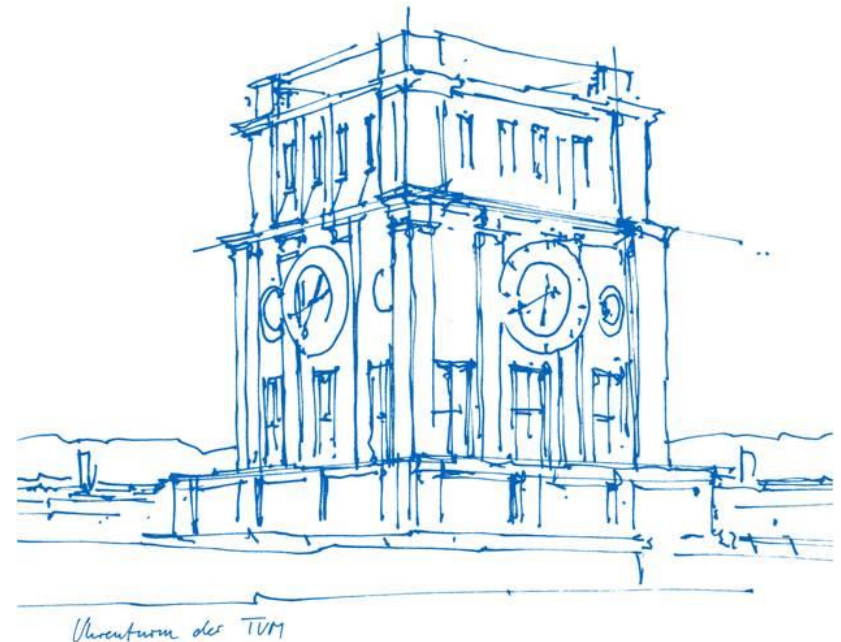


Seminar Advanced Topics of Quantum Computing

Technische Universität München

Munich, 17. November 2023



Circuit Simulation

Statevector simulator with Python

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Munich, 17. November 2023



Content of Seminar Work

1. Quantum circuit model in general
2. Quantum Information
 - Vectors
 - Unitary matrices
3. Quantum circuit basic gates examples
4. Statevector simulation on Python

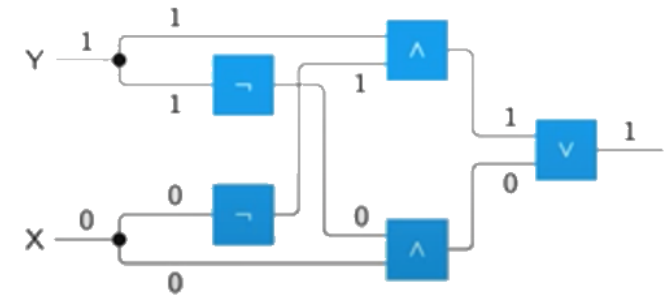
Quantum Circuits Model

Circuit – general model of computation:

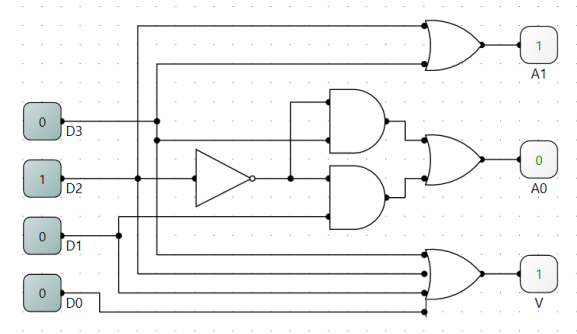
- Wires carry information
- Gates represent operations
- Circuits are always acyclic
- Information flows from left to right

Quantum algorithms are most commonly described by a **Quantum circuit**:

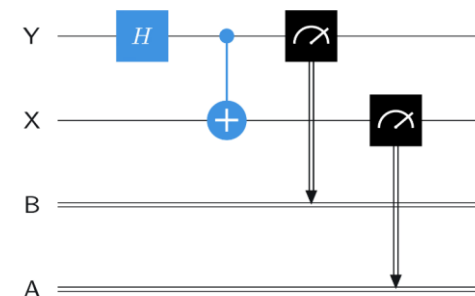
- Wires represent qubits
- Gates represent:
 - unitary operations
 - measurements



Boolean logic



Electrical engineering



Quantum circuit

- Quantum states are represented by **vectors**,
Operations are represented by **unitary matrices**
- Standard basis measurements
- Unitary operations (Gates)

$$v = \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix} \text{ Euclidean norm}$$

$$\|v\| = \sqrt{\sum_{k=1}^n |\alpha_k|^2}.$$

Quantum state vectors

A quantum state of a system is represented by a **column vector** (state set Σ), similar to probabilistic states

1. The entries of a quantum state vector are **complex numbers**.
2. The sum of the **absolute values squared** of the entries of a quantum state vector is 1.

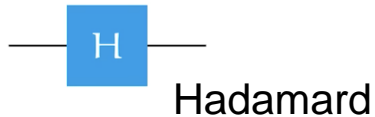
$$|\psi\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_n \end{pmatrix} \frac{1}{\sqrt{|\Sigma|}} \sum_{a \in \Sigma} |a\rangle,$$

Dirac notation quantum state vector:
number of elements in Σ

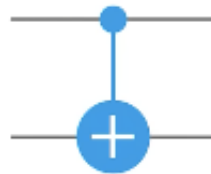
Basic Quantum Gates (=Unitary operations on qubits):

- are operations applied to a qubit that changes the quantum state of the qubit for quantum computation to solve the problem

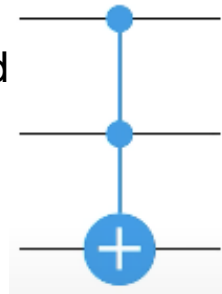
Single-qubit gates:



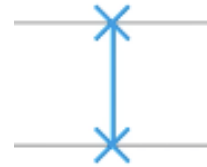
Multi-qubit gates:



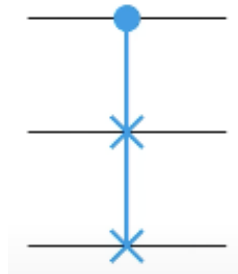
Controlled- NOT



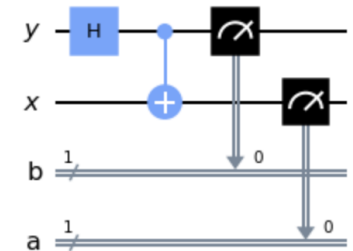
Toffoli gate**



Swap gate



Fredkin gate



**Double controlled-NOT gate (CCX), has two control qubits and one target. It applies a NOT to the target only when both controls are in state $|1\rangle$

The rotation operators are defined as:

$$R_x(\theta) = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -i \sin\left(\frac{\theta}{2}\right) \\ -i \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix}$$

$$R_y(\theta) = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix}$$

$$R_z(\theta) = \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix}$$

Parametric gate: the matrix depends on the *parameter*, which should be passed together *with the qubits on which the gate should act*

are generated by exponentiation of the Pauli matrices according to:

$$\exp(iAx) = \cos(x) I + i \sin(x) A$$

where A is one of the three Pauli Matrices.

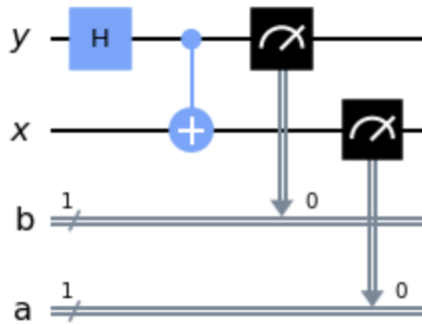
- Rz rotation operator can also be expressed as

$$\begin{pmatrix} e^{i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix} \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}$$

which differs from the definition above by a global phase only.

Examples of operation on information using gates

- **Hadamard Gate** perform first operation, **Controlled -NOT** the second



- Control- Y qubit
- Target- X qubit

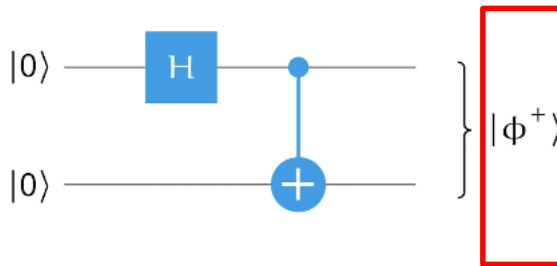
time
multiplication

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \end{pmatrix}.$$

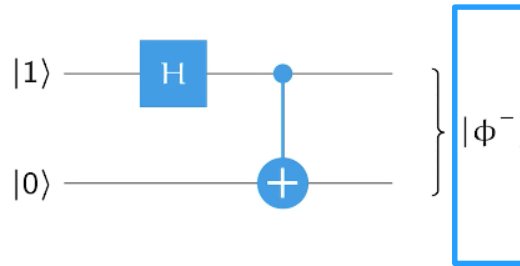
1. Controlled-NOT 2. Hadamard

Explanation of calculations

Run qubit at ket $|0\rangle, |0\rangle$

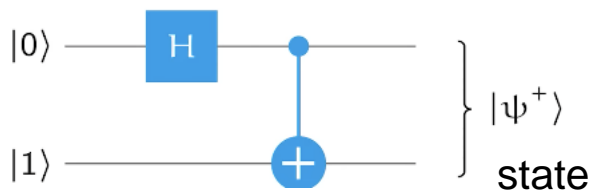


Run qubit at ket $|1\rangle, |0\rangle$

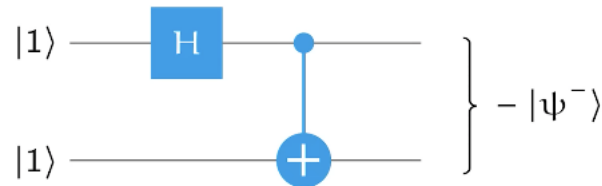


$$\begin{aligned} U|00\rangle &= |\phi^+\rangle \\ U|01\rangle &= |\phi^-\rangle \\ U|10\rangle &= |\psi^+\rangle \\ U|11\rangle &= -|\psi^-\rangle \end{aligned}$$

Run qubit at ket $|0\rangle, |1\rangle$

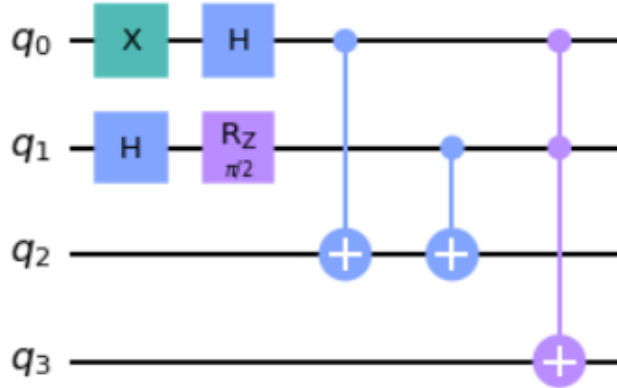


Run qubit at ket $|1\rangle, |1\rangle$



$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \end{pmatrix}$$

Statevector simulator with Python



```
import numpy as np
import matplotlib.pyplot as plt
```

```
q = QuantumCircuit(4)
q.x(0) # NOT gate on Q0
q.h(0) # Hadamard gate on Q0
q.h(1) # Hadamard gate on Q1
q.rz(np.pi/2, 1) # RZ gate on Q1
q.cx(0, 2) # Controlled NOT gate Q0 -> Q2
q.cx(1, 2) # Controlled NOT gate Q1 -> Q2
q.ccx(0, 1, 3) # Toffoli gate Q0 & Q1 -> Q3
print("State vector:\n", q.get_statevector())
print("Measurements:\n", q.measure(5))
q.draw_measures()
```

State vector:

```
[ 0.35355339-0.35355339j  0.      +0.j      0.      +0.j
  0.      +0.j      0.      +0.j      0.      +0.j
  0.35355339+0.35355339j  0.      +0.j      0.      +0.j
  0.      +0.j      -0.35355339+0.35355339j  0.      +0.j
  0.      +0.j      -0.35355339-0.35355339j  0.      +0.j
  0.      +0.j      ]
```

I built Python statevector simulator use Qiskit as a reference to understand, what it is doing under the hood

https://github.com/MarinaZuzu/Test_-Quantum-Computing-Seminar/tree/main

Class QuantumCircuit

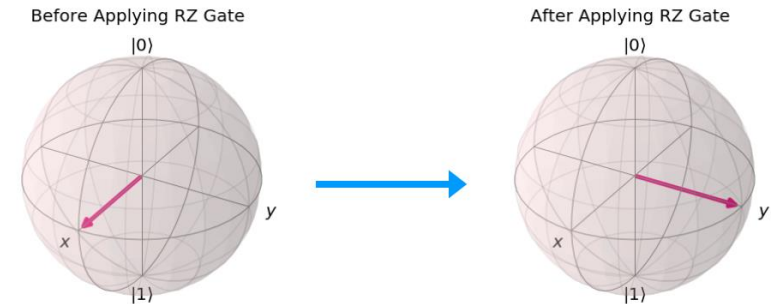
```
# Class QuantumCircuit
class QuantumCircuit:
    def __init__(self, qubits):
        if qubits < 1:
            raise Exception("qubits should be more than zero")
        self.qubits = qubits
        self.measures = {}

    # Init state vector
    self.state_vector = np.zeros((2**qubits), dtype=complex)
    # Start from state "0000"
```

Parametric gate (RZ) simulation

- The gate matrix depends on the parameter
- Parameter (phi) passed together with the qubits
- RZ-gate is a single-qubit rotation about the Z axis

$$RZ(\lambda) = \exp\left(-i\frac{\lambda}{2}Z\right) = \begin{pmatrix} e^{-i\frac{\lambda}{2}} & 0 \\ 0 & e^{i\frac{\lambda}{2}} \end{pmatrix}$$



```
def rz(self, phi, q0):

    if not self.__check_param(q0):
        raise Exception("wrong parameter")

    # Init RZ gate matrix
    RZ = np.array([[np.exp(-0.5j*phi), 0], [0, np.exp(0.5j*phi)]], dtype=complex) # rz(phi, 0)
    print("\nRZ gate base matrix:\n", RZ)

    # Adjust RZ gate matrix for circuit size
    I = np.eye(2**(self.qubits - 1))
    RZI = np.kron(RZ, I)
    print("\nRZ gate matrix for qubit 0:\n", RZI)

    # reorder to qbit q0
    perm = self.__get_perm(q0)
    G = self.__reorder_gate(RZI, perm)
    print("\nRZ gate matrix for qubit {}: \n".format(q0), G)

    # calculate new state vector
    self.state_vector = np.matmul(G, self.state_vector)
```

Measurement of qubit's states simulation

- Sampling from the statevector
- Measure all qubits
- Result of a single measurement as a bitstring

```
def measure(self, shots):

    # calculate probability distribution
    distribution = abs(self.state_vector)**2
    print("Distribution:\n", distribution)

    # perform measures with a random sample function
    self.measures = {}
    for i in range(shots):
        sample = np.random.choice(len(distribution), p=distribution)
        key = f"{sample:0{self.qubits}b}" # single measurement as a bitstring
        if key in self.measures:
            self.measures[key] += 1
        else:
            self.measures[key] = 1

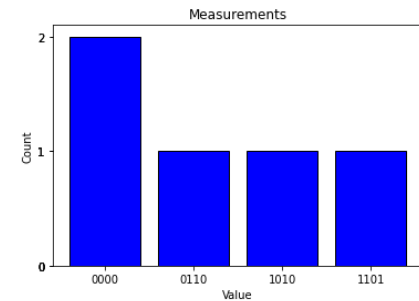
    # sort the dictionary
    self.measures = dict(sorted(self.measures.items()))
    return self.measures
```

```
print("State vector:\n", q.get_statevector())
print("Measurements:\n", q.measure(5))
q.draw_measures()
```

```
State vector:
[ 0.35355339-0.35355339j  0.          +0.j          0.          +0.j
  0.          +0.j          0.          +0.j          0.          +0.j
  0.35355339+0.35355339j  0.          +0.j          0.          +0.j
  0.          +0.j          -0.35355339+0.35355339j  0.          +0.j
  0.          +0.j          -0.35355339-0.35355339j  0.          +0.j
  0.          +0.j          ]
```

```
Distribution:
[0.25 0.  0.  0.  0.  0.  0.25 0.  0.  0.  0.25 0.  0.  0.25
 0.  0. ]
```

```
Measurements:
{'0000': 2, '0110': 1, '1010': 1, '1101': 1}
```

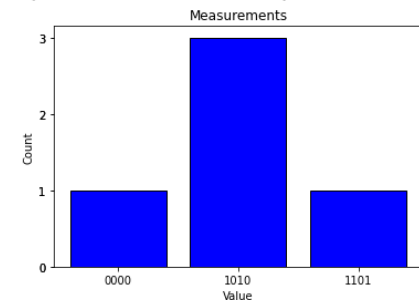


```
print("State vector:\n", q.get_statevector())
print("Measurements:\n", q.measure(5))
q.draw_measures()
```

```
State vector:
[ 0.35355339-0.35355339j  0.          +0.j          0.          +0.j
  0.          +0.j          0.          +0.j          0.          +0.j
  0.35355339+0.35355339j  0.          +0.j          0.          +0.j
  0.          +0.j          -0.35355339+0.35355339j  0.          +0.j
  0.          +0.j          -0.35355339-0.35355339j  0.          +0.j
  0.          +0.j          ]
```

```
Distribution:
[0.25 0.  0.  0.  0.  0.  0.25 0.  0.  0.  0.25 0.  0.  0.25
 0.  0. ]
```

```
Measurements:
{'0000': 1, '1010': 3, '1101': 1}
```



Thank you!



1. <https://www.quantum-inspire.com/kbase/what-is-a-quantum-algorithm>
2. <https://learning.quantum-computing.ibm.com/tutorial/composer-user-guide>
3. [https://colab.research.google.com/github/MarinaZuzu/Test_-Quantum-Computing-Seminar/blob/main/sim-wrapped-inclass%20\(2\).ipynb#scrollTo=f3d7774f-1f7a-416d-a57a-857e84c7c0c5](https://colab.research.google.com/github/MarinaZuzu/Test_-Quantum-Computing-Seminar/blob/main/sim-wrapped-inclass%20(2).ipynb#scrollTo=f3d7774f-1f7a-416d-a57a-857e84c7c0c5)