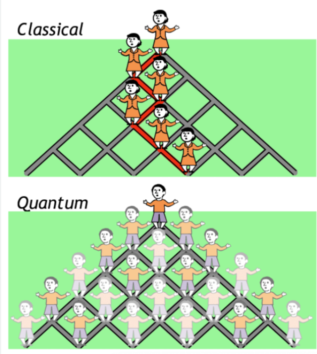
Lecture Topic: Quantum Walks and Quantum Replacements of Monte Carlo Sampling

Quantum (Random) Walks



Introduction to Quantum Walks

- **Quantum walks** form a fundamental concept of quantum mechanics;
- Distinct perspective on random processes compared to their classical counterparts;
- Quantum walks, and algorithms that utilize them, have several important features...

Speedups

- Quantum walks often show quadratic speedups
- Sometimes show exponential speedups (e.g. the Hidden Flat Problem you can find on the lecture notes)
- Quantum walks form a model of universal (quantum) computation

Definitions

- Quantum walk: process on a graph $G = (V, E)$
- V is the set of vertices and E the set of edges of G
- Basis states $|x\rangle$, $x \in V$

In what follows, for simplicity, let $G = \mathbb{Z}$.

Our task is to find a “rule” as to evolve a quantum state labeled by its position to some other (neighboring) position.

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The “naive” unitaries

Consider $U \in U(N)$ such that

$$\begin{aligned} U : \mathcal{H}_G &\to \mathcal{H}_G \\ |x\rangle &\mapsto a|x-1\rangle + b|x\rangle + c|x+1\rangle \end{aligned} \tag{1.1}$$

which conveys the information for the potential that $|x\rangle$

1. moves left with some amplitude $a \in \mathbb{C}$,
2. stays at the same place with amplitude $b \in \mathbb{C}$,
3. moves right with amplitude $c \in \mathbb{C}$.

Consistency

The quantum walk process needs exhibit **consistent behavior across all vertices**:

That is, a, b and c should be independent of $x \in V$ (similarly to how the probabilities of moving left/right are independent of x in the classical random walk). Unfortunately, this definition does not work.

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The coin space

Solution: additional "coin" space: $|i, x\rangle$ for $i \in \{0, 1\}$, $x \in \mathbb{Z}$, with Hilbert spaces $\mathcal{H}_{\mathrm{C}}, \mathcal{H}_{\mathrm{W}}$. At each step, we perform two unitary operations:

(1) A **coin flip** operation $C : \mathcal{H}_{\mathrm{C}} \to \mathcal{H}_{\mathrm{C}}$ which "puts" the walker in superposition, so it walks all possible paths simultaneously.

(2) Followed by a **shift** operation $S : \mathcal{H}_{\mathrm{W}} \to \mathcal{H}_{\mathrm{W}}$ the operator responsible for the actual walk on G.

$$C|i, x\rangle = \begin{cases} a|0, x\rangle + b|1, x\rangle & \text{if } i = 0, \\ c|0, x\rangle + d|1, x\rangle & \text{if } i = 1. \end{cases} \tag{1.2}$$

$$S|i, x\rangle = \begin{cases} |0, x+1\rangle & \text{if } i = 0, \\ |1, x-1\rangle & \text{if } i = 1. \end{cases} \tag{1.3}$$

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Hadamard walker

If we choose for C the Hadamard matrix:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{1.4}$$

we have a 'Hadamard walker" while S can be explicitly described as follows:

$$S = \left(|0\rangle\langle 0| \otimes \sum_{x=-\infty}^{\infty} |x+1\rangle\langle x| \right) + \left(|1\rangle\langle 1| \otimes \sum_{x=-\infty}^{\infty} |x-1\rangle\langle x| \right). \tag{1.5}$$

The walker's unitary step and asymmetry

A *step of a quantum walk* amounts to the unitary $U = SC \in U(N)$.

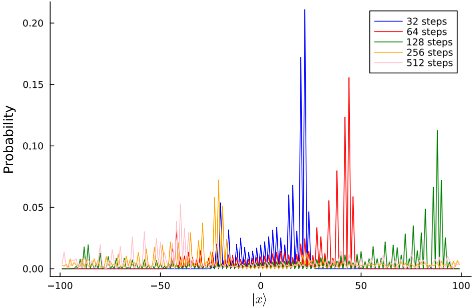

Figure: Probability distribution of quantum walk, starting at $|+, 0\rangle$, after different numbers of steps.

Bias

The quantum walker's initial state is the product of the coin state and the position state.

The former state, $|i\rangle$, controls the direction in which the walker moves. Therefore, the choice of coin operator leads to vastly different constructive and destructive interference patterns.

This behavior is in stark contrast to a classical random walk, where the walker has equal probability of moving left or right at each step, and there is no preference or bias for either direction. The **bias** in a quantum walk is a unique characteristic of the underlying physics.

Example $G = \mathbb{Z}$

Example in a bounded subset of the integer line with $C = H$. It is common to assume that the walker starts at position $x = 0$ with the coin state being the $|0\rangle$ or $|1\rangle$ state.

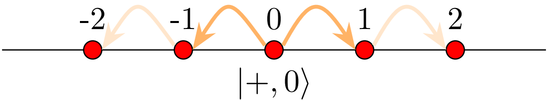

Figure: Beginning a quantum walk, after the coin operator has been applied, at $|+, 0\rangle$, by applying $C = H$ on $|0, 0\rangle$, on the $\mathbb{Z}$-line.

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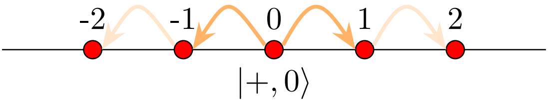

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For ease of notation, we denote the r-th application of the quantum walk operator U by $U^{(r)}|\psi_{r-1}\rangle$.

The quantum walk amounts to the following set of operations:

- Select coin operator $C = H$
- Initialize the state (position of the walker): $|\mathbf{0}\rangle = |0\rangle_{\mathrm{C}} \otimes |0\rangle_{\mathrm{W}} = |0,0\rangle$ (or $|1,0\rangle$)
- for $r \in \mathbb{N}$ repeat $U^r|\mathbf{0}\rangle$ as:
  - Apply the coin operator: $C|\mathbf{0}\rangle$
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Therefore, the initial state is $|\mathbf{0}\rangle \equiv |\psi_0\rangle$ and we obtain

$$|\psi_1\rangle = \frac{|0,-1\rangle + |0,1\rangle}{\sqrt{2}} \tag{1.6}$$

$$|\psi_2\rangle = \frac{|0,-2\rangle + |1,0\rangle + |0,0\rangle - |1,2\rangle}{2} \tag{1.7}$$

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This state is not symmetric around the origin and the probability distributions will not be centered at the origin. This is clear from Fig. 1.1. As a matter of fact the standard deviation of the walker, after r iterations of U is:

$$\sigma(r) \approx 0.54r \tag{1.9}$$

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Standard deviation

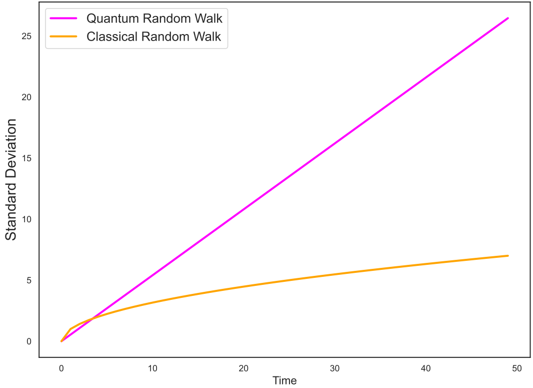

Figure: The standard deviation of a classical versus quantum walk as a function of the steps.

Balistic behavior of the quantum walker

Often we say that the quantum walkers showcase a **ballistic bheaviour**;

the rapid, linear spread of the probability distribution of the quantum walker's position over time, contrasting sharply with the slower, diffusive spreading observed in classical random walks.

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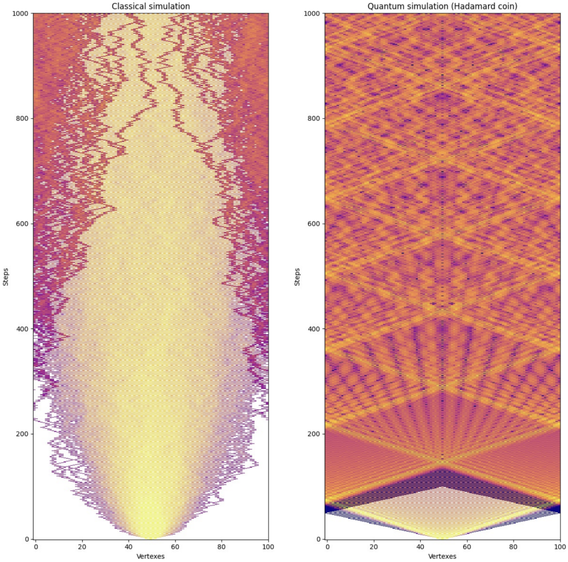
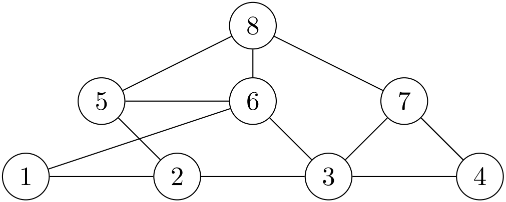
The walker's efficiency



Quantum Walks Graphs

Quantum Walk on a Complete Graph



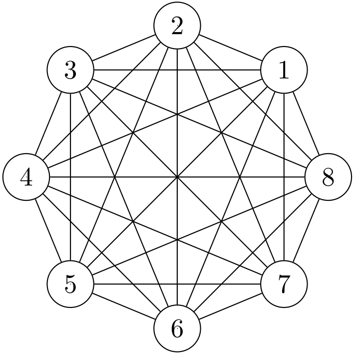


Figure: An asymmetric non-complete graph $G = (8, 10)$ and its symmetric completion $\overline{G} = K_8$.

Example $G = K_4$

Easy-to-work-with graph, the complete graph K_4 with 4 vertices and 6 edges and perform such *search*.

Let us commence with a classical random walk on K_4 wherein we are looking to "find" the marked vertex $\#2$ (but we do not know it). In the Fig. next we display the success probability after 1 and 2 steps.

Classical walk on $G = K_4$

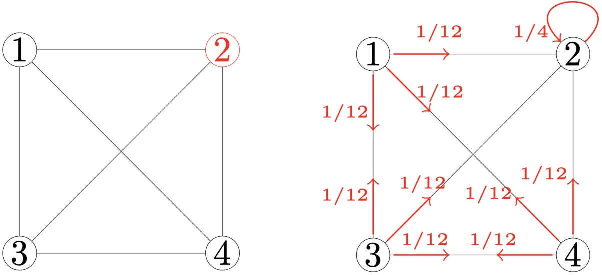
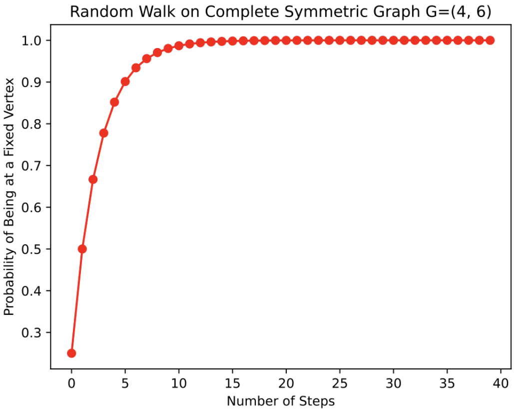


Figure: Left: At step 1 the probability that the walker "lands" on vertex #2 is 1/4. Right: At step 2 the probability that the walker "lands" on vertex #2 is 1/2. The loop in vertex #2 denotes that this vertex is a trap: it allows us to know the walker landed on the marked vertex and the walker is not allowed to attain any other state.

Success Probability

Overall, the trend for the success probability continues, and we observe the behavior of the walker. For large N, the success probability of $1/2$ is reached after $\mathcal{O}(N)$ steps.



Quantum Grover Walks on K_4

We have to implement the coin and shift operators. Diagrammatically at step 0 we are back at the initial state of the classical walk. In total we have 12 amplitudes to consider;

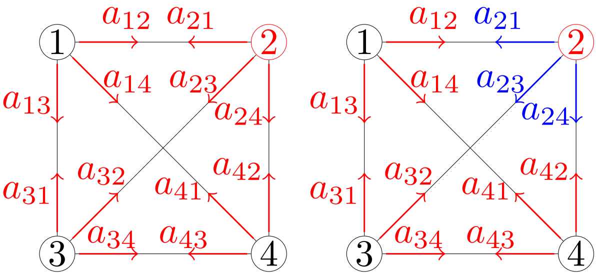


Figure: Left: the state of the quantum walk is a superposition of the amplitudes $a_{ij} \in \mathbb{C}$, for all $i, j \in V(K_4)$. Once the oracle is applied the marked state's amplitudes obtain a negative sign (marked with blue and in analogy with Grover's operator).

Quantum Grover Walks on K_4

Initially, we have $a_{ij} = \frac{1}{\sqrt{12}}$ for all i, j.

Then, the coin flip operator C, which here is taken to be Grover's diffusion operator, amounts to marking the state we look for, assigning a negative sign to the corresponding amplitudes. The marking is done by assuming access to an oracle O (essentially the same oracle found in Grover's operator) that is able to perform this operation. Then, it changes the direction of adjacent red-blue pair vertices.

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Quantum Grover Walks on K_4

Then S reverses the amplitude values along their mean at each vertex. For example, the mean of the vertex #1 after application of C is

$$\mu_{12} = \frac{a_{21} + a_{13} + a_{14}}{3}. \tag{1.10}$$

Therefore, S amounts to a map $S : a_{ij} \mapsto a'_{ij} = \mu_{12} - a_{ij}$, for the three pairs $\{21, 13, 14\}$. Of course, this is applied to all amplitudes for all vertices.

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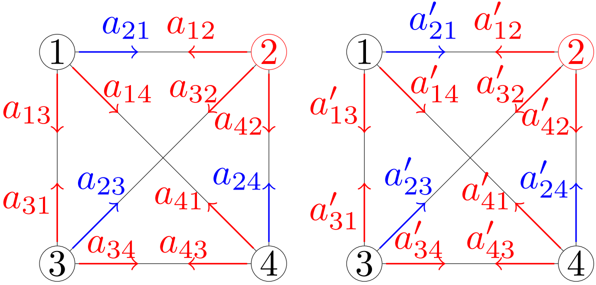

Figure: Left: Coin operator is applied and reverses the relevant amplitudes. The shift operator reverses these amplitudes along their means.

Quantum Grover Walks on K_4

In the second step, we already get the amplitude asymmetry resulting from the oracle flipping the signs of the marked vertex followed by C and then S. As a result, one observes that:

$$\text{probability of success at step 1} = \frac{11}{108} \approx 0.1 \tag{1.11}$$

$$\text{probability of success at step 2} = \frac{25}{36} \approx 0.7 \tag{1.12}$$

$$\text{probability of success at step 3} = \ldots \tag{1.13}$$

Quantum Grover Walks on K_4

Overall, for a large number of vertices N, the probability that the walker lands on the marked vertex is $1/2$ is given after $\pi\sqrt{N}$ steps and therefore the run-time is $\mathcal{O}(\sqrt{N})$. This marks another example in which quantum walks portray a quadratic speedup over classical random walks.

Szegedy Walks

Szegedy Walks

Consider an undirected and unweighted graph G. Szegedy's quantum walk occurs on the edges of the bipartite double cover of the original graph.

If the original graph is G, then its bipartite double cover is the graph tensor product $G \times K_2$ which duplicates the vertices into two partite sets X and Y.

A vertex in X is connected to a vertex in Y if and only if they are connected in the original graph;

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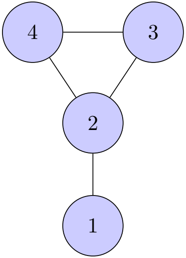

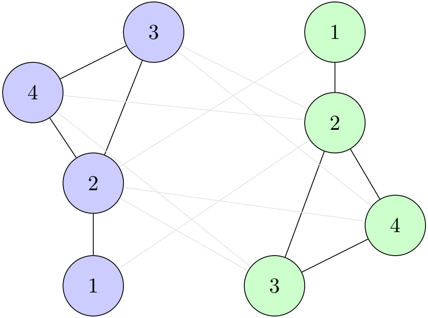

Figure: Left: A graph G. Right: The bipartite double cover of G. The double cover contains double the number of edges.

Szegedy Walks

The Hilbert space of a Szegedy walk: $\mathbb{C}^{2|E|}$.

Let us denote a walker on the edge connecting $x \in X$ with $y \in Y$ as $|x, y\rangle$. Then the computational basis is:

$$|x, y\rangle, \qquad x \in X, y \in Y, x \sim y \tag{1.14}$$

where $x \sim y$ denotes that the vertices x and y are adjacent.

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Szegedy Walks

Szegedy's walk is defined by repeated applications of the unitary

$$U = R_2 R_1, \tag{1.15}$$

where

$$R_1 = 2 \sum_{x \in X} |\phi_x\rangle \langle \phi_x| - \mathbf{1} \tag{1.16}$$

$$R_2 = 2 \sum_{y \in Y} |\psi_y\rangle \langle \psi_y| - \mathbf{1}, \tag{1.17}$$

are reflection operators and

$$|\phi_x\rangle = \frac{1}{\sqrt{\deg(x)}} \sum_{y \sim x} |x, y\rangle \tag{1.18}$$

$$|\psi_y\rangle = \frac{1}{\sqrt{\deg(y)}} \sum_{x \sim y} |x, y\rangle \tag{1.19}$$

Szegedy Walks

Before:

- $\deg(x)$ is the degree of vertex x
- $y \sim x$ denotes the sums over the neighbors of x

Observe that $|\phi_x\rangle$ is the equal superposition of edges incident to $x \in X$, and $|\psi_y\rangle$ is the equal superposition of edges incident to $y \in Y$.

Here, there is an equivalent of the "inversion about the mean" operation of Grover's algorithm, which we also saw previously in the context of walks over K_4. The reflection R_1 goes through each vertex in X and reflects the amplitude of its incident edges about their average amplitude, and R_2 similarly does this for the vertices in Y.

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Szegedy Walks

Classically: search for a marked vertex on G amounts to randomly walks until a marked vertex is found (then walker freezes)

Quantumly: Szegedy's quantum walk searches by quantizing this random walk with absorbing vertices and the resulting bipartite double cover. Search is performed by repeatedly applying the unitary

$$\widetilde{U} = \widetilde{R}_2 \widetilde{R}_1, \tag{1.20}$$

where the tilde distinguishes in that we are searching for absorbing vertices. At unmarked vertices they act as $\widetilde{R}_j = R_j$ simply by inverting the amplitudes of the edges around their average at each vertex. At the marked vertices, similarly to the K_4 case, they act by flipping the signs of the amplitudes of all incident edges. A similar search can be performed using Grover's diffusion operator.

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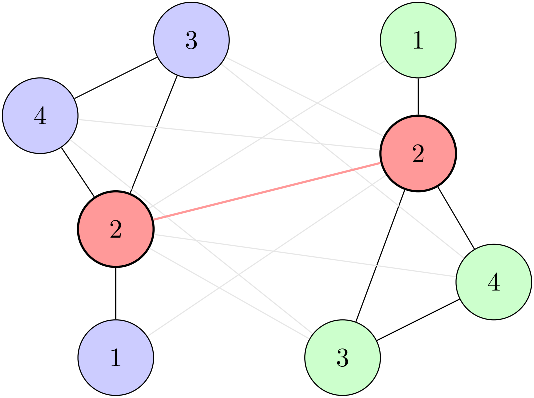

Figure: The marked state corresponds to vertex #2 which is an absorbing vertex: $\langle 2_Y | 2_X \rangle = \langle 2_X | 2_Y \rangle = 0$.

Continuous-time Quantum Walks

Continuous-time Quantum Walks

Continuous-time random walk but **quantum**..

Will allow us later to understand the **universality of quantum walks**.

Continuous-time Quantum Walks

Continuous-time random walk on a graph $G = (V, E)$ with adjacency matrix A defined as:

$$A_{i,j} = \begin{cases} 1, & (i,j) \in E \\ 0, & (i,j) \notin E \end{cases} \tag{1.21}$$

for every pair $i, j \in V$. In this definition we do not allow self-loops therefore the diagonal of A is zero.

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There is another matrix associated with G that is of equal importance, the Laplacian of G defined as:

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$$\frac{\mathrm{d}}{\mathrm{d}t} p_i(t) = \sum_{j \in V} L_{jk} p_j(t). \tag{1.23}$$

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Observe that

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_{j\in V} p_j(t) = \sum_{j,k\in V} L_{jk}p_k(t) = 0 \tag{1.24}$$

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Instead of probabilities of Eq. (1.24) we can insert the amplitudes $q_j(t) = \langle j \mid \psi(t) \rangle$ where $\{|j\rangle : j \in V\}$ is an orthonormal basis $\mathcal{H}$. Then, we obtain the equation:

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The solution of reads:

$$U(t) = e^{-\imath Ht} = e^{-\imath Lt}, \tag{1.28}$$

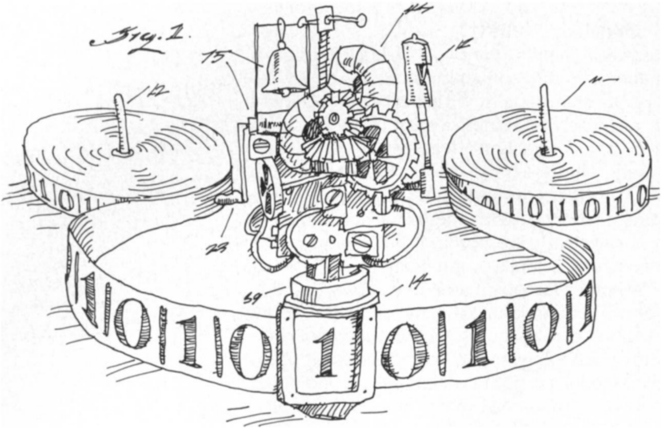
and the evolution of an initial state from $t = 0$ to some arbitrary time t is given by:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle. \tag{1.29}$$

Exponential speedups using Quantum Walks

(see notes)

Universality of Quantum Qalks



Universality of Quantum Walks

- Quantum walks form a universal model of computation [Childs; 0806.1972].
- We will show this using the concept of the **universal computation graph**.
- Universality: any problem solved by a gate-based quantum computer also solved by a quantum walk.
- In principle, any quantum algorithm we have seen previously can be recast as a quantum walk algorithm.

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Consider a (continuous) walker on $G = \mathbb{Z}$ where the basis states are $|x\rangle$ with Hamiltonian $H_G = A_G$.

By solving the eigenvalue equation we find that **the eigenstates** of H_G are the momentum states $|k\rangle$; the states that satisfy

$$\langle x|k\rangle = e^{-\imath kx}, \tag{1.30}$$

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In momentum space, with orthogonal states $|\phi_k\rangle \equiv |k\rangle$, we know that

$$|k\rangle = \sum_{x\in\mathbb{Z}} e^{-\imath kx}|x\rangle. \tag{1.31}$$

These **momentum states** however (as is usual with Fourier bases) are not normalizable (think as maps $E(G) \to \mathbb{C}$).

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Next, let us consider a finite graph G and create out of it an infinite graph with adjacency matrix H by attaching semi-infinite lines to M of its vertices.

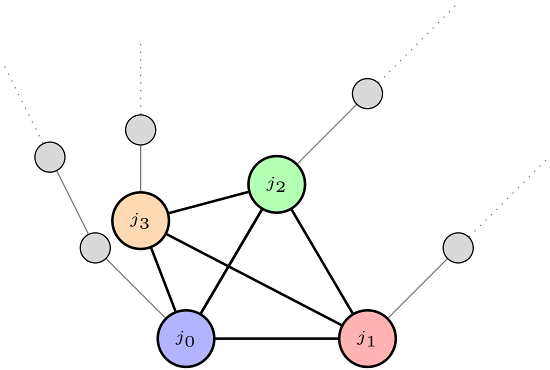

Figure: Universal computation graph.

Universality of Quantum Walks

The states living on the j-th line are labeled $|x, j\rangle$.

$|x, j\rangle$ corresponds to the state where x is allowed to walk along the j-th line. The eigenstates of H_G for each line j must be a superposition of the form of Eq. (1.31) with momenta k taking any of the values:

- $\pm k$ with eigenvalues $2\cos(k)$,
- $k = \pm i\kappa$ and eigenvalue $2\cosh(\kappa)$,
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For numerous reasons, Childs truncates $|k\rangle$ such that it has support over a finite number of vertices. Denote the truncated state supported over L vertices as

$$|k\rangle_L := \frac{1}{\sqrt{L}} \sum_{x=1}^{L} e^{-\imath kx} |x\rangle \tag{1.33}$$

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In the physics literature, such states are called **wave packets** and the sign of the exponential denotes the direction of the wave;

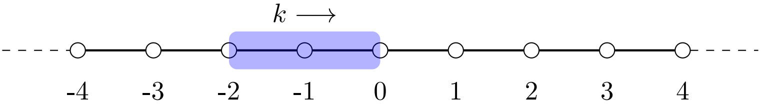

Figure: A wave packet supported over 3 vertices moving coming from the (far) left.

The infinite line in the figure above becomes a **universal computation graph** by inserting in some vertex a finite graph G.

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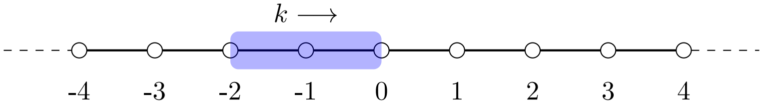

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As seen in Fig. 1.13. In principle, one can prepare a wave packet as the one with momentum k and let it propagate.

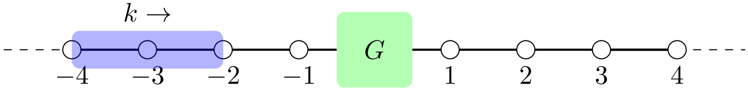

Figure: Inserting a finite graph G into the integer line, yields a one-dimensional universal computation graph.

G serves as a **quantum obstacle** in the propagation of the wave packet.

Universality of Quantum Walks

This amounts to a dynamic scattering process. Let us denote this incoming (to G) wave packet as

$$|w(k)\rangle_{\mathrm{L}} \quad \text{if the wave packet comes from the left,} \tag{1.34}$$
$$|w(k)\rangle_{\mathrm{R}} \quad \text{if the wave packet comes from the right.} \tag{1.35}$$

The dynamics correspond to the following equations:

$$\langle x_{\mathrm{L}}|w_{\mathrm{L}}(k)\rangle = e^{-\imath kx} + R_{\mathrm{L}}(k)e^{\imath kx} \tag{1.36}$$
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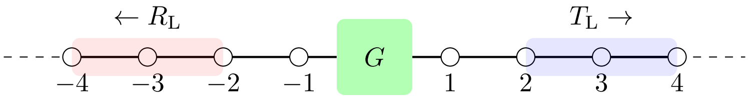

Figure: Part of the wave packet will be reflected and part will be transfered through G. The coefficients $R_{\mathrm{L,R}}, T_{\mathrm{L,R}}$ are called reflection and transfer coefficients.

Universality of Quantum Walks

For every scattering process, as the one above, there is a scattering matrix S. In this case,

$$S = \begin{pmatrix} R_{\mathrm{L}} & T_{\mathrm{L}} \\ R_{\mathrm{R}} & T_{\mathrm{R}} \end{pmatrix}, \tag{1.39}$$

and it is an element of $U(2)$.

More generally, an arbitrary number of semi-infinite lines can be considered as in Fig. 1.11 with an arbitrary graph G. If there are N semi-infinite lines, then $S \in U(N)$.

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It is possible to encode a qubit state by considering two universal computation diagrams in one dimension:

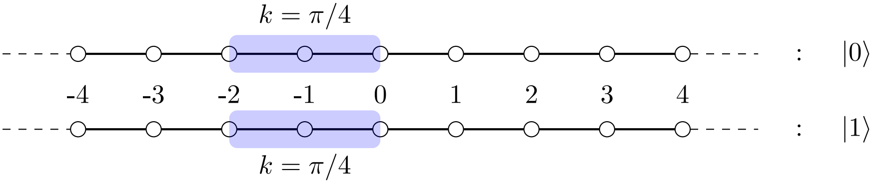

Figure: A single qubit can be represented by two infinite lines and momentum $\pi/4$. The qubit is in the $|0\rangle$ state if the wavepacket propagates in the top line and in the $|1\rangle$ state if at the bottom.

Universality of Quantum Walks

As before, we can insert a graph G with 4 semi-infinite lines as in Fig. 1.16.

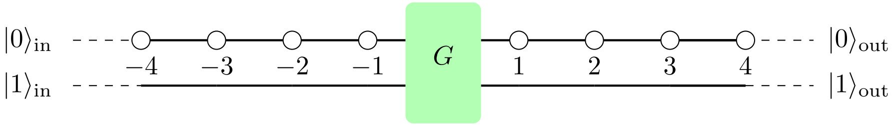

Figure: A two-qubit unitary U can be encoded through G to be implemented as a quantum walk.

Universality of Quantum Walks

A unitary is implemented by inserting a graph G such that its corresponding S-matrix has the structure

$$S = \begin{pmatrix} 0 & U^\dagger \\ U & 0 \end{pmatrix}, \tag{1.40}$$

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Childs showed it is possible to implement the unitaries

$$U_{\pi/4} = \begin{pmatrix} e^{-\imath\pi/4} & 0 \\ 0 & 1 \end{pmatrix}, \quad U_{\mathrm{b}} = -\frac{\imath}{\sqrt{2}} \begin{pmatrix} 1 & -\imath \\ -\imath & 1 \end{pmatrix}, \tag{1.41}$$

which form a universal gate set for one-qubit operations; up to a certain precision ε, any single-qubit gate can be implemented by a string of these two unitaries.

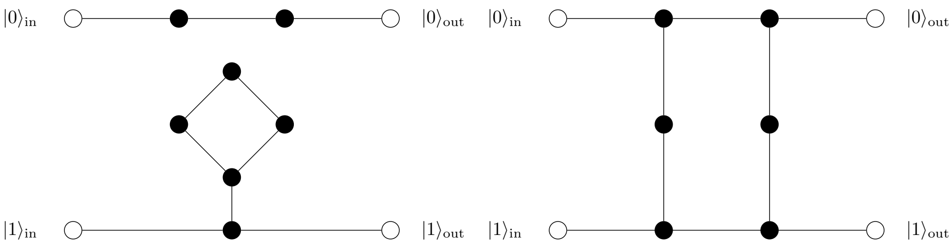

Figure: The graphs encoding $U_{\pi/4}$ and U_{b}.

Universality of Quantum Walks

This construction was further generalized to n-qubit gates proving that quantum walks form a universal model of computation.

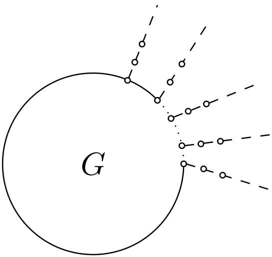

Figure: The graph G obtained by attaching N semi-infinite paths to a graph G.

Universality of Quantum Walks

By considering a finite graph G and attaching $N/2 = n$ pairs of semi-infinite paths, we are able to encode n qubits. Eventually, it is possible to encode any n-qubit unitary to a graph G to obtain a quantum walk equivalent of any arbitrary circuit.

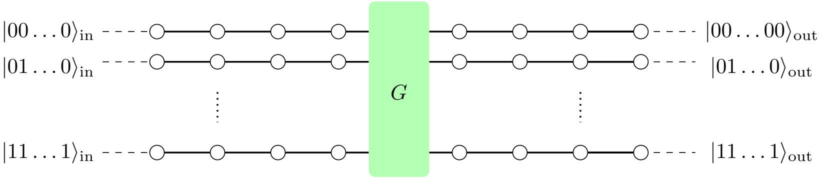

Figure: If G is chosen to encode a desired unitary $U \in U(n)$ the circuit can be implemented by a quantum walk.

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Worry not since [Childs, Gosset, Webb 2013] showed that by considering **multiparticle quantum walk** one requires a $\mathrm{poly}(n)$ sized graph G!

However the construction of 2-qubit gates (and above) is quite more involved since, as you can imagine, it requires scattering of 2 particle states or higher. We leave this as an exercise.

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You might be worried that for 2^n-dimensional states we require 2×2^n semi-infinite lines. Thus a graph G of size $\mathcal{O}(2^n)$.

Worry not since [Childs, Gosset, Webb 2013] showed that by considering **multiparticle quantum walk** one requires a $\mathrm{poly}(n)$ sized graph G!

However the construction of 2-qubit gates (and above) is quite more involved since, as you can imagine, it requires scattering of 2 particle states or higher. We leave this as an exercise.

Quantum Walks