An Introduction to Quantum Computing

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Two-State Qubits

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Before entering Qubits in details we take a look at the Schrödingers equation:

- The smallest unit of information in Quantum Computing is the Quantum-bit or Qubit.
- A Qubit represents the state of the wavefunction $|\phi\rangle$ in Schrödingers equation at a specific time.
- A single Qubit may be in the “on” state ($|1\rangle$) or it may be in the “off” state ($|0\rangle$) or any linear combination thereof.
- Schrödingers equation, which describes how the state of a quantum mechanical system evolves in time is linear. Hence, linear combinations of solutions are also valid solutions.

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Schrödingers Equation and Impact:

- **Schrödingers Equation:**

$$\frac{\partial\,|\psi(t)\rangle}{\partial t} = -i\,\frac{\widehat{H}\,|\psi(t)\rangle}{\hbar} = -i\,\frac{2\,\pi\,\widehat{H}\,|\psi(t)\rangle}{h} \qquad (1)$$

  where $\hbar$ is the reduced Planck constant $\hbar = h/(2\pi)$, and $\widehat{H}(t)$ is the Hamiltonian of the system.
- Schrödingers Equation describes how the state changes in time depending on the Hamiltonian.
- Eq. (1) can be slightly rewritten as:

$$i\,\hbar\,\frac{\partial}{\partial t}|\psi(t)\rangle = \widehat{H}\,|\psi(t)\rangle \qquad (2)$$

  which is a first order linear differential equation.

A quantum system is a system that obeys the laws and postulates of quantum mechanics

- A single qubit, two-state quantum system can be described by two orthonormal basis vectors using Dirac *braket* notation:

$$\mathrm{ket}(0) = |0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad \mathrm{ket}(1) = |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{3}$$

- Say we have a unitary transformation described by the unitary transfer matrix Q:

$$Q = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{4}$$

As an example, applying $|0\rangle$ to the matrix Q leads to $Q\,|0\rangle$.

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Qubit states:

- The two basis state vectors $|0\rangle$ and $|1\rangle$ form two orthonormal basis states $\{|0\rangle, |1\rangle\}$.
- The orthonormal basis states $\{|0\rangle, |1\rangle\}$ are jointly called the computational basis, which spans two-dimensional linear vector (Hilbert) space of the qubit.
- A pure qubit state is a coherent superposition of the basis states – a single qubit can thus be described as a linear combination of $|0\rangle$ and $|1\rangle$:

$$|\psi\rangle = a_0|0\rangle + a_1|1\rangle$$

where a_0 and a_1 are complex probability amplitudes.

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A pure quantum state is described by:

- A quantum state $|\psi\rangle$ is a high-dimensional vector in Hilbert space.
- In the following, we use $|0\rangle$ and $|1\rangle$ as basis states – the set of basis states $\{|0\rangle, |1\rangle\}$ must be orthogonal but can otherwise be randomly chosen.
- The state $|\psi\rangle$ is referred to as being a pure state if its length is unity, i.e. $\langle\psi|\psi\rangle = 1$ or equivalently $\||\psi\rangle\|^2 = 1$.

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A qubit can represent two pure states, but also:

- in a superposition state between the two pure states.
- individual measuring of a state is random, while probabilities can be predicted via quantum mechanics.
- entanglement with another qubit.

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Properties of BITS and QUBITS:

CLASSICAL BITS (BITS)	QUANTUM BITS (QUBITS)
A single bit can be either state 0 or state 1	A qubit can be in basis/core state $\|0\rangle$, in basis/core state $\|1\rangle$ or any state being a linear (potentially complex) combination of the two
Can be measured completely	Can be measured partly with given probability
Unchanged states after measurement	States are changed by measurement
A bit can be copied	A qubit cannot be copied
A bit can be erased	A qubit cannot be erased

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A quantum system is a system that obeys the laws and postulates of quantum mechanics:

- Dirac *braket* notation → 'ket':

$$\mathrm{ket}(v) = |v\rangle = v = \begin{bmatrix} v_0 \\ v_1 \\ \vdots \\ v_n \end{bmatrix} \tag{5}$$

- Dirac *braket* notation → 'bra':

$$\mathrm{bra}(u) = \langle u| = u^\dagger = [u_0^*, u_1^*, \ldots, u_n^*] \tag{6}$$

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- Dirac *braket* notation → 'inner product':

$$\langle u|v\rangle = \langle u| \cdot |v\rangle = (u, v) = \langle u, v\rangle = u^\dagger\, v \qquad (7)$$

$$= u_0^*\, v_0 + u_1^*\, v_1 + \cdots + u_n^*\, v_n \qquad (8)$$

- Dirac *braket* (*ketbra*) notation → 'outer product':

$$|v\rangle\,\langle u| = v\, u^\dagger \qquad (9)$$

$$= \begin{bmatrix} v_0 \\ v_1 \\ \vdots \\ v_n \end{bmatrix} [u_0^*, u_1^*, \ldots, u_n^*] \qquad (10)$$

$$= \begin{bmatrix} u_0^*\, v_0 & u_1^*\, v_0 & \cdots & u_n^*\, v_0 \\ u_0^*\, v_1 & u_1^*\, v_1 & \cdots & u_n^*\, v_1 \\ \vdots & \vdots & \ddots & \vdots \\ u_0^*\, v_n & u_1^*\, v_n & \cdots & u_n^*\, v_n \end{bmatrix} \qquad (11)$$

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Matrix Density (more follows later):

- In quantum mechanics, a density matrix (or density operator) is a matrix that describes the quantum state of a physical system. It allows for the calculation of the probabilities of the outcomes of any measurement performed upon this system. It is a generalization of the more usual state vectors or wavefunctions: density matrices can also represent mixed states. Mixed states arise in two situations:
  - when the preparation of the system is not fully known, and thus one must deal with a statistical ensemble of possible preparations, and
  - when one wants to describe a physical system that is entangled with another, without describing their combined state (system interacting with an environment).
- Density matrices are thus crucial tools when dealing with mixed states, such as quantum statistical mechanics, quantum decoherence, and quantum information.

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A quantum system is a system that obeys the laws and postulates of quantum mechanics[1]:

1. The system's state at a given time is described by a wave function vector, $\psi(t)$, in a complex vector space.
2. $\psi(t)$ evolves over time as Schrödingers wave equation.
3. Each measurable system attribute that can be measured is represented by a linear operator on its vector space.

[1] https://physics.stackexchange.com/questions/505541/what-is-a-quantum-system

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A quantum system is a system that obeys the laws and postulates of quantum mechanics[2]:

4. The act of measuring an observable of the system causes the system's wave function to "collapse" to an eigenstate of the corresponding operator. The result of the measurement will be the eigenvalue of that eigenstate.
5. The probability that a measurement of an observable of the system at a given time will return a given value is the squared modulus of the complex amplitude of the projection of its wave function (immediately before the measurement) onto the corresponding eigenstate.

[2] https://physics.stackexchange.com/questions/505541/what-is-a-quantum-system

Characteristics:

- The example demonstrates how a single qubit can be initialized to a certain state vector.
- Assuming we have an orthonormal set of basis vectors $|0\rangle$ and $|1\rangle$ given by:

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{12}$$

- The state of the qubit q is thus:

$$\begin{aligned} |\psi\rangle &= a_0\,|0\rangle + a_1\,|1\rangle && (13) \\ &= a_0 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + a_1 \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} && (14) \end{aligned}$$

Both $|\psi\rangle = [a_0,\, a_1]^{\mathrm{T}}$ and $\langle\psi| = [a_0^*,\, a_1^*]$ are named *statevectors*.

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Example 1: Qubit Initialization

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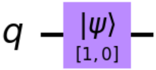
istate0.py:

```
#

# Import tools
from qiskit import QuantumCircuit, assemble, Aer
from qiskit.visualization import plot_histogram, plot_bloch_vector
from math import sqrt, pi

# Create a quantum circuit with one qubit
qc = QuantumCircuit(1)

# Define initial_state as |1> ; apply initialisation to the 0th qubit ; draw circuit
initial_state1 = [1, 0]
qc.initialize(initial_state1, 0)
qc.draw('mpl', filename="Lectures/#3/initial_state/results/state0")
```

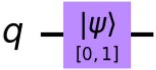
Two-State Qubits
Example 1: Qubit Initialization

The following provides three initializations of q statevectors.

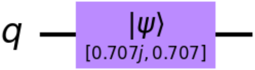
- Initialize qubit q to the statevector $|\psi\rangle = [1,\ 0]^{\mathrm{T}}$:



- Initialize qubit q to the statevector $|\psi\rangle = [0,\ 1]^{\mathrm{T}}$:



- Initialize qubit q to the statevector $|\psi\rangle = \frac{1}{\sqrt{2}}\,[i,\ 1]^{\mathrm{T}}$:



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Characteristics:

- The example demonstrates how a single qubit can be initialized to a certain state vector. This is identical to Example 1.
- Next is that we simulate (with quantum noise . . . or?) and estimate the possible outcomes by printing.
- The state of the qubit q is thus simulated.

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meas_statevector.py:

```python
# Import relevant packages, functions, ...
from qiskit import QuantumCircuit, Aer
from qiskit.visualization import plot_histogram, plot_bloch_vector
from math import sqrt, pi, log2
import os

# Define a function to map from statevector to dictionary
def statevector_to_dict(sv):
    bit_mask = f"0{int(log2(len(sv)))}b"
    return {format(i, bit_mask): v.real for i, v in enumerate(sv)}

# Define quantum circuit and some initial statevectors
Q_circuit = QuantumCircuit(1)  # Create a quantum circuit with one qubit
initial_state0 = [0, 1]    # Define initial_state as |1>
initial_state1 = [1, 0]    # Define initial_state as |0>
initial_state2 = [1/sqrt(2), 1/sqrt(2)]

# Apply initialisation operation to the 0th qubit
Q_circuit.initialize(initial_state2, 0)
Q_circuit.draw('mpl', filename="Lectures/#3/measurement/results/init_state")
```


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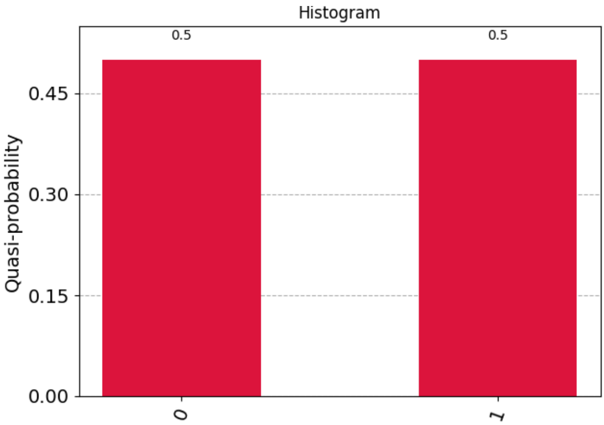
meas_statevector.py:

```python
# Run the quantum circuit on a statevector simulator backend
simulator = Aer.get_backend('statevector_simulator')

# Create a Quantum program for execution
job = simulator.run(Q_circuit)
result = job.result()
outputstate = result.get_statevector(Q_circuit, decimals=3)
print(outputstate)

# Map statevector to dictionary
sv_dict = statevector_to_dict(outputstate.data)
plot_histogram(sv_dict, legend=None, color=['crimson'], title="Histogram", filename="
    Lectures/#3/measurement/results/hist")
```

meas_statevector.py:



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Qgates:

- A quantum gate (quantum logic gate) is a functional unit (matrix) that transfer input state/states to an output state according to the properties of the quantum gate.
- A number of connected (normally different) qgates form a qcircuit that implements an algorithm. This is similar to low-level electronics using connected binary gates (OR, AND, XOR etc.) to achieve a logical desired link between input variables (states) and output variables (states).
- Due to normalization constraints, any gate operation U must be unitary:

$$UU^\dagger = U^\dagger U = I, \quad U, I \in \mathbb{C}^{2^N \times 2^N} \tag{15}$$

where U is a complex square matrix, $U^\dagger$ is the conjugate transpose of U, and I is the identity matrix.

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A unitary matrix $U \in \mathbb{C}^{2^N \times 2^N}$ has the following properties:

- Given two complex vectors $u, v \in \mathbb{C}^{2^N \times 1}$, multiplication preserves the inner product: $\langle u|v\rangle = \langle U\,u|U\,v\rangle$.
- U is normal, i.e. $UU^\dagger = U^\dagger U$.
- U is diagonalizable meaning that U can be decomposed as $U = A\Delta A^\dagger$ where A is unitary, and Δ is unitary and diagonal.
- $|\det(U)| = 1$ meaning that $\det(U)$ is on the unit circle of the complex plane.
- The eigenspaces of U are orthogonal.
- $U = \exp\left[i\,H\right]$ where $i = \sqrt{-1}$ and H is a Hermitian matrix.

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Qgates:

- To compute the output state we start by defining input basis states as vectors:

$$|\mathbf{0}\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad |\mathbf{1}\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{16}$$

- Say we have a unitary transformation described by the unitary transfer matrix Q:

$$Q = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{17}$$

Specifically, this matrix is referred to as the Pauli-X Qgate.

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Qgates:

- Applying the input state $|0\rangle$ to the transformation matrix Q leads to:

$$|0\rangle \longrightarrow Q\,|0\rangle = Q\begin{bmatrix}1\\0\end{bmatrix} = |1\rangle \qquad (18)$$

- Applying the input state $|1\rangle$ to the transformation matrix Q leads to:

$$|1\rangle \longrightarrow Q\,|1\rangle = Q\begin{bmatrix}0\\1\end{bmatrix} = |0\rangle \qquad (19)$$

- This means that $|0\rangle \xrightarrow{Q} |1\rangle$ and $|1\rangle \xrightarrow{Q} |0\rangle$. In other words, the Pauli-X Qgate flips the state.

Operator	Symbol	Matrix	Comments
Pauli-X	$\mathbf{X}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	Pauli matrices: $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \in \mathbb{C}^{2\times 2}$. All are Hermitian ($\mathbf{M} = \mathbf{M}^\dagger$), involutory ($\mathbf{M}^2 = \mathbf{I}$) and unitary ($\mathbf{M}\mathbf{M}^\dagger = \mathbf{M}^\dagger\mathbf{M} = \mathbf{I}$).[3]
Pauli-Y	$\mathbf{Y}$	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$	
Pauli-Z	$\mathbf{Z}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$	
Hadamard	$\mathbf{H}$	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$	
Phase	$\mathbf{S}$	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$	

[3] For more details see Nielsen & Chuang: “Quantum Computation and Quantum Information”, Cambridge University Press, 2010.

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