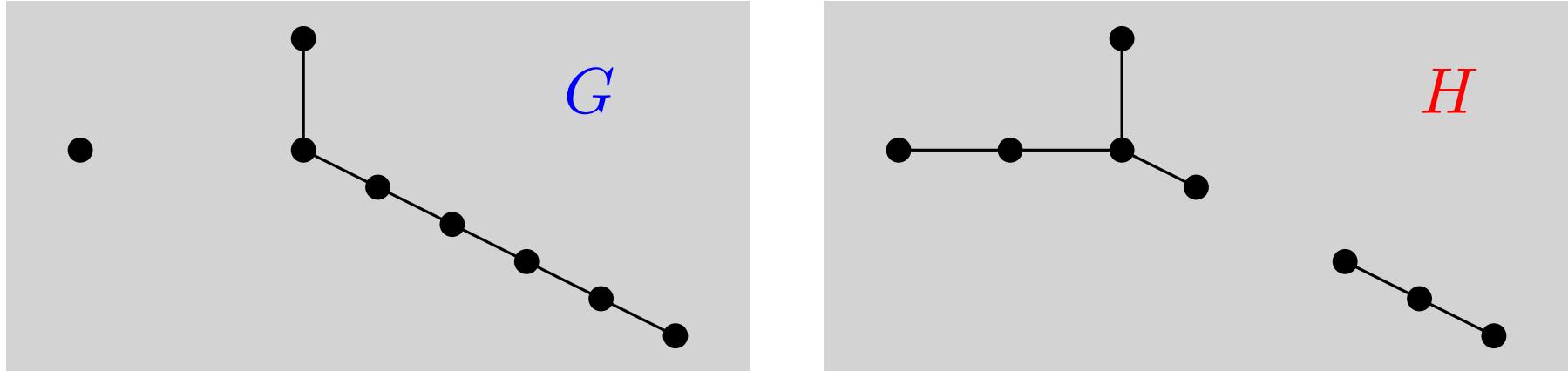
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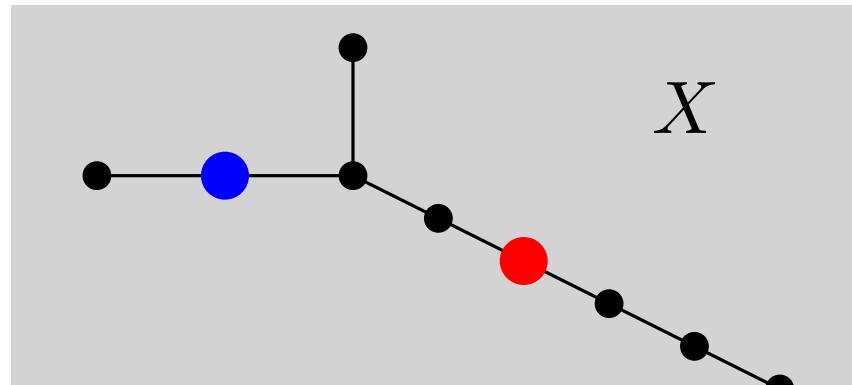
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But this is also given by the (y, y) entry of $A(Y)^k$.

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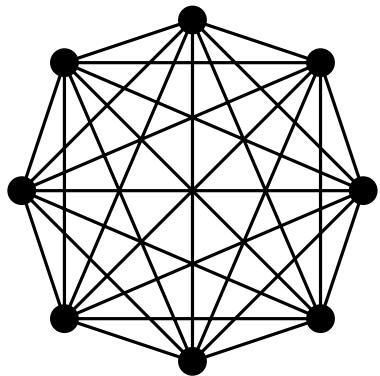
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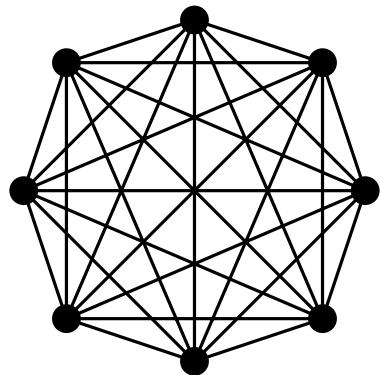
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Non-examples



Complete graph K_n

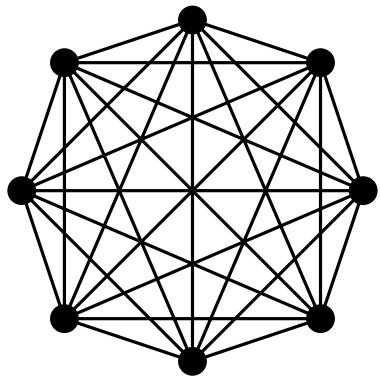
Non-examples



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Every pair of vertices is cospectral.

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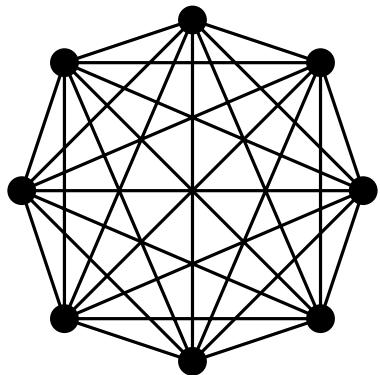


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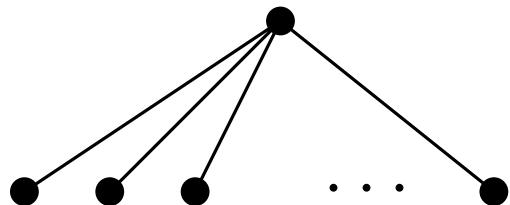
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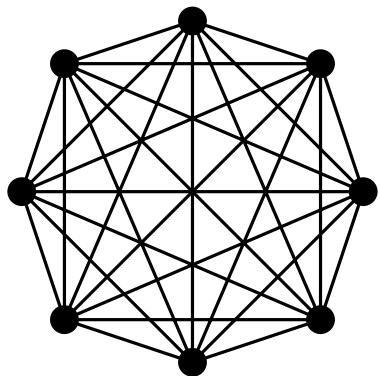
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Star graph $K_{1,n}$

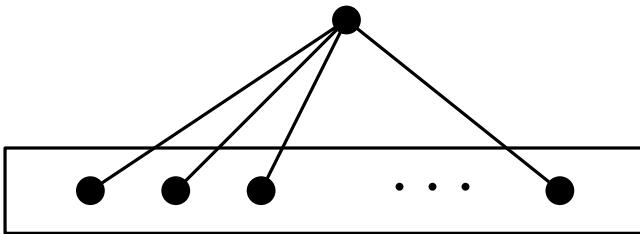
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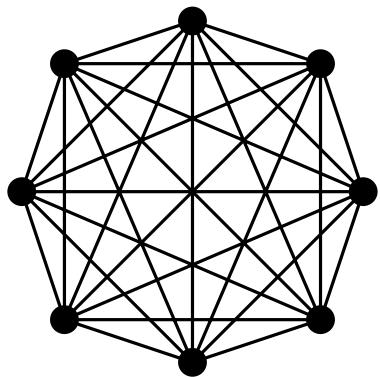
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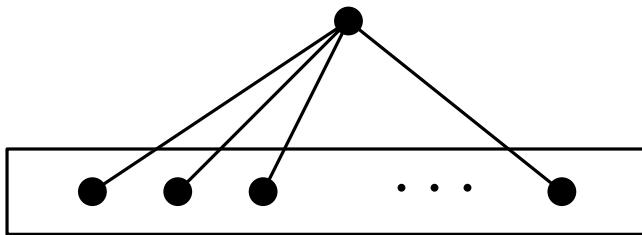


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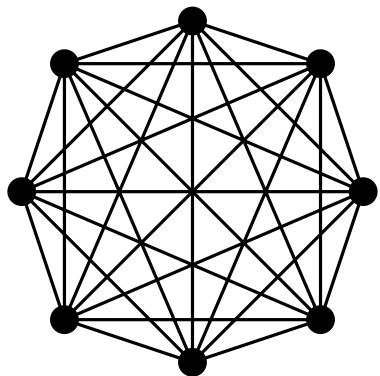
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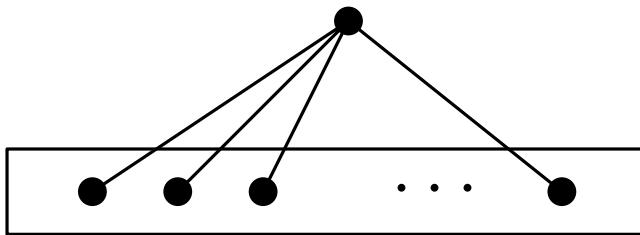
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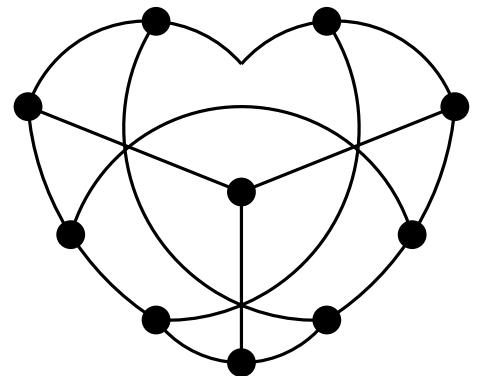
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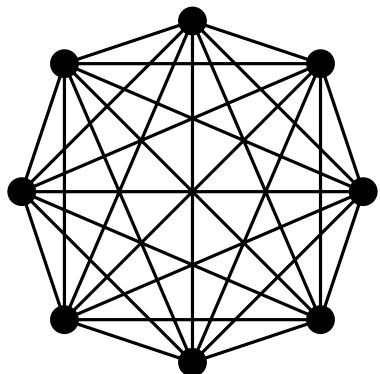


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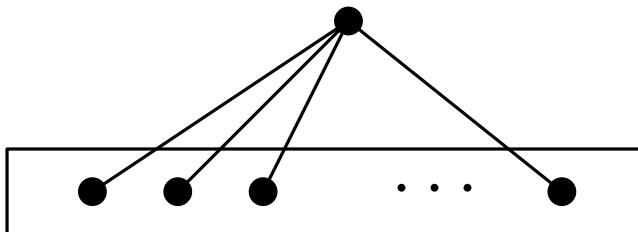
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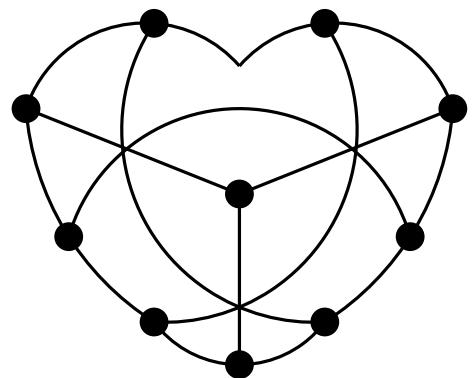
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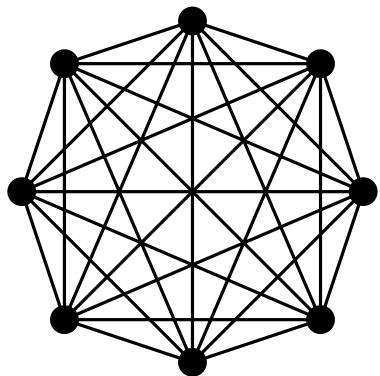
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The Petersen graph

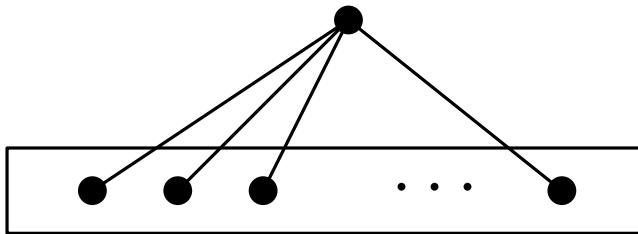
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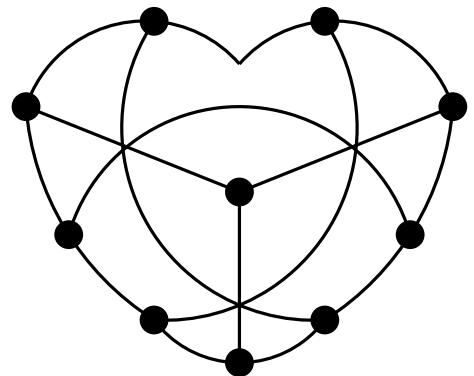
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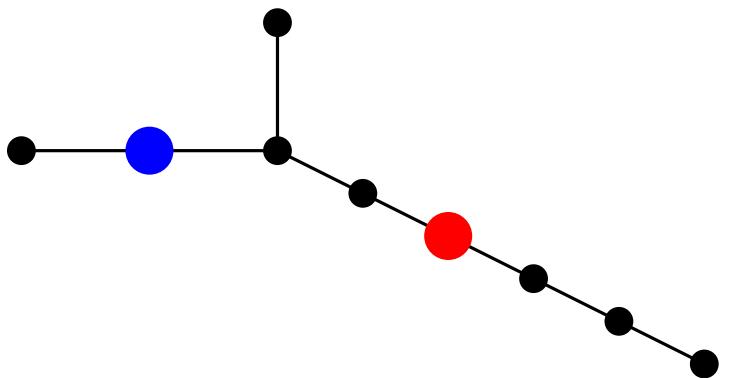


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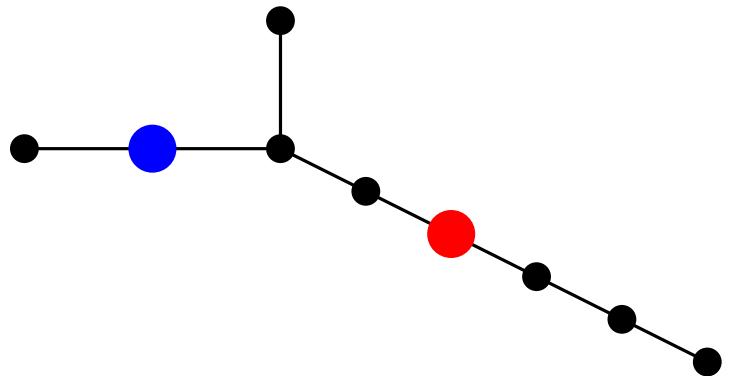
(Any primitive strongly regular graph)

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Examples

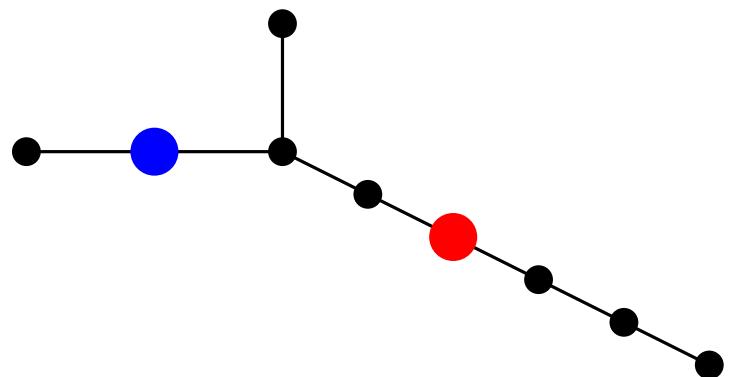


Examples



u, v cospectral and X has simple eigenvalues $\Rightarrow u, v$ strongly cospectral

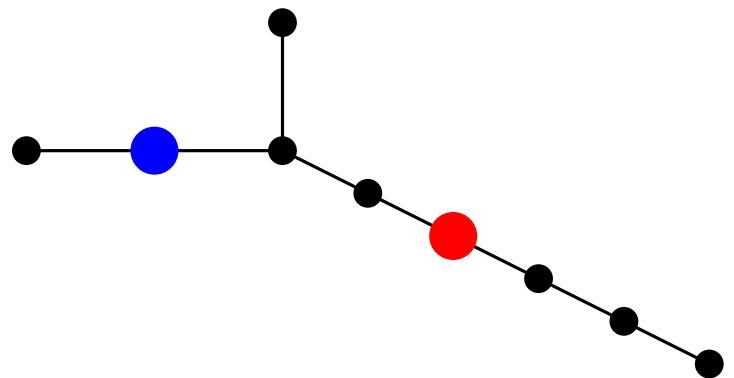
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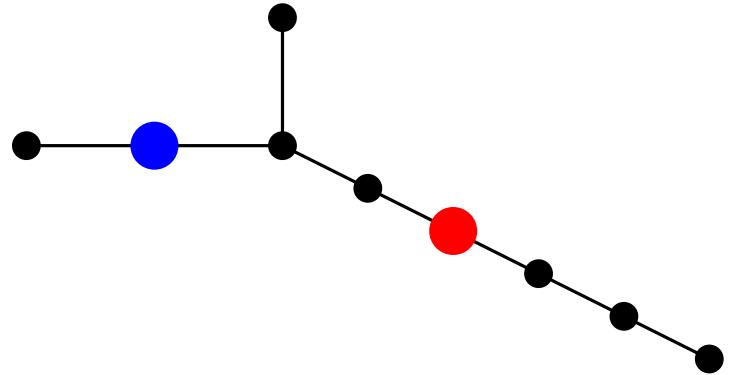
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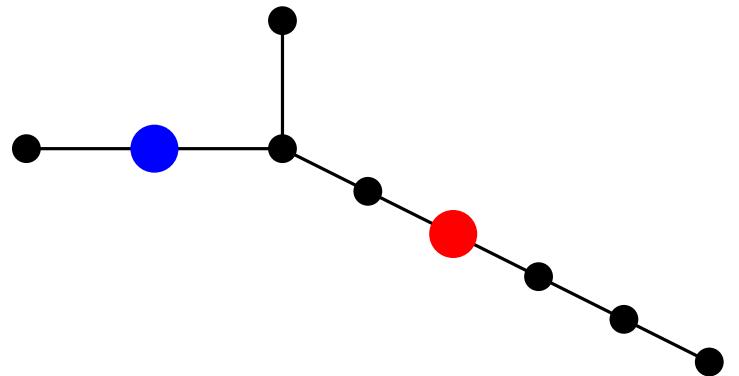
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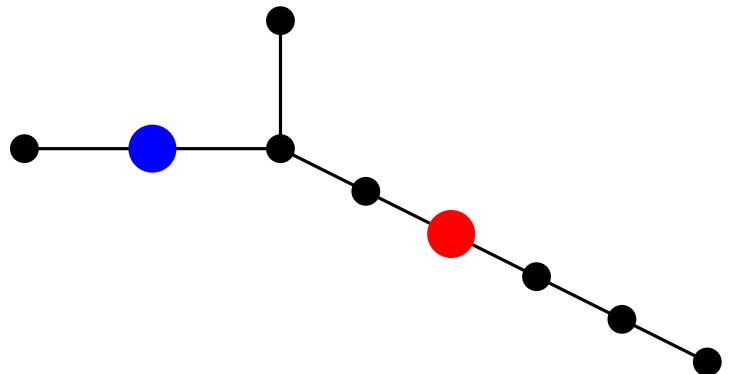
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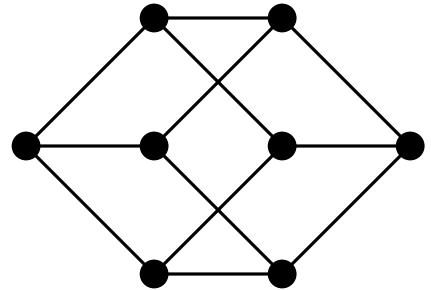
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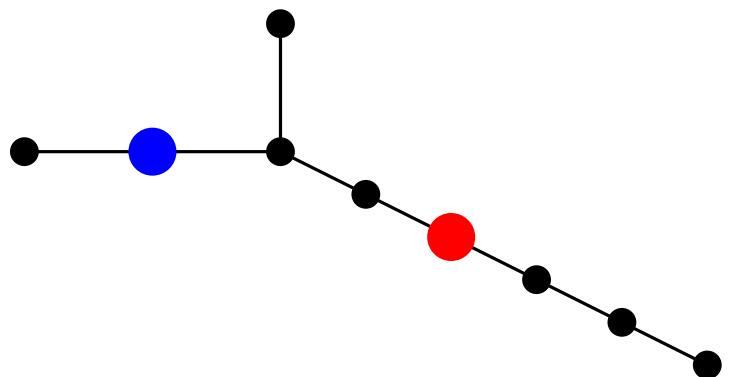
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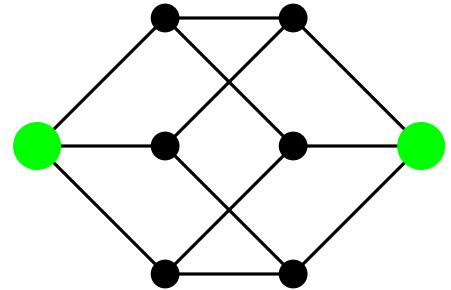
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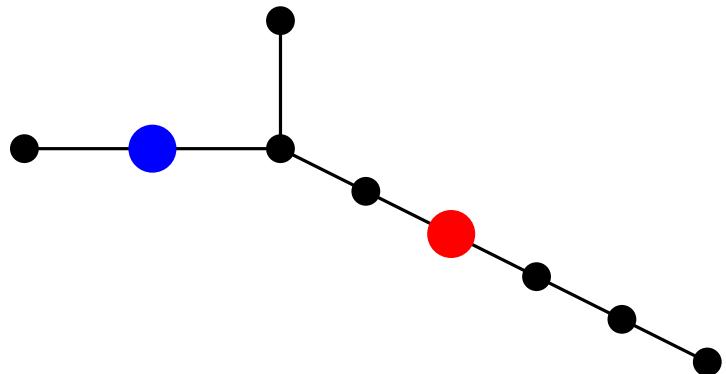


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Antipodal vertices in the hypercube

Examples



u, v cospectral and X has simple eigenvalues $\Rightarrow u, v$ strongly cospectral

Theorem

Suppose B belongs to an association scheme. The following are equivalent.

- (1) there exists x and y strongly cospectral mates w.r.t. B ;
- (2) there exists j such that A_j is a permutation matrix of order two with no fixed points; and
- (3) every $x \in V$ has a strongly cospectral mate with respect to B .

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Theorem (Godsil 2012)

If the continuous-time quantum walk on G admits perfect state transfer from u to v then u, v are strongly cospectral.

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Theorem (Guo & Schmeits 2022+)

If the vertex face quantum walk on G admits perfect state transfer from u to v at time τ then u, v are strongly cospectral with respect B_d for all d divisors of τ . In particular, they are strongly cospectral w.r.t. B_1 .

(Orthogonal) Symmetries of Graphs

Orthogonal symmetries

UvA

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$$Qe_u = Qe_v, \quad Q^2 = I, \quad Q \text{ is a polynomial in } A.$$

Since $AQ = QA$, we can call Q an orthogonal symmetry of the graph.

Orthogonal symmetries

Let X be a graph with adjacency matrix $A = \sum_{r=0}^d \theta_r E_r$.

Vertices u, v in a graph X are **cospectral vertices** if

$$(E_r)_{u,u} = (E_r)_{v,v} \text{ for } r = 0, \dots, d.$$

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In all the examples listed so far, the strongly cospectral vertices come in pairs.

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u

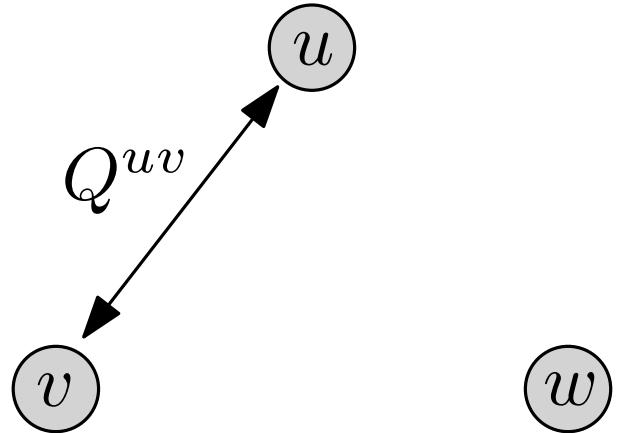
v

w

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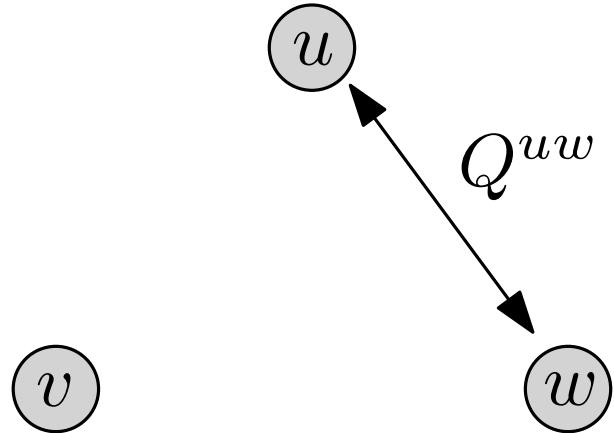
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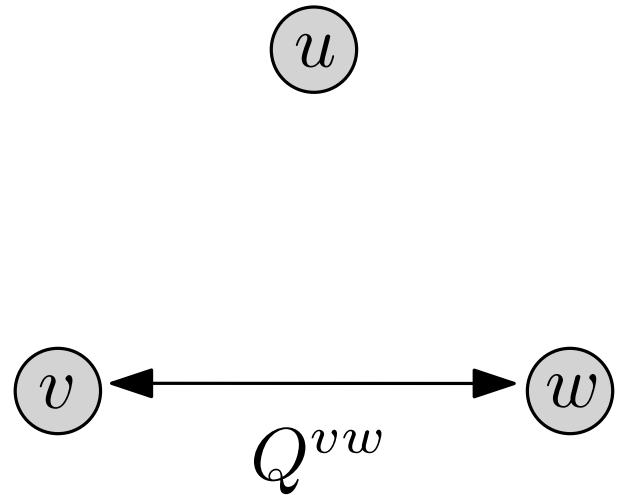
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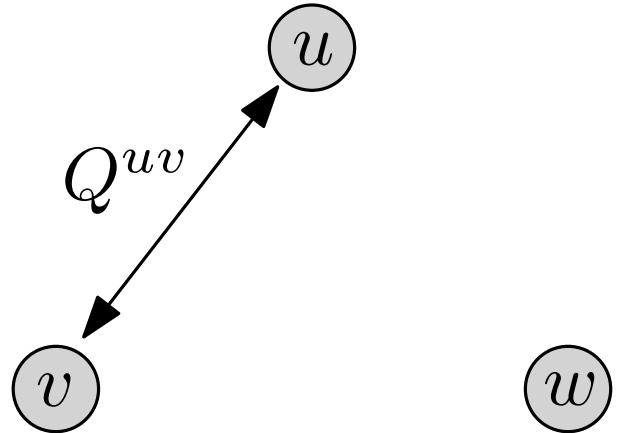
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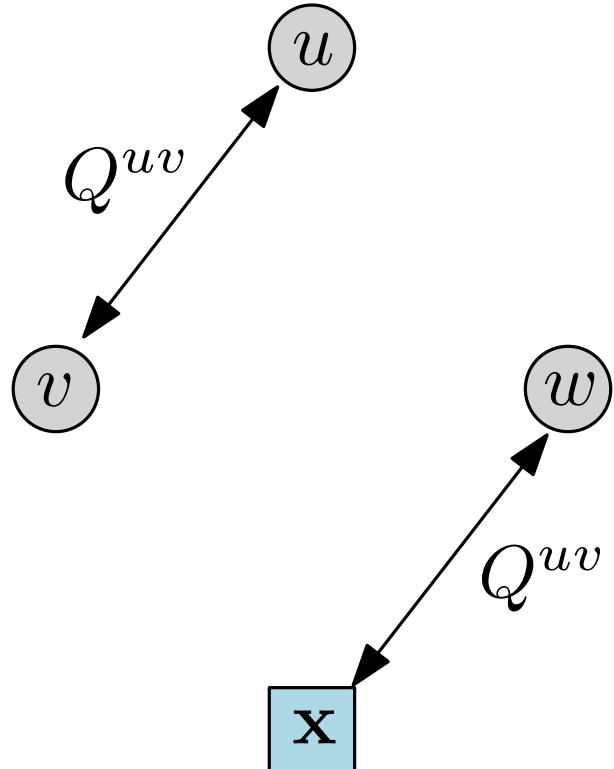


Where does Q^{uv} send e_w ?

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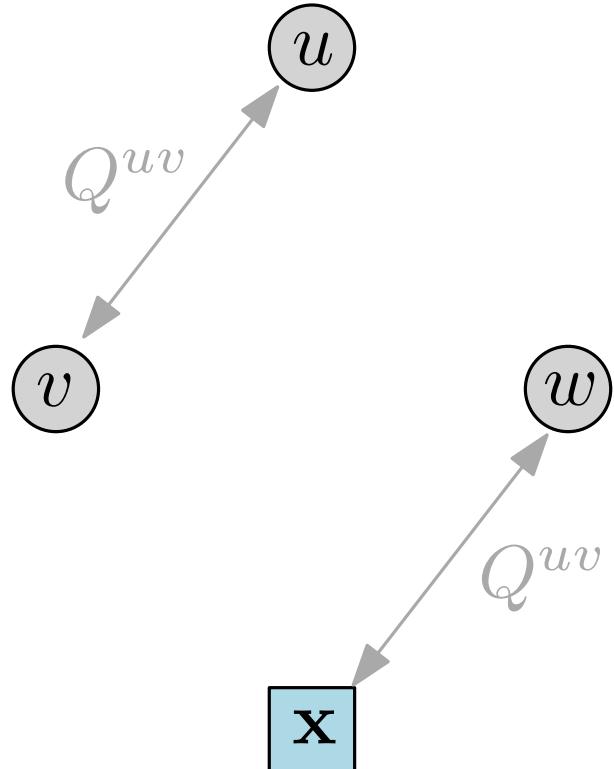


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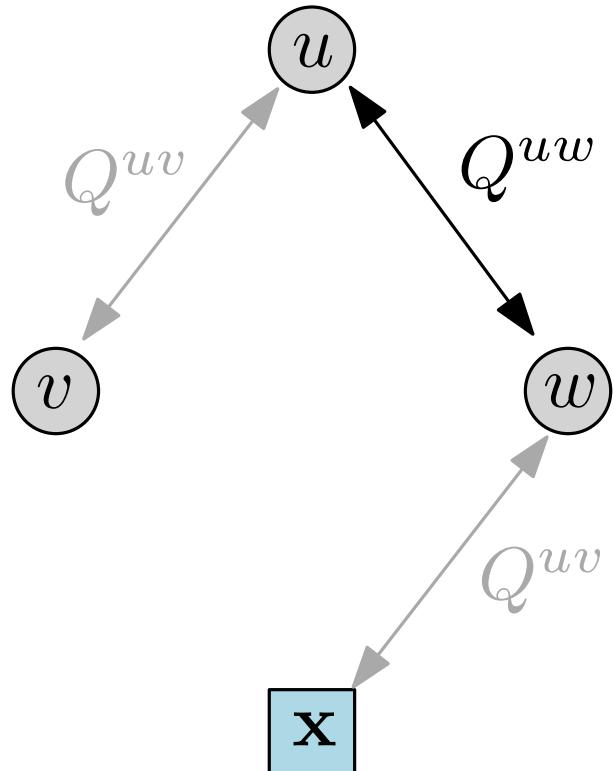
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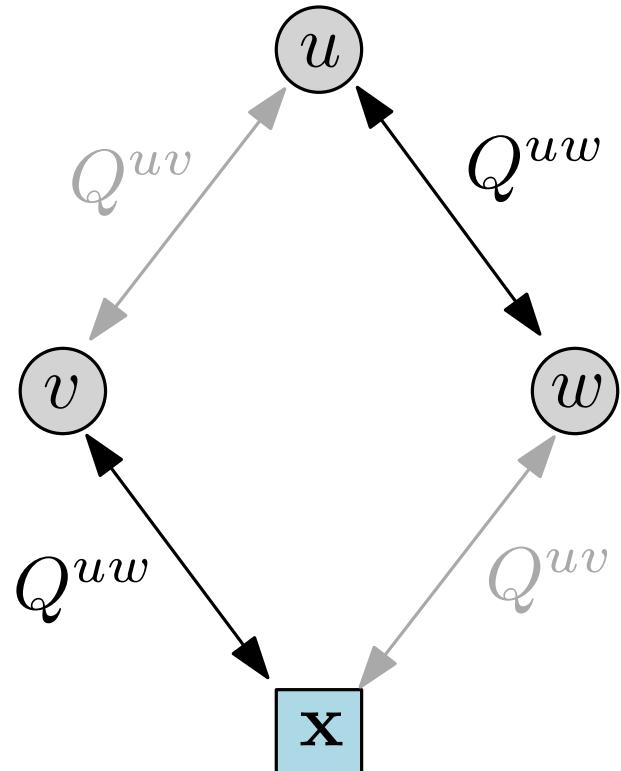
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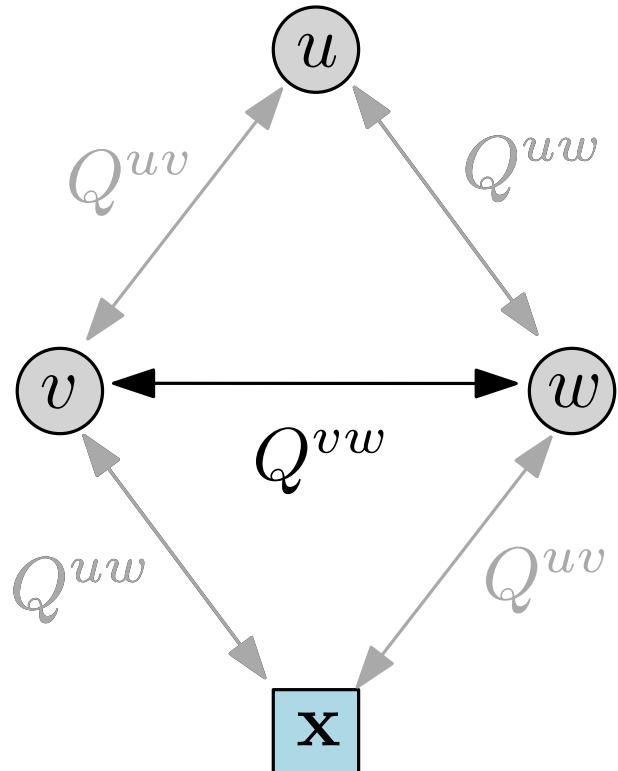
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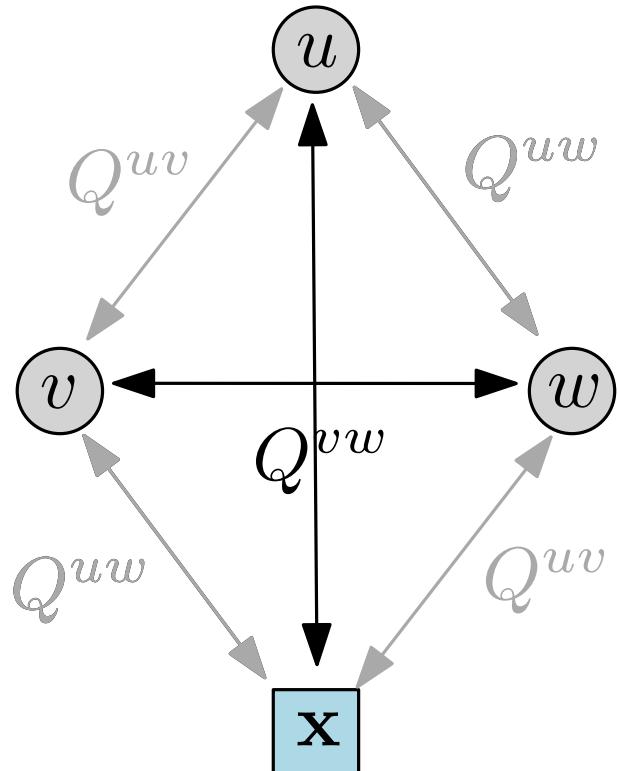
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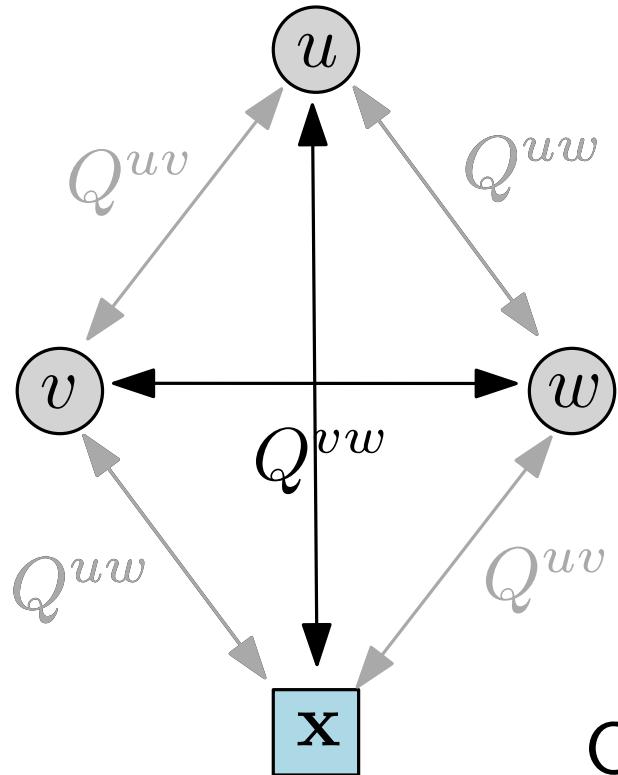
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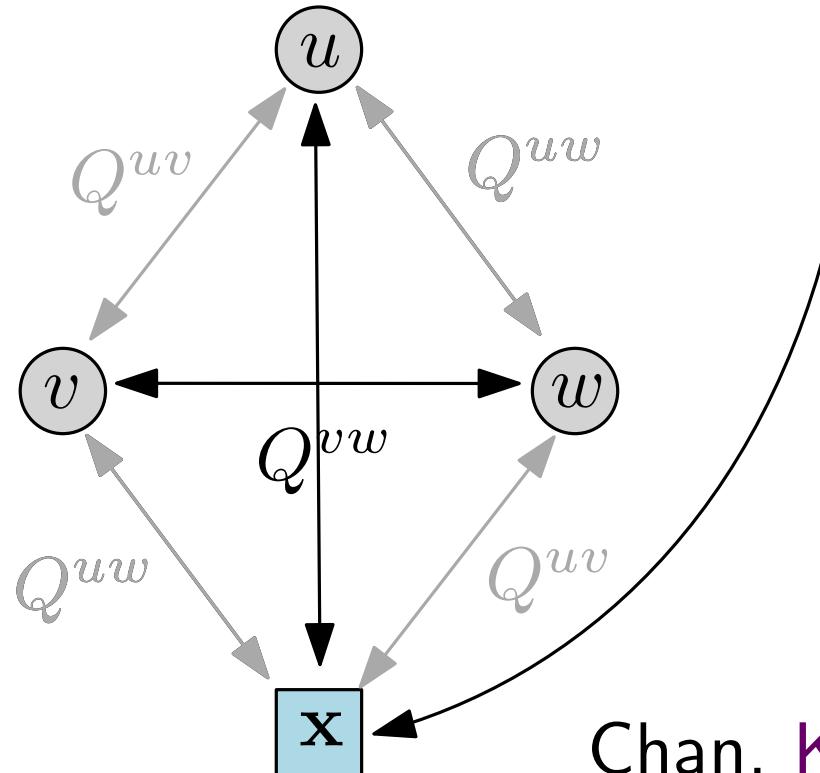


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This vector x is an example of a **phantom mate**.

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Summary

- One can study quantum walks using linear algebraic graph theory and prove properties about the walk using algebraic properties of the graph.

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- One can study quantum walks using linear algebraic graph theory and prove properties about the walk using algebraic properties of the graph.
- In the process of doing this, various new (completely classical) graph properties arise and provide interesting combinatorial problems.

Thanks!

