Quantum Computing

1. Qubits

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References

- B Schumacher, M Westmoreland. **Quantum Processes Systems**, and Information. Cambridge University Press, 2010.
- MA Nielsen, IL Chuang. **Quantum Computation and Quantum Information**. Cambridge University Press, 2002.

Quantum Computers

- IBM Q Experience - https://quantum-computing.ibm.com/
- D-Wave LEAP - https://www.dwavesys.com/take-leap

Simulators

- **Quirk** - https://algassert.com/quirk
- **QuTIP** - http://qutip.org/
- **Qiskit** - https://qiskit.org/
- **Quantum Computing Playground** - http://www.quantumplayground.net/
- Many more... https://quantiki.org/wiki/list-qc-simulators

[1]:
```
from qutip import *
from qutip.qip.operations import *
import numpy as np
```

Qubits

- A qubit is $|\Phi\rangle = a|0\rangle + b|1\rangle$, $a, b \in \mathbb{C}$
  - Forms a vector space over $\mathbb{C}^2$ with basis

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

  - Normalised: $a^2 + b^2 = 1$
  - Point (ϕ, θ) on the Bloch sphere (ignoring global phase γ)

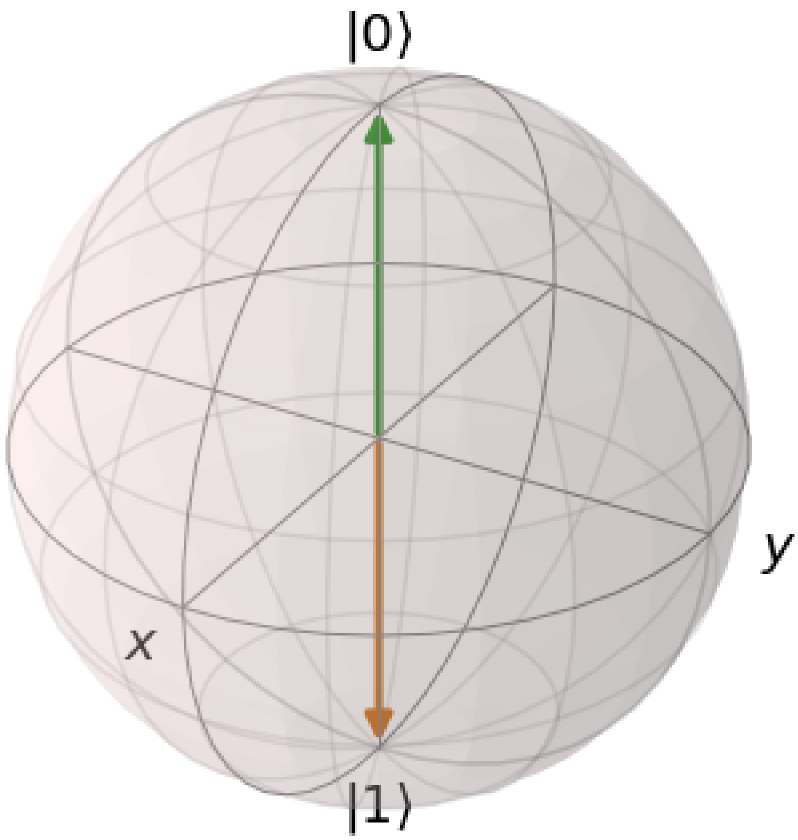
$$a = e^{i\gamma} \cos\left(\frac{\phi}{2}\right), b = e^{i(\gamma+\theta)} \sin\left(\frac{\phi}{2}\right)$$

- Qubit is in **superposition** of $|0\rangle$ and $|1\rangle$
  - with probability a^2 in $|0\rangle$ and probability b^2 in $|1\rangle$

[2]:
```
Zero = basis(2,0)
One = basis(2,1)
print(Zero,"\n",One)
```

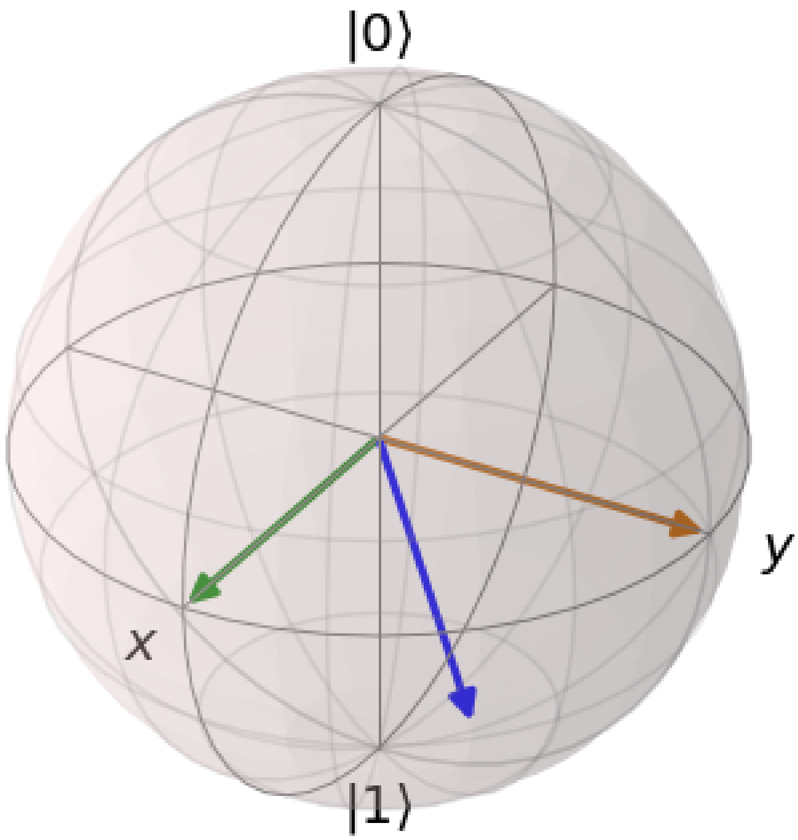
```
b = Bloch()
b.add_states([Zero,One])
b.show()
```

```
Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[1.]
 [0.]]
 Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
Qobj data =
[[0.]
 [1.]]
```



[3]:
```
psi_x = (Zero + (1+0j) * One).unit()
psi_y = (Zero + (0+1j) * One).unit()
psi_z = (Zero + (1+1j) * One).unit()

b = Bloch()
b.add_states([psi_x,psi_y,psi_z])
b.show()
```



Single Qubit Gates

- (Pure) quantum program for a single qubit: **rotation on the Bloch sphere**
  - This is a unitary operator U (bounded, linear, $UU^\dagger = U^\dagger U = I$)
  - Could be constructed from individual operations (gates; unitary operators)
  - Change the phase (rotation around z axis)
  - Change the probability of being in $|0\rangle$ or $|1\rangle$ (rotation around x or y axis)
  - Or arbitrary combinations of these
- E.g. the **Hadamard gate**

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

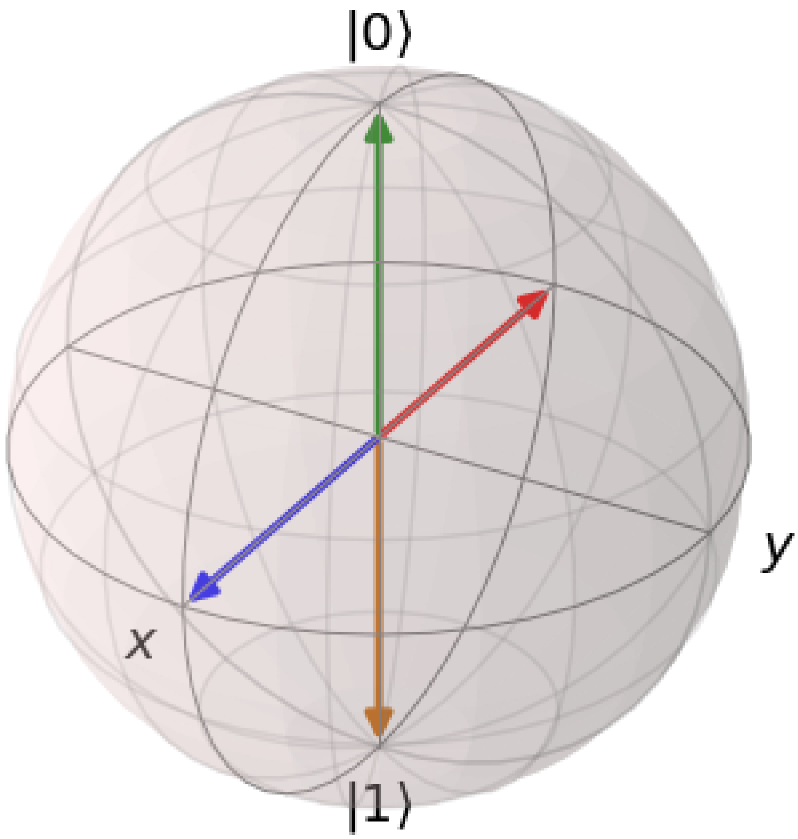
  - Used to put qubits into a superposition state: map $|0\rangle$ to $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |+\rangle$
  - Also $|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle$
  - $\pi/2$ rotation about Z, then $\pi/2$ rotation about Y axis
  - $|+\rangle, |-\rangle$ forms the **superposition/Hadamard basis** (compared to $|0\rangle, |1\rangle$ Z basis)

[4]:
```
H = 1/np.sqrt(2) * Qobj([[1,1],[1,-1]]) # or H = snot()

Psi0 = H * ket("0") # or Zero
```

```
Psi1 = H * ket("1") # or One

b = Bloch()
b.add_states([ket("0"),ket("1"),Psi0,Psi1])
b.show()
```



Common Single Qubit Gates

- Pauli gates: half turn (π) around X, Y, Z axis

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \qquad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

- Hadamard gate

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

- ^1/2 ($\pi/2$), ^1/4 ($\pi/4$), ^1/8 ($\pi/8$) Pauli gates, etc.; e.g. the phase gate

$$S = Z^{\frac{1}{2}} = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}; SS = Z$$

- General single qubit gate

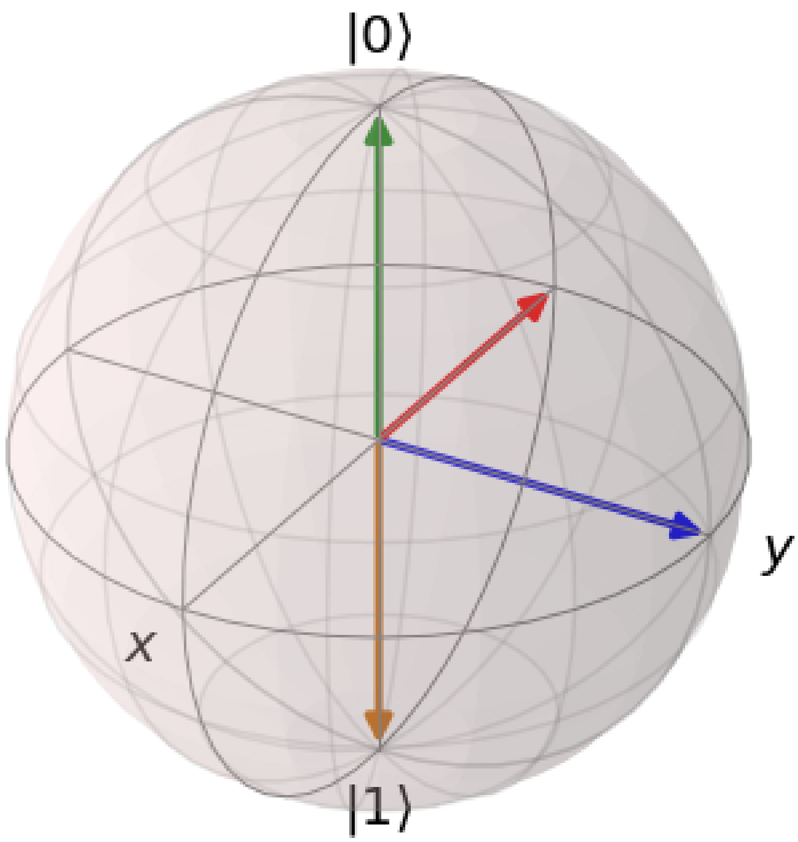
$$U = \begin{bmatrix} \cos(\theta/2) & -e^{i\lambda}\sin(\theta/2) \\ e^{i\phi}\sin(\theta/2) & e^{i\lambda+i\phi}\cos(\theta/2) \end{bmatrix}$$

- Note, any quantum gate U must be a unitary operation: $UU^{\dagger} = I$

[5]:
```
X = sigmax()
Y = sigmay()
Z = sigmaz()

Psi1 = Y * ket("0")
Psi2 = X.sqrtm() * Psi1
Psi3 = Z.sqrtm() * Psi2

b = Bloch()
b.add_states([ket("0"),Psi1,Psi2,Psi3])
b.show()
```



- Quirk

Measurements

- Non-unitary part of quantum programs (projective) to read out state (probabilisitic, dependent on measurement basis)
- A quantum measurment is described by a set of measurement operators $\{M_m\}$
  - Index m refers to the measurement outcome (e.g. 0, 1)
- Probability that the results m occurs for a state $|\Psi\rangle$ is

$$p_m = \langle\Psi|M_m^\dagger M_m|\Psi\rangle$$

  - $\langle\Psi|$ is $|\Psi\rangle$ (column vector; ket) as row vector (complex conjugate transpose; dagger; bra)
- The state of the system after the measurement, resulting in m, is

$$\frac{M_m|\Psi\rangle}{\sqrt{p_m}}$$

- The opeartors must satisfy the completeness equation

$$\sum_m \frac{M_m|\Psi\rangle}{\sqrt{p_m}} = I$$

Projective Measurements

- Simplest type of measurements, where $M_m^2 = M_m$
- Measurement operators for the "Z basis":

$$M_0 = |0\rangle\langle 0| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$M_1 = |1\rangle\langle 1| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

- For $|\Psi\rangle = a|0\rangle + b|1\rangle$: * $p_0 = \langle\Psi|M_0^\dagger M_0|\Psi\rangle = a^2$ * $p_1 = \langle\Psi|M_1^\dagger M_1|\Psi\rangle = b^2$

[6]:
```
M0 = ket("0") * bra("0")
M1 = ket("1") * bra("1")

print(M0.full()); print(M1.full()) # .full() to simplify output
```

```
[[1.+0.j 0.+0.j]
 [0.+0.j 0.+0.j]]
[[0.+0.j 0.+0.j]
 [0.+0.j 1.+0.j]]
```

[7]:
```
Psi = (ket("0") + ket("1")).unit()  # |+>
p_0 = Psi.dag() * (M0.dag() * M0) * Psi
p_1 = Psi.dag() * (M1.dag() * M1) * Psi

print(p_0.full(),p_1.full())
```

```
[[0.5+0.j]] [[0.5+0.j]]
```

[8]:
```
Psi = (ket("0") - ket("1")).unit() # |->
p_0 = Psi.dag() * (M0.dag() * M0) * Psi
```

```
p_1 = Psi.dag() * (M1.dag() * M1) * Psi

print(p_0.full(),p_1.full())
```

```
[[0.5+0.j]] [[0.5+0.j]]
```

- Measurement operators for the superposition basis

$$M_+ = |+\rangle\langle+| = \frac{1}{2}\begin{bmatrix}1 & 1\\1 & 1\end{bmatrix}$$

$$M_- = |-\rangle\langle-| = \frac{1}{2}\begin{bmatrix}1 & -1\\-1 & 1\end{bmatrix}$$

[9]:
```
MP = (ket("0") + ket("1")).unit () * (bra("0") + bra("1")).unit ()
MM = (ket("0") - ket("1")).unit () * (bra("0") - bra("1")).unit ()

print(MP.full()); print(MM.full())
```

```
[[0.5+0.j 0.5+0.j]
 [0.5+0.j 0.5+0.j]]
[[ 0.5+0.j -0.5+0.j]
 [-0.5+0.j  0.5+0.j]]
```

[10]:
```
Psi = (ket("0") + ket("1")).unit()
p_P = Psi.dag() * (MP.dag() * MP) * Psi
p_M = Psi.dag() * (MM.dag() * MM) * Psi

print(p_P.full(),p_M.full())
```

```
[[1.+0.j]] [[0.+0.j]]
```

[11]:
```
Psi = (ket("0") - ket("1")).unit()
p_P = Psi.dag() * (MP.dag() * MP) * Psi
p_M = Psi.dag() * (MM.dag() * MM) * Psi

print(p_P.full(),p_M.full())
```

```
[[0.+0.j]] [[1.+0.j]]
```

Measurement basis

- Some states are not distinguishable in a particular measurement basis
  - Cannot distinguish phase of $|+\rangle$ and $|-\rangle$ when measuring in the Z basis
  - That means we can never know the full quantum state (cf. Heisenberg uncertainty)
- We cannot arbitrarily specify the measurement basis (usually it is fixed to the Z basis)
  - So how can we distinguish between $|+\rangle$ and $|-\rangle$?
  - Try it with this quirk circuit.
- Understand probability vs. phase vs. measurement basis
  - E.g. z-axis rotations in the Z vs superposition measurement basis
  - Circuit

Multiple Qubits

- Tensor product of single qubit states
  - Two qubit states: $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$
  - Three qubit states: $|000\rangle$, $|001\rangle$, $|010\rangle$, $|011\rangle$, …
  - Qubits from right-to-left are top-down in the circuit (right-most/top bit is the least significant bit; but not always used consistently)
- Single states:
  - $\Psi_0 = a|0\rangle + b|1\rangle$
  - $\Psi_1 = c|0\rangle + d|1\rangle$
  - $\Psi_2 = e|0\rangle + f|1\rangle$
- To combine qubits, take **tensor product** states:

$$\Psi_{10} = \Psi_1 \otimes \Psi_0 = ca|0_1 0_0\rangle + cb|0_1 1_0\rangle + da|1_1 0_0\rangle + db|1_1 1_0\rangle \tag{1}$$

$$\Psi_2 \otimes \Psi_{10} = eca|0_2 0_1 0_0\rangle + ecb|0_2 0_1 1_0\rangle + eda|0_2 1_1 0_0\rangle + edb|0_2 1_1 1_0\rangle \tag{2}$$

$$+ fca|1_2 0_1 0_0\rangle + fcb|1_2 0_1 1_0\rangle + fda|1_2 1_1 0_0\rangle + fdb|1_2 1_1 1_0\rangle \tag{3}$$

- Note $|0_1\rangle \otimes |0_0\rangle = |0_1 0_0\rangle = |00\rangle$, …

Entanglement

- The tensor product space contains all states with correlations between measurements of individual qubits
  - Some are classical (cf. classical probabilities, e.g. iid vs. hidden rules)
  - Some are stronger/weaker (quantum)
- Quantum correlations are the essence of **entanglement**
  - Knowledge about the measurment result of one qubit perfectly predicts the measurement outcome of another qubit
  - E.g. $\frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$, $\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$
  - Note, such states are not representable as a (tensor) product of single qubits (we need something else to get these states)

CNOT - a Two-Qubit Gate

- Controlled-not (CNOT) gate:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} (a|0_c 0_t\rangle + b|0_c 1_t\rangle + c|1_c 0_t\rangle + d|1_c 1_t\rangle) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$$

$$= a|0_c 0_t\rangle + b|0_c 1_t\rangle + d|1_c 0_t\rangle + c|1_c 1_t\rangle = \begin{bmatrix} a & b & d & c \end{bmatrix}^t$$

  - Careful with pure vector notation and qubit basis order (it is in order of decimal value of basis-bits); usually better to keep the states instead of only using vectors
- Apply a NOT gate (the X gate) to the target qubit only if the control qubit is $|1\rangle$
  - Circuit

Full Entanglement Circuit with Operators

- Creating entanglement with CNOT gates
  - Entanglement Circuit

- Compute the linear operator for this
  - $\otimes$ as **tensor product** (**Kronecker product**) on the linear operators, e.g.:

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \otimes \begin{bmatrix} W & X \\ Y & Z \end{bmatrix} = \left[\begin{array}{cc|cc} aW & aX & bW & bX \\ aY & aZ & bY & bZ \\ \hline cW & cX & dW & dX \\ cY & cZ & dY & dZ \end{array}\right]$$

- CNOT on 2 qubit circuit, where qubit 1 is control and qubit 0 is target:

$$\mathrm{CNOT} = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes X = \mathrm{CNOT}(2, 1, 0)$$

  - Note operator on top-most / right-most (least significant) qubit is right-most in tensor product

- For qubit 1 as control and qubit 0 as target we get

[12]:
```
print(np.real( (tensor( ket("0")*bra("0"), qeye(2) ) + tensor( ket("1")*bra("1"),␣
↪sigmax()) ).full() ))
```

```
[[1. 0. 0. 0.]
 [0. 1. 0. 0.]
 [0. 0. 0. 1.]
 [0. 0. 1. 0.]]
```

- For qubit 0 as control and qubit 1 as target we get

[13]:
```
print(np.real( (tensor( qeye(2), ket("0")*bra("0") ) + tensor(sigmax(),␣
↪ket("1")*bra("1")) ).full() ))
```

```
[[1. 0. 0. 0.]
 [0. 0. 0. 1.]
 [0. 0. 1. 0.]
 [0. 1. 0. 0.]]
```

- So the full circuit is described by the following matrix operations:

[14]:
```
H = snot() * np.sqrt(2) # Remove normalisation for ease of reading
X = sigmax()
XH = tensor(X,H)

print(X.full()," x"); print(H.full()," ="); print(XH.full())
```

```
[[0.+0.j 1.+0.j]
 [1.+0.j 0.+0.j]]  x
[[ 1.+0.j  1.+0.j]
 [ 1.+0.j -1.+0.j]]  =
[[ 0.+0.j  0.+0.j  1.+0.j  1.+0.j]
 [ 0.+0.j  0.+0.j  1.+0.j -1.+0.j]
 [ 1.+0.j  1.+0.j  0.+0.j  0.+0.j]
 [ 1.+0.j -1.+0.j  0.+0.j  0.+0.j]]
```

[15]:
```
CNOT = tensor( qeye(2), ket("0")*bra("0") ) + tensor(sigmax(), ket("1")*bra("1") )
CIRCUIT = CNOT*XH

print('CNOT*(X x H) ='); print(CIRCUIT.full())
```

```
CNOT*(X x H) =
[[ 0.+0.j  0.+0.j  1.+0.j  1.+0.j]
 [ 1.+0.j -1.+0.j  0.+0.j  0.+0.j]
 [ 1.+0.j  1.+0.j  0.+0.j  0.+0.j]
 [ 0.+0.j  0.+0.j  1.+0.j -1.+0.j]]
```

[16]:
```
print((CIRCUIT * ket("00") / np.sqrt(2)).full()) # divive by sqrt(2) to normalise (see␣
↪above)
```

```
[[0.        +0.j]
 [0.70710678+0.j]
 [0.70710678+0.j]
 [0.        +0.j]]
```

Multi-Qubit Gates

- Any arbitrary unitary transformation on n qubits can be constructed from single qubit gates and CNOT.
  - Still useful to have other gates
- Generalise CNOT to applying other single qubit gates U:

$$|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U$$

[17]:
```
U = snot()
print((tensor(ket("0")*bra("0"),qeye(2)) + tensor(ket("1")*bra("1"),U)).full())
```

```
[[ 1.        +0.j  0.        +0.j  0.        +0.j  0.        +0.j]
 [ 0.        +0.j  1.        +0.j  0.        +0.j  0.        +0.j]
 [ 0.        +0.j  0.        +0.j  0.70710678+0.j  0.70710678+0.j]
 [ 0.        +0.j  0.        +0.j  0.70710678+0.j -0.70710678+0.j]]
```

- Anti-controlled single qubit gates:

$$|1\rangle\langle 1| \otimes I + |0\rangle\langle 0| \otimes U$$

[18]:
```
U = sigmax()
print((tensor(ket("1")*bra("1"),qeye(2)) + tensor(ket("0")*bra("0"),U)).full())
```

```
[[0.+0.j 1.+0.j 0.+0.j 0.+0.j]
 [1.+0.j 0.+0.j 0.+0.j 0.+0.j]
 [0.+0.j 0.+0.j 1.+0.j 0.+0.j]
 [0.+0.j 0.+0.j 0.+0.j 1.+0.j]]
```

- Or use multiple controls (same with anti-controls)

$$(|00\rangle\langle 00| + |01\rangle\langle 01| + |10\rangle\langle 10|) \otimes I + |11\rangle\langle 11| \otimes U$$

[19]:
```
U = sigmax()
print(np.real(␣
↪(tensor((ket("00")*bra("00")+ket("01")*bra("01")+ket("10")*bra("10")),qeye(2)) + \
                tensor(ket("11")*bra("11"),U)                                         ␣
↪          ).full() ))
```

```
[[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. 0. 1.]
[0. 0. 0. 0. 0. 0. 1. 0.]]
```

Circuit Diagrams and Operators

- Sort top-down qubits in quantum circuit to right-to-left tensor product to get the state
  - Least significant bit is right-most in ket and top-most in circuit
- Take tensor product (Kronecker product) of stacked gates on qubits where top-down order becomes right-to-left order in product
  - For any quantum wire without a gate insert a 2×2 identity matrix
  - Can ignore qubits not involved at all (for simplicitly)
    - until they become relevant (then expand with tensor product; careful to not mix up the order)
- Resulting operators from left-to-right in circuit are (matrix) multiplied right-to-left to get operator of circuit
  - Initial state (usually $|0...0\rangle$) is multiplied from the right with the opeartor
  - Note, initial sate $|0...0\rangle$ means the first column of the full operator defines the result
- Can ignore normalisation (and normalise in the end such that matrix is unitary or state vector represents probabilities / squares sum up to one)
- Note, in the matrix-vector represetnation with the Z basis, the order of the entries in the vector is determined by the decimal value of the qubit
- Use numpy and/or qutip to compute full circuit operators, etc.
  - Mapping of basis states gives a clue of what basic circuits are doing
- There are other ways to order this and can use different basis, so be careful

More Operations

- There is no quantum operation that can copy a qubit (**no cloning theorem**)
  - All operations must be unitary (if they aren't, they are not purely quantum)
  - Meassurements are not unitary (but destroy the quantum state)
- There is a gate to swap the state between two qubits
  - swap (or linked "x" in the circuit)
- Identical circuits for multi-controlled gates
  - There are multiple options to create the same full operator from individual gates (depending on which gates you have available; various sets of gates are universal / can generate all possible unitary operators/circuits)

Density Matrices

- Density matrix of state $|\Psi\rangle$ is simply $|\Psi\rangle\langle\Psi|$
  - Diagonal elements contain probabilities of being in the specific states (trace/sum of diagonal elements is 1)
  - Off-diagonal elements are the coherences (coupling between the states)
  - E.g. Density Example