Quantum Computing

A Gentle Introduction to Grover's Algorithm

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v1.0

Outline

Outline

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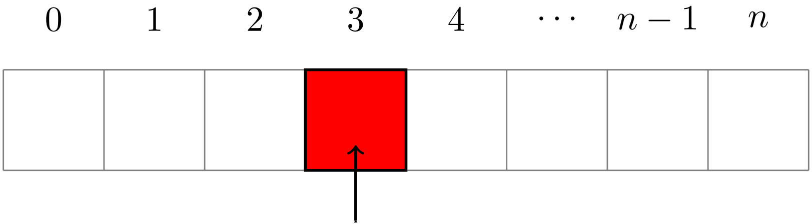
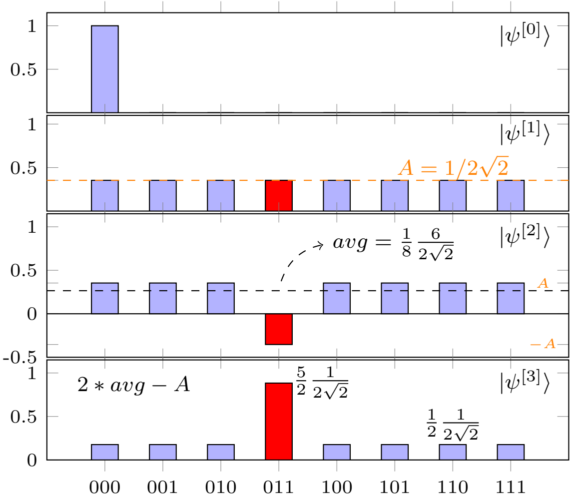
Grover's algorithm: Motivation

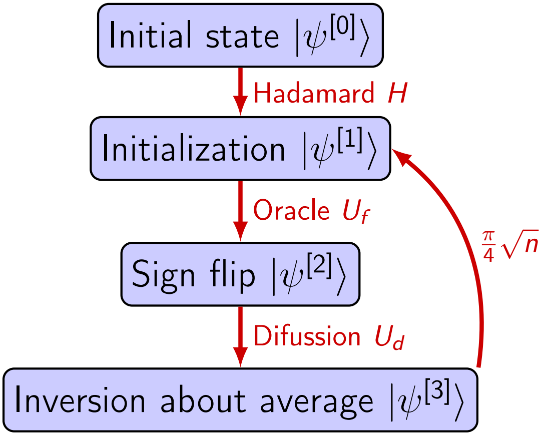
Grover's algorithm performs a search over an unorder set of 2^n items fo find the unique element that satisfies some condition

- Classic approach: $\sum_{i=1}^{n} \frac{1}{n} i = \frac{n+1}{1} \Rightarrow \mathcal{O}(n)$
- Quantum approach: $(\ldots) \Rightarrow \mathcal{O}(\sqrt{n})$



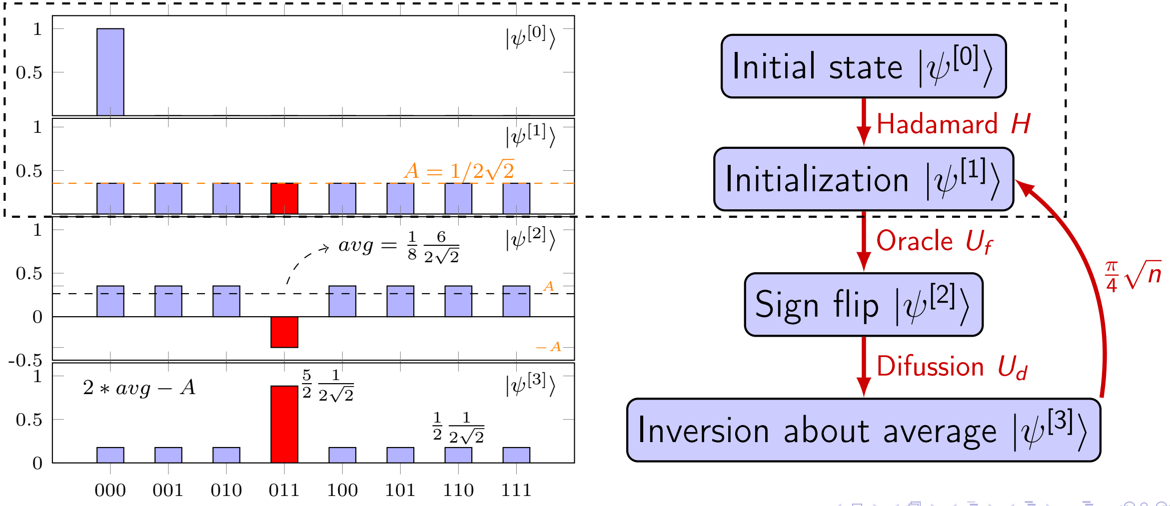
Grover's algorithm: Outline





Outline

Initialization



Initialization

We find a method (unitary operator) to have all the states with the same probability (*principle of superposition*).

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We find a method (unitary operator) to have all the states with the same probability (*principle of superposition*).

$$\begin{aligned}
\left(I^{\otimes n} \otimes X\right) |0\rangle_{n+1} &= |0\rangle_n \otimes |1\rangle \\
H^{\otimes(n+1)} \left[\left(I^{\otimes n} \otimes X\right) |0\rangle_{n+1}\right] &= H^{\otimes n} |0\rangle_n \otimes H |1\rangle \\
&= \sum_{j \in \{0,1\}^n} \frac{1}{\sqrt{2^n}} |j\rangle_n \otimes \frac{1}{\sqrt{2}} \left(|0\rangle - |1\rangle\right) \\
&= \sum_{j \in \{0,1\}^n} \alpha_j |j\rangle_n \otimes \frac{1}{\sqrt{2}} \left(|0\rangle - |1\rangle\right) \\
&= |\psi^{[1]}\rangle
\end{aligned}$$

Initialization

3-qubit example: Set ancillary qubit to $|1\rangle$

$$
\begin{aligned}
\left(I^{\otimes 3} \otimes X\right)|0\rangle_{3+1} &= I^{\otimes 3}|0\rangle_3 \otimes X|0\rangle \\
&= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\
&= |0\rangle_3 \otimes |1\rangle
\end{aligned}
$$

Initialization

3-qubit example: Apply Hadamard gate

$$
\begin{aligned}
|\psi^{[1]}\rangle &= H^{\otimes(3+1)}\left[(I^{\otimes 3}\otimes X)\,|0\rangle_{n+1}\right] \\
&= H^{\otimes 3}\,|0\rangle_3 \otimes H\,|1\rangle \\
&= \frac{1}{\sqrt{2^3}}\begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\
1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\
1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\
1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\
1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\
1 & -1 & -1 & 1 & -1 & 1 & 1 & -1
\end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix}
\end{aligned}
$$

Initialization

3-qubit example: Apply Hadamard gate

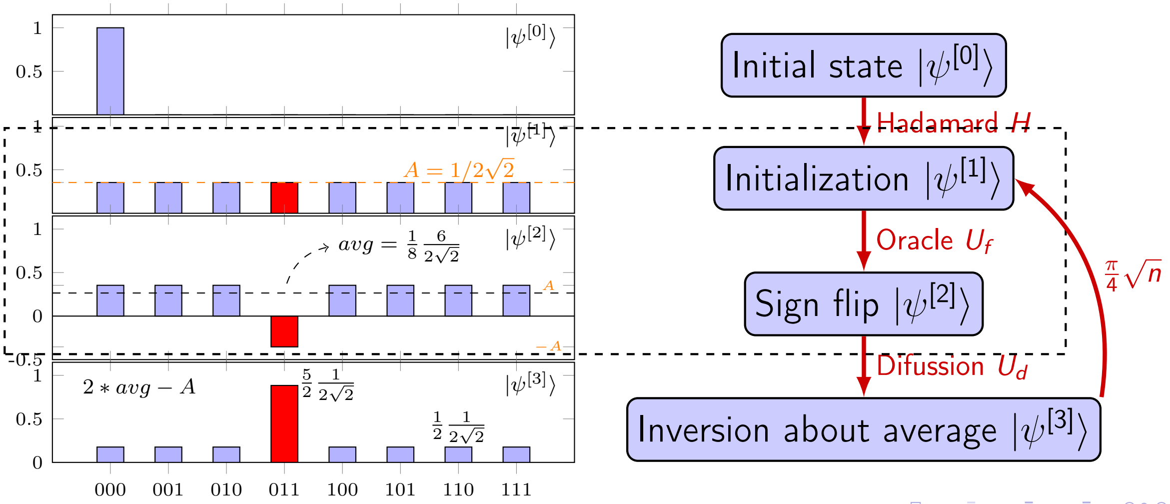
$$
\begin{aligned}
|\psi^{[1]}\rangle &= \frac{1}{\sqrt{2^3}}(11111111)^{\dagger} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \\
&= [\frac{1}{2\sqrt{2}}|000\rangle + \frac{1}{2\sqrt{2}}|001\rangle + \frac{1}{2\sqrt{2}}|010\rangle + \frac{1}{2\sqrt{2}}|011\rangle \\
&+ \frac{1}{2\sqrt{2}}|100\rangle + \frac{1}{2\sqrt{2}}|101\rangle + \frac{1}{2\sqrt{2}}|110\rangle + \frac{1}{2\sqrt{2}}|111\rangle] \\
&\otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)
\end{aligned}
$$

Initialization

3-qubit example: Summary

$$
\begin{aligned}
|\psi^{[1]}\rangle &= H^{\otimes(3+1)}\left[(I^{\otimes 3}\otimes X)\,|0\rangle_{n+1}\right] \\
&= [\frac{1}{2\sqrt{2}}\,|000\rangle + \frac{1}{2\sqrt{2}}\,|001\rangle + \frac{1}{2\sqrt{2}}\,|010\rangle + \frac{1}{2\sqrt{2}}\,|011\rangle \\
&+ \frac{1}{2\sqrt{2}}\,|100\rangle + \frac{1}{2\sqrt{2}}\,|101\rangle + \frac{1}{2\sqrt{2}}\,|110\rangle + \frac{1}{2\sqrt{2}}\,|111\rangle] \\
&\otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right) \\
&= \sum_{j\in\{0,1\}^n} \frac{1}{\sqrt{2^n}}\,|j\rangle_n \otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right) = |\psi^{[1]}\rangle
\end{aligned}
$$

Sign flip


$|\psi^{[0]}\rangle$
$|\psi^{[1]}\rangle$
$A = 1/2\sqrt{2}$
$|\psi^{[2]}\rangle$
$avg = \frac{1}{8}\,\frac{6}{2\sqrt{2}}$
A
$-A$
$|\psi^{[3]}\rangle$
$2 * avg - A$
$\frac{5}{2}\,\frac{1}{2\sqrt{2}}$
$\frac{1}{2}\,\frac{1}{2\sqrt{2}}$
000 001 010 011 100 101 110 111
Initial state $|\psi^{[0]}\rangle$
Hadamard H
Initialization $|\psi^{[1]}\rangle$
Oracle U_f
Sign flip $|\psi^{[2]}\rangle$
Difussion U_d
Inversion about average $|\psi^{[3]}\rangle$
$\frac{\pi}{4}\sqrt{n}$

Sign flip

We find a method (unitary operator) which flip the sign of the state of interest.

Sign flip

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Quantum Oracle

It is defined the operator U_f:

$$U_f : |j\rangle_n \otimes |y\rangle_1 \rightarrow |j\rangle_n \otimes |y \oplus f(j)\rangle_1 ,$$

where $\oplus$ is the sum operator in mod 2, and $f(j) = \left\{ \begin{array}{cc} 1 & j = l \\ 0 & j \neq l \end{array} \right\}$

A	B	XOR
0	0	0
0	1	1
1	0	1
1	1	0

Sign flip

We apply U_f (*Quantum Oracle*) to the previous state $\psi^{[1]}$

$$
\begin{aligned}
\left|\psi^{[2]}\right\rangle &= U_f \left|\psi^{[1]}\right\rangle \\
&= U_f \left(\sum_{j\in\{0,1\}^n} \alpha_j \left|j\right\rangle_n \otimes \frac{1}{\sqrt{2}} \left(\left|0\right\rangle - \left|1\right\rangle \right) \right) \\
&= U_f \left(\alpha_l \left|l\right\rangle_n \otimes \frac{1}{\sqrt{2}} \left(\left|0\right\rangle - \left|1\right\rangle \right) + \sum_{j\in\{0,1\}^n;\, j\neq l} \alpha_j \left|j\right\rangle_n \otimes \frac{1}{\sqrt{2}} \left(\left|0\right\rangle - \left|1\right\rangle \right) \right) \\
&= \left(-\alpha_l \left|l\right\rangle_n + \sum_{j\in\{0,1\}^n;\, j\neq l} \alpha_j \left|j\right\rangle_n \right) \otimes \frac{1}{\sqrt{2}} \left(\left|0\right\rangle - \left|1\right\rangle \right)
\end{aligned}
$$

Sign flip

We apply U_f (*Quantum Oracle*) to the previous state $\psi^{[1]}$

$$
\begin{aligned}
|\psi^{[2]}\rangle &= U_f\,|\psi^{[1]}\rangle \\
&= U_f\left(\sum \alpha_j\,|j\rangle_n \otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)\right) \\
&= U_f\left(\alpha_l\,|l\rangle_n \otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right) + \sum_{j\in\{0,1\}^n;\ j\neq l} \alpha_j\,|j\rangle_n \otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)\right) \\
&= \left(-\alpha_l\,|l\rangle_n + \sum_{j\in\{0,1\}^n;\ j\neq l} \alpha_j\,|j\rangle_n\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)
\end{aligned}
$$

sign flip!

Sign flip

We apply U_f (*Quantum Oracle*) to the previous state $\psi^{[1]}$

$$
\begin{aligned}
|\psi^{[2]}\rangle &= U_f |\psi^{[1]}\rangle \\
&= U_f \left(\sum \alpha_j |j\rangle_n \otimes \frac{1}{\sqrt{2}} \left(|0\rangle - |1\rangle \right) \right) \\
&= U_f \left(\alpha_l |l\rangle_n \otimes \frac{1}{\sqrt{2}} \left(|0\rangle - |1\rangle \right) + \sum_{j \in \{0,1\}^n;\, j \neq l} \alpha_j |j\rangle_n \otimes \frac{1}{\sqrt{2}} \left(|0\rangle - |1\rangle \right) \right) \\
&= \left(\boxed{-\alpha_l |l\rangle_n} + \sum_{j \in \{0,1\}^n;\, j \neq l} \alpha_j |j\rangle_n \right) \otimes \boxed{\frac{1}{\sqrt{2}} \left(|0\rangle - |1\rangle \right)}
\end{aligned}
$$

sign flip!

Extra qubit!

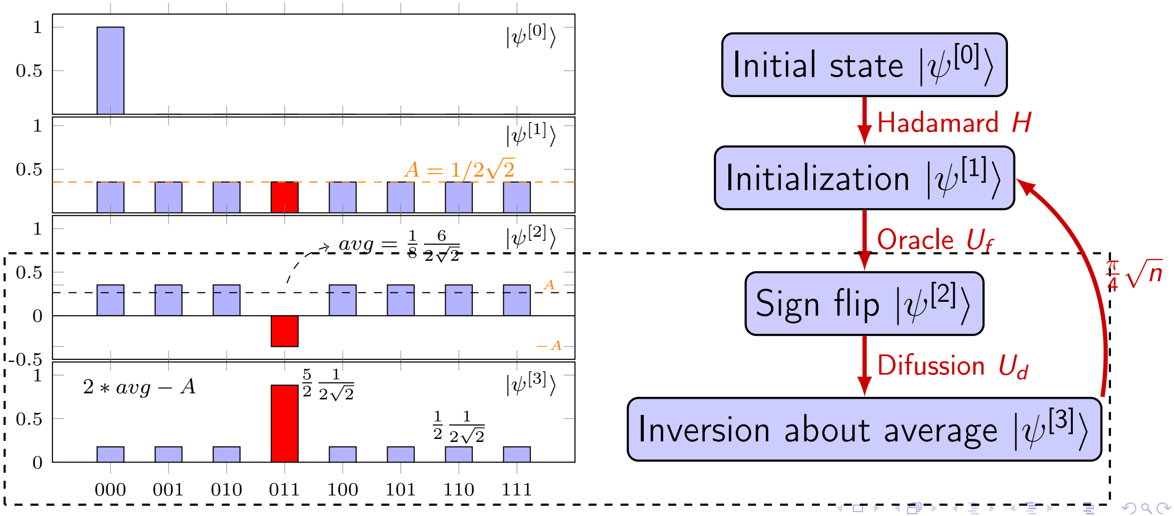
Sign flip[1]

3-qubit example: Quantum Oracle

$$
\begin{aligned}
|\psi^{[2]}\rangle &= U_f\,|\psi^{[1]}\rangle \\
&= [\frac{1}{2\sqrt{2}}\,|000\rangle + \frac{1}{2\sqrt{2}}\,|001\rangle + \frac{1}{2\sqrt{2}}\,|010\rangle - \frac{1}{2\sqrt{2}}\,|011\rangle \\
&+ \frac{1}{2\sqrt{2}}\,|100\rangle + \frac{1}{2\sqrt{2}}\,|101\rangle + \frac{1}{2\sqrt{2}}\,|110\rangle + \frac{1}{2\sqrt{2}}\,|111\rangle] \\
&\otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)
\end{aligned}
$$

[1] This slide shows the result of applying U_f but not how is applied. This is because this step of the algorithm depends on the specific problem.

Inversion about average



Inversion about the average

We find a method (unitary operator) to invert the amplitude about the average

Inversion about the average

We find a method (unitary operator) to invert the amplitude about the average

$$\sum_{j\in\{0,1\}^n} \alpha_j \left|j\right\rangle_n \xrightarrow{U_d} \sum_{j\in\{0,1\}^n} \left(2 \left(\sum_{k\in\{0,1\}^n} \frac{\alpha_k}{2^n} \right) - \alpha_j \right) \left|j\right\rangle_n ,$$

where $\sum_{k\in\{0,1\}^n} \frac{\alpha_k}{2^n}$ is the average.

$$\sum_{k\in\{0,1\}^n} \frac{\alpha_k}{2^n} = \frac{1}{2^3} \frac{6}{2\sqrt{2}}$$

Inversion about the average

Difusion operator

$$U_d = \begin{pmatrix} \frac{2}{2^n} & \frac{2}{2^n} & \cdots & \frac{2}{2^n} \\ \frac{2}{2^n} & \frac{2}{2^n} & \cdots & \frac{2}{2^n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{2}{2^n} & \frac{2}{2^n} & \cdots & \frac{2}{2^n} \end{pmatrix} - I^{\otimes n} = \cdots = -H^{\otimes n} D H^{\otimes n}, \qquad (1)$$

where $D = diag\left(-1, 1, 1, \cdots, 1\right)$

Inversion about the average

3-qubit example: Difussion operator in python

```
>>> import numpy as np
>>> H1 = 1/np.sqrt(2)*np.array([[1,1],[1, -1]]) # Hadamard operator 1 qubit
>>> H2 = np.kron(H1,H1) # Hadamard operator 2 qubit
>>> H3 = np.kron(H2,H1) # Hadamard operator 3 qubit

>>> D = np.eye(8) # Diagonal operator
>>> D[0,0] = -1

>>> Ud = -np.dot(np.dot(H3,D),H3) # Difussion operator
>>> psi_2 = 1/(2*np.sqrt(2))*np.array([1,1,1,-1,1,1,1,1]) # psi_2

>>> psi_3 = np.dot(Ud,psi_2)
>>> print(psi_3)
array([0.176 , 0.176 , 0.176 , 0.883, 0.176, 0.176, 0.176, 0.176])
```

Inversion about the average

3-qubit example: Difussion operator

$$|\psi^{[3]}\rangle = U_d \, |\psi^{[2]}\rangle$$

$$|\psi^{[3]}\rangle = -\frac{1}{8}\frac{1}{2\sqrt{2}}\begin{pmatrix} 6 & -2 & -2 & -2 & -2 & -2 & -2 & -2 \\ -2 & 6 & -2 & -2 & -2 & -2 & -2 & -2 \\ -2 & -2 & 6 & -2 & -2 & -2 & -2 & -2 \\ -2 & -2 & -2 & 6 & -2 & -2 & -2 & -2 \\ -2 & -2 & -2 & -2 & 6 & -2 & -2 & -2 \\ -2 & -2 & -2 & -2 & -2 & 6 & -2 & -2 \\ -2 & -2 & -2 & -2 & -2 & -2 & 6 & -2 \\ -2 & -2 & -2 & -2 & -2 & -2 & -2 & 6 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \\ 1 \\ -1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{4\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 5 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

Measurement & Repetition

For the first iteration we measure

$$\boxed{\begin{array}{ccccccc} \alpha_{011} & = & \frac{5}{2}\frac{1}{2\sqrt{2}} & \longrightarrow & \|\alpha_{011}\|^2 & \simeq & 78,12\% \\ \alpha_j & = & \frac{1}{2}\frac{1}{2\sqrt{2}} & \longrightarrow & \|\alpha_j\|^2 & \simeq & 3,12\% \quad (j \neq |011\rangle) \end{array}}$$

The optimal number of repetitions $R \simeq \frac{\pi}{4}\sqrt{n} \simeq 2.2$. For the second iteration (Oracle & Diffusion) we have:

$$\boxed{\begin{array}{ccccccc} \alpha_{011} & = & \frac{11}{4}\frac{1}{2\sqrt{2}} & \longrightarrow & \|\alpha_{011}\|^2 & \simeq & 94,5\% \\ \alpha_j & = & \frac{-1}{4}\frac{1}{2\sqrt{2}} & \longrightarrow & \|\alpha_j\|^2 & \simeq & 0,78\% \quad (j \neq |011\rangle) \end{array}}$$

Outline

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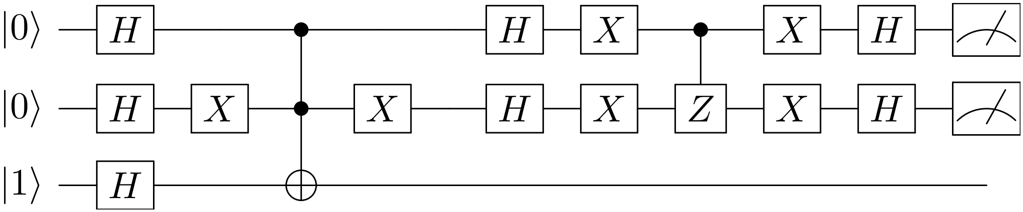
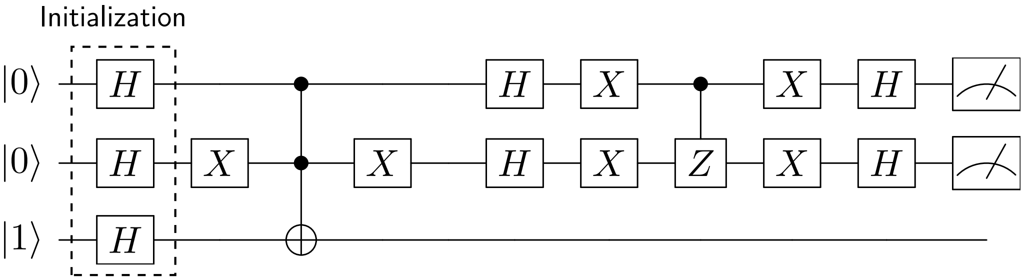
2-Qubit Quantum Circuit



2-Qubit Quantum Circuit

Initialization



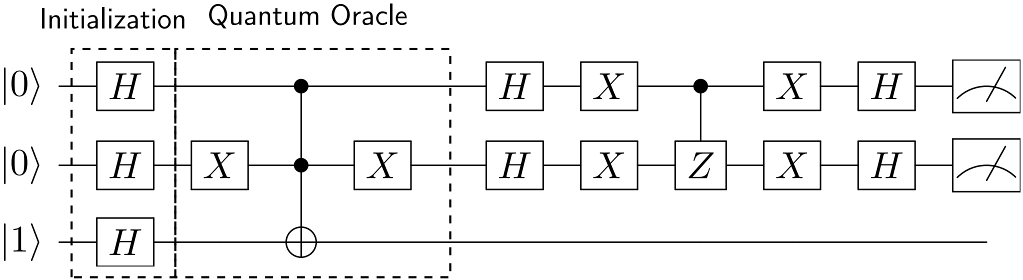
2-Qubit Quantum Circuit

Initialization

$$
\begin{aligned}
\psi^{[0]} &= |001\rangle \\
\psi^{[1]} &= H^{\otimes 3}\psi^{[0]} \\
&= \frac{1}{\sqrt{8}}\left(|000\rangle + |010\rangle + |100\rangle + |110\rangle - |001\rangle - |011\rangle - |101\rangle - |111\rangle\right)
\end{aligned}
$$

2-Qubit Quantum Circuit

Quantum Oracle



2-Qubit Quantum Circuit

Quantum Oracle

$$U_f = (I \otimes X \otimes I) \cdot T \cdot (I \otimes X \otimes I) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

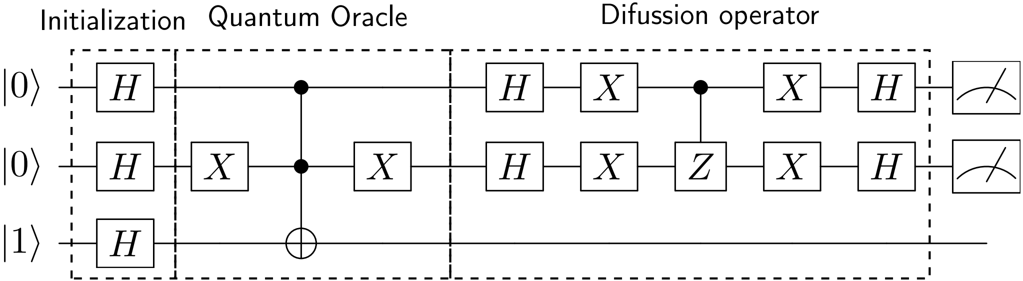
2-Qubit Quantum Circuit

Quantum Oracle

$$
\begin{aligned}
\psi^{[1]} &= \frac{1}{\sqrt{8}}\left(|000\rangle + |010\rangle + |100\rangle + |110\rangle - |001\rangle - |011\rangle - |101\rangle - |111\rangle\right) \\
\psi^{[2]} &= U_f \left|\psi^{[1]}\right\rangle \\
&= \frac{1}{\sqrt{8}}\left(|000\rangle + |010\rangle + |101\rangle + |110\rangle - |001\rangle - |011\rangle - |100\rangle - |111\rangle\right) \\
&= \frac{1}{\sqrt{8}}\left(|00\rangle + |01\rangle - |10\rangle + |11\rangle\right) \otimes \left(|0\rangle - |1\rangle\right) \\
&= \frac{1}{2}\left(|00\rangle + |01\rangle - |10\rangle + |11\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)
\end{aligned}
$$

2-Qubit Quantum Circuit

Difussion Operator



2-Qubit Quantum Circuit

Diffusion Operator

$$U_d = (H \otimes H) \cdot (X \otimes X) \cdot (CZ)\,(X \otimes X) \cdot (H \otimes H) = \frac{1}{4}\begin{pmatrix} 2 & -2 & -2 & -2 \\ -2 & 2 & -2 & -2 \\ -2 & -2 & 2 & -2 \\ -2 & -2 & -2 & 2 \end{pmatrix}$$

$$\psi^{[3]} = U_d \psi^{[2]}$$

$$\frac{1}{8}\begin{pmatrix} 2 & -2 & -2 & -2 \\ -2 & 2 & -2 & -2 \\ -2 & -2 & 2 & -2 \\ -2 & -2 & -2 & 2 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{8}\begin{pmatrix} 2 & -2 & 2 & -2 \\ -2 & 2 & 2 & -2 \\ -2 & -2 & -2 & -2 \\ -2 & -2 & 2 & 2 \end{pmatrix} \rightarrow \begin{pmatrix} 0 \\ 0 \\ -1 \\ 0 \end{pmatrix} = -\left|10\right\rangle$$

Outline

Implementation

Next slides show the implementation of the algorithm in two different ways:

1. Using *qiskit* framework. In this case we have a simulated quantun backend. The reader can copy & run the code in python in order to reproduce the experiment
2. Building the gates directly in Quantum IBM computer

In both cases we will observe a histogram with an unique state ($|10\rangle$)

IBM Implementation: Qiskit

Backend & Quantum Registers

```
from qiskit import *
from qiskit import QuantumCircuit
from qiskit.circuit.quantumcircuit import QuantumCircuit
from qiskit.visualization import plot_histogram

backend = BasicAer.get_backend('qasm_simulator')
#backend = BasicAer.get_backend('statevector_simulator')

'''Quantum register
https://quantumcomputing.stackexchange.com/questions/4907/
qiskit-is-there-any-way-to-discard-the-results-of-a-measurement'''

q = QuantumRegister(2, 'q')
a = QuantumRegister(1, 'a')
c = ClassicalRegister(2, 'c')
```

IBM Implementation: Qiskit

Quantum Circuit

```
#Circuit
circ = QuantumCircuit(q,a,c) # type: qiskit.circuit.quantumcircuit.QuantumCircuit

# ===== prepare the states: psi^{[0]} =====
circ.iden(q[0])
circ.iden(q[1])
circ.x(a[0])

#===== Initialization: psi^{[1]} =====
circ.h(q[0])
circ.h(q[1])
circ.h(a[0])
circ.barrier(q)

#===== Sign flip: psi^{[2]} =====
circ.x(q[0])
circ.ccx(q[0], q[1], a[0])
circ.x(q[0])

circ.barrier(q)

#===== Inversion about average: psi^{[3]} =====
circ.h(q[0])
circ.h(q[1])
circ.x(q[0])
circ.x(q[1])
```

IBM Implementation: Qiskit

Measurement

```
#===== Meaurement =====
circ.measure(q,c)

#job
job = execute(circ, backend=backend, shots=1000)
result = job.result()

#circuit
figure = circ.draw(output='mpl')
figure.savefig('../data/images/qiskit-circuit.png')

#histogram
counts = result.get_counts(circ)
print("Total counts:")
print(counts)

figure = plot_histogram(counts)
figure.savefig('../data/images/qiskit-histogram.png')
```

IBM Implementation: Qiskit

Measurement

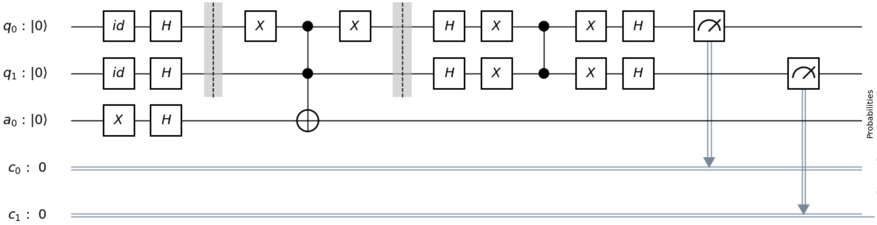


Figure: Quantum Circuit

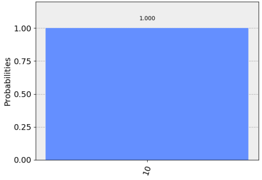


Figure: Histogram

IBM Implementation: Quantum Experience

https://www.research.ibm.com/ibm-q/technology/experience/

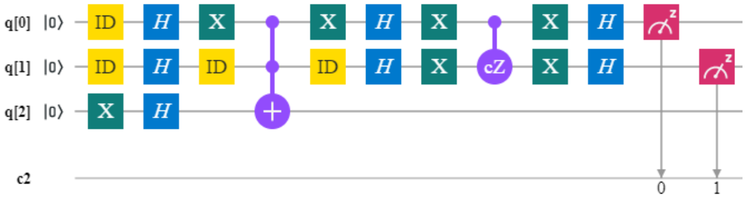


Figure: Quantum Circuit

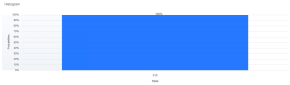


Figure: Histogram

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