Lecture 2: Quantum circuits, entanglement and measurements

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Quantum computing: operations

- Operations on a single qubit must be represented as 2×2 unitary matrices U: $U^\dagger U = I$
- Pauli matrices

$$I \equiv \sigma_0 \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad X \equiv \sigma_1 \equiv \sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$Y \equiv \sigma_2 \equiv \sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad Z \equiv \sigma_3 \equiv \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- Pauli X acts as a NOT gate: $|0\rangle \to |1\rangle$ and $|1\rangle \to |0\rangle$

Quantum computing: operations

Hadamard	H	$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$
Pauli-X	X	$\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$
Pauli-Y	Y	$\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}$
Pauli-Z	Z	$\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$
Phase	S	$\begin{bmatrix}1 & 0\\ 0 & i\end{bmatrix}$
$\pi/8$	T	$\begin{bmatrix}1 & 0\\ 0 & e^{i\pi/4}\end{bmatrix}$

Nielsen, Chuang, Ch. 4

Quantum computing: operations

- Rotations around x, y, z axes:

$$R_x(\theta) \equiv e^{-i\theta X/2} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}X = \begin{bmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$

$$R_y(\theta) \equiv e^{-i\theta Y/2} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}Y = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$

$$R_z(\theta) \equiv e^{-i\theta Z/2} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}Z = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}.$$

- Any unitary U can be represented as (Z-Y decomposition)

$$U = e^{i\alpha}R_z(\beta)R_y(\gamma)R_z(\delta)$$

Eigenvalues, eigenvectors and diagonalization

- *Eigenvalues* and *eigenvectors* of a linear operator A

$$A|v\rangle = v|v\rangle$$

- An operator A is called *normal* if $AA^\dagger = A^\dagger A$
- An operator is normal if and only if it is diagonalizable (spectral decomposition theorem)
- A diagonalizable operator A has a diagonal representation

  $A = \sum_i \lambda_i |i\rangle\langle i|$, where λ_i are the eigenvalues and $|i\rangle$ are the orthonormal set of eigenvectors of A
- The computational basis = eigenvectors of Z and

$$Z = |0\rangle\langle 0| - |1\rangle\langle 1|$$

Code in Qiskit

In [1]:

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

# create a circuit with one qubit
qc = qiskit.QuantumCircuit( 1 )

# add some gates
qc.x( 0 )
qc.y( 0 )
qc.z( 0 )
qc.h( 0 )

# draw
qc.draw( "mpl", scale=1.5 )
```

Out[1]:

Tensor products

- Let V, W be inner product spaces of dimension m, n. Then $V \otimes W$ is a $m \cdot n$ dimensional vector space whose elements are linear combinations of tensor products $|v\rangle \otimes |w\rangle$ of elements $|v\rangle \in V$ and $|w\rangle \in W$
- Notation: $|v\rangle \otimes |w\rangle \equiv |v\rangle |w\rangle \equiv |v, w\rangle \equiv |vw\rangle$
- The tensor product satisfies the following properties:
  - respects addition in V and W
  - respects scalar multiplication in V and W
- The inner product on $V \otimes W$

$$\left(\sum_i a_i |v_i\rangle \otimes |w_i\rangle, \sum_j b_j |v'_j\rangle \otimes |w'_j\rangle \right) \equiv \sum_{ij} a_i^* b_j \langle v_i | v'_j\rangle \langle w_i | w'_j\rangle$$

Tensor products

- Linear operators on $V \otimes W$ are defined as

$$(A \otimes B)\left(\sum_i a_i |v_i\rangle \otimes |w_i\rangle\right) \equiv \sum_i a_i \, A|v_i\rangle \otimes B|w_i\rangle$$

- In matrix representation we can use the *Kronecker product*: if A is $m \times n$ and B is $p \times q$ matrices then $A \otimes B$ is a $mp \times nq$ matrix
- For example $X \otimes Y$

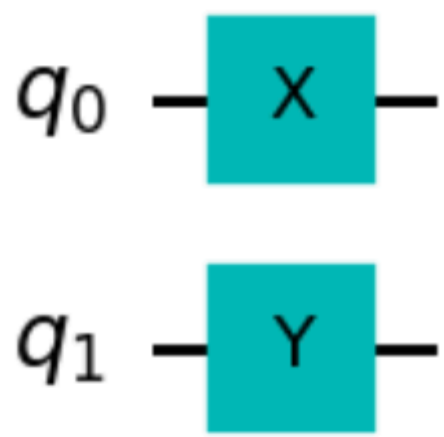
$$X \otimes Y = \begin{pmatrix} 0 \cdot Y & 1 \cdot Y \\ 1 \cdot Y & 0 \cdot Y \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}$$

Code in Qiskit

In [2]:

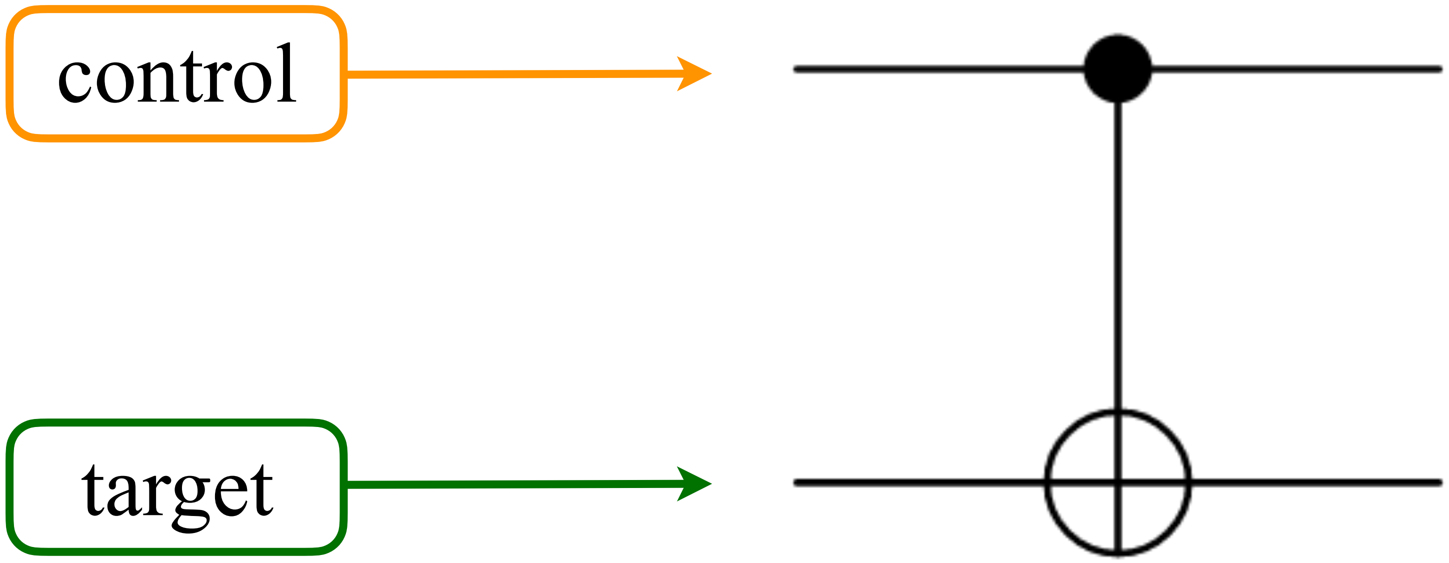
```
# create a circuit with two qubits
qc = qiskit.QuantumCircuit( 2 )

# add some gates
qc.x( 0 )
qc.y( 1 )

# draw
qc.draw( "mpl", scale=1.5 )
```

Out[2]:



Controlled operations

- Controlled-NOT or CNOT gate: $|c\rangle|t\rangle \rightarrow |c\rangle|c \oplus t\rangle$

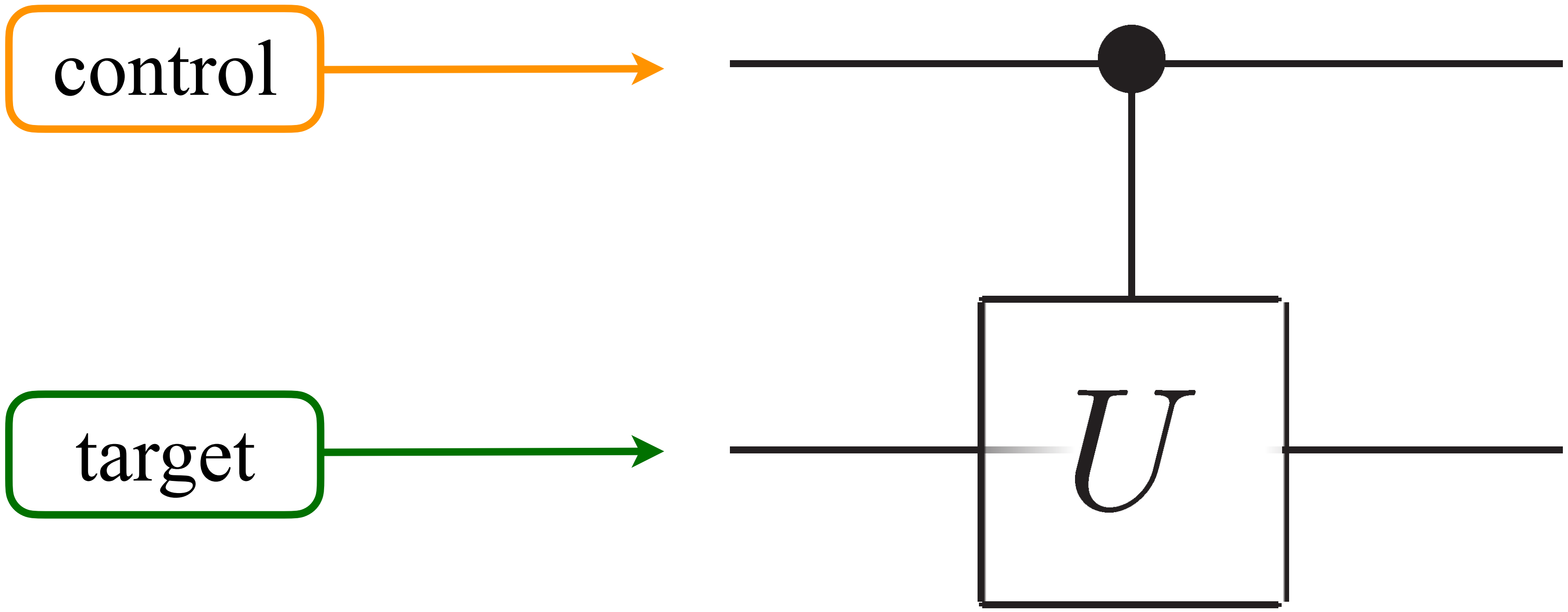


- CNOT = controlled-X

$$CX = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes X = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Controlled operations

- A general controlled-U gate: $|c\rangle|t\rangle \to |c\rangle U^c|t\rangle$



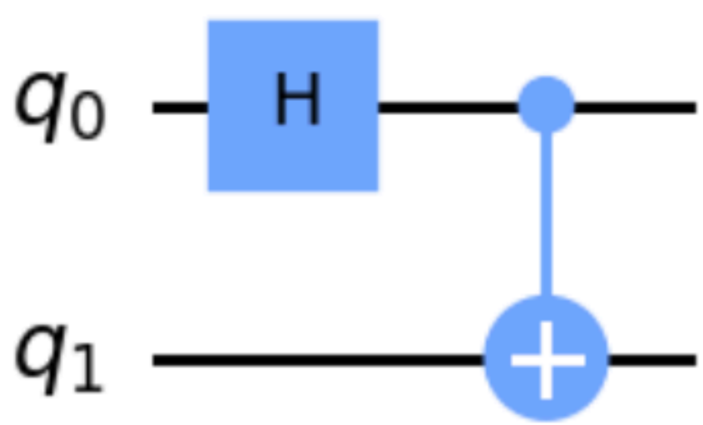
- ***Single qubit gates and the CNOT gate are universal — any unitary operation on n qubits can be implemented with these gates and thus they are universal for quantum computation***

Circuit with CNOT

In [3]:

```
# create a circuit with two qubits
qc = qiskit.QuantumCircuit( 2 )

# add some gates
qc.h( 0 )
qc.cx( 0, 1 )

# draw
qc.draw( "mpl", scale=1.5 )
```

Out[3]:



Circuit with CNOT

- By convention the qubits are initialized in $|0\rangle$ state
- We start with $|0\rangle \otimes |0\rangle \equiv |00\rangle$
- The Hadamard gate: $|0\rangle \to (|0\rangle + |1\rangle)/\sqrt{2}$, thus we get

$$|00\rangle \to (|0\rangle + |1\rangle)/\sqrt{2} \otimes |0\rangle \equiv (|00\rangle + |10\rangle)/\sqrt{2}$$

- The CNOT gate:

$$\left(|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes X\right)\left(|0\rangle \otimes |0\rangle/\sqrt{2} + |1\rangle \otimes |0\rangle/\sqrt{2}\right)$$

$$= \left(|0\rangle \otimes |0\rangle/\sqrt{2} + |1\rangle \otimes |1\rangle/\sqrt{2}\right) \equiv (|00\rangle + |11\rangle)/\sqrt{2}$$

- The final state for the two qubits cannot be represented as a tensor product of single qubit states — it is an *entangled* state:

$$(|00\rangle + |11\rangle)/\sqrt{2} \neq (\alpha|0\rangle + \beta|1\rangle) \otimes (\gamma|0\rangle + \delta|1\rangle)$$

Spin-1/2 addition

- Recall:

  $$\vec{S} = \frac{\hbar}{2}\vec{\sigma} \qquad \text{and we can identify } |0\rangle = |\uparrow\rangle \text{ and } |1\rangle = |\downarrow\rangle$$

- For two spin-1/2 particles the total spin operator is $\vec{S} = \vec{S}_1 + \vec{S}_2$ (or more carefully $\vec{S} = \vec{S}_1 \otimes I + I \otimes \vec{S}_2$) and the simultaneous eigenstates of total S_z and $\vec{S}^2$ are

  $$|s=0, m_s=0\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$$
  $$|s=1, m_s=-1\rangle = |\downarrow\downarrow\rangle$$
  $$|s=1, m_s=0\rangle = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$$
  $$|s=1, m_s=1\rangle = |\uparrow\uparrow\rangle$$

Spin-1/2 addition

- The state that we construct with the Hadamard and CNOT gate is nothing else as one of the triplet states $|s = 1, m_s = 0\rangle$
- In the context of quantum computing such entangled states are often called the *Bell states*

Measurements

- By convention measurements are performed in the computational basis and the measurement operators are:

$$M_0 = |0\rangle\langle 0| \quad \text{and} \quad M_1 = |1\rangle\langle 1|$$

- The probability of an outcome $m = 0,1$ is

$$p(m) = \langle\psi|M_m^\dagger M_m|\psi\rangle = \langle\psi|M_m|\psi\rangle$$

and the state collapses to $|0\rangle$ or $|1\rangle$

- By construction the measurement operators satisfy the completeness relation $\sum_{m=0,1} M_m^\dagger M_m = I$

- Let $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ be the state before the measurement, then

$$p(0) = |\alpha|^2 \quad \text{and} \quad p(1) = |\beta|^2$$

Projective measurements

- Consider an observable O which is a Hermitian operator on the state space. Then there is a spectral decomposition $O = \sum_m \lambda_m P_m$ where λ_m is the eigenvalue of O and P_m is the projector onto the eigenspace of O with eigenvalue λ_m
- The expectation value of O on state $|\psi\rangle$ is

$$\langle\psi|O|\psi\rangle = \langle\psi|\sum_m \lambda_m P_m|\psi\rangle = \sum_m \lambda_m \langle\psi|P_m|\psi\rangle = \sum_m \lambda_m p(m)$$

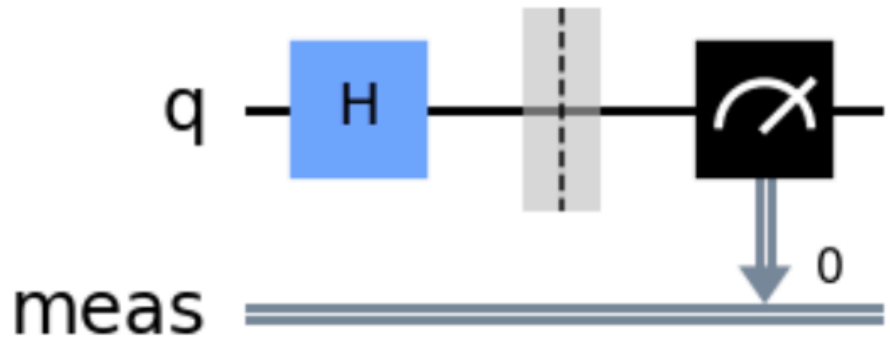
- The measurement in the computational basis is essentially $\langle\psi|Z|\psi\rangle = 1 \cdot |\langle 0|\psi\rangle|^2 + (-1) \cdot |\langle 1|\psi\rangle|^2 = p(0) - p(1)$

Code in Qiskit

In [4]:

```
# create a circuit
qc = qiskit.QuantumCircuit( 1 )

# add some gates
qc.h( 0 )

# add the measurement
qc.measure_all()

# draw
qc.draw( "mpl", scale=1.5 )
```

Out[4]:



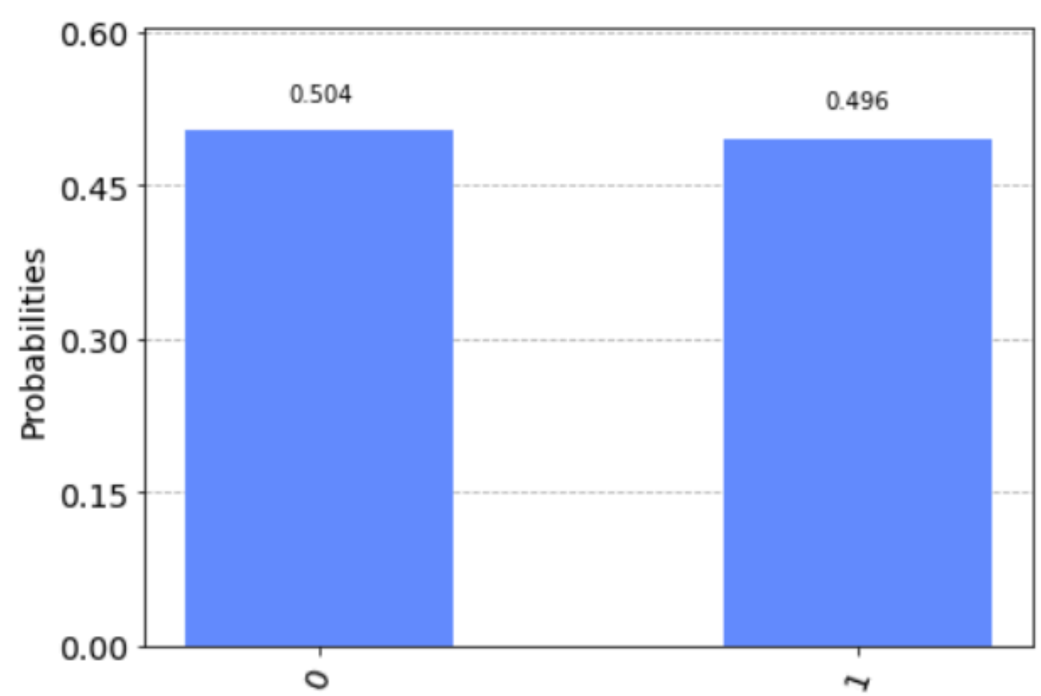
Code in Qiskit

In [5]:

```
# simulate

# number of repetitions
N = 10000

backend = qiskit.Aer.get_backend( 'qasm_simulator' )
job = qiskit.execute( qc, backend, shots=N )
result = job.result()

measurements = result.get_counts( qc )
print( measurements )
qiskit.visualization.plot_histogram( measurements )
```

```
{'0': 5038, '1': 4962}
```

Out[5]:



Density matrix

- Consider measuring an operator A on state $|\psi\rangle$
- Using some orthonormal basis $|\phi_i\rangle$:

$$\langle\psi|A|\psi\rangle = \langle\psi|\sum_i |\phi_i\rangle\langle\phi_i|A|\psi\rangle = \sum_i \langle\phi_i|\left(A|\psi\rangle\langle\psi|\right)|\phi_i\rangle \equiv \mathrm{tr}(A\rho)$$

$$\mathrm{tr}(\ldots) \equiv \sum_i \langle\phi_i|\ldots|\phi_i\rangle \quad \text{and} \quad \rho = |\psi\rangle\langle\psi| \text{ — } \textit{density matrix}$$

- If a state can be described by a state vector, it is called a *pure state*
- If we have an *ensemble* of pure states where the system can be in state $|\psi_\alpha\rangle$ with probability p_α, it is called a *mixed state*
- Density matrix allows one to also describe mixed states:

$$\rho = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$$

Density matrix

- Evolution:

$$\rho = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha| \rightarrow \sum_\alpha p_\alpha U|\psi_\alpha\rangle\langle\psi_\alpha|U^\dagger = U\rho U^\dagger$$

- Measurement:

$$p(m) = \sum_\alpha p(m|\alpha)\, p_\alpha = \sum_\alpha p_\alpha \mathrm{tr}(M_m^\dagger M_m |\psi_\alpha\rangle\langle\psi_\alpha|) = \mathrm{tr}(M_m^\dagger M_m \rho)$$

- The density matrix after measurement:

$$\rho_m = \frac{M_m \rho M_m^\dagger}{\mathrm{tr}(M_m^\dagger M_m \rho)}$$

Density matrix

- Properties:

$$\mathrm{tr}(\rho) = \sum_\alpha p_\alpha \mathrm{tr}(|\psi_\alpha\rangle\langle\psi_\alpha|) = \sum_\alpha p_\alpha = 1$$

$$\langle\phi|\rho|\phi\rangle = \sum_\alpha p_\alpha \langle\phi|\psi_\alpha\rangle\langle\psi_\alpha|\phi\rangle = \sum_\alpha p_\alpha |\langle\phi|\psi_\alpha\rangle|^2 \geq 0,$$

i.e. ρ is a positive operator

- For a pure state:

$$\mathrm{tr}(\rho^2) = \mathrm{tr}(|\psi\rangle\langle\psi|\psi\rangle\langle\psi|) = \mathrm{tr}(|\psi\rangle\langle\psi|) = 1$$

- For a mixed state:

$$\mathrm{tr}(\rho^2) < 1$$

Reduced density matrix

- Consider two physical systems A and B described by the density matrix ρ^{AB}
- The *reduced* density matrix for system A is defined as

  $$\rho^A \equiv \mathrm{tr}_B(\rho^{AB})$$

  with the *partial trace* over system B defined as

  $$\mathrm{tr}_B(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) \equiv |a_1\rangle\langle a_2|\,\mathrm{tr}(|b_1\rangle\langle b_2|)$$

- For a product state $\rho^{AB} = \rho \otimes \sigma$ we get $\rho^A = \mathrm{tr}(\rho \otimes \sigma) = \rho$ as expected
- For an entangled state, e.g.

  $$\rho = 1/2\,(|00\rangle + |11\rangle)(\langle 00| + \langle 11|)$$

  we get $\rho^A = I/2$, i.e. a mixed (!) state

Conclusion

- Quantum computing requires a programming model that follows the rules of quantum mechanics
- Universal quantum computers (i.e. universal set of gates) are possible
- The hope is that quantum computing would allow one to solve problems that require amount of classical computing that scales exponentially with the number of degrees of freedom in the problem