

# Quantum Computing

## Exercises: Quantum walks

1. At each time step, a quantum walk corresponds to a unitary map  $U \in U(N)$  such that

$$U : \mathcal{H}_G \rightarrow \mathcal{H}_G$$
$$|x\rangle \mapsto a|x-1\rangle + b|x\rangle + c|x+1\rangle$$

Show that  $U$  is unitary if and only if one of the following three conditions is true:

- (a)  $|a| = 1, b = c = 0,$
- (b)  $|b| = 1, a = c = 0,$
- (c)  $|c| = 1, a = b = 0.$

Using the unitarity of the operator we know that:

$$\langle x | \underbrace{U^\dagger U}_I | y \rangle = \delta_{xy} \quad (1)$$

So, for instance, for the following states, we have:

$$\langle x-1 | U^\dagger U | x+1 \rangle = (a \langle x-2 | + b \langle x-1 | + c \langle x |) (a | x \rangle + b | x+1 \rangle + c | x+2 \rangle) = 0$$

The only term surviving being  $c \langle x | a | x \rangle = ac = 0$

$$\langle x | U^\dagger U | x+1 \rangle = (a \langle x-1 | + b \langle x | + c \langle x+1 |) (a | x \rangle + b | x+1 \rangle + c | x+2 \rangle) = 0$$

The non-vanishing terms now are

$$\begin{cases} b \langle x | a | x \rangle \Rightarrow ab \\ c \langle x+1 | b | x+1 \rangle \Rightarrow bc \end{cases} \Rightarrow ab + bc = 0$$

$$\langle x | U^\dagger U | x \rangle = (a \langle x-1 | + b \langle x | + c \langle x+1 |) (a | x-1 \rangle + b | x \rangle + c | x+1 \rangle) = 0$$

Lastly, the system to be solved is:

$$\begin{cases} ac = 0 \\ ab + bc = 0 \\ a^2 + b^2 + c^2 = 1 \end{cases} \quad (2)$$

2. Demonstrate that the shift operator  $S$ , as defined in

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

is equivalent to

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

Applying directly the first definition of the operator to the state  $|i, x\rangle$ , we get the second one:

$$\begin{aligned} S|i, x\rangle &= \left( |0\rangle \overbrace{\langle 0|}^{\delta_{0i}} |i\rangle \otimes \underbrace{\sum_{k=-\infty}^{\infty} |k+1\rangle \langle k|}_{|x+1\rangle} |x\rangle \right) + \left( |1\rangle \overbrace{\langle 1|}^{\delta_{1i}} |i\rangle \otimes \underbrace{\sum_{k=-\infty}^{\infty} |k-1\rangle \langle k|}_{|x-1\rangle} |x\rangle \right) \\ &= \begin{cases} |0\rangle \otimes |x+1\rangle & \text{if } i = 0, \\ |1\rangle \otimes |x-1\rangle & \text{if } i = 1. \end{cases} = \begin{cases} |0, x+1\rangle & \text{if } i = 0, \\ |1, x-1\rangle & \text{if } i = 1. \end{cases} \end{aligned}$$

3. In the lecture notes, starting at the state  $|\psi_0\rangle = |0\rangle |0\rangle$ , we have seen how to obtain the successive states up to  $|\psi_3\rangle$  by using the unitary operator  $U = S(H \otimes I)$ . Derive  $|\psi_4\rangle$  for the walker on the finite subset of  $\mathbb{Z}$ .

The previous states  $|\psi_{1..3}\rangle$  can be found also in R. Portugal, Quantum walks and search algorithms (3.19).

$$|\psi_4\rangle = U|\psi_3\rangle = \frac{1}{2\sqrt{2}}[2U|01\rangle + U|11\rangle + \dots]$$

$$U|01\rangle = S(H \otimes I)|01\rangle = S\left|\frac{|0\rangle+|1\rangle}{\sqrt{2}}1\right\rangle = \frac{1}{\sqrt{2}}[S|01\rangle + S|11\rangle] = \frac{1}{\sqrt{2}}[|02\rangle + |10\rangle]$$

$$U|11\rangle = S(H \otimes I)|11\rangle = S\left|\frac{|0\rangle-|1\rangle}{\sqrt{2}}1\right\rangle = \frac{1}{\sqrt{2}}[S|01\rangle - S|11\rangle] = \frac{1}{\sqrt{2}}[|02\rangle - |10\rangle]$$

$$U|03\rangle = \frac{1}{\sqrt{2}}[|02\rangle - |10\rangle]$$

$$U|1-3\rangle = \frac{1}{\sqrt{2}}[|0-2\rangle - |1-4\rangle]$$

$$U|0-1\rangle = \frac{1}{\sqrt{2}}[|00\rangle - |0-2\rangle]$$

$$|\psi_4\rangle = \frac{1}{4}[|10\rangle + 3|02\rangle + |12\rangle - |00\rangle - |1-4\rangle + |04\rangle]$$

4. Show that the formula from the lecture notes,  $H|k\rangle = 2\cos(k)|k\rangle$  holds, by performing the discrete Fourier transform in the computational basis states.

For the walker on the line, every state  $|x\rangle$  is only connected to its adjacent states  $|x \pm 1\rangle$ , that is, its adjacency matrix,  $A$ , is defined by:

$$\begin{cases} \langle x|A|x \pm 1\rangle = 1 \\ \langle x|A|y\rangle = 0, y \neq x \pm 1 \end{cases} \quad (3)$$

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

Changing from the computational basis to the Fourier basis, we have:

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} e^{ikx} |x\rangle, \quad \langle k| = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} e^{-ikx} \langle x|, \quad \text{where } k = \frac{2\pi\kappa}{N}$$

Now, taking the matrix element of the adjacency matrix and identifying it with the hamiltonian:

$$\begin{aligned} \langle k| \underbrace{A}_{=H} |k'\rangle &= \frac{1}{N} \sum_{x=0}^{N-1} e^{-ikx} \langle x| H \sum_{x=0}^{N-1} e^{ik'x} |x\rangle = \frac{1}{N} \sum_{x=0}^{N-1} e^{-ikx} e^{ik'(x+1)} + e^{-ikx} e^{ik'(x-1)} = \\ &= \frac{1}{N} \sum_{x=0}^{N-1} e^{-ix(k-k')} e^{ik'} + e^{-ix(k-k')} e^{-ik'} = \underbrace{(e^{ik'} + e^{-ik'})}_{2\cos k} \underbrace{\frac{1}{N} \sum_{x=0}^{N-1} e^{-ix(k-k')}}_{\delta_{\kappa\kappa'}} \end{aligned}$$

Where in the last equation, we have made use of the partial sum,  $s_n$ , of a geometric series:

$$s_n = ar^0 + ar^1 + \dots + ar^{n-1} \quad (4)$$

$$= \sum_{k=0}^{n-1} ar^k = \sum_{k=1}^n ar^{k-1} \quad (5)$$

$$= \begin{cases} a \left( \frac{1-r^n}{1-r} \right), & \text{for } r \neq 1 \\ an, & \text{for } r = 1 \end{cases} \quad (6)$$

$$\frac{1}{N} \sum_{x=0}^{N-1} e^{-ix(k-k')} = \frac{1}{N} \sum_{x=0}^{N-1} (e^{-i(k-k')})^x = \begin{cases} \frac{1-e^{\frac{2\pi i}{N}(\kappa-\kappa')N}}{1-e^{\frac{2\pi i}{N}(\kappa-\kappa')}} = 0 \\ \frac{N}{N} = 1 \end{cases} = \delta_{\kappa\kappa'}$$