

# Quantum Mechanics I: Basic Principles

Michael A. Nielsen

University of Queensland

**"I ain't no physicist but I know what matters"  
- Popeye the Sailor**

**Goal of this and the next lecture:** to introduce all the basic elements of quantum mechanics, using examples drawn from quantum information science.

# What is quantum mechanics?

It is a *framework* for the development of physical theories.

It is *not* a complete physical theory in its own right.

Applications software

Operating system

Specific rules

Quantum mechanics

Quantum  
electrodynamics (QED)



QM consists of *four mathematical postulates* which lay the ground rules for our description of the world.

Newtonian gravitation

Newton's laws of motion

# How successful is quantum mechanics?

It is *unbelievably* successful.

Not just for the small stuff!

QM crucial to explain why stars shine, how the Universe formed, and the stability of matter.

No deviations from quantum mechanics are known

Most physicists believe that any "theory of everything" will be a quantum mechanical theory



A conceptual issue, the so-called "measurement problem", remains to be clarified.

Attempts to describe gravitation in the framework of quantum mechanics have (so far) failed.

# The structure of quantum mechanics

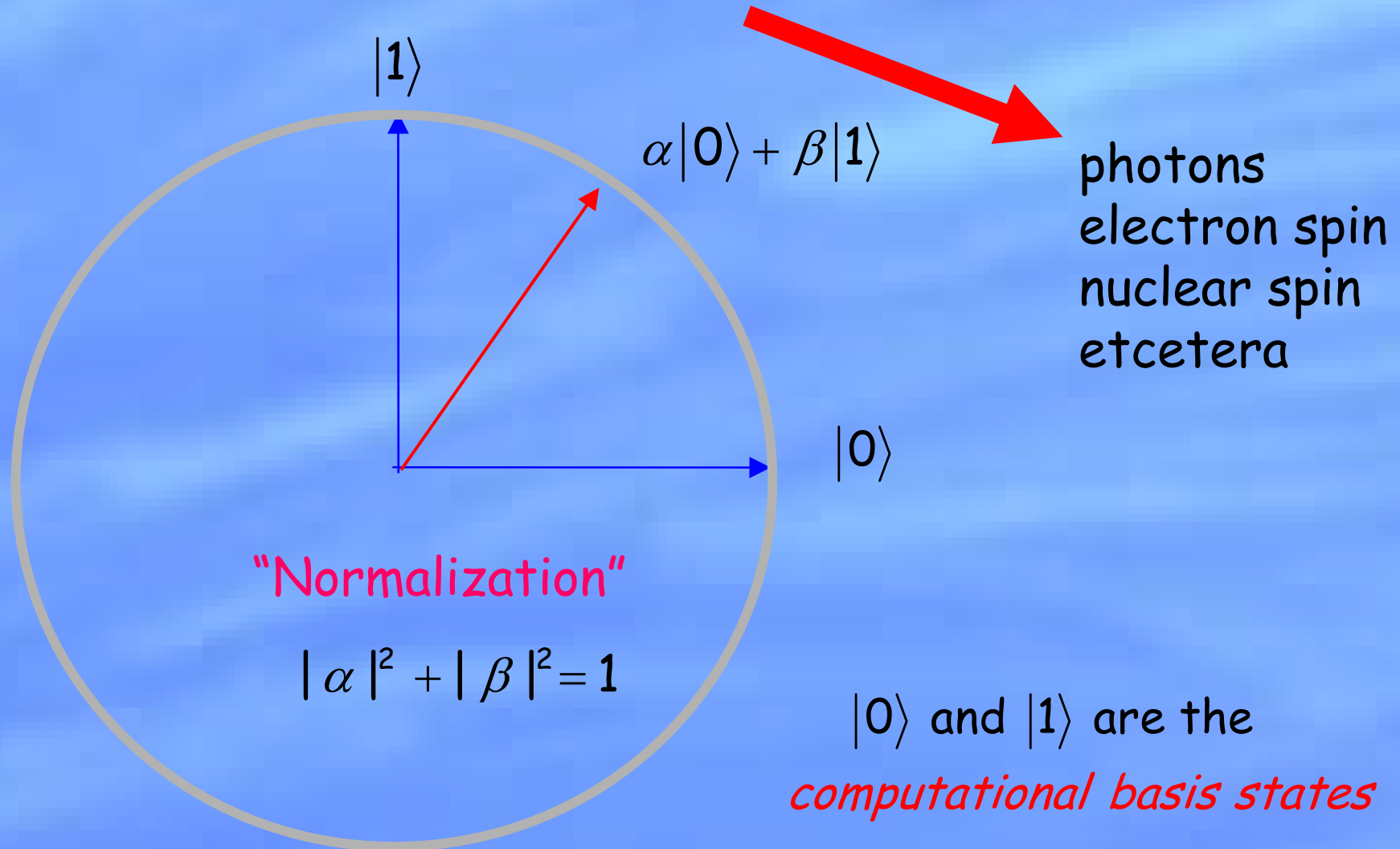
*linear algebra*

*Dirac notation*  $|\psi\rangle, \langle\phi|, \langle A\rangle$

*4 postulates of  
quantum mechanics*

1. How to describe quantum states of a closed system.  
"state vectors" and "state space"
2. How to describe quantum dynamics.  
"unitary evolution"
3. How to describe measurements of a quantum system.  
"projective measurements"
4. How to describe quantum state of a composite system.  
"tensor products"

# Example: **qubits** (two-level quantum systems)



"All we do is draw little arrows on a piece of paper - that's all."  
- Richard Feynman

# Postulate 1: Rough Form

Associated to any quantum system is a complex vector space known as **state space**.

The **state** of a closed quantum system is a unit vector in state space.

Example: we'll work mainly with qubits, which have state space  $\mathbb{C}^2$ .

$$\alpha|0\rangle + \beta|1\rangle \equiv \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

Quantum mechanics **does not** prescribe the state spaces of specific systems, such as electrons. That's the job of a physical theory like quantum electrodynamics.

# A few conventions

We write vectors in state space as:  $|\psi\rangle$  ( $= \vec{\psi}$ )

This is the *ket* notation.

nearly

We *always* assume that our physical systems have *finite-dimensional* state spaces.

$$|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle + \alpha_2 |2\rangle + \dots + \alpha_{d-1} |d-1\rangle$$

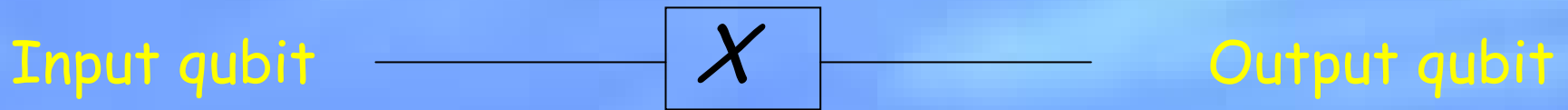
$$= \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_{d-1} \end{bmatrix}$$

**Qudit**

$\mathbb{C}^d$

# Dynamics: quantum logic gates

Quantum not gate:



$$X|0\rangle = |1\rangle; \quad X|1\rangle = |0\rangle.$$

$$\alpha|0\rangle + \beta|1\rangle \rightarrow ?$$

$$\alpha|0\rangle + \beta|1\rangle \rightarrow \alpha|1\rangle + \beta|0\rangle$$

Matrix representation:

$$X = \begin{array}{c} |0\rangle \\ |1\rangle \end{array} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

General dynamics of a closed quantum system (including logic gates) can be represented as a **unitary matrix**.



# Unitary matrices

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

Hermitian conjugation; taking the adjoint

$$A^\dagger = (A^*)^T = \begin{bmatrix} a^* & c^* \\ b^* & d^* \end{bmatrix}$$

$A$  is said to be unitary if  $AA^\dagger = A^\dagger A = I$

We usually write unitary matrices as  $U$ .

Example:

$$XX^\dagger = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I$$

# Nomenclature tips

matrix  
=  
(linear) operator  
=  
(linear) transformation  
=  
(linear) map  
=  
quantum gate (modulo unitarity)

## Postulate 2

The **evolution** of a **closed quantum system** is described by a **unitary transformation**.

$$|\psi'\rangle = U|\psi\rangle$$

# Why unitaries?

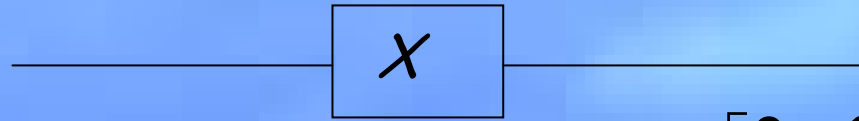
Unitary maps are the only linear maps that preserve normalization.

$$|\psi'\rangle = U|\psi\rangle \text{ implies } \|\psi'\rangle\| = \|U|\psi\rangle\| = \|\psi\rangle\| = 1$$

**Exercise:** prove that unitary evolution preserves normalization.

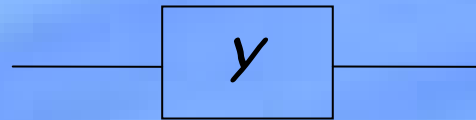
# Pauli gates

X gate (AKA  $\sigma_x$  or  $\sigma_1$ )



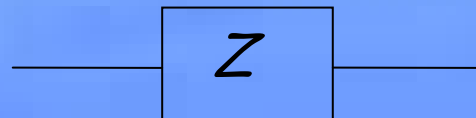
$$X|0\rangle = |1\rangle; \quad X|1\rangle = |0\rangle; \quad X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Y gate (AKA  $\sigma_y$  or  $\sigma_2$ )



$$Y|0\rangle = i|1\rangle; \quad Y|1\rangle = -i|0\rangle; \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

Z gate (AKA  $\sigma_z$  or  $\sigma_3$ )



$$Z|0\rangle = |0\rangle; \quad Z|1\rangle = -|1\rangle; \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Notation:  $\sigma_0 \equiv I$

**Exercise:** prove that  $XY=iZ$

**Exercise:** prove that  $X^2=Y^2=Z^2=I$

# Measuring a qubit: a rough and ready prescription

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

Quantum mechanics DOES NOT allow us to determine  $\alpha$  and  $\beta$ .

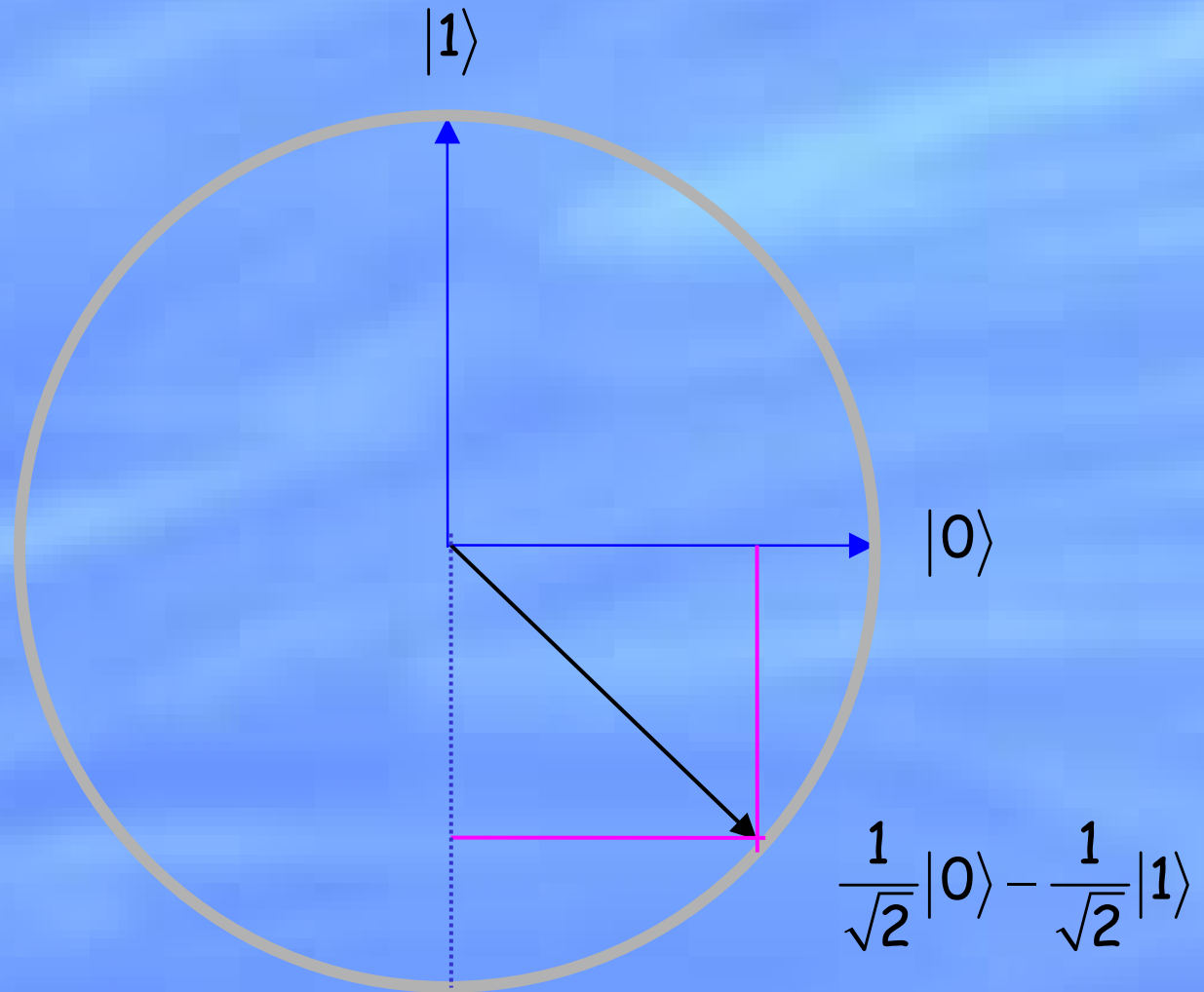
We can, however, read out limited information about  $\alpha$  and  $\beta$ .

“Measuring in the computational basis”

$$P(0) = |\alpha|^2; \quad P(1) = |\beta|^2$$

Measurement **unavoidably disturbs** the system, leaving it in a state  $|0\rangle$  or  $|1\rangle$  determined by the outcome.

# Measuring a qubit



$$P(0) = P(1) = \frac{1}{2}$$



# More general measurements

Let  $|e_1\rangle, \dots, |e_d\rangle$  be an orthonormal basis for  $\mathcal{C}^d$ .

A "measurement of  $|\psi\rangle$  in the basis  $|e_1\rangle, \dots, |e_d\rangle$ " gives result  $j$  with probability  $P(j) = \left| \langle e_j | \psi \rangle \right|^2$ .

Reminder: 
$$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} \cdot \begin{bmatrix} \chi \\ \delta \end{bmatrix} \equiv \alpha^* \chi + \beta^* \delta$$

Measurement **unavoidably disturbs** the system, leaving it in a state  $|e_j\rangle$  determined by the outcome.

# Qubit example

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

Introduce orthonormal basis

$$|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \quad |-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

$$\text{Pr}(+) = \left| \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \cdot \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \right|^2 = \left| \frac{\alpha + \beta}{\sqrt{2}} \right|^2 = \frac{|\alpha + \beta|^2}{2}$$

$$\text{Pr}(-) = \frac{|\alpha - \beta|^2}{2}$$

# Inner products and duals

"Young man, in mathematics you don't understand things, you just get used to them." - John von Neumann

The inner product is used to define the **dual** of a vector  $|\psi\rangle$ .

If  $|\psi\rangle$  lives in  $\mathcal{C}^d$  then the **dual** of  $|\psi\rangle$  is a function  $\langle\psi|: \mathcal{C}^d \rightarrow \mathcal{C}$  defined by  $\langle\psi|(|\phi\rangle) \equiv |\psi\rangle \bullet |\phi\rangle$

Simplified notation:  $\langle\psi|\phi\rangle$

**Example:**  $\langle 0 | (\alpha | 0 \rangle + \beta | 1 \rangle) = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \bullet \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha$

Properties:  $\langle a | b \rangle = \langle b | a \rangle^*$ , since  $(|a\rangle, |b\rangle) = (|b\rangle, |a\rangle)^*$

$$A|b\rangle \leftrightarrow \langle b|A^\dagger, \text{ since } (A|b\rangle, |c\rangle) = (|b\rangle, A^\dagger|c\rangle) = \langle b|A^\dagger|c\rangle$$

## Duals as row vectors

Suppose  $|a\rangle = \sum_j a_j |j\rangle$  and  $|b\rangle = \sum_j b_j |j\rangle$ . Then

$$\begin{aligned}\langle a|b\rangle &= (\langle a|, |b\rangle) = \sum_j a_j^* b_j \\ &= \begin{bmatrix} a_1^* & a_2^* & \dots \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \end{bmatrix}\end{aligned}$$

This suggests the very useful **identification** of  $\langle a|$  with the row vector  $\begin{bmatrix} a_1^* & a_2^* & \dots \end{bmatrix}$ .

## Postulate 3: rough form

If we measure  $|\psi\rangle$  in an orthonormal basis  $|e_1\rangle, \dots, |e_d\rangle$ , then we obtain the result  $j$  with probability  $P(j) = |\langle e_j | \psi \rangle|^2$ .

The measurement **disturbs** the system, leaving it in a state  $|e_j\rangle$  determined by the outcome.

# The measurement problem

Quantum system



Measuring apparatus

Rest of the Universe



Postulates 1 and 2



Postulate 3

**Research problem:** solve the measurement problem.

# Irrelevance of “global phase”

Suppose we measure  $|\psi\rangle$  in the orthonormal basis  $|e_1\rangle, \dots, |e_d\rangle$ .

Then  $\Pr(j) = |\langle e_j | \psi \rangle|^2$ .

Suppose we measure  $e^{i\theta} |\psi\rangle$  in the orthonormal basis  $|e_1\rangle, \dots, |e_d\rangle$ .

Then  $\Pr(j) = |\langle e_j | e^{i\theta} |\psi\rangle|^2 = |\langle e_j | \psi \rangle|^2$ .

The **global phase factor**  $e^{i\theta}$  is thus **unobservable**, and we may identify the states  $|\psi\rangle$  and  $e^{i\theta} |\psi\rangle$ .

# Revised postulate 1

Associated to any quantum system is a complex **inner product space** known as state space.

The state of a closed quantum system is a unit vector in state space.

**Note:** These inner product spaces are often called **Hilbert spaces**.



# Multiple-qubit systems

$$\alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

Measurement in the computational basis:  $P(x,y) = |\alpha_{xy}|^2$

General state of  $n$  qubits:  $\sum_{x \in \{0,1\}^n} \alpha_x |x\rangle$

Classically, requires  $O(2^n)$  bits to describe the state.

**“Hilbert space is a big place” - Carlton Caves**

“Perhaps [...] we need a mathematical theory of quantum automata. [...] the quantum state space has far greater capacity than the classical one: [...] in the quantum case we get the exponential growth [...] the quantum behavior of the system might be much more complex than its classical simulation.” - Yu Manin (1980)

# Postulate 4

The state space of a composite physical system is the **tensor product** of the state spaces of the component systems.

**Example:** Two-qubit state space is  $\mathcal{C}^2 \otimes \mathcal{C}^2 = \mathcal{C}^4$

Computational basis states:  $|0\rangle \otimes |0\rangle$ ;  $|0\rangle \otimes |1\rangle$ ;  $|1\rangle \otimes |0\rangle$ ;  $|1\rangle \otimes |1\rangle$

Alternative notations:  $|0\rangle|0\rangle$ ;  $|0,0\rangle$ ;  $|00\rangle$ .

## Properties

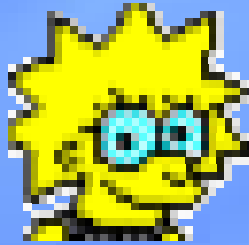
$$z(|v\rangle \otimes |w\rangle) = (z|v\rangle) \otimes |w\rangle = |v\rangle \otimes (z|w\rangle)$$

$$(|v_1\rangle + |v_2\rangle) \otimes |w\rangle = |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle$$

$$|v\rangle \otimes (|w_1\rangle + |w_2\rangle) = |v\rangle \otimes |w_1\rangle + |v\rangle \otimes |w_2\rangle$$

# Some conventions implicit in Postulate 4

Alice



Bob



If Alice prepares her system in state  $|a\rangle$ , and Bob prepares his in state  $|b\rangle$ , then the joint state is  $|a\rangle \otimes |b\rangle$ .

Conversely, if the joint state is  $|a\rangle \otimes |b\rangle$  then we say that Alice's system is **in the state  $|a\rangle$** , and Bob's system is **in the state  $|b\rangle$** .

$$|a\rangle \otimes |b\rangle = (e^{i\theta} |a\rangle) \otimes (e^{-i\theta} |b\rangle)$$

**"Alice applies the gate  $U$  to her system"** means that  $(U \otimes I)$  is applied to the joint system.

$$(A \otimes B)|v\rangle \otimes |w\rangle = A|v\rangle \otimes B|w\rangle$$

# Examples

Suppose a NOT gate is applied to the second qubit of the state  $\sqrt{0.4}|00\rangle + \sqrt{0.3}|01\rangle + \sqrt{0.2}|10\rangle + \sqrt{0.1}|11\rangle$ .

The resulting state is

$$\begin{aligned} & (\mathcal{I} \otimes X) \left( \sqrt{0.4}|00\rangle + \sqrt{0.3}|01\rangle + \sqrt{0.2}|10\rangle + \sqrt{0.1}|11\rangle \right) \\ &= \sqrt{0.4}|01\rangle + \sqrt{0.3}|00\rangle + \sqrt{0.2}|11\rangle + \sqrt{0.1}|10\rangle. \end{aligned}$$

**Worked exercise:** Suppose a two-qubit system is in the state  $0.8|00\rangle + 0.6|11\rangle$ . A NOT gate is applied to the second qubit, and a measurement performed in the computational basis. What are the probabilities for the possible measurement outcomes?

# Quantum entanglement

Alice

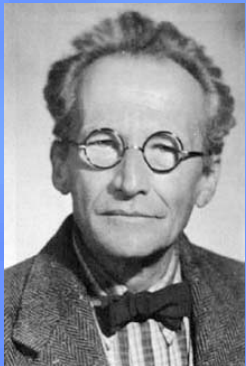


Bob



$$|\psi\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

$$\begin{aligned} |\psi\rangle \neq |a\rangle|b\rangle \quad & |\psi\rangle = (\alpha|0\rangle + \beta|1\rangle)(\gamma|0\rangle + \delta|1\rangle) \\ & = \alpha\gamma|00\rangle + \beta\gamma|10\rangle + \alpha\delta|01\rangle + \beta\delta|11\rangle \\ & \rightarrow \beta = 0 \text{ or } \gamma = 0. \end{aligned}$$



Schroedinger (1935): "I would not call [entanglement] *one* but rather *the* characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought."

# Summary

**Postulate 1:** A closed quantum system is described by a unit vector in a complex inner product space known as state space.

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

$$|\psi'\rangle = U|\psi\rangle$$

**Postulate 3:** If we measure  $|\psi\rangle$  in an orthonormal basis  $|e_1\rangle, \dots, |e_d\rangle$ , then we obtain the result  $j$  with probability

$$P(j) = |\langle e_j | \psi \rangle|^2.$$

The measurement disturbs the system, leaving it in a state  $|e_j\rangle$  determined by the outcome.

**Postulate 4:** The state space of a composite physical system is the tensor product of the state spaces of the component systems.