



# Ch2: Quantum Mechanics for Quantum Computing



### Dirac notations

Dirac notations (also called bra-ket notations) are specifically designed to ease algebraic calculations that frequently come up in quantum mechanics:

Notation	Description
$z^*$	Complex conjugate of the complex number $z$ . $(1 + i)^* = 1 - i$
$ \psi\rangle$	Vector. Also known as a <i>ket</i> .
$\langle\psi $	Vector dual to $ \psi\rangle$ . Also known as a <i>bra</i> .
$\langle\varphi \psi\rangle$	Inner product between the vectors $ \varphi\rangle$ and $ \psi\rangle$ .
$ \varphi\rangle \otimes  \psi\rangle$	Tensor product of $ \varphi\rangle$ and $ \psi\rangle$ .
$ \varphi\rangle \psi\rangle$	Abbreviated notation for tensor product of $ \varphi\rangle$ and $ \psi\rangle$ .
$A^*$	Complex conjugate of the $A$ matrix.
$A^T$	Transpose of the $A$ matrix.
$A^\dagger$	Hermitian conjugate or adjoint of the $A$ matrix, $A^\dagger = (A^T)^*$ . $\begin{bmatrix} a & b \\ c & d \end{bmatrix}^\dagger = \begin{bmatrix} a^* & c^* \\ b^* & d^* \end{bmatrix}.$
$\langle\varphi A \psi\rangle$	Inner product between $ \varphi\rangle$ and $A \psi\rangle$ . Equivalently, inner product between $A^\dagger \varphi\rangle$ and $ \psi\rangle$ .



### Dirac notations

- Ket-vector:

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix}$$

- Bra-vector:

$$\langle\psi| = (\psi_1^*, \psi_2^*, \dots, \psi_N^*)$$

- Hermitian conjugate:

$$|\psi\rangle^\dagger = \langle\psi|$$



### Dirac notations

- Inner-product: 
$$\langle \phi | \psi \rangle = (\phi_1^*, \phi_2^*, \dots, \phi_N^*) \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix} = \phi_1^* \psi_1 + \phi_2^* \psi_2 + \dots + \phi_N^* \psi_N$$

- Outer-product: 
$$|\psi\rangle\langle\phi| = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix} (\phi_1^*, \phi_2^*, \dots, \phi_N^*) = \begin{pmatrix} \psi_1 \phi_1^* & \psi_1 \phi_2^* & \cdots & \psi_1 \phi_N^* \\ \psi_2 \phi_1^* & \psi_2 \phi_2^* & \cdots & \psi_2 \phi_N^* \\ \vdots & \vdots & \ddots & \vdots \\ \psi_N \phi_1^* & \psi_N \phi_2^* & \cdots & \psi_N \phi_N^* \end{pmatrix}$$



### Dirac notations

- Tensor-product of vector:

$$|\psi\rangle \otimes |\phi\rangle = |\psi, \phi\rangle = \begin{pmatrix} \psi_1 \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{pmatrix} \\ \psi_2 \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{pmatrix} \\ \vdots \\ \psi_N \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{pmatrix} \end{pmatrix} = \begin{pmatrix} \psi_1 \phi_1 \\ \psi_1 \phi_2 \\ \vdots \\ \psi_2 \phi_1 \\ \psi_2 \phi_2 \\ \vdots \\ \psi_N \phi_N \end{pmatrix}$$

## State space

**Postulate 1:** Associated to any isolated physical system is a complex vector space with inner product (that is, a Hilbert space) known as the state space of the system. The system is completely described by its state vector, which is a unit vector in the system's state space.

## State space

**Postulate 1:** Associated to any isolated physical system is a complex vector space with inner product (that is, a Hilbert space) known as the state space of the system. The system is completely described by its state vector, which is a unit vector in the system's state space.

The simplest quantum mechanical system, and the system which we will be most concerned with, is the qubit:

- State-vector:  $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$
- Probability amplitudes:  $\alpha, \beta \in \mathbb{C}$
- Normalization:  $|\alpha|^2 + |\beta|^2 = 1$

- Orthonormal set of basis vectors:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

also known as computational basis states in QC



### Unitary evolution

**Postulate 2:** The time evolution of a closed quantum system is described by a unitary transformation:



## Unitary evolution

**Postulate 2:** The time evolution of a closed quantum system is described by a unitary transformation:

- State evolution:  $|\psi(t_2)\rangle = U_{12} |\psi(t_1)\rangle$
- Unitary:  $UU^\dagger = I$

## Unitary evolution

**Postulate 2:** The time evolution of a closed quantum system is described by a unitary transformation:

- State evolution:  $|\psi(t_2)\rangle = U_{12} |\psi(t_1)\rangle$
- Unitary:  $UU^\dagger = I$

Note that unitary implies reversibility – the converse doesn't hold true. Thus no heat dissipation arises when performing a quantum computation – Landauer's principle.

## Unitary evolution

**Postulate 2 bis:** The time evolution of a closed quantum system is described by the Schrödinger equation:

$$i\hbar \frac{d|\psi\rangle}{dt} = H |\psi\rangle \Rightarrow |\psi(t_2)\rangle = e^{\frac{-iH(t_2-t_1)}{\hbar}} |\psi(t_1)\rangle = U_{12} |\psi(t_1)\rangle$$

- $H$ : Hamiltonian of the system – an operator corresponding to the sum of the kinetic energies plus the potential energies of the system.
- Exponential operator: unitary evolution

## Unitary evolution

**Postulate 2 bis:** The time evolution of a closed quantum system is described by the Schrödinger equation:

$$i\hbar \frac{d|\psi\rangle}{dt} = H |\psi\rangle \Rightarrow |\psi(t_2)\rangle = e^{\frac{-iH(t_2-t_1)}{\hbar}} |\psi(t_1)\rangle = U_{12} |\psi(t_1)\rangle$$

- $H$ : Hamiltonian of the system – an operator corresponding to the sum of the kinetic energies plus the potential energies of the system.
- Exponential operator: unitary evolution

Any unitary operator  $U$  can be realized in the form  $U = e^{iH}$  where  $H$  is some hermitian operator ( $H = H^\dagger$ ). **Actual physics systems that realize necessary Hamiltonians are not yet our interest.**

## Quantum measurement – General measurement

**Postulate 3:** Quantum measurements are described by a collection  $\{M_m\}$  of measurement operators. These are operators acting on the state space of the system being measured. The index “m” refers to the measurement outcomes that may occur in the experiment. If the state of the quantum system is  $|\psi\rangle$  immediately before the measurement then the probability that result “m” occurs is given by:

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

- The state of the system after the measurement is: 
$$\frac{M_m |\psi\rangle}{\sqrt{\langle \psi | M_m^\dagger M_m | \psi \rangle}}$$
- The measurement operators satisfy the completeness equation: 
$$\sum_m M_m^\dagger M_m = I$$



### Quantum measurement – Projective measurement

For many applications of quantum computation and quantum information we will be concerned primarily with projective measurements. Projective measurements are special cases of general measurements when the measurement operators are Hermitian and orthogonal projectors:

$$P_m^\dagger = P_m$$

$$P_m^2 = P_m$$

$$P_m P_{m'} = P_m \delta_{m,m'}$$

Then the probability that result “m” occurs is given by:

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

- The state of the system after the measurement is:  $\frac{P_m |\psi\rangle}{\sqrt{p(m)}}$

- The measurement operators satisfy the completeness equation:  $\sum_m P_m = I$

## Quantum measurement – Projective measurement

Example:  $|\psi\rangle = \sqrt{\frac{2}{3}} |0\rangle + \sqrt{\frac{1}{3}} |1\rangle$

## Quantum measurement – Projective measurement

Example:  $|\psi\rangle = \sqrt{\frac{2}{3}}|0\rangle + \sqrt{\frac{1}{3}}|1\rangle$

The projectors for this state are:

$$P_0 = |0\rangle\langle 0|$$

$$P_1 = |1\rangle\langle 1|$$

and we verify:

$$P_0^2 = |0\rangle\langle 0|0\rangle\langle 0| = |0\rangle\langle 0| = P_0$$

$$P_1^2 = |1\rangle\langle 1|1\rangle\langle 1| = |1\rangle\langle 1| = P_1$$



## Quantum measurement – Projective measurement

Example:  $|\psi\rangle = \sqrt{\frac{2}{3}}|0\rangle + \sqrt{\frac{1}{3}}|1\rangle$

The probabilities of getting a 0 or a 1 after measurement are:

$$\begin{aligned} p(0) &= \|P_0 |\psi\rangle\|^2 = \langle\psi|0\rangle\langle 0|\psi\rangle = \left(\sqrt{\frac{2}{3}}\langle 0| + \sqrt{\frac{1}{3}}\langle 1|\right) |0\rangle\langle 0| \left(\sqrt{\frac{2}{3}}|0\rangle + \sqrt{\frac{1}{3}}|1\rangle\right) \\ &= \left(\sqrt{\frac{2}{3}}\langle 0|0\rangle + \sqrt{\frac{1}{3}}\langle 1|0\rangle\right) \left(\sqrt{\frac{2}{3}}\langle 0|0\rangle + \sqrt{\frac{1}{3}}\langle 0|1\rangle\right) = \frac{2}{3} \end{aligned}$$

$$\begin{aligned} p(1) &= \|P_1 |\psi\rangle\|^2 = \langle\psi|1\rangle\langle 1|\psi\rangle = \left(\sqrt{\frac{2}{3}}\langle 0| + \sqrt{\frac{1}{3}}\langle 1|\right) |1\rangle\langle 1| \left(\sqrt{\frac{2}{3}}|0\rangle + \sqrt{\frac{1}{3}}|1\rangle\right) \\ &= \left(\sqrt{\frac{2}{3}}\langle 0|1\rangle + \sqrt{\frac{1}{3}}\langle 1|1\rangle\right) \left(\sqrt{\frac{2}{3}}\langle 1|0\rangle + \sqrt{\frac{1}{3}}\langle 1|1\rangle\right) = \frac{1}{3} \end{aligned}$$

## Quantum measurement – Projective measurement

Example:  $|\psi\rangle = \sqrt{\frac{2}{3}}|0\rangle + \sqrt{\frac{1}{3}}|1\rangle$

Suppose we got result 0, the state of system after the measurement is:

$$|\psi'\rangle = \frac{P_0|\psi\rangle}{\sqrt{p(0)}} = \frac{|0\rangle\langle 0|(\sqrt{\frac{2}{3}}|0\rangle + \sqrt{\frac{1}{3}}|1\rangle)}{\sqrt{\frac{2}{3}}} = \frac{|0\rangle(\sqrt{\frac{2}{3}}\langle 0|0\rangle + \sqrt{\frac{1}{3}}\langle 0|1\rangle)}{\sqrt{\frac{2}{3}}} = \frac{\sqrt{\frac{2}{3}}|0\rangle}{\sqrt{\frac{2}{3}}} = |0\rangle$$

## Quantum measurement – Projective measurement

Projective measurements have many nice properties. In particular, it is very easy to calculate average values for projective measurements:

$$E(M) = \sum_m m p(m) = \sum_m m \langle \psi | P_m | \psi \rangle = \langle \psi | \left( \sum_m m P_m \right) | \psi \rangle = \langle \psi | M | \psi \rangle \equiv \langle M \rangle$$

## Quantum measurement – Projective measurement

Projective measurements have many nice properties. In particular, it is very easy to calculate average values for projective measurements:

$$E(M) = \sum_m m p(m) = \sum_m m \langle \psi | P_m | \psi \rangle = \langle \psi | \left( \sum_m m P_m \right) | \psi \rangle = \langle \psi | M | \psi \rangle \equiv \langle M \rangle$$

**Example:**  $|\psi\rangle = \sqrt{\frac{2}{3}}|0\rangle + \sqrt{\frac{1}{3}}|1\rangle$  and  $M = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$\begin{aligned} \langle Z \rangle &= \langle \psi | \left( |0\rangle\langle 0| - |1\rangle\langle 1| \right) | \psi \rangle \\ &= \langle \psi | 0 \rangle \langle 0 | \psi \rangle - \langle \psi | 1 \rangle \langle 1 | \psi \rangle \\ &= p(0) - p(1) \\ &= \frac{2}{3} - \frac{1}{3} = \frac{1}{3} \end{aligned}$$



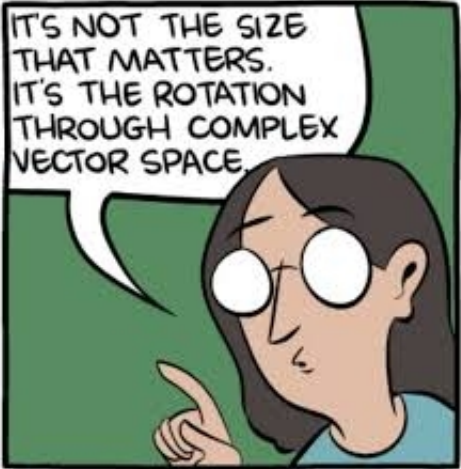
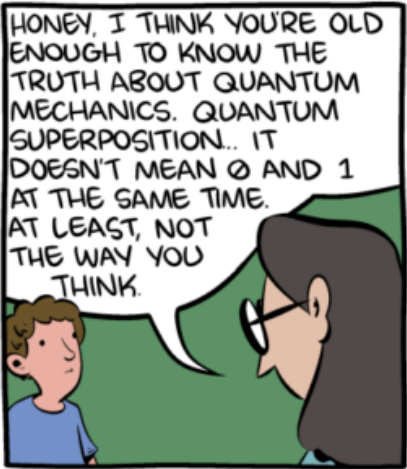
# 2.3 bits, p-bits, q-bits

## Bits

## Probabilistic bits

## Quantum bits

State (single-unit)	Bit $x \in \{0, 1\}$	Stochastic vector $\vec{s} = p_0\vec{0} + p_1\vec{1}$ $p_0, p_1 \in \mathbb{R}_+$ $p_0 + p_1 = 1$	Complex vector $\vec{\psi} = \alpha_0\vec{0} + \alpha_1\vec{1}$ $\alpha_0, \alpha_1 \in \mathbb{C}$ $ \alpha_0 ^2 +  \alpha_1 ^2 = 1$
------------------------	-------------------------	--	--





# 2.3 bits, p-bits, q-bits

	Bits	Probabilistic bits	Quantum bits
State (single-unit)	Bit $x \in \{0, 1\}$	Stochastic vector $\vec{s} = p_0 \vec{0} + p_1 \vec{1}$ $p_0, p_1 \in \mathbb{R}_+$ $p_0 + p_1 = 1$	Complex vector $\vec{\psi} = \alpha_0 \vec{0} + \alpha_1 \vec{1}$ $\alpha_0, \alpha_1 \in \mathbb{C}$ $ \alpha_0 ^2 +  \alpha_1 ^2 = 1$
State (multi-unit)	Bit-string $x \in \{0, 1\}^n$	Stochastic vector $\vec{s} = \{p_x\}_{x \in \{0, 1\}^n}$	Complex vector $\vec{\psi} = \{\alpha_x\}_{x \in \{0, 1\}^n}$



# 2.3 bits, p-bits, q-bits

	Bits	Probabilistic bits	Quantum bits
State (single-unit)	Bit $x \in \{0, 1\}$	Stochastic vector $\vec{s} = p_0 \vec{0} + p_1 \vec{1}$ $p_0, p_1 \in \mathbb{R}_+$ $p_0 + p_1 = 1$	Complex vector $\vec{\psi} = \alpha_0 \vec{0} + \alpha_1 \vec{1}$ $\alpha_0, \alpha_1 \in \mathbb{C}$ $ \alpha_0 ^2 +  \alpha_1 ^2 = 1$
State (multi-unit)	Bit-string $x \in \{0, 1\}^n$	Stochastic vector $\vec{s} = \{p_x\}_{x \in \{0, 1\}^n}$	Complex vector $\vec{\psi} = \{\alpha_x\}_{x \in \{0, 1\}^n}$
Operations	Boolean logic	Stochastic matrices $\sum_{j=1}^S P_{i,j} = 1$	Unitary matrices $UU^\dagger = I$



# 2.3 bits, p-bits, q-bits

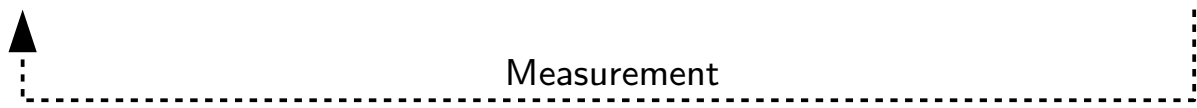
	Bits	Probabilistic bits	Quantum bits
State (single-unit)	Bit $x \in \{0, 1\}$	Stochastic vector $\vec{s} = p_0 \vec{0} + p_1 \vec{1}$ $p_0, p_1 \in \mathbb{R}_+$ $p_0 + p_1 = 1$	Complex vector $\vec{\psi} = \alpha_0 \vec{0} + \alpha_1 \vec{1}$ $\alpha_0, \alpha_1 \in \mathbb{C}$ $ \alpha_0 ^2 +  \alpha_1 ^2 = 1$
State (multi-unit)	Bit-string $x \in \{0, 1\}^n$	Stochastic vector $\vec{s} = \{p_x\}_{x \in \{0, 1\}^n}$	Complex vector $\vec{\psi} = \{\alpha_x\}_{x \in \{0, 1\}^n}$
Operations	Boolean logic	Stochastic matrices $\sum_{j=1}^S P_{i,j} = 1$	Unitary matrices $UU^\dagger = I$
Component Ops	Boolean gates	Tensor products of matrices	Tensor products of matrices





# 2.3 bits, p-bits, q-bits

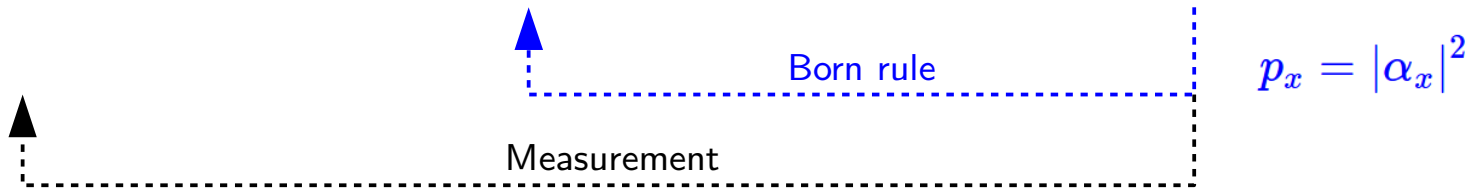
	Bits	Probabilistic bits	Quantum bits
State (single-unit)	Bit $x \in \{0, 1\}$	Stochastic vector $\vec{s} = p_0 \vec{0} + p_1 \vec{1}$ $p_0, p_1 \in \mathbb{R}_+$ $p_0 + p_1 = 1$	Complex vector $\vec{\psi} = \alpha_0 \vec{0} + \alpha_1 \vec{1}$ $\alpha_0, \alpha_1 \in \mathbb{C}$ $ \alpha_0 ^2 +  \alpha_1 ^2 = 1$
State (multi-unit)	Bit-string $x \in \{0, 1\}^n$	Stochastic vector $\vec{s} = \{p_x\}_{x \in \{0, 1\}^n}$	Complex vector $\vec{\psi} = \{\alpha_x\}_{x \in \{0, 1\}^n}$
Operations	Boolean logic	Stochastic matrices $\sum_{j=1}^S P_{i,j} = 1$	Unitary matrices $UU^\dagger = I$
Component Ops	Boolean gates	Tensor products of matrices	Tensor products of matrices





## 2.3 bits, p-bits, q-bits

	Bits	Probabilistic bits	Quantum bits
State (single-unit)	Bit $x \in \{0, 1\}$	Stochastic vector $\vec{s} = p_0 \vec{0} + p_1 \vec{1}$ $p_0, p_1 \in \mathbb{R}_+$ $p_0 + p_1 = 1$	Complex vector $\vec{\psi} = \alpha_0 \vec{0} + \alpha_1 \vec{1}$ $\alpha_0, \alpha_1 \in \mathbb{C}$ $ \alpha_0 ^2 +  \alpha_1 ^2 = 1$
State (multi-unit)	Bit-string $x \in \{0, 1\}^n$	Stochastic vector $\vec{s} = \{p_x\}_{x \in \{0, 1\}^n}$	Complex vector $\vec{\psi} = \{\alpha_x\}_{x \in \{0, 1\}^n}$
Operations	Boolean logic	Stochastic matrices $\sum_{j=1}^S P_{i,j} = 1$	Unitary matrices $UU^\dagger = I$
Component Ops	Boolean gates	Tensor products of matrices	Tensor products of matrices





## 2.3 bits, p-bits, q-bits

	Bits	Probabilistic bits	Quantum bits
State (single-unit)	Bit $x \in \{0, 1\}$	Stochastic vector $\vec{s} = p_0 \vec{0} + p_1 \vec{1}$ $p_0, p_1 \in \mathbb{R}_+$ $p_0 + p_1 = 1$	Complex vector $\vec{\psi} = \alpha_0 \vec{0} + \alpha_1 \vec{1}$ $\alpha_0, \alpha_1 \in \mathbb{C}$ $ \alpha_0 ^2 +  \alpha_1 ^2 = 1$
State (multi-unit)	Bit-string $x \in \{0, 1\}^n$	Stochastic vector $\vec{s} = \{p_x\}_{x \in \{0, 1\}^n}$	Complex vector $\vec{\psi} = \{\alpha_x\}_{x \in \{0, 1\}^n}$
Operations	Boolean logic	Stochastic matrices $\sum_{j=1}^S P_{i,j} = 1$	Unitary matrices $UU^\dagger = I$
Component Ops	Boolean gates	Tensor products of matrices	Tensor products of matrices

