

# **Introduction to Quantum Computing**

**Qubits, gates and circuits**

**Juan de Gracia, PhD. Researcher at RISE Research Institutes of Sweden**

# About me

## Juan de Gracia

- PhD in Quantum Chemistry from KTH Royal Institute of Technology
- Postdoc in Quantum Computing at WACQT (Chalmers)
- Researcher in Multiscale modeling in KTH (PDC).
- Researcher in HPC and QC in RISE Research Institutes of Sweden.



# Quick outline

- Why quantum is quantum?
- 0 and 1 and everything in the between: **Superposition**
- Qubits make friends using tensor products: **Entanglement**
- What do I do with this? Gates and **Interference**

**Why quantum is quantum?**

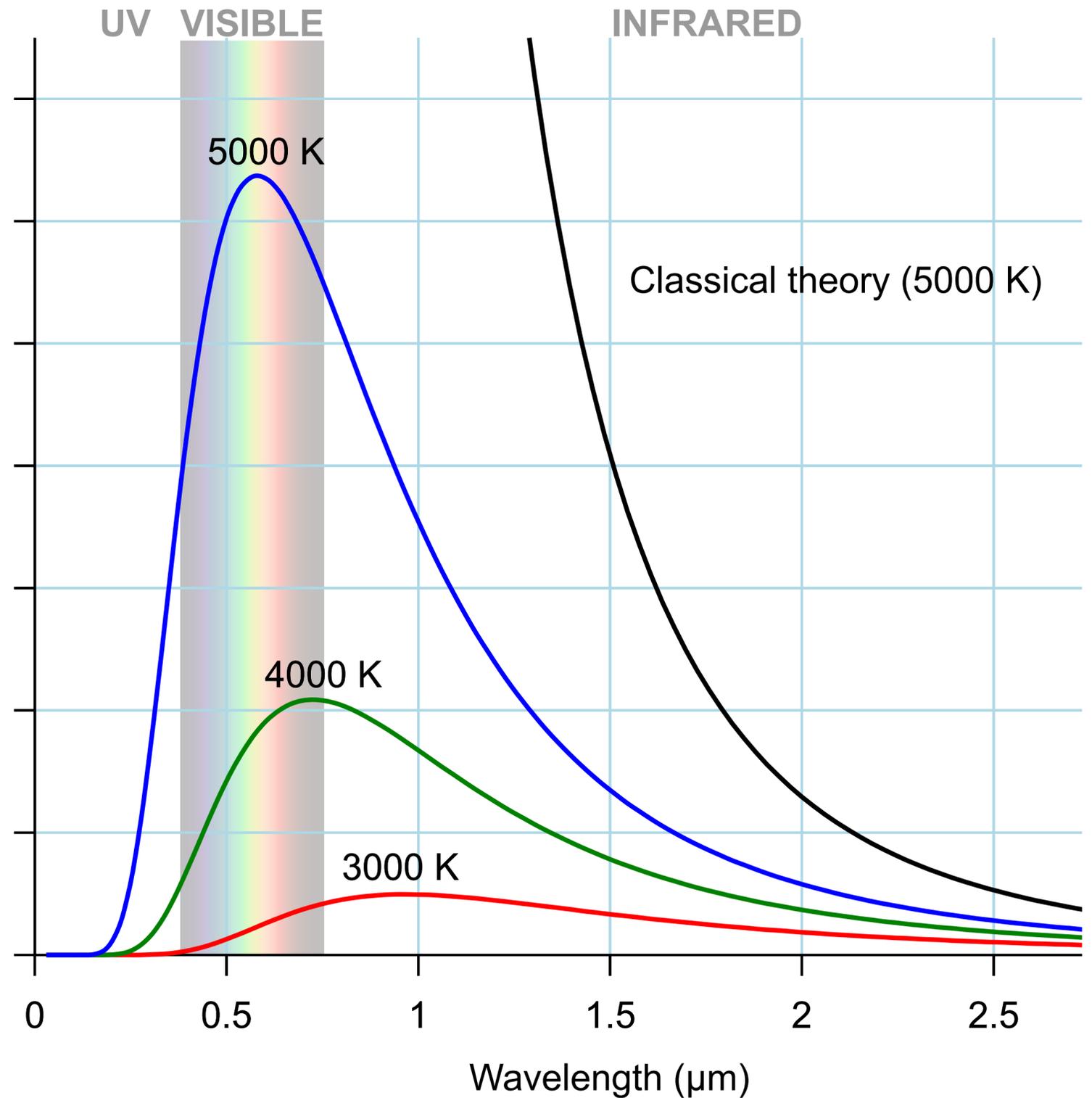
# Classical mechanics doesn't work!

- Classical theory: Rayleigh-Jeans Law. Imagine a black body composed by tiny springs that vibrate at any frequency.

- All frequencies are allowed (all energies). The average energy per oscillator is  $\langle E \rangle = kT$

- $$u(\lambda, T) = \frac{8\pi}{\lambda^4} kT$$

- Energy density goes to infinity near UV: Ultraviolet catastrophe!



# A bit like machine learning does:

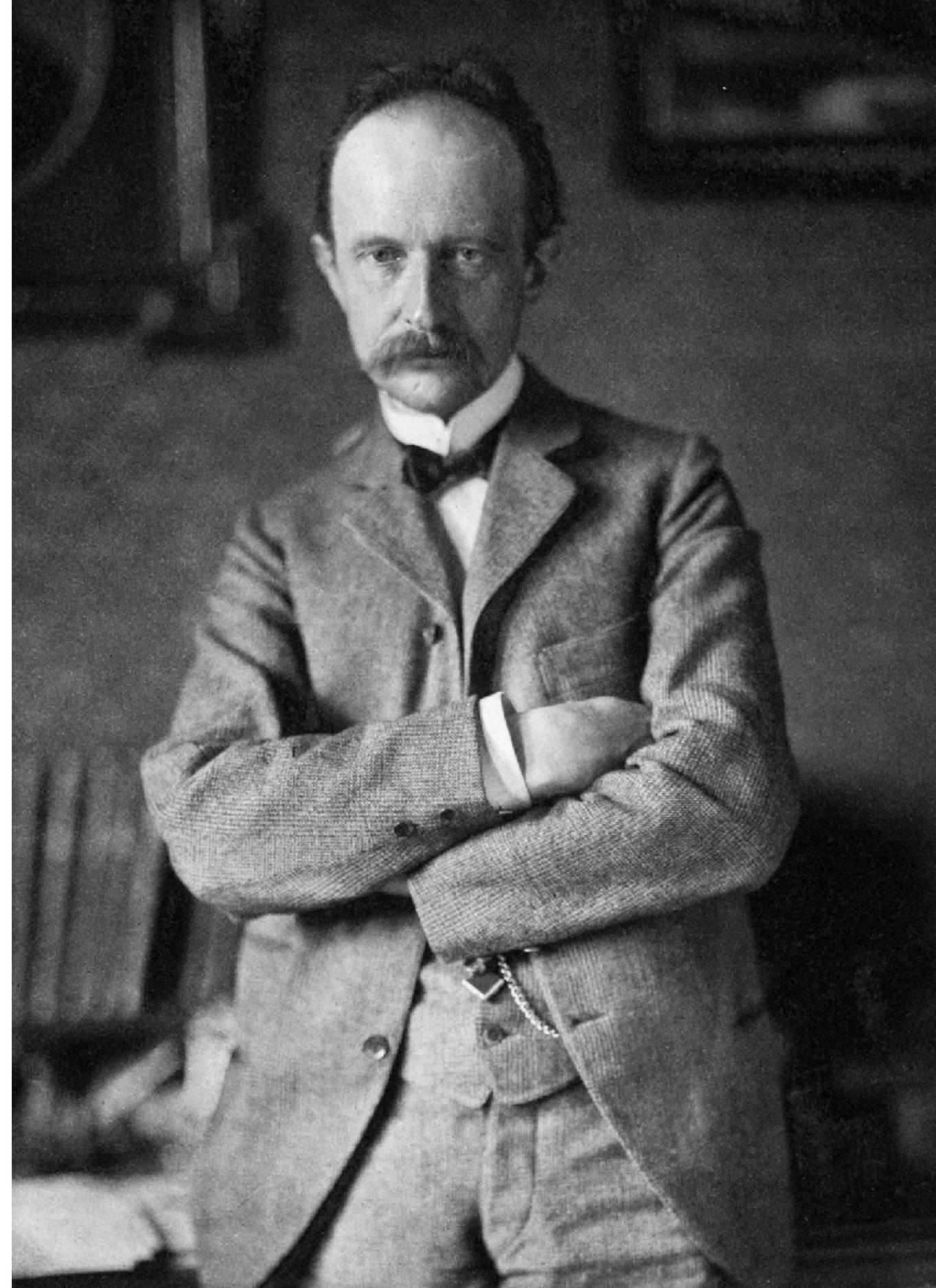
- When Planck wanted to study physics, one of his professors told him “*in physics, almost everything is already discovered; all that remains is to fill in a few holes.*”
- If the Rayleigh–Jeans law doesn’t match, maybe I can tweak the formula to make it fit.

- $E_n = nh\nu; n = 1, 2, 3, \dots$  and  $\langle E \rangle = \frac{h\nu}{e^{h\nu/kT} - 1}$

- Now the oscillators vibrate in a **quantized manner and the energy is Quantized >>> Quantum Mechanics**

- $u(\lambda, T) = \frac{8\pi hc}{\lambda^5} \cdot \frac{1}{e^{hc/\lambda kT} - 1}$

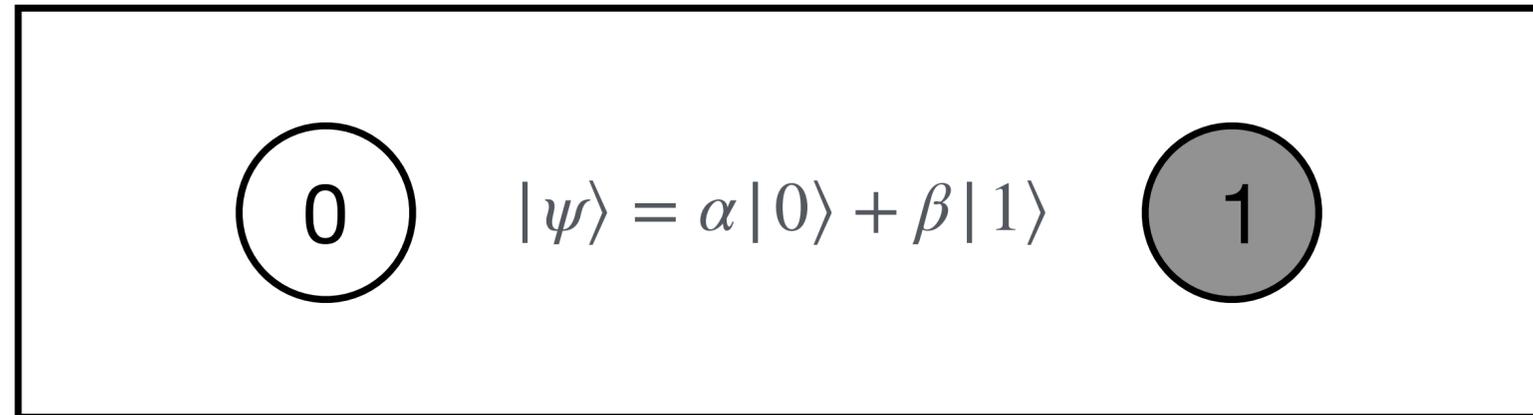
- Exp and theory matches. At lower frequencies Planck and RJ coincides.  $e^{h\nu/kT} \approx 1 + \frac{h\nu}{kT}$



**0 and 1 and everything in  
between**

# 0 and 1 and everything in between

Quantum and classical bits



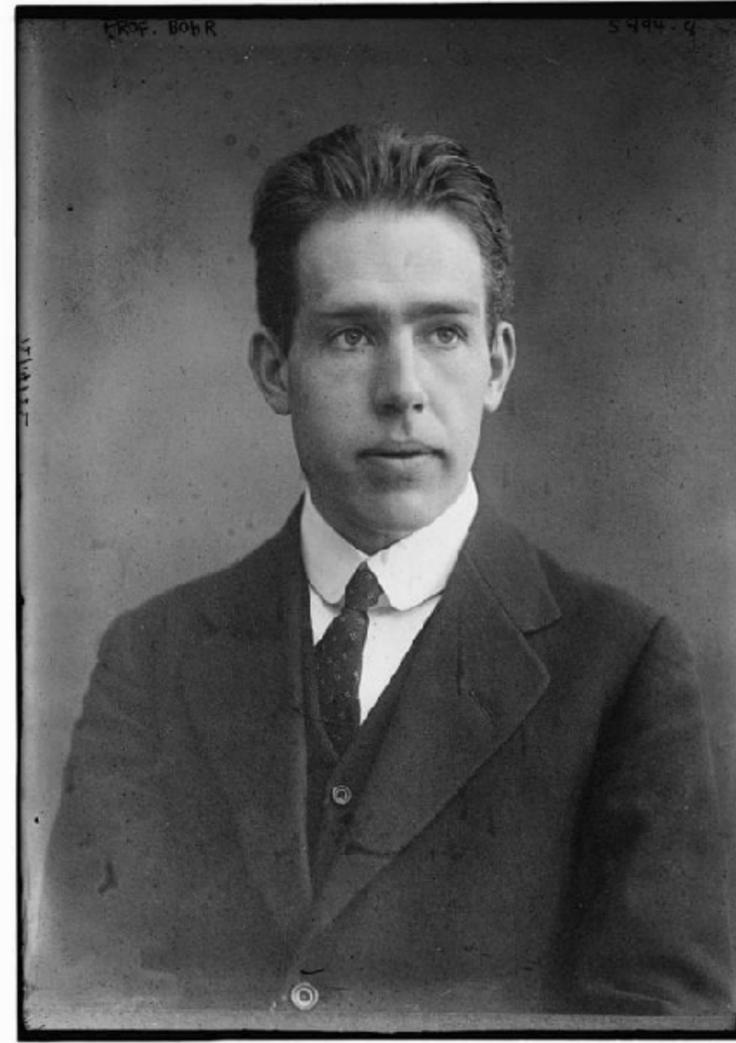
A diagram illustrating a quantum state  $|\psi\rangle$  as a superposition of two basis states,  $|0\rangle$  and  $|1\rangle$ . The state  $|\psi\rangle$  is represented by the equation  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ . The basis state  $|0\rangle$  is shown as a white circle with the number 0 inside, and the basis state  $|1\rangle$  is shown as a gray circle with the number 1 inside. The entire diagram is enclosed in a black rectangular border.

Where are  $\alpha, \beta \in \mathbb{C}$  called **complex amplitudes** and  $|0\rangle, |1\rangle$  are the **orthonormal** basis vectors

# What are the complex amplitudes?

Or how shall we interpret quantum mechanics

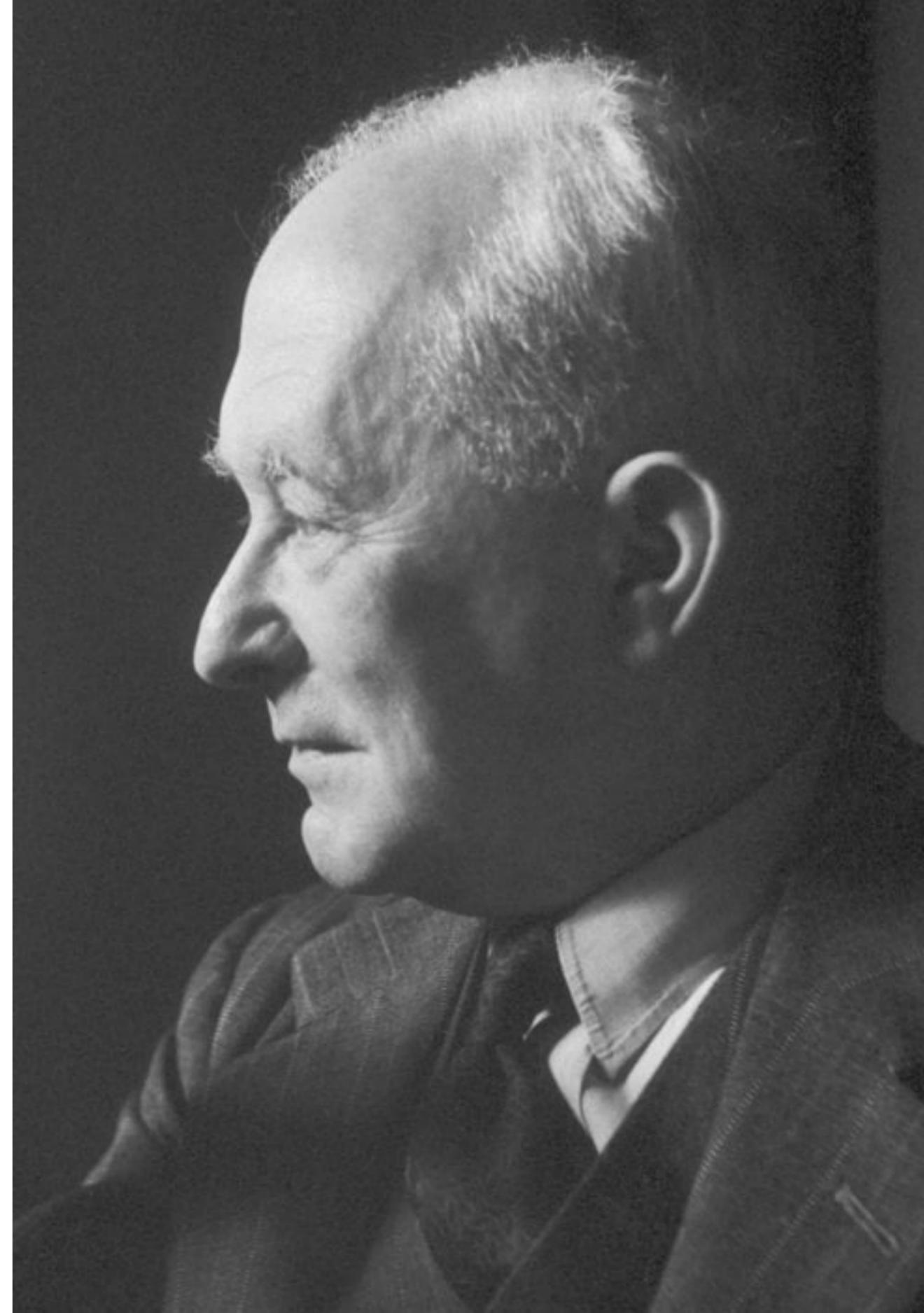
- The meaning of the wave function was not entirely clear after formulated by Schrödinger.
- Niels Bohr and Werner Heisenberg established the current interpretation of quantum mechanics (Copenhagen interpretation) says: ***A quantum system doesn't have definite properties until it's measured. The wavefunction gives only probabilities of possible outcomes, and measurement causes it to collapse into one of them.***



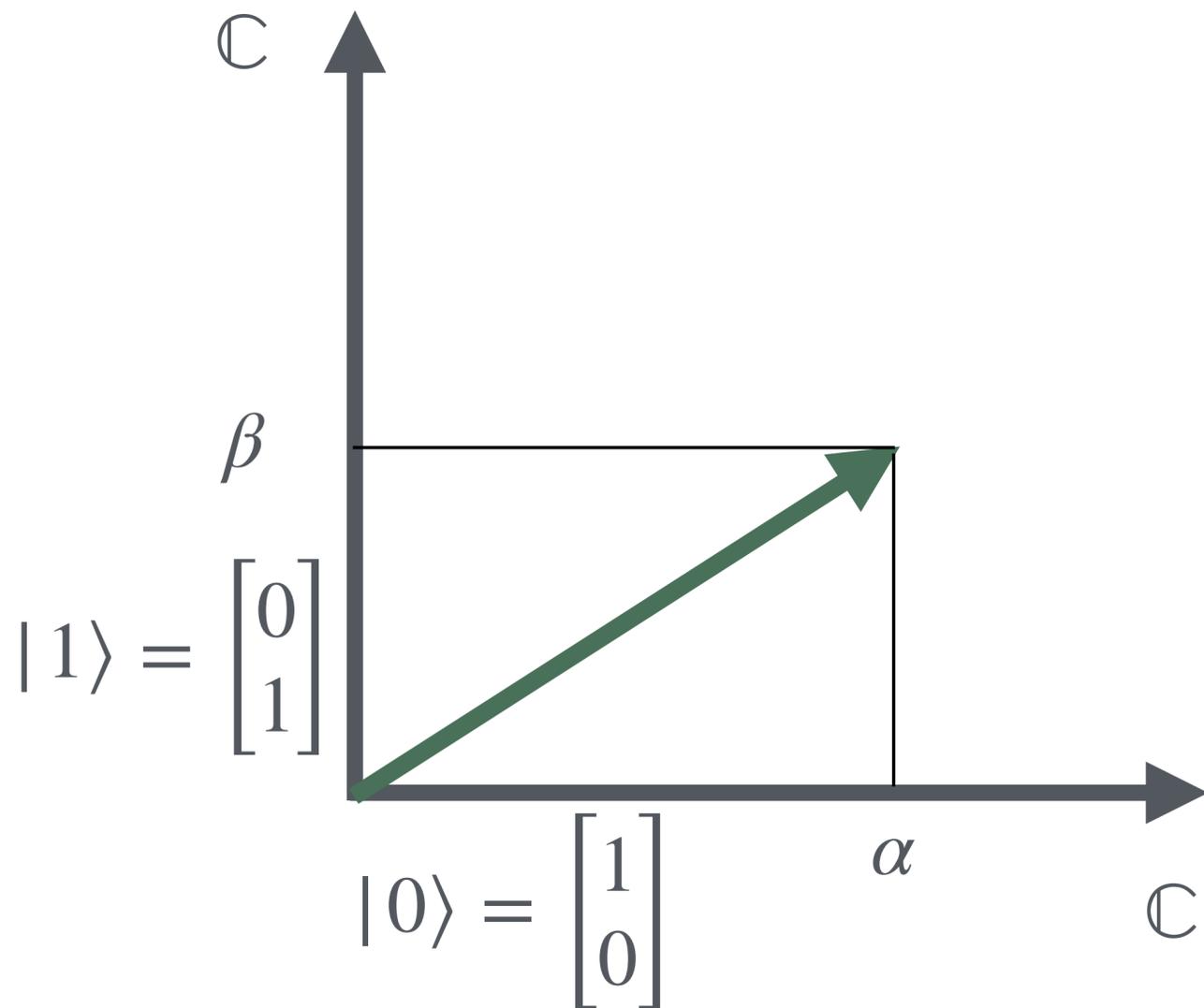
# What are the complex amplitudes?

## Or how shall we interpret quantum mechanics

- Max Born (1926) nailed down the probabilistic interpretation of the wave function (Born rule) as one of the postulates of Quantum Mechanics.
- The Born rule says that the square of the wavefunction's amplitude gives the probability of finding a particle in a particular state.
- $P(x) = |\psi(x)|^2$
- Apply this to the qubit state (normalized)  
 $\langle \psi | \psi \rangle = (\alpha^* \langle 0 | \beta^* \langle 1 |)(\alpha | 0 \rangle + \beta | 1 \rangle) = |\alpha|^2 + |\beta|^2 = 1$
- This means that  $|\alpha|^2, |\beta|^2$  are the probabilities to collapse in  $|0\rangle, |1\rangle$  respectively.



# Geometric representation



0

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

1

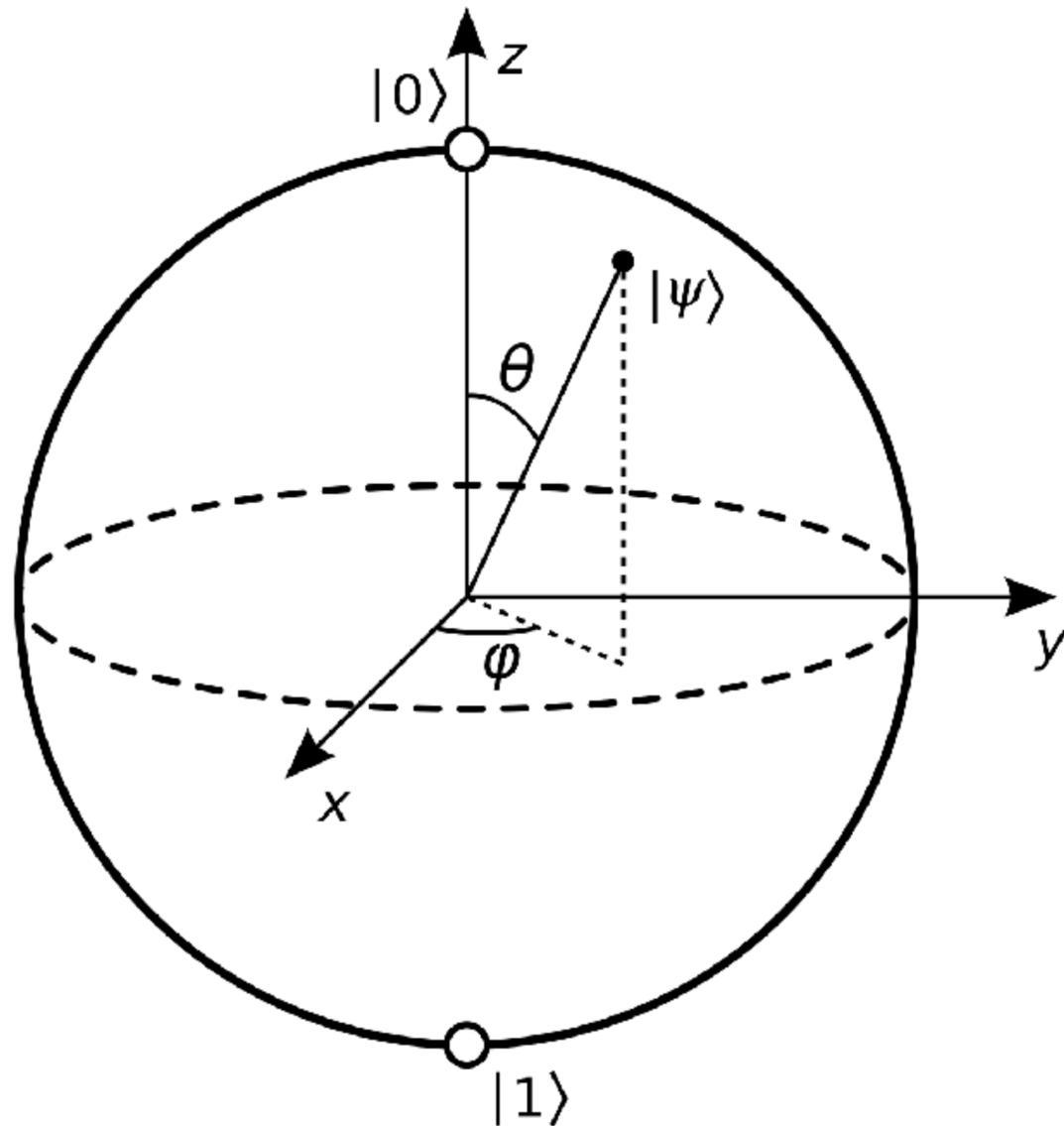
$$|\psi\rangle = \alpha \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} x \\ yi \\ z \\ ki \end{bmatrix}$$

Issue here:

Since  $\alpha, \beta \in \mathbb{C}$  those numbers have 2 components.

**The accurate geometric representation requires 4D!**

# Geometric representation



$$\textcircled{0} \quad |\psi\rangle = \alpha|0\rangle + \beta|1\rangle \quad \textcircled{1}$$

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$

## Bloch Sphere:

Since  $\phi, \theta \in \mathbb{R}$  we can do a 3D representation of a qubit

- $\theta$  represents the relative weight between (probability)  $|0\rangle$  and  $|1\rangle$ .
- $\phi$  represents the relative phase between  $|0\rangle$  and  $|1\rangle$ .

# How do we measure?

## Superposition

- The qubit is a linear combination of the basis states  $|0\rangle$  and  $|1\rangle$  or a **superposition** of the basis states.
- $|\alpha|^2, |\beta|^2$  are the probabilities to measure in  $|0\rangle, |1\rangle$  respectively.
- We need to measure in  $|0\rangle, |1\rangle$  basis.
- Done by **projection operators**  $P_0 = |0\rangle\langle 0|$ ,  $P_1 = |1\rangle\langle 1|$
- Then the probabilities are:  $P(0) = \langle \psi | P_0 | \psi \rangle = |\alpha|^2$ ,  $P(1) = \langle \psi | P_1 | \psi \rangle = |\beta|^2$ .
- Measuring gives only  $|0\rangle, |1\rangle$ , measuring many times gives the probabilities >> In a **Quantum computer one can recreate the superposition** but never measuring it directly because **measuring destroy the quantum state!**

**Qubits make friends using tensor  
products**

# Constructing a 2-Qubit system

$$|\psi_1\rangle = \alpha_1 |0\rangle + \beta_1 |1\rangle$$

$$|\psi_2\rangle = \alpha_2 |0\rangle + \beta_2 |1\rangle$$

$$|\psi_1\psi_2\rangle = ?$$

# The tensor product

## Definition

$$|\psi_1\rangle = \begin{bmatrix} \alpha_1 \\ \beta_1 \end{bmatrix}$$

$$|\psi_2\rangle = \begin{bmatrix} \alpha_2 \\ \beta_2 \end{bmatrix}$$

$$|\psi_1\psi_2\rangle = |\psi_1\rangle \otimes |\psi_2\rangle = \begin{bmatrix} \alpha_1\alpha_2 \\ \alpha_1\beta_2 \\ \beta_1\alpha_2 \\ \beta_1\beta_2 \end{bmatrix}$$

# The tensor product

## In computational basis

$$|\psi_1\rangle = \alpha_1 |0\rangle + \beta_1 |1\rangle$$

$$|\psi_2\rangle = \alpha_2 |0\rangle + \beta_2 |1\rangle$$

$$|\psi_1\psi_2\rangle = \alpha_1\alpha_2 |00\rangle + \alpha_1\beta_2 |01\rangle + \beta_1\alpha_2 |10\rangle + \beta_1\beta_2 |11\rangle$$

The new space has dimension  $2^2 = 4$ . In general, a system of  $N$  qubits has dimension  $2^N$  by the nature of tensor products.

This means that the amount of information that a **quantum state can encode increases exponentially with the number of qubits!**

If you mean storing an arbitrary 128-qubit state vector classically: it needs  $2^{128}$  complex amplitudes. With 16 bytes per complex double  $\rightarrow 2^{128} \times 16 = 16 \times 2^{128} = 2^4 \times 2^{128} = 2^{132}$  bytes  $\approx$  **5.44 quadrillion yottabytes.**

# Separable and non-separable states

$$|\psi_1\rangle = \alpha_1 |0\rangle + \beta_1 |1\rangle$$

$$|\psi_2\rangle = \alpha_2 |0\rangle + \beta_2 |1\rangle$$

$$|\psi_1\psi_2\rangle = \alpha_1\alpha_2 |00\rangle + \alpha_1\beta_2 |01\rangle + \beta_1\alpha_2 |10\rangle + \beta_1\beta_2 |11\rangle$$

If a 2-qubit state can be written as the tensor product of two states we say the state is **separable**.

On the contrary, if a 2-qubit state cannot be written as the tensor product of 2 states then is **non-separable or entangled!**

$$|\psi_1\psi_2\rangle \neq \alpha_1\alpha_2 |00\rangle + \alpha_1\beta_2 |01\rangle + \beta_1\alpha_2 |10\rangle + \beta_1\beta_2 |11\rangle$$

# The Bell state

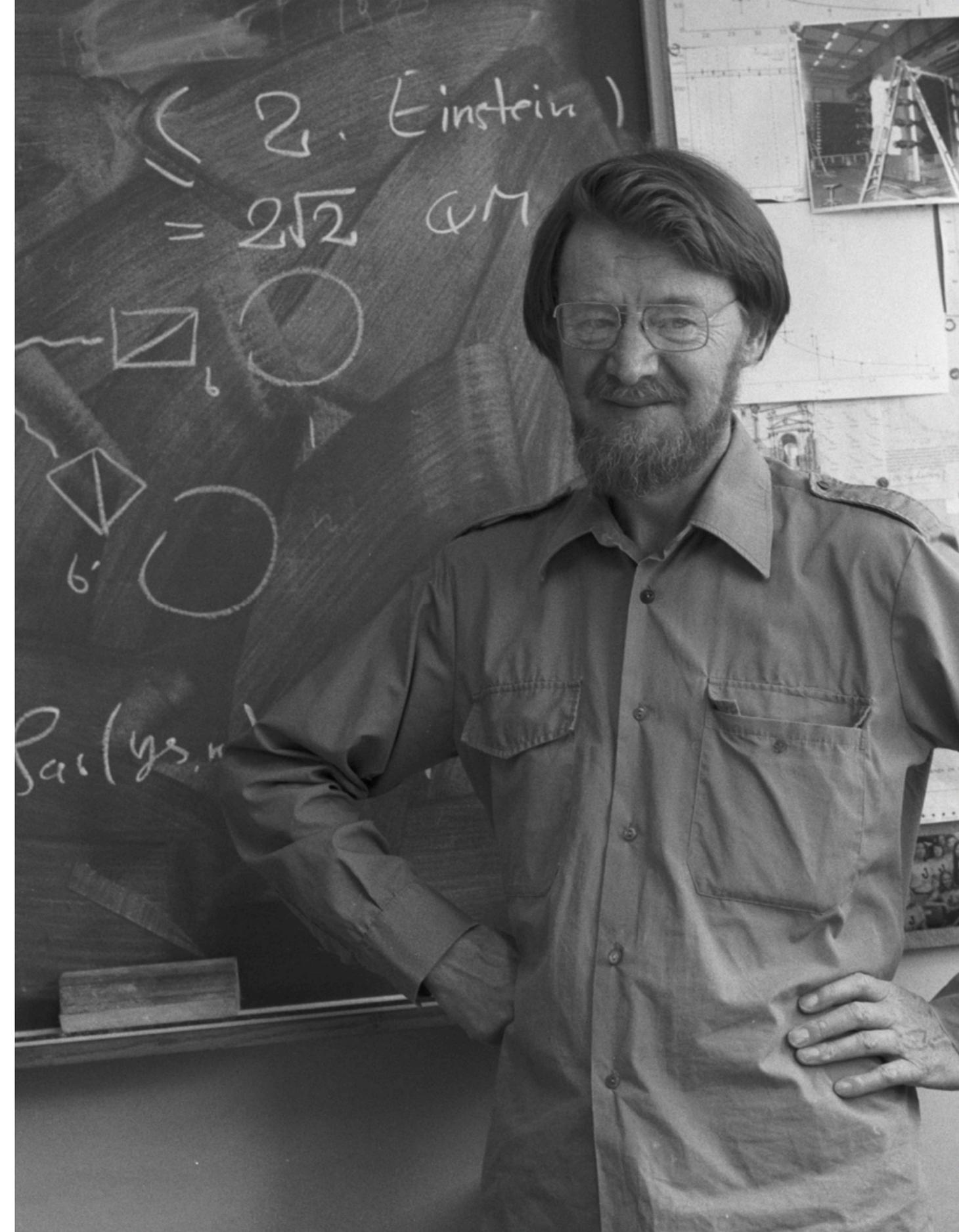
$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

The **entanglement** shows when we measure (remember projection operators). So, measuring the first qubit gives:

$$P_0|\Phi^+\rangle = \frac{1}{\sqrt{2}}|00\rangle, P_1|\Phi^+\rangle = \frac{1}{\sqrt{2}}|11\rangle$$

This means that we have 50% chance to measure  $|00\rangle$  or  $|11\rangle$  and as we can see the **measuring the first qubit determines the second qubit** >> **Realization of entanglement**

But there is no communication possible because the outcome of the measurement is still random with a 50% chance >> **No-communication theorem**



**What do I do with this?**

# Unitary operators

- The time evolution of an isolated quantum system is always described by a unitary operator
- Unitarity implies two things:
  1. The probability is preserved
  2. The transformation is reversible
- A matrix  $U$  is unitary if:  $U^\dagger U = U U^\dagger = I$  being  $I$  the identity matrix and  $U^\dagger$  the conjugate transpose
- Example:  $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ , complex conjugate:  $\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$ , and the transpose:  $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = Y$
- The matrix  $Y$  is not only unitary but also **Hermitian**  $Y^\dagger = Y$ . Observables in Quantum Mechanics are Hermitian.

# Basic unitary operators

## The Pauli Matrices

- As we saw, a single qubit can be represented as a vector inside a unit sphere (Bloch sphere)
- A unitary operator over a qubit represents a **rotation in the sphere.**
- The basic generators of rotations are the **Pauli matrices:**

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

- These are the most basic 1 qubit gates and generates **any rotation.**

# Unitary operators create interference

- When a unitary transformation mixes amplitudes, some outcomes are amplified by constructive interference while others are suppressed by destructive interference. This selective reinforcement of desired computational paths is what gives quantum algorithms their power.

- Let's take an arbitrary unitary:  $U = \begin{pmatrix} u_{00} & u_{01} \\ u_{10} & u_{11} \end{pmatrix}$

- And an arbitrary qubit:  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

- $U|\psi\rangle = \begin{pmatrix} u_{00}\alpha + u_{01}\beta \\ u_{10}\alpha + u_{11}\beta \end{pmatrix} = \psi'_0|0\rangle + \psi'_1|1\rangle$

- This operation puts new amplitudes to the qubit state, meaning both different probabilities and different phases. The phases cause **Interference**

- $P_0 = |\psi'_0|^2 = |u_{00}\alpha + u_{01}\beta|^2 = |u_{00}\alpha|^2 + |u_{01}\beta|^2 + 2|u_{00}\alpha||u_{01}\beta|\cos(\Delta\phi)$

- $\Delta\phi$  is the **Phase difference**:

- If  $\Delta\phi = 0$ ,  $\cos(0) = 1$  >> **constructive interference**

- If  $\Delta\phi = \pi$ ,  $\cos(\pi) = -1$  >> **destructive interference**

# 1-Qubit gates

Gate	$ 0\rangle$	$ 1\rangle$
$X$ (Pauli-X)	$ 1\rangle$	$ 0\rangle$
$Y$ (Pauli-Y)	$i 1\rangle$	$-i 0\rangle$
$Z$ (Pauli-Z)	$ 0\rangle$	$- 1\rangle$
$H$ (Hadamard)	$\frac{1}{\sqrt{2}}( 0\rangle +  1\rangle)$	$\frac{1}{\sqrt{2}}( 0\rangle -  1\rangle)$
$S$ (Phase)	$ 0\rangle$	$i 1\rangle$
$T$ ( $\pi/8$ gate)	$ 0\rangle$	$e^{i\pi/4} 1\rangle$
$R_x(\theta)$	$\cos\frac{\theta}{2} 0\rangle - i\sin\frac{\theta}{2} 1\rangle$	$-i\sin\frac{\theta}{2} 0\rangle + \cos\frac{\theta}{2} 1\rangle$
$R_y(\theta)$	$\cos\frac{\theta}{2} 0\rangle - \sin\frac{\theta}{2} 1\rangle$	$\sin\frac{\theta}{2} 0\rangle + \cos\frac{\theta}{2} 1\rangle$
$R_z(\theta)$	$e^{-i\theta/2} 0\rangle$	$e^{i\theta/2} 1\rangle$

# 2-Qubit Gates

## Controlled gates

General form

$$C(U) = \begin{bmatrix} I & 0 \\ 0 & U \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & u_{00} & u_{01} \\ 0 & 0 & u_{10} & u_{11} \end{bmatrix}$$

They are controlled because they act if a control qubit takes the value  $|1\rangle$

$$\text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\text{CZ} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$C(P(\phi)) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{pmatrix}$$

# 2-Qubit Gates

## Swap gates

$$\text{SWAP}|a, b\rangle = |b, a\rangle, \quad \text{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$i\text{SWAP}|a, b\rangle = i|b, a\rangle, \quad \text{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

# 2-qubit gates

Gate	Action on Computational Basis
<b>CNOT</b> (Controlled-X)	$ 00\rangle \rightarrow  00\rangle,  01\rangle \rightarrow  01\rangle,$ $ 10\rangle \rightarrow  11\rangle,  11\rangle \rightarrow  10\rangle$
<b>CZ</b> (Controlled-Z)	$ 00\rangle \rightarrow  00\rangle,  01\rangle \rightarrow  01\rangle,$ $ 10\rangle \rightarrow  10\rangle,  11\rangle \rightarrow - 11\rangle$
<b>SWAP</b>	$ 00\rangle \rightarrow  00\rangle,  01\rangle \rightarrow  10\rangle,$ $ 10\rangle \rightarrow  01\rangle,  11\rangle \rightarrow  11\rangle$
<b>iSWAP</b>	$ 00\rangle \rightarrow  00\rangle,  01\rangle \rightarrow i 10\rangle,$ $ 10\rangle \rightarrow i 01\rangle,  11\rangle \rightarrow  11\rangle$
<b>Controlled-H</b>	$ 00\rangle \rightarrow  00\rangle,  01\rangle \rightarrow  01\rangle,$ $ 10\rangle \rightarrow \frac{1}{\sqrt{2}}( 10\rangle +  11\rangle),$ $ 11\rangle \rightarrow \frac{1}{\sqrt{2}}( 10\rangle -  11\rangle)$
<b>Controlled-Phase</b> ( $CP(\phi)$ )	$ 00\rangle \rightarrow  00\rangle,  01\rangle \rightarrow  01\rangle,$ $ 10\rangle \rightarrow  10\rangle,  11\rangle \rightarrow e^{i\phi} 11\rangle$
<b>Bell creation</b> (H on qubit 0, then CNOT)	$ 00\rangle \rightarrow \frac{1}{\sqrt{2}}( 00\rangle +  11\rangle)$

**Those are all the basic ingredients  
to make circuits and algorithms.  
Have fun!**