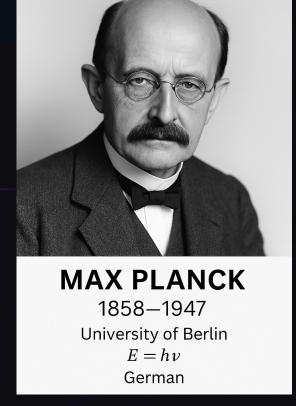


## Welcome to the Quantum Frontier

## GOALS:

- 1) Quantum Computation isn't magic
- 2) Give a sense of the ideas behind it
- 3) Show you how to run quantum programs



Not to turn you into a quantum physicist in 2 hours

There will be a variety of levels of presentation – everyone will get lost at some point.



# Why Quantum? Why Now? Classical limits Moore's Law pl Simulation bottl Quantum opportu Simulating mole Solving hard se Hybrid algorithr Qis "Learning" quantum computing in 2012

Why Quantum? Why Now?

#### Classical limits

- Moore's Law plateau
- Simulation bottlenecks

#### Quantum opportunities

- Simulating molecules
- Solving hard search problems
- Hybrid algorithms for near-term utility



Qiskit



# Logging into Hopper



First login to the Linux workstation in front of you. Your CARC username is on the sign in sheet.

If you have logged in before use your existing password

This is an "important step" so don't let me move on until you have logged in

# Logging into Hopper



ssh vanilla@hopper.alliance.unm.edu

Should prompt you for a password...

Don't let me move on until you are able to login.

Replace vanilla with your name (unless your last name is Ice)

```
[vanilla@hopper ~] $ git clone https://lobogit.unm.edu/CARC/workshops.git Cloning into 'workshops'...
remote: Enumerating objects: 132, done.
remote: Counting objects: 100% (75/75), done.
remote: Compressing objects: 100% (43/43), done.
remote: Total 132 (delta 33), reused 74 (delta 32), pack-reused 57
Receiving objects: 100% (132/132), 57.58 KiB | 3.60 MiB/s, done.
Resolving deltas: 100% (51/51), done.
```

Rather than make you write shell scripts lets just download some we wrote for this workshop...

```
[vanilla@hopper workshops]$ git stash
[vanilla@hopper workshops]$ git pull
```

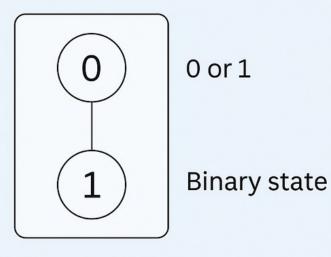
```
[vanilla@hopper ~]$ cd workshops
[vanilla@hopper workshops]$ module load miniconda3
[vanilla@hopper workshops]$
conda env create --file quantum_computing/conda_envs/quantum-computing.yml
Type "yes" to installing when prompted
```

Let's setup the quantum packages we need with conda

# From Bits to Qubits

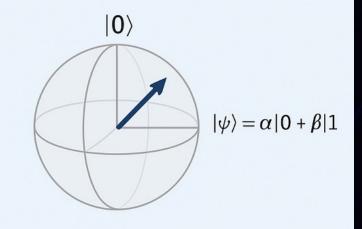
## From Bits to Qubits

### **Classical Bit**



Binary state

### **Quantum Qubit**



Superposition
Probabilistic until measured

## Supremacy vs Advantage vs Utility: What's the Difference?

Term	Definition	Goal	Usefulness	Example
Quantum Supremacy	A quantum computer solves at least one problem faster than any classical computer, regardless of practicality.	Prove quantum capabilities	X The problem may be artificial	Google's Sycamore chip (random circuit sampling)
Quantum Advantage	A quantum system outperforms classical approaches on a specific, structured problem.	Demonstrate task-specific performance	Possibly useful	Early VQE on small molecules
Quantum Utility	A quantum device solves a <b>real-world</b> problem better than classical methods, justifying its use.	Provide practical value	Clearly useful	As of today: None

# What Quantum Computing Can Do

# WHAT QUANTUM COMPUTING CAN DO



# Efficient factoring of large integers

- Shor's algorithm breaks RSA



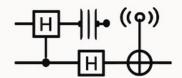
# Quadratic speedup for search problems

- Grover's algorithm



## Simulation of quantum systems

Molecules, condensed matter, photonics



## Hybrid optimisation & ML workflows

 Variational algorithms, quantum classifiers

# What Quantum Computing Can't Do Faster

#### Limitation

- X Not faster at everything
- X Not yet fault-tolerant
- X Not scalable (yet)
- X Not a replacement for classical computing

#### **Notes**

No speedup for all problems—only specific types

NISQ era = noisy hardware, limited depth

Current devices = tens to hundreds of noisy qubits\*

Best as a **co-processor**, not a universal upgrade

# How to factor 2048 bit RSA integers in 8 hours using 20 million noisy qubits

Craig Gidney<sup>1</sup> and Martin Ekerå<sup>2</sup>

 <sup>1</sup>Google Inc., Santa Barbara, California 93117, USA
 <sup>2</sup>KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden Swedish NCSA, Swedish Armed Forces, SE-107 85 Stockholm, Sweden

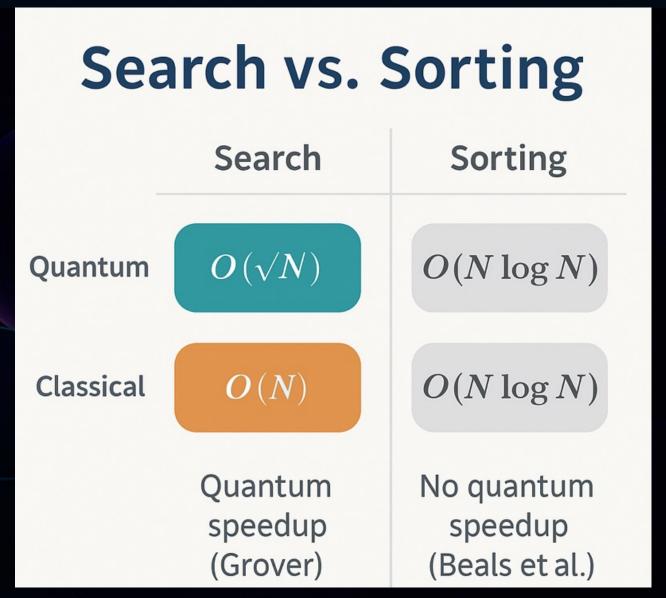
We significantly reduce the cost of factoring integers and computing discrete logarithms in finite fields on a quantum computer by combining techniques from Shor 1994, Griffiths-Niu 1996, Zalka 2006, Fowler 2012, Ekerå-Håstad 2017, Ekerå 2017, Ekerå 2018, Gidney-Fowler 2019, Gidney 2019. We estimate the approximate cost of our construction using plausible physical assumptions for large-scale superconducting

Craig Gidney and Martin Ekerå. How to factor 2048 bit RSA integers in 8 hours using 20 million noisy qubits. Quantum, 5, 433 (2021). https://doi.org/10.22331/q-2021-04-15-433

Not faster(and adds overhead) for Sorting, matrix multiplication, numerical integration.

# What Quantum Computing Can't Do Faster

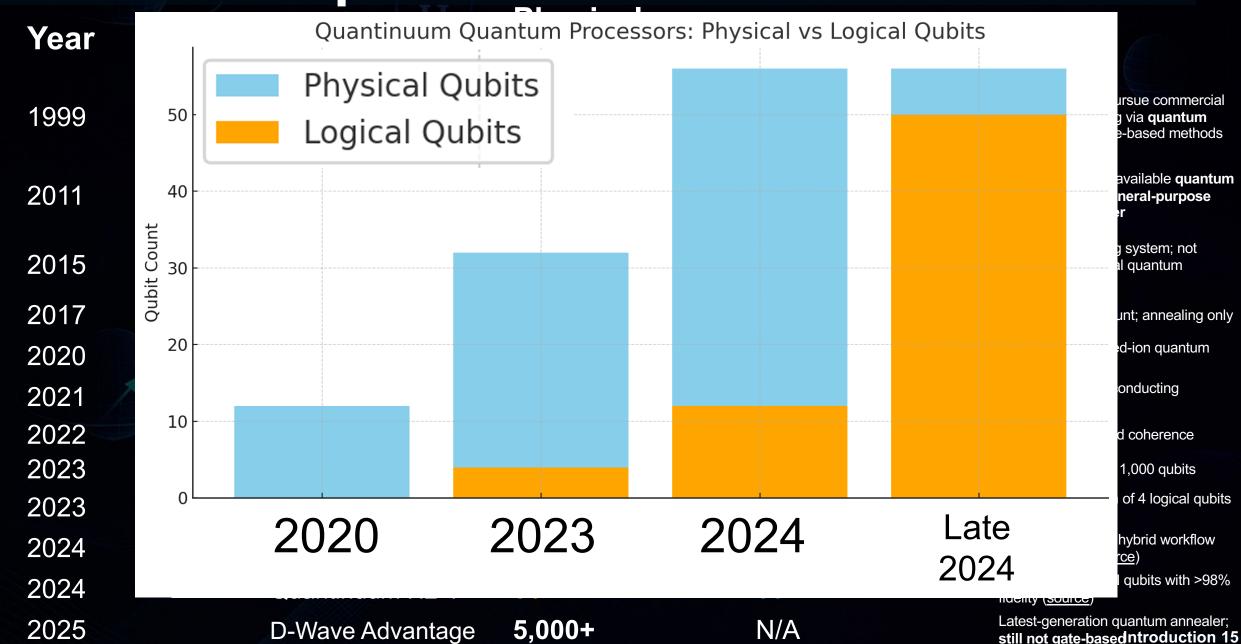
Beals, R., Buhrman, H., Cleve, R., Mosca, M., & de Wolf, R. (2001). Quantum lower bounds by polynomials. Journal of the ACM, 48(4), 778–797. https://doi.org/10.1145/502090.502097



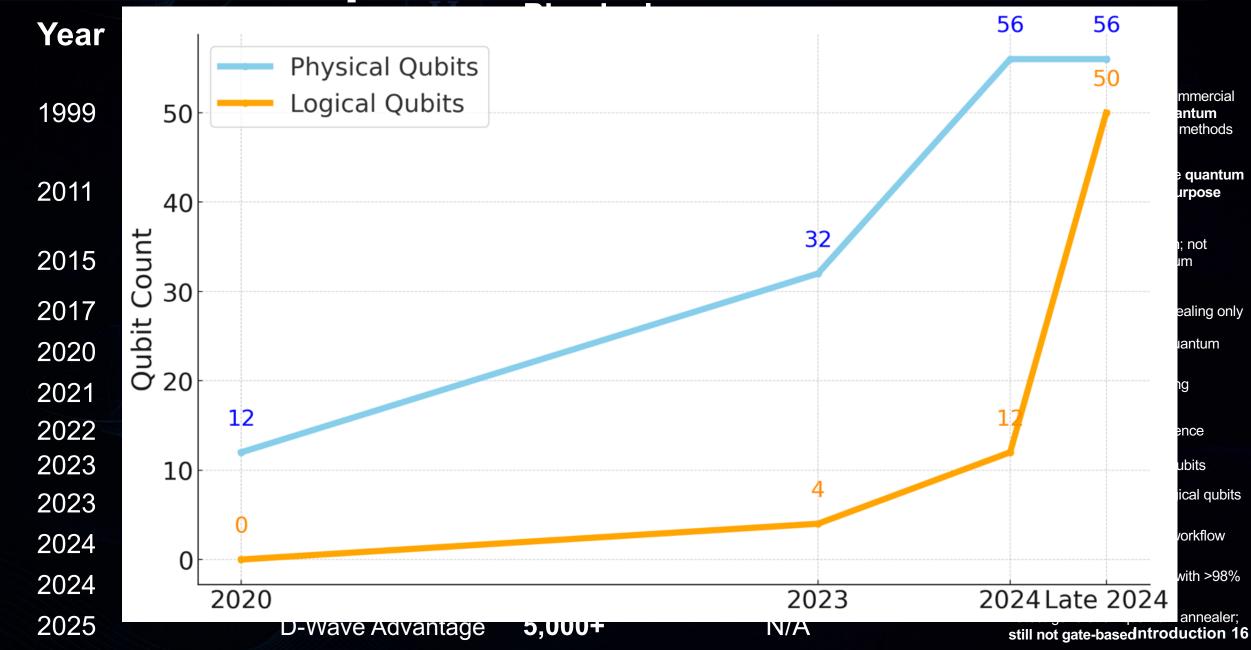
# Hardware improvement in Qubits

Year	Name	Physical Qubits	<b>Logical Qubits</b>	Notes
1999	D-Wave founded	N/A	N/A	First company to pursue commercial quantum computing via <b>quantum annealing</b> , not gate-based methods
2011	D-Wave One	~128	N/A	First commercially available quantun annealer; not a general-purpose quantum computer
2015	D-Wave 2X	~1,000	N/A	Quantum annealing system; not capable of universal quantum algorithms
2017	D-Wave 2000Q	~2,048	N/A	Expanded qubit count; annealing only
2020	Quantinuum H1-1	12	N/A	Gate-based, trapped-ion quantum computer
2021	IBM Eagle	127	N/A	Gate-based superconducting processor
2022	IBM Osprey	433	N/A	Increased scale and coherence
2023	IBM Condor	1,121	N/A	First IBM chip over 1,000 qubits
2023	Quantinuum H2	32	4	First demonstration of 4 logical qubits (source)
2024	Quantinuum H2-1	56	12	12 logical qubits in hybrid workflow with Microsoft (source)
2024	Quantinuum H2-1	56	50	Achieved 50 logical qubits with >98% fidelity (source)
2025	D-Wave Advantage	5,000+	N/A	Latest-generation quantum annealer; still not gate-basedntroduction 1

# Hardware improvement in Qubits



# Hardware improvement in Qubits



## Why HPC Cares About Quantum and Quantum Needs HPC

Category	High Performance Computing (HPC)		
Cost	~\$1–10M (e.g. Easley: \$1.5M)*		

~\$1–10M (e.g. Easley: \$1.5M)\*

Remote job scheduler

Shared systems managed by

scheduler

Large remote scarce systems

Needed

Primarily researchers

Runs quantum simulators

### Quantum Computing (QC)

~\$100M+ per system

Remote job scheduler

Shared systems managed by

scheduler

Large remote scarce systems

Needed

Still experimental

HPC for simulations

**Access** 

**Users** 

**P** Hardware

Use Today

**Training** 

Link

Both HPC and Quantum are expensive, specialised, and require expert support. Until large fault-tolerant QCs exist, HPC is where most quantum computing algorithms actually run. Introduction 17

<sup>\*</sup>doesn't fit on a desk

# Classical vs Quantum Thinking

Classical Thinking

Bits: 0 or 1

Logic is deterministic

Measurement reveals truth

Copying is easy

State is local and separable

Errors are binary and correctable

**Quantum Thinking** 

Qubits: 0 and 1 (superposition)

Logic is probabilistic\*

Measurement changes the system

No-cloning: copying is forbidden

State can be entangled and nonlocal

Errors are subtle, continuous, and must be detected differently

# The Quantum Revolution

## **Foundations of Quantum Science**



Erwin Schrödinger 1887–1961 Austrian University of Vienna

$$ih\partial\Psi = H\Psi$$



Max Born 1882–1970 German University of Göttingen

$$|\psi|^2$$



Werner Heisenberg 1901–1976 German University of Leipzig

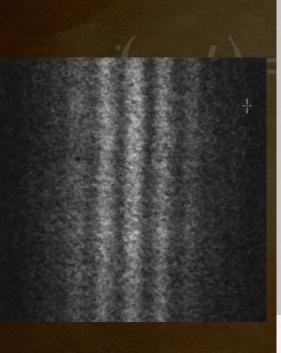
$$\Delta x \, \Delta p \ge \frac{h}{2}$$

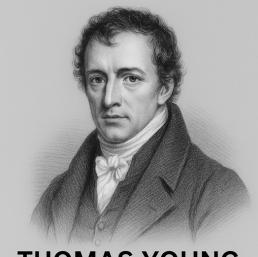


Louis de Broglie 1892–1987 French Collège de France

$$\lambda = \frac{h}{p}$$

# Photons interfere with one another like waves do





#### **THOMAS YOUNG**

1773-1829 **British Physicist** 

 $\lambda = \frac{d \sin \theta}{n}$ 

**Royal Society** 

Thomas Young's interference experiments confirmed the wave nature of light, laying crucial groundwork for the later discovery of wave-particle duality.

#### PHILOSOPHICAL

### TRANSACTIONS.

I. The Bakerian Lecture. Experiments and Calculations relative to physical Optics. By Thomas Young, M. D. F.R.S.

Read November 24, 1803.

EXPERIMENTAL DEMONSTRATION OF THE GENERAL LAW OF THE INTERFERENCE OF LIGHT.

In making some experiments on the fringes of colours accompanying shadows, I have found so simple and so demonstrative a proof of the general law of the interference of two portions of light, which I have already endeavoured to establish, that I think it right to lay before the Royal Society, a short statement of the facts which appear to me so decisive. The proposition

#### Demonstration of single-electron buildup of an interference pattern

A. Tonomura, J. Endo, T. Matsuda, and T. Kawasaki Advanced Research Laboratory, Hitachi, Ltd., Kokubunji, Tokyo 185, Japan

H. Ezawa

Department of Physics, Gakushuin University, Mejiro, Tokyo 171, Japan

(Received 17 December 1987; accepted for publication 22 March 1988)

The wave-particle duality of electrons was demonstrated in a kind of two-slit interference experiment using an electron microscope equipped with an electron biprism and a positionsensitive electron-counting system. Such an experiment has been regarded as a pure thought experiment that can never be realized. This article reports an experiment that successfully recorded the actual buildup process of the interference pattern with a series of incoming single electrons in the form of a movie.

#### I. INTRODUCTION

The two-slit interference experiment with electrons is frequently discussed in textbooks on quantum mechanics, and is referred to as "impossible, absolutely impossible to explain in any classical way, and has in it the heart of quantum mechanics." In this experiment (see Fig. 1), electrons incident on a wall with two slits pass through the slits and are detected one by one on a screen behind them. Accumulation of successive single electrons detected at the screen builds up an interference pattern. According to the interpretation in quantum mechanics, a single electron can pass through both of the slits in a wave form called "probability amplitude" when the uncertainty of the electron position in the wall plane covers the two slits, and when no observation is made of the electron at either one of the slits. The electron is then detected as a particle at a point somewhere on the screen according to the probability distribution of the interference pattern. However, if the electron is caught when passing through the slits, it takes place at either one of the two slits, never both, and the probability distribution on the screen will be completely different.

Although in textbooks this experiment is talked about as

a matter of fact, "this experiment has never been done in just this way, since the apparatus would have to be made on an impossibly small scale," as Feynman points out. However, this is not necessarily true. In fact, several attempts have been made up to now; Zeilinger et al.2 confirmed the

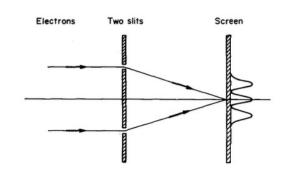


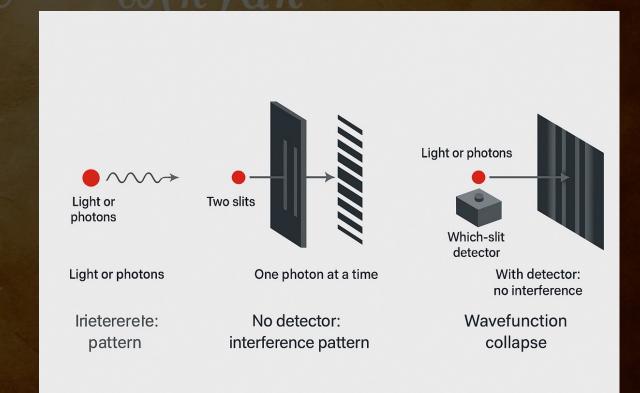
Fig. 1. Two-slit electron interference experiment.

Einstein (1905): Light quanta (photons) to explain the photoelectric effect

•de Broglie (1924): Hypothesised that matter (like electrons) also has wave properties

Davisson-Germer (1927): Confirmed electron diffraction, validating de Broglie

Bohr, Heisenberg, Schrödinger (1920s): Formalised the quantum framework



117

Einstein (1905): Light quanta (photons) to explain the photoelectric effect •de Broglie (1924): Hypothesised that matter (like electrons)

#### Demonstration of si

A. Tonomura, J. Endo Advanced Research Labora

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(Received 17 December

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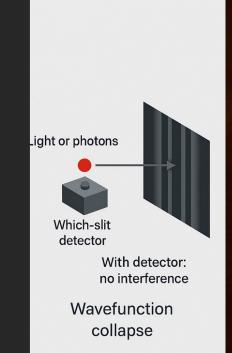
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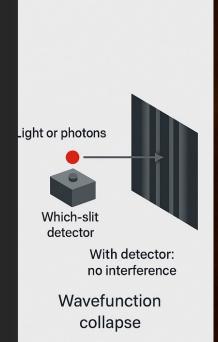
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The single-photon double-slit experiment shows that quantum particles don't follow independent paths— each one behaves like a wave exploring all possibilities, and this principle underlies quantum computing.

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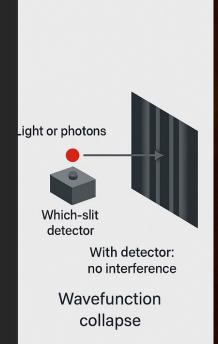
Although in textbooks this ex

Next we will build up a set of properties that we can exploit to solve some problems faster than a classical computer can.

BTW – All classical computers are also quantum. It's just that didn't know how to build them in a way that let's us exploit that fact.

ectron diffraction,

: Formalised the



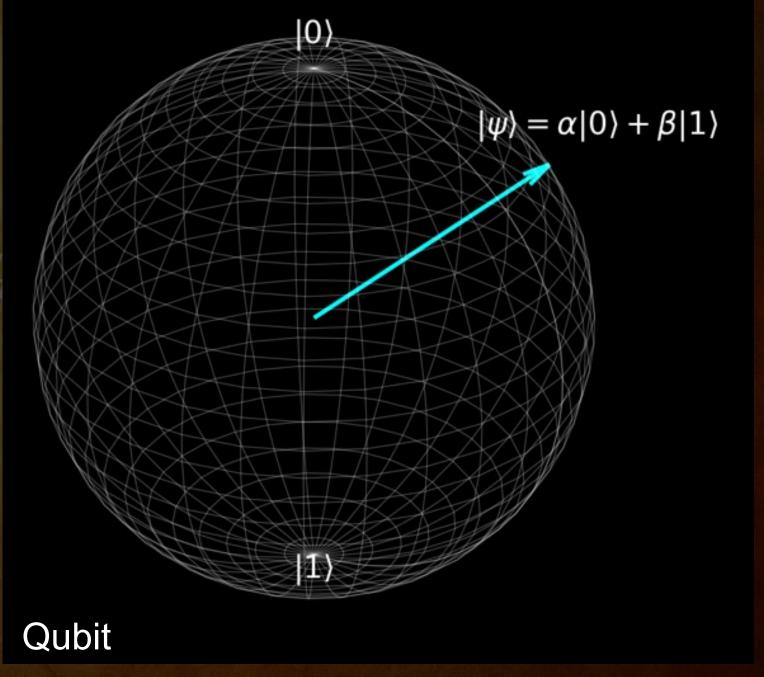
# Superposition

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

This expression is the quantum equivalent of a wave function: it describes a qubit's state as a superposition of basis states, not a single bit value. Psi the quantum state vector and is a linear combination of 0 and 1 the "ket" here just means a column vector.

$$|0\rangle = \begin{bmatrix} 1\\0 \end{bmatrix} \quad \text{and} \quad |1\rangle = \begin{bmatrix} 0\\1 \end{bmatrix}$$

A qubit isn't just 0 or 1—it's like a wave that can be both at once, with weights that tell us how likely each outcome is when we measure it.



# Superposition

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

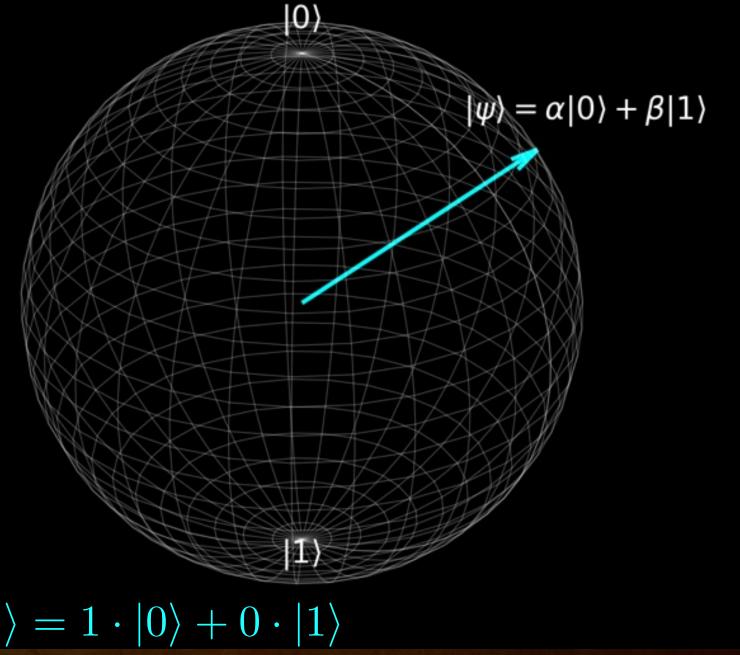
$$|0\rangle = \begin{bmatrix} 1\\0 \end{bmatrix} \quad \text{and} \quad |1\rangle = \begin{bmatrix} 0\\1 \end{bmatrix}$$

We map the position on the sphere with the Bloch formula:

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

E.g for Theta = 0:

We map the position on the sphere with the Bloch formula: 
$$|\psi\rangle=\cos\left(\frac{\theta}{2}\right)|0\rangle+e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle$$
 E.g for Theta = 0: 
$$|\psi\rangle=\cos(0)|0\rangle+\sin(0)|1\rangle=1\cdot|0\rangle+0\cdot|1\rangle$$



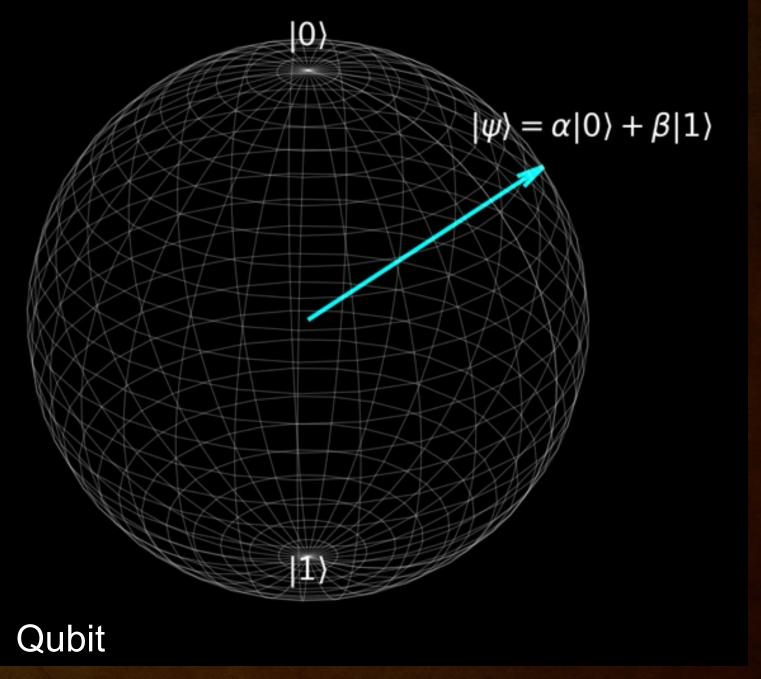
# Superposition

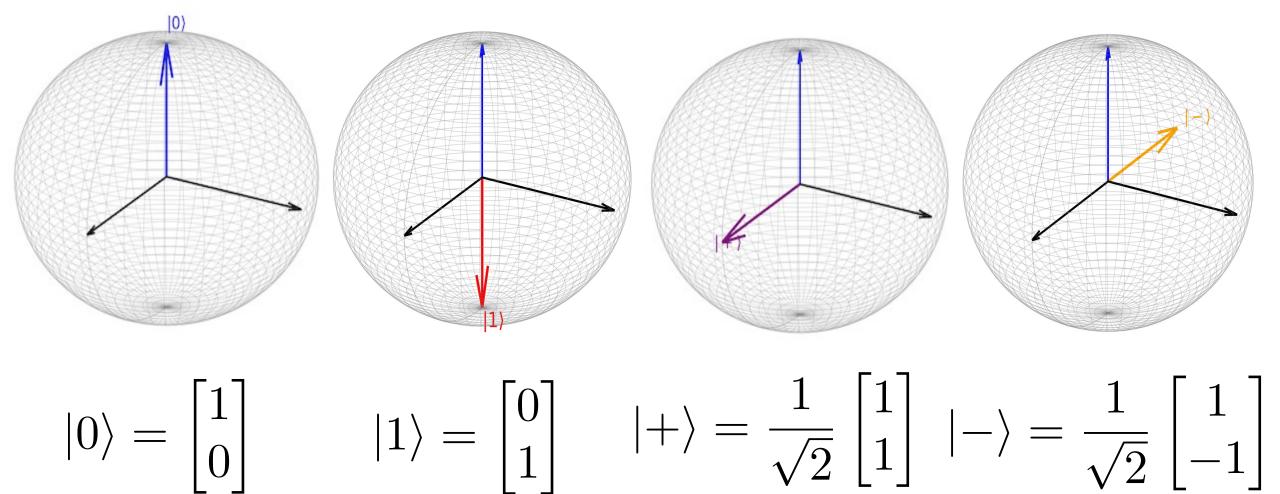
$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

A qubit isn't just 0 or 1—it's like a wave that can be both at once, with weights that tell us how likely each outcome is when we measure it.

The formula is Dirac notation for mapping the superposition to a sphere.

$$\Delta(x,t) = \frac{R}{2} |\psi$$





**Standard Basis** 

**Hadamard Basis** 

# Quantum Interference

### Concept

Like in waves

Constructive

Destructive

Why it matters

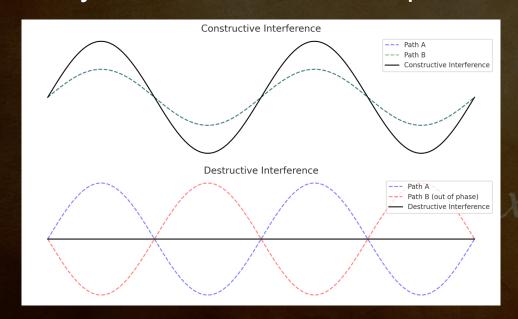
### Quantum Interference

Quantum amplitudes can add or cancel

Amplitudes reinforce, increasing outcome probability

Amplitudes cancel, suppressing outcomes

Used in quantum algorithms to find correct answers faster





# **Unitary Evolution & Reversibility**

#### **Classical Systems**

Many processes are **irreversible** (e.g. XOR, erasure)

Bit states collapse or overwrite

Logic gates may lose information

Example: NAND cannot be undone

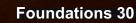
#### **Quantum Systems**

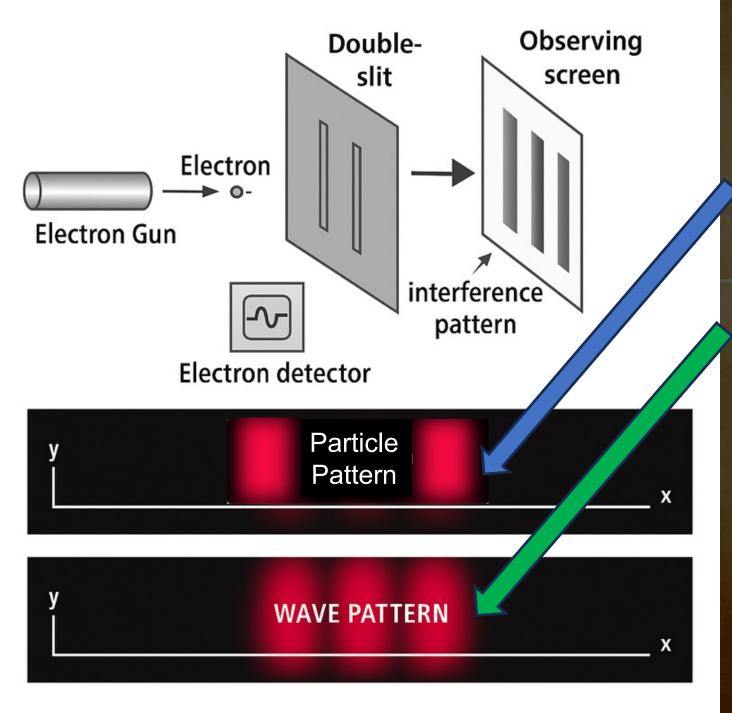
All quantum operations must be **reversible** 

Qubit states evolve smoothly under unitary gates

Quantum gates preserve information (unitary)

Example: Hadamard, CNOT can be reversed





With measurement (Electron detector let's us know whether an electron went through a particular slit): interference disappears

Without measurement: wave interference pattern appears

Mirrors quantum computing: coherence enables interference

**Measurement = collapse** 

**Decoherence = unintended collapse** 

# Measurement Collapses the Wavefunction

- •Measurement collapses the quantum state into  $|0\rangle or |1\rangle$ \* Collapse is probabilistic and irreversible
- •Decoherence is unintentional measurement by the environment
- Quantum computation must preserve coherence until final measurement
- •Unitary operations preserve coherence, which allows quantum superpositions to evolve and interfere. Measurement and decoherence both break coherence, collapsing or scrambling those superpositions.

\* Recall this notation just means  $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$  and  $|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$  which is a definite point on the surface of the Bloch sphere representing the qubit

# Decoherence: When Quantum Becomes Classical

- Wavefunction collapse is what we observe when we measure a quantum system.
- •Decoherence is a physical explanation for why quantum states lose superposition without measurement due to entanglement with the environment.
- •BTW this is why sticking a cat into a box with cyanide and a cesium atom trigger wouldn't really put the cat in a superposition of live and dead, unless the box it is in isolates the contents from the rest of the universe at a quantum level.

# Born's Rule

A **shot** is one run of the circuit from initial state preparation to final measurement.

We need multiple shots to converge on a solution.

Alex?

- Quantum states are described by amplitudes
- A qubit state:  $|\psi\rangle=\alpha|0\rangle+\beta|1\rangle$
- Born's Rule connects amplitudes to measurable outcomes
- The probability of measuring  $|i\rangle$  is:

$$P(i) = |\langle i|\psi\rangle|^2$$

- Measurement outcomes are inherently probabilistic
- The same circuit run multiple times can give different results
- More shots → clearer statistics
- Why it matters:
- It's how we extract classical data from a quantum system
- Underlies all circuit outputs, from Bell states to Shor's algorithm

# Summary: What We Know

We have seen that the double-slit experiment revealed a fundamental property of the universe.

Until measurement or decoherence objects\* exist as a wave function governed by Schrodinger's equation. This means they exist in all possible states simultaneously.

When unintended interactions with the environment occur, or an intended measurement occurs, the wave function collapses into just one of the states.

Quantum computers maintain that Wave function state of qubits in order to perform computations faster.

e.g. Bucky Ball made of 240 Carbon atoms. Fein, Y., et al. (2019). "Quantum superposition of molecules beyond 25 kDa." Nature Physics, 15, 1242-1245. DOI: 10.1038/s41567-019-0663-9

# From Bits to Qubits

## MATHEMATICAL FOUNDATIONS



David Hilbert 1862–1943 Göttingen Germany Hilbert Space

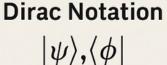
 $\psi_1, \psi_2 \in H$ 



Neumann
1903-1957
IAS
Hungary
von Neumann
Entropy  $-Tr\langle \rho \log p \rangle$ 



Paul
Dirac
1902-1984
Cambridge
U.K.
Dirac Notatio





Bell 1928-1990 CERN U.K. Bell Inequality |E(a,b)+E(a,b)+E(a',) $-E(a',b)| \le 2$ 

# Quantum Gates: Basic Building Blocks

Gates must be reversable

Logical "not" is reversable. If you see not(x) = 1, you know that x must be 0

Logical "or" is not reversable. or(x,y)=1 doesn't fix whether x was 1 or y was 1.

Nothing irreversible can happen in Schrodinger's world.



Operating on bits involve flipping some on/off value: A low high voltage on a wire, magnetizing a small region on an iron coated disk, or laser writing pits into a surface. These encode 0s and 1s.

We manipulate the 0s and 1s with binary operators following an deterministic algorithm,

In quantum computing: Qubits are a superposition of 0 and 1 that defines the surface of a sphere.

We modify the qubit by changing the probability amplitudes that define where the qubit is likely to be on the Bloch sphere when we measure it.

So quantum operations are usually not writing a 0 or 1 it is applying a rotation on the vector that defines the qubit.

So rather than writing 01+01=10 as we would adding binary numbers, we might rotate the qbit about the x axis by angle theta with the RX(theta) operator.

# Н

# **Quantum Gates: Basic Building Blocks**

A lot of quantum operations (gates) are analogous to classical gates.

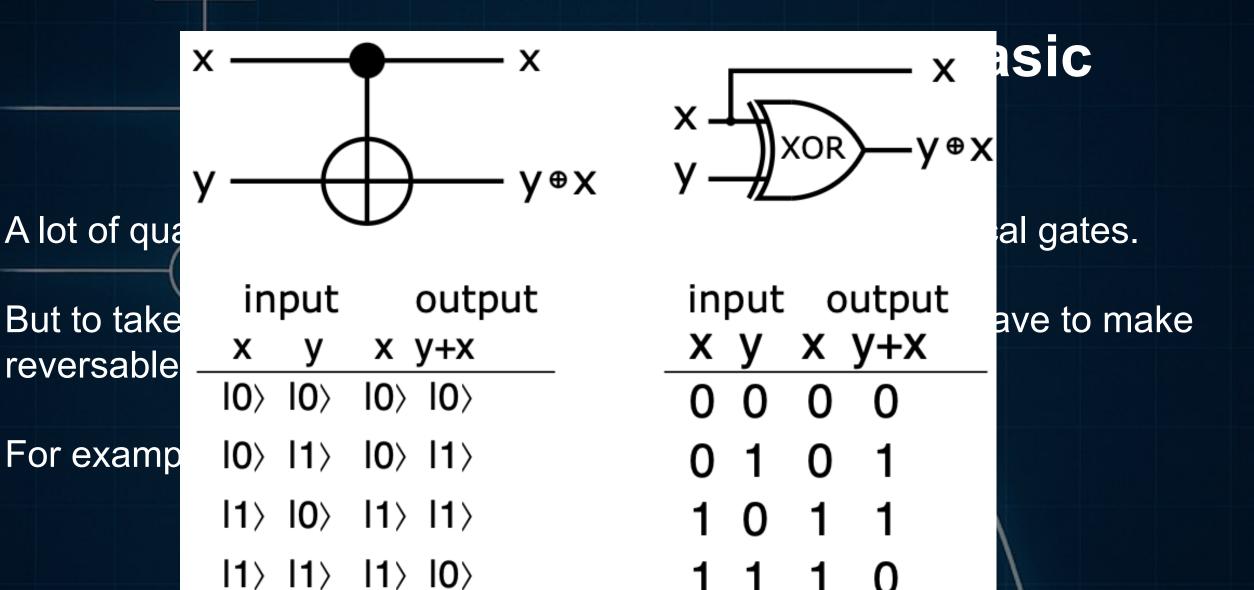
But to take advantage of superposition and coherence we have to make reversable versions.

For example, exclusive or (xor) is not reversable ...

$$xor(0,0) = 0$$
,  $xor(0,1) = 1$ 

$$xor(1,0) = 1, xor(1,1) = 0$$

If you get a 1 you don't know which of the inputs was 1



But control xor is – we output the value of one of the inputs to make it reversable

	Symbol	Name	Description	Matrix Representation
	I	Identity	Does nothing to the qubit	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
	X	Pauli-X	Bit-flip gate (like NOT)	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
	Y	Pauli-Y	Bit & phase flip	$egin{bmatrix} ar{0} & -ar{i} \ i & 0 \end{bmatrix}$
	$\mathbf{Z}$	Pauli-Z	Phase flip gate	$egin{bmatrix} 1 & 0 \ 0 & -1 \end{bmatrix}$
	$\mathcal{D}_{\mathrm{H}}$	Hadamard	Creates superposition	$rac{1}{\sqrt{2}}egin{bmatrix} 1 & ec{1} \ 1 & -1 \end{bmatrix}$
	S	Phase Gate	Applies phase of $i$	$egin{bmatrix} ar{1} & 0 \ 0 & i \end{bmatrix}$
F.7	T	$\pi/8 \text{ Gate}$	Applies phase of $e^{i\pi/4}$	$egin{bmatrix} 1 & 0 \ 0 & e^{i\pi/4} \end{bmatrix}$
$ 1\rangle$	$\overline{\mathrm{RX}(\theta)}$	X-Rotation	Rotates around X-axis by $\theta$	$\cos\left(\frac{\theta}{2}\right)I - i\sin\left(\frac{\theta}{2}\right)X$
$ 0\rangle =  0\rangle$	$\mathrm{RY}( heta)$	Y-Rotation	Rotates around Y-axis by $\theta$	$\cos\left(rac{ ilde{ heta}}{2} ight)I-i\sin\left(rac{ ilde{ heta}}{2} ight)Y$
	$\mathrm{RZ}(\theta)$	Z-Rotation	Rotates around Z-axis by $\theta$	$egin{bmatrix} 1 & 0 \ 0 & e^{i heta} \end{bmatrix}$
$\begin{bmatrix} 0 \end{bmatrix}$	$\overline{\text{CX}}$	CNOT	Controlled-X gate	Acts on 2 qubits: flips target if control is $ 1\rangle$
$ 1\rangle =  1 $	CZ	Controlled-Z	Applies Z if control is $ 1\rangle$	Diagonal matrix with -1 at bottom right
	SWAP	Swap	Swaps two qubits	Interchanges the two states

Table 1: Common Unitary Quantum Gates

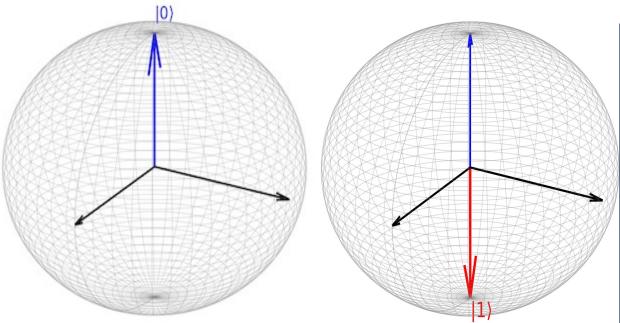


# Hadamard and the Birth of Superposition

One of the most important operators is H, the Hadamard operator. This is the operator that places qbits into superposition so they obey Schrodinger's equation.

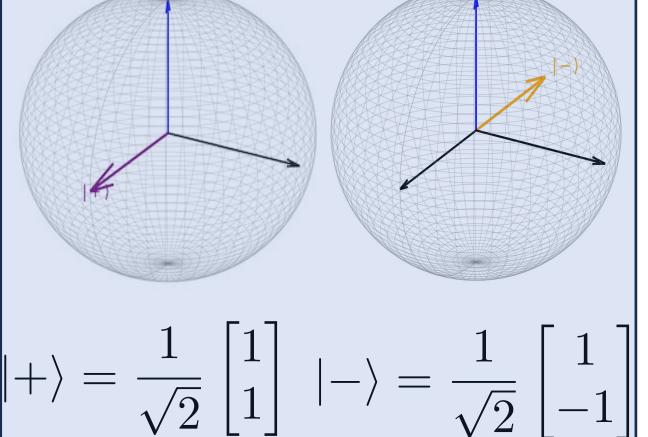
$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

•The gate itself became standardised in quantum algorithms through the work of **David Deutsch** (1985), **Peter Shor**, and others developing quantum logic circuits.



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

## **Standard Basis**



## **Hadamard Basis**

This is how we put the qubits into superposition

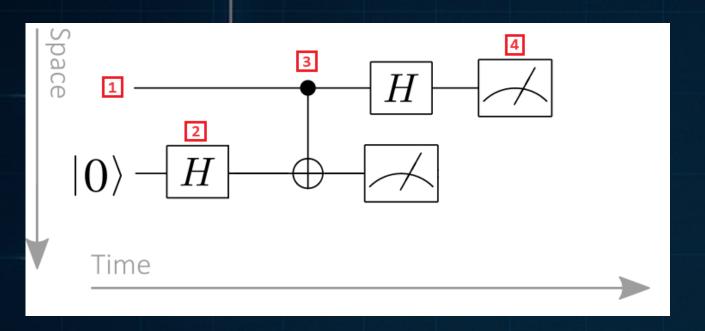


- Controlled gates act conditionally on the control qubit state
- Most common: apply a gate only if control qubit is in  $|1\rangle$
- Examples:
  - CNOT: flips the target qubit if control is  $|1\rangle$
  - $\mathbb{C}\mathbf{Z}$ : flips the phase of the target if control is  $|1\rangle$
  - Toffoli (CCNOT): flips the target if two controls are  $|1\rangle$
- Enables entanglement, conditional logic, and quantum interference flow
  Quantum Logic & Circuits 44



# Quantum Circuit Diagrams 101

- Qubit wires: horizontal lines (top to bottom = different qubits)
- Time flows left to right
- •Boxes = gates (e.g., H, X, Z, etc.)
- •Dots and lines = control and target (e.g., CNOT)
- •Measurement shown with \( \times \) or [M]



- 1. **Qubit Registers** Horizontal lines represent qubits. Top to bottom = Qubit 0, Qubit 1, etc.
- 2. Quantum Gate Boxes apply quantum operations. The H gate here puts the qubit into superposition.
- 3. Controlled Gate The CNOT gate uses a control (filled circle) and a target (plus in a circle). It flips the target qubit if the control is  $|1\rangle$ .
- 4. **Measurement** Meter symbols measure qubits, collapsing them to classical bits (0 or 1).

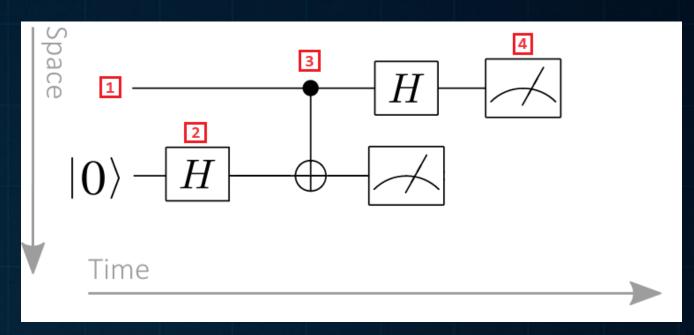
  https://learn.microsoft.com/en-us/azure/quantum/concepts-circuits

1. Hadamard gate on qubit 0:

$$|0\rangle \xrightarrow{H} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

 $\rightarrow$  Now the state is:

$$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle$$



2. CNOT gate, with:

Control: qubit 0

Target: qubit 1

 $\rightarrow$  This flips the second qubit only when the first is  $|1\rangle$ 

Final state: 
$$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

Controlled not gate:





# No-Cloning

### **No-Cloning Theorem**

It is **not** possible to copy an **arbitrary unknown** quantum state This contrasts with classical information, which can be duplicated freely

### **Implications**

Reinforces quantum information's fragility Enables secure communication (e.g., quantum key distribution)

Forces new strategies:

entanglement, teleportation, error correction

# Schrödinger vs Classical Logic Flow

- Classical logic: follows a branching flow conditionals like if/else determine discrete paths through a program.
- Quantum logic: evolves smoothly and reversibly via Schrödinger's equation; all possibilities evolve in superposition.
- Measurement: collapses the superposition into a definite classical state the only irreversible step.

$$i\hbar \frac{d}{dt} \ket{\psi(t)} = \hat{H} \ket{\psi(t)}$$

Quantum evolution is continuous, reversible, and governed by unitary
transformations.

Quantum Evolution is continuous, reversible, and governed by unitary
Quantum Logic & Circuits 49

# **Building a Superposition Circuit**

Let's walk through how we build a quantum state that explores many possibilities in parallel.

We always begin with qubits in the  $|0\rangle$  state. These are like classical bits set to 0.

By applying a Hadamard gate to each qubit, we turn each  $|0\rangle$  into  $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ .

If we do this to n qubits, we get a superposition over all  $2^n$  possible combinations.

Mathematically, this is written as:  $H^{\otimes n}|0\rangle^{\otimes n}=\frac{1}{\sqrt{2^n}}\sum_{x=0}^{2^n}|x\rangle$  Each  $|x\rangle$  represents a possible bitstring.

# Summary: Thinking in Quantum Logic

Qubits can be in superpositions: not just 0 or 1, but both

Operations are reversible and unitary (no information is lost)

Entanglement creates strong correlations beyond classical limits

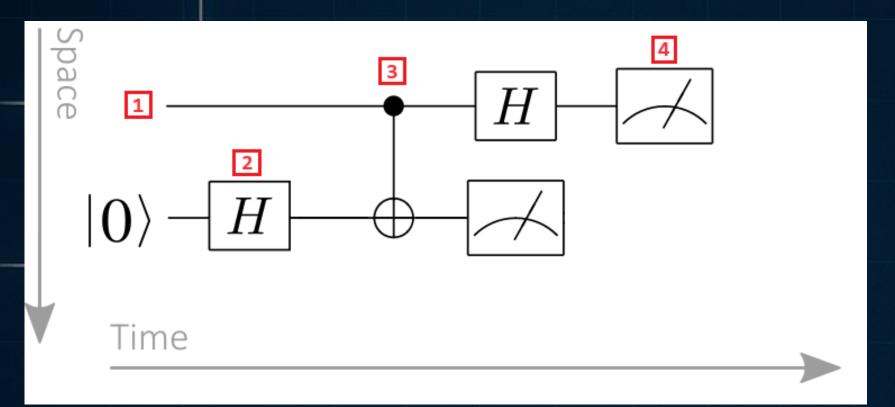
Measurement collapses a quantum state to a classical outcome

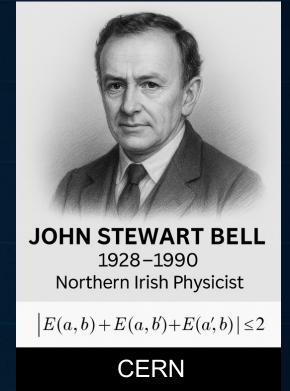
No cloning: we can't copy unknown quantum states

Quantum computation uses interference, not branching, to find answers

# What Is Entanglement?

- Entanglement links qubits so their states are no longer independent
- Measuring one immediately affects the other, no matter the distance
- Entangled states cannot be described as separate parts
- Enables key quantum protocols: teleportation, superdense coding, QKD





This simple circuit creates a **Bell state**—an entangled pair of qubits. Measuring one qubit immediately determines the result of the other, no matter how far apart they are. It's the foundation of quantum teleportation, superdense coding, and quantum key distribution.

## **Meet the Bell States**

#### Meet the Bell States

The four maximally entangled two-qubit states:

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

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

$$\Psi^{+} = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle)$$

$$\Psi^{-} = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle)$$

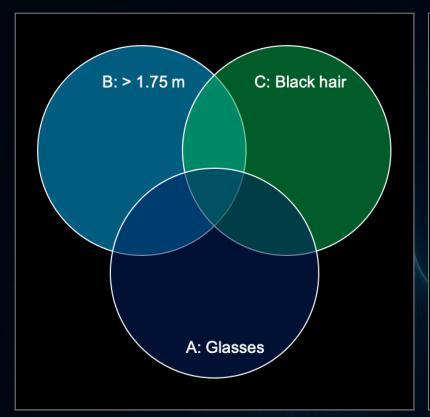
Now we are dealing with two qubits

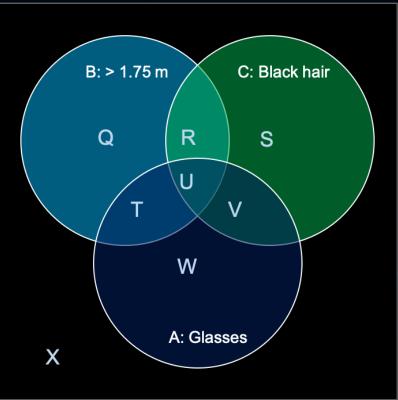
 $|10\rangle$ 

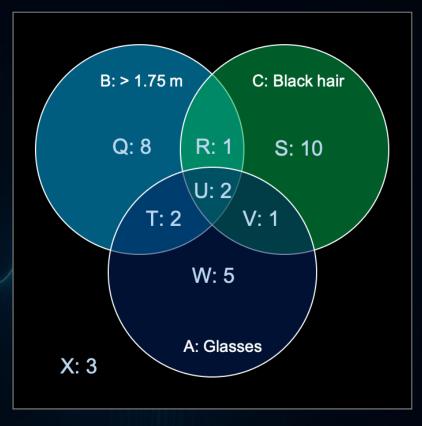
Means one qubit is in state [0,1] and the other is in state [1,0]

- Perfect correlation or anti-correlation when measured
- Basis for quantum communication, teleportation, and error correction

## **Bell's Theorem**

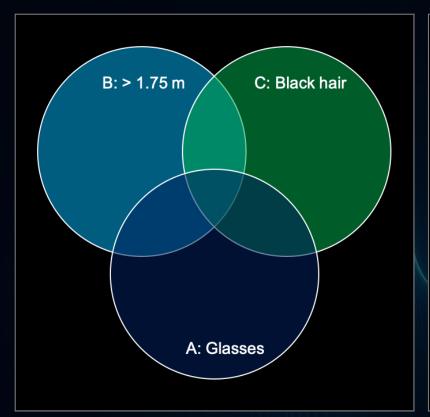


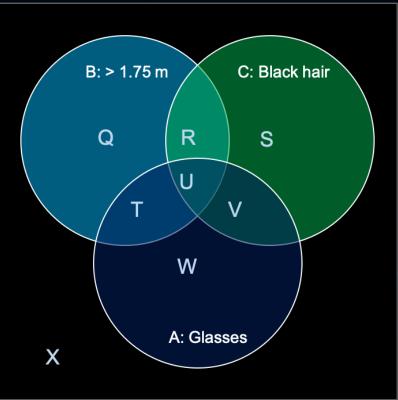


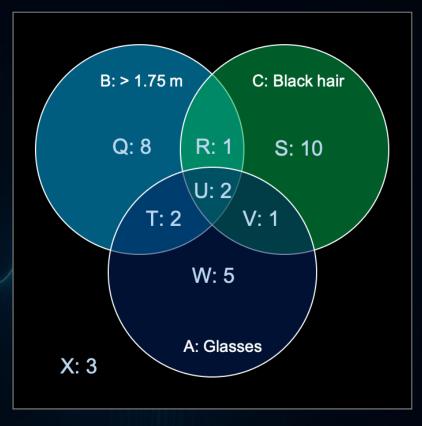


The number of people who are in A but not B, plus the number who are in B but not C, must be greater than or equal to the number who are in A but not C.

## **Bell's Theorem**







The number of people who wear glasses but are shorter than 1.75 m, plus those who are taller than 1.75 m but don't have black hair, should be at least as many as those who wear glasses and don't have black hair.

## Bell's Theorem: Spooky Action at a Distance

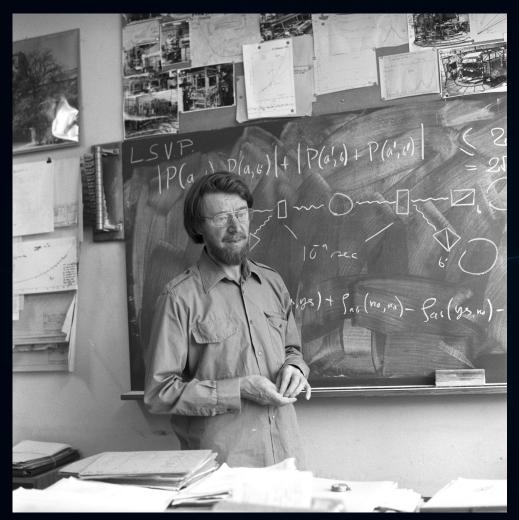
- Classical physics assumes:
  - Locality: no influence travels faster than light
  - Realism: properties exist before measurement
- Bell's theorem shows that quantum predictions can violate inequalities based on these assumptions
- Experiments confirm: entangled particles do not follow classical rules
- Quantum mechanics is either **nonlocal**, **non-real**, or both

 $E(a,b) = \langle A(a) \cdot B(b) \rangle$  in the classical world where E ranges from -1 (anticorrelated) to +1 (perfect correlation).

Bell's Inequality: 
$$|E(a,b) - E(a,b')| + |E(a',b) + E(a',b')| \le 2$$

Quantum mechanics can produce results up to  $2\sqrt{2}$ 

## **Bell Inequality in Action**



John Clauser, b 1942 Lawrence BerkleyLabs and UC Berkley, American

- Entangled photon pairs sent to Alice and Bob
- Each chooses random detector angles: a, a', b, b'
- Compute correlations:

• CHSH\*inequality:

$$S = |E(a,b) - E(a,b')| + |E(a',b) + E(a',b')| \le 2$$

- Classical physics:  $S \leq 2$
- Quantum mechanics:  $S \leq 2\sqrt{2} \approx 2.828$
- Experimental results:  $S \approx 2.4-2.8$
- Confirms violation of classical realism and locality

\*1969, John Clauser, Michael Horne, Abner Shimony, and Richard Holt developed a more experimentally testable version inequality.

# One or more of the following assumptions is wrong...

## Reject Locality

- → Maybe particles communicate faster than light.
- Reject Reality
- → Particles don't have definite properties until measured.
- Reject Free Will (Superdeterminism)
- → Everything—including our measurement choices—was predetermined; the universe is fully scripted.

Giustina, M. et al. Significant-loophole-free test of Bell's theorem with entangled photons. Phys. Rev. Lett. 2015, Vol. 115, 25040.38.

## **Entanglement vs Classical Correlation**

Origin

**Description** 

**Measurement Effect** 

Copyable

Limitations

**Example** 

#### **Classical Correlation**

Shared cause or common information

Probabilistic — based on known values

Measuring one doesn't affect the other

Yes, information can be cloned

Can't violate Bell's inequality

Two people given matching socks either blue or red.

Knowing the colour or one sock implies the colour of the other one

#### **Quantum Entanglement**

Joint quantum preparation (e.g. Bell state)

No classical description — shared quantum state

Measuring one collapses the state of the other

No — copying violates the nocloning theorem

Violates Bell's inequality (experimentally confirmed)

$$\frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right)$$

## The Quantum Edge

## Superposition

→ A quantum system can explore many states at once

## Entanglement

→ Correlations stronger than anything classically possible

### Interference

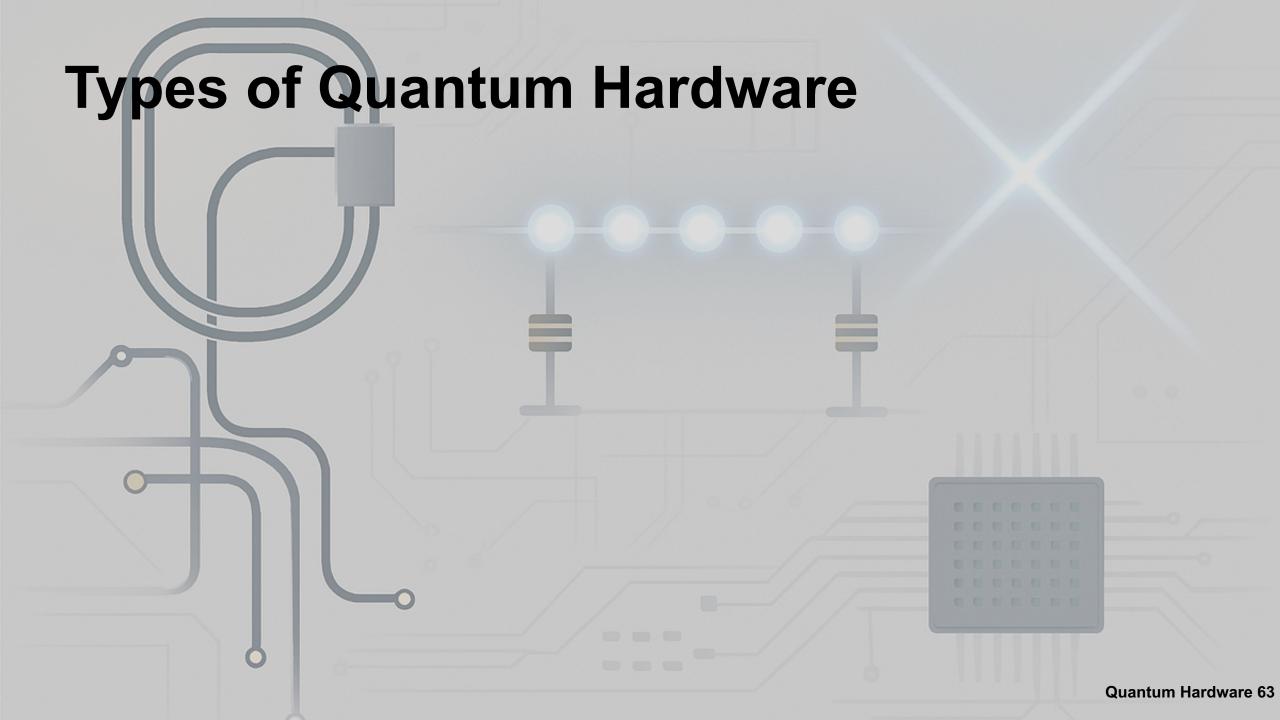
→ Amplifies correct paths, cancels the wrong ones

# From Theory to Physical Qubits

In 1993 Seth Lloydd described a method for building the first quantum computer.

"Arrays of pulsed, weakly coupled quantum systems ... the basic unit in the array could be a quantum dot, a nuclear spin, ... or any multistate quantum system that interacts locally with its neighbors and can be compelled to switch between states with resonant pulses of light."

S. Lloyd, A potentially realizable quantum computer, Science, 261(5128): 1569-1571, 1993.

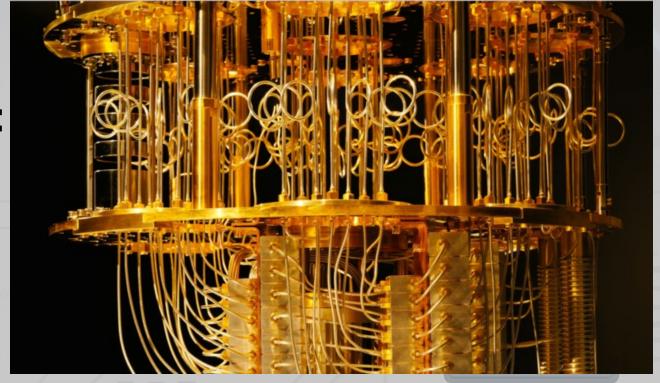


# **Superconducting Qubits**

•Description: Utilize superconducting circuits at cryogenic temperatures to perform quantum

operations.

- •Notable Companies:
- ·IBM
- ·Google
- Rigetti Computing
- ·Intel



Superconducting quantum processor suspended in a cryostat for ultra-cold operation and precise qubit measurement.

## **Trapped Ion Qubits**

Description: Employ ions confined and manipulated using

electromagnetic fields.

- •Notable Companies:
- ·lonQ
- Quantinuum
- Honeywell

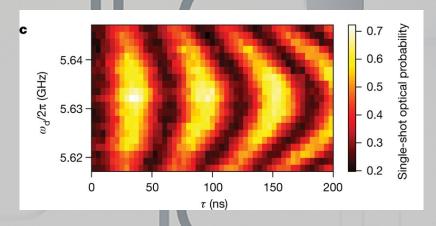


Ion trap quantum processor housed in an ultra-high vacuum chamber, used to isolate and control individual trapped ion qubits.

## Measurement in Hardware

### **Superconducting qubits**

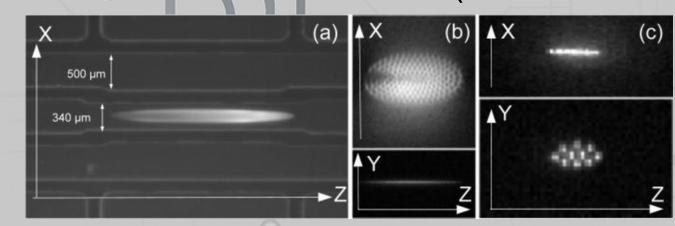
Readout via resonator frequency shift (microwave cavity QED)



Delaney, R. D., et al. "Superconducting-qubit readout via low-backaction electro-optic transduction." *Nature* 606.7914 (2022): 489-493.

### **Trapped ions**

• Fluorescence detection (ions emit or don't under laser illumination)



Szymanski, B., et al. "Large 2D Coulomb crystals in a radio frequency surface ion trap." *arXiv preprint arXiv:1201.2584* (2012).

Other Quantum Computer Implementation

#### **Photonic Qubits**

Use photons for quantum computations, often at room temperature.

- PsiQuantum
- Xanadu
- ORCA Computing

#### **Neutral Atom Qubits**

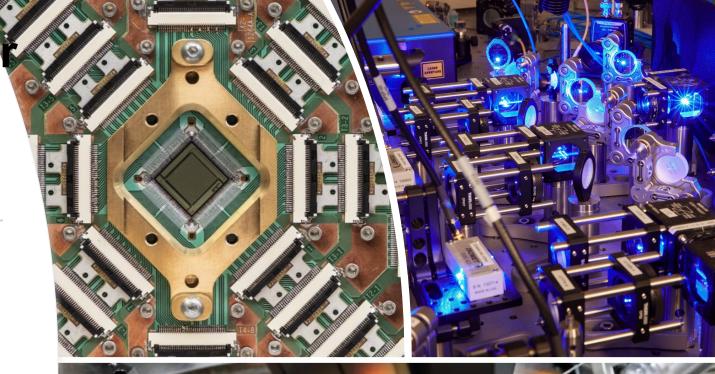
Neutral atoms trapped in optical lattices or tweezers.

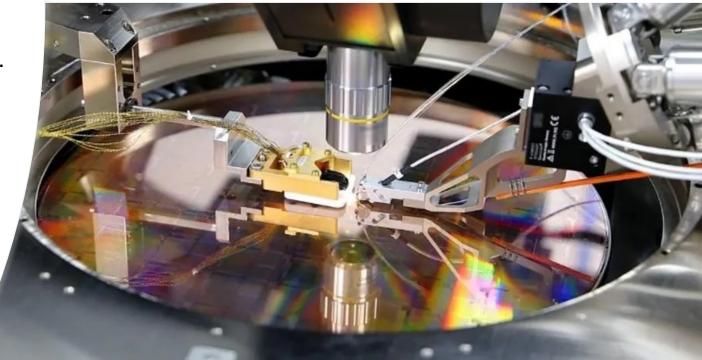
- QuEra Computing
- ColdQuanta
- Atom Computing

#### **Quantum Annealers**

Specialized devices for optimization problems, leveraging quantum tunneling.

D-Wave Systems





## From Theory to Programming

- •Quantum Mechanics provides the rules
  Schrödinger equation, unitary evolution, measurement
- Quantum Circuits encode those rules
   Gates represent unitary operators; circuits evolve qubit states

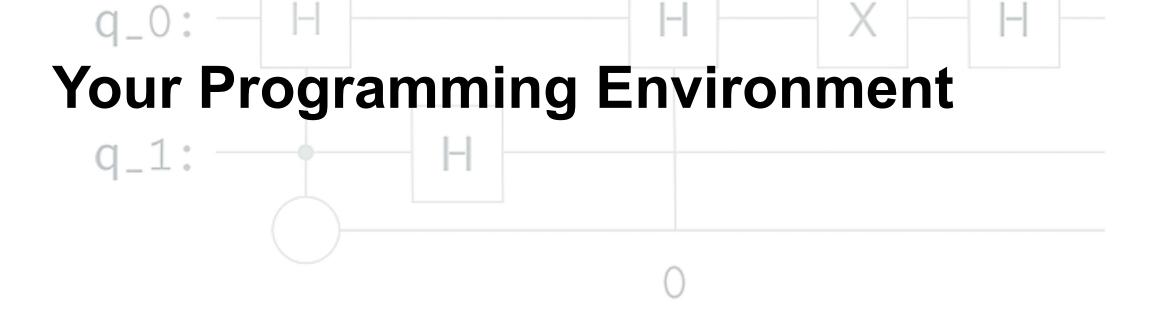
### **Quantum Programming Languages**

Qiskit (IBM)

Cirq (Google)

Braket (Amazon)

Ocean (D-Wave, for annealing)



## Qubits, Gates, and Circuits in Code (Cirq)

```
import cirq
# Create a quantum circuit with two qubits
q0, q1 = cirq.LineQubit.range(2)
# Define the circuit
circuit = cirq.Circuit(
cirq.H(q0), # Hadamard gate on q0
cirq.CNOT(q0, q1), # CNOT gate (entanglement)
cirq.measure(q0, q1) # Measurement
# Simulate the circuit
simulator = cirq.Simulator()
result = simulator.run(circuit, repetitions=10)
# Print results
print("Cirq Circuit:")
print(circuit)
print("Measurement Results:")
print(result)
```

## Qubits, Gates, and Circuits in Code (Cirq)

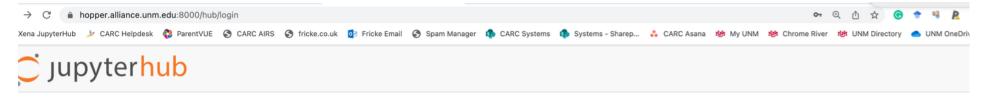
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```

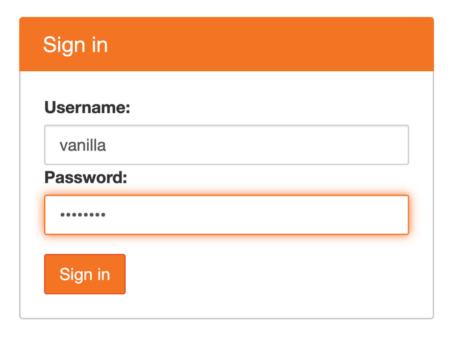
The outputs are the same for both qubits.

They are not communicating through wires or any other "real" connection.

Recall Bell's three hypotheses...

## Now it's your turn Go to https://hopper.alliance.unm.edu:8000



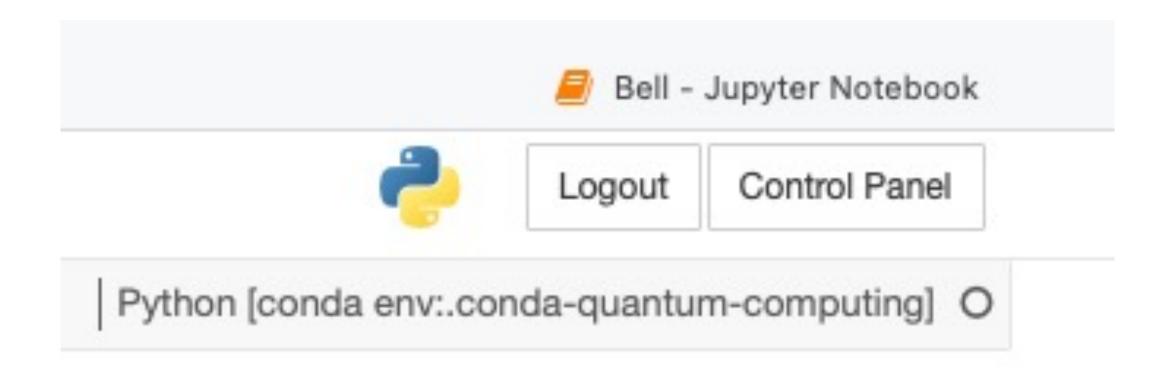


#### **Server Options**

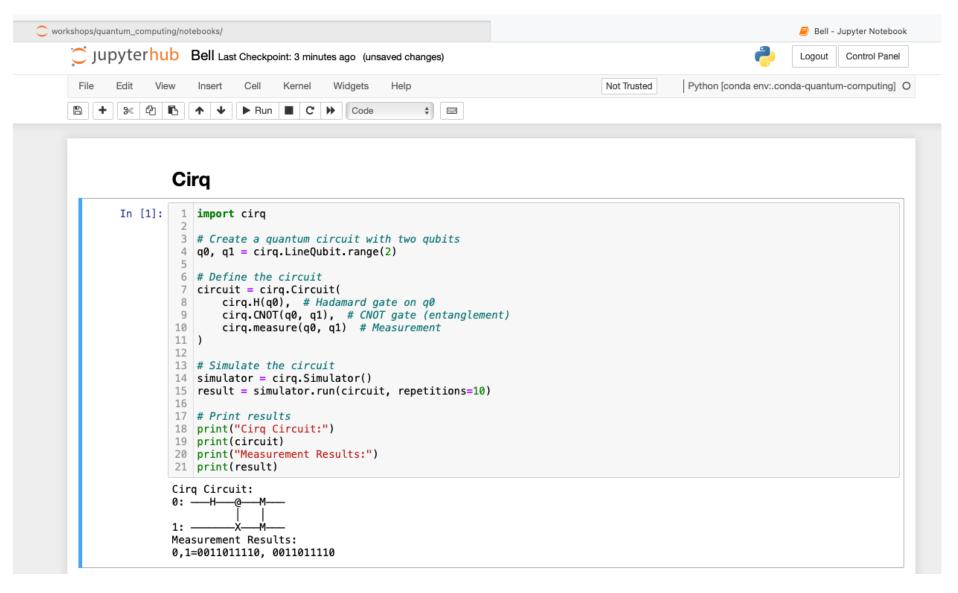




Click on Bell.ipynb



Double check you have this kernel loaded



# Qubits, Gates, and Circuits in Code (qiskit)

Now we will entangle three qubits with qiskit and then measure their correlation.

```
import numpy as np
from giskit import QuantumCircuit

# 1. A quantum circuit for preparing the quantum state |000> + i |111> / √2
qc = QuantumCircuit(3)
qc.h(0)  # generate superposition
qc.p(np.pi / 2, 0)  # add quantum phase
qc.cx(0, 1)  # 0th-qubit-Controlled-NOT gate on 1st qubit
qc.cx(0, 2)  # 0th-qubit-Controlled-NOT gate on 2nd qubit
```

## Qubits, Gates, and Circuits in Code (qiskit)

```
# 2. Add the classical output in the form of measurement of all qubits
qc_measured = qc.measure_all(inplace=False)
# 3. Execute using the Sampler primitive
from qiskit.primitives import StatevectorSampler
sampler = StatevectorSampler()
job = sampler.run([qc_measured], shots=1000)
result = job.result()
print(f" > Counts: {result[0].data['meas'].get_counts()}")
> Counts: {'111': 508, '000': 492}
```

The **StatevectorEstimator** computes properties **analytically** from the full quantum state, not just from sampling.

# Qubits, Gates, and Circuits in Code (qiskit)

```
# 4. Define the observable to be measured from gisClassical bound (Bell's Inequality): operator  |\langle XXY\rangle + \langle XYX\rangle + \langle YXX\rangle - \langle YYY\rangle| \leq 2  # 5. Exe from gis estimato Quantum mechanical prediction (maximum): job = es  |\langle XXY\rangle + \langle XYX\rangle + \langle YXX\rangle - \langle YYY\rangle| = 4  print(f" > Expectation values: {result[0].data.evs}")
```

> Expectation values: 4.000376620708558

### $q_0:$

### Simulators and Emmulators

q\_1: ---

#### Simulators

- Run exact mathematical models of quantum states
- Ideal and noise-free
- •• Good for small systems (up to ~30–35 qubits)
- Examples: StatevectorSimulator, QasmSimulator

#### Emulators

- Add realistic noise models and decoherence
- Useful for testing error mitigation and circuit robustness
- Closer to how real hardware behaves
- Often used with device-specific noise profiles

 $C_1$ 



### $q_0:$

### How to Access Real Quantum Devices

### $q_1$ :

#### **IBM Quantum (Qiskit)**

Sign up at <u>quantum-computing.ibm.com</u>
Free tier includes several 5–7 qubit devices
Use IBMProvider to submit jobs via Qiskit

#### Quantinuum, Xanadu, QuEra, etc.

Access often through API keys or cloud portals Some offer free trials, most are enterprise or researchfacing

#### **Amazon Braket (AWS)**

Access devices from IonQ, OQC, Rigetti
Requires AWS account and setup of a Braket notebook instance
Pay-as-you-go pricing

#### Google (Cirq)

Access to real hardware is limited

Most public Cirq usage is simulator-based

Quantum Computing Service access is via partnerships or Google collaborators

 $C_1$ 

# **Quantum Algorithms**

- Quantum algorithms use quantum phenomena
- → Superposition, interference, entanglement, and measurement
- Different structure than classical algorithms
- → Operate on qubit states, not deterministic bit states
- → Exploit probability amplitudes to steer computation
- Goal: amplify correct answers, cancel out wrong ones

# **Quantum Algorithms**

### **Practical Quantum Computation**

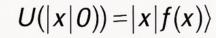


Richard Feynman (1918–1988) American Caltech

"Nature isn't classical, dammit!"



David Deutsch (b. 1953) British University of Oxford





Peter Shor (bon1959) American MIT

 $O((\log N)^2(\log \log N))$ (log log log N))

## Deutsch's Algorithm

#### Problem:

Given a function  $f: \{0,1\} \to \{0,1\}$ , determine whether it is **constant** or **bal-anced**.

Classical approach: Requires 2 evaluations of f. Quantum advantage: Requires only 1 quantum evaluation using superposition and interference.

#### Key Steps:

- Apply Hadamard gates to create superposition.
- Use a quantum oracle to evaluate f(0) and f(1) simultaneously.
- Apply Hadamard to interfere the outputs.
- Measure to determine whether f is constant or balanced.

## Deutsch's Algorithm

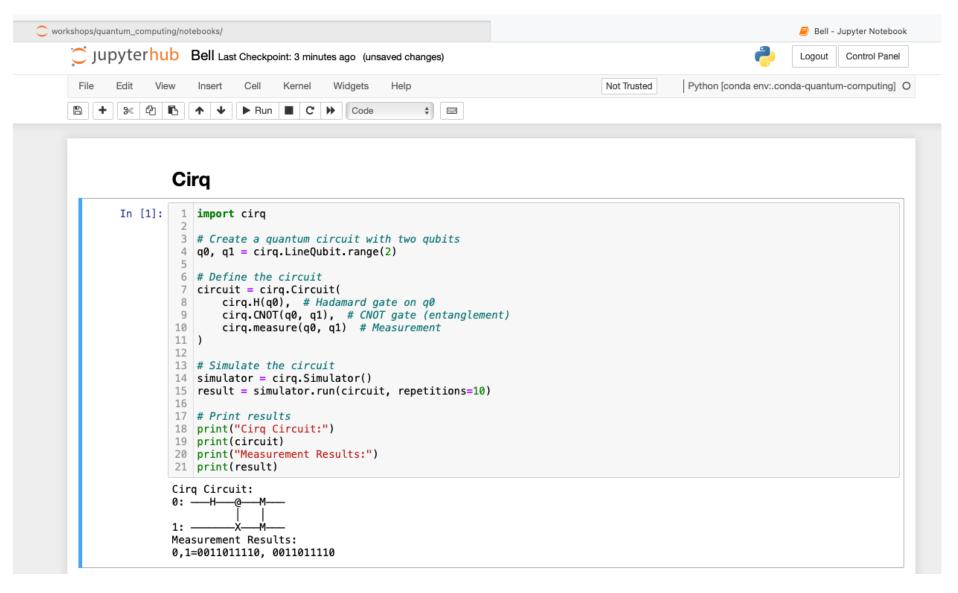
```
Qiskit-style pseudocode:
from qiskit import QuantumCircuit
qc = QuantumCircuit(2, 1)
qc.h([0, 1])
                   # Superposition
qc.cx(0, 1)
                   # Oracle (e.g., balanced case)
qc.h(0)
                   # Interference
qc.measure(0, 0) # Measure first qubit
```

Classical Computer takes needs to test the function twice.

Quantum Computer only needs to test it once.

### Interpretation:

- Measure  $0 \to f$  is constant
- Measure  $1 \to f$  is balanced



# Deutsch-Jozsa Algorithm

Given a function

$$f: \{0,1\}^n \to \{0,1\}$$

guaranteed to be either:

- Constant: the output is the same for all  $2^n$  inputs, or
- Balanced: the output is 0 for exactly half of the inputs, and 1 for the other half,

determine which case applies using as few evaluations of f as possible.

In other words, we generalize to the case where the problem size is n instead of 2.

# Deutsch-Jozsa Algorithm

In the worst case, a classical algorithm needs to evaluate up to:  $2^{n-1} + 1$  times to be sure—because you could see  $2^{n-1}$  zeros before hitting a one.

The Deutsch–Jozsa algorithm requires exactly 1 call to the quantum oracle. All  $2^n$  inputs are explored in superposition, and quantum interference reveals the answer after a single evaluation.

Input Size n	Classical (Worst Case)	Quantum
1 011101 1	2	1
2 0 1 0 0 1 0 1 1 0	3	
31 0 0 1 1 1 1 0	5	
n <sup>1 0 1 1 0 1 0</sup>	$2^{n-1}+1$	1 /
100	$\approx 6.3 \times 10^{29}$	Quantum Algorithms 88

# **Quantum Fourier Transform (QFT)**

- Quantum analogue of the Discrete Fourier Transform (DFT)
  Maps amplitudes to frequency components in the quantum state
- Operates on a quantum register Transforms basis states  $|x\rangle$  into a superposition of phase-encoded states

Core tool in algorithms like:

- Shor's Algorithm (factoring)
- Quantum Phase Estimation
- Hidden Subgroup Problems

Exponential speedup:

QFT uses  $O(n^2)$  gates vs. classical DFT's  $O(n2^n)$  operations

# Quantum Phase Estimation (QPE)

Goal: Estimate the phase  $\phi$  in an eigenvalue equation:

$$U|\psi\rangle = e^{2\pi i\phi}|\psi\rangle$$

Why it matters:

QPE is the quantum routine that allows us to find periodicity (used in Shor's Algorithm), eigenvalues (in quantum chemistry), and simulate quantum systems.

1 1 1 0 1 1

QPE uses QFT<sup>-1</sup> to decode a phase from a quantum state.

The phase is stored as a pattern of amplitudes, and the inverse QF7 translates this
interference pattern into a readable binary number.

## Shor's Algorithm

- Goal: Factor a large integer N efficiently
- Classical complexity: Exponential time
- Quantum complexity: Polynomial time (with high probability)
- •Key insight:
- •Reduces factoring to a **period-finding** problem
- •Quantum subroutine:

Uses Quantum Phase Estimation (QPE) and the Quantum Fourier Transform (QFT)

- Breaks RSA encryption
- •(Because RSA's security depends on factoring being hard)

## Variational Quantum Eigensolver

Goal: Approximate the ground state energy of a quantum system (e.g., molecules, spin chains, Hamiltonians)

Hybrid approach:

- Quantum computer prepares parameterised quantum states
- Classical optimizer adjusts parameters to minimise energy
- Uses the variational principle:

$$E(\theta) = \langle \psi(\theta) | H | \psi(\theta) \rangle \ge E_0$$

 $\rightarrow$  The lowest measured energy gives an upper bound on the true ground state  $E_0$ 



## Variational Quantum Eigensolver

### Circuit:

- Ansatz (parameterised gate sequence)
- Measurement of expectation values of H

### Why VQE Works:

- •Real quantum devices can prepare rich entangled states
- •Classical computers handle non-convex optimisation
- Together, they explore a large space of trial wavefunctions

## Why Quantum Error Correction Is Necessary

#### **Qubits are fragile**

- Easily disturbed by noise, temperature, or stray electromagnetic fields
- Suffer from decoherence, bit-flip, and phase-flip errors

#### **No-cloning theorem**

We can't make backup copies of quantum states like in classical RAM

### Gate operations and measurements are imperfect

- Error rates per operation are often 0.1–1%, and these errors accumulate
- Quantum algorithms require thousands or millions of gates
- → Without correction, noise overwhelms computation

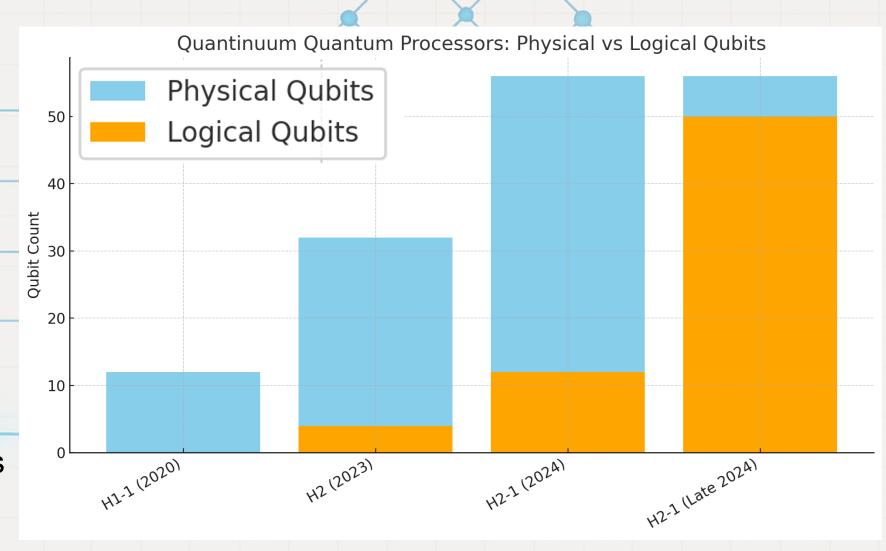
### QEC uses redundancy across multiple qubits

- One logical qubit = many physical qubits
- Errors are detected and corrected without collapsing the state

## How We Protect Quantum Information

Encode 1 logical qubit into many physical qubits Redundancy allows detection and correction of errors.

E.g. **Steane code** – uses 7 physical qubits per logical qubit



# Summary: Quantum computing is real, and rapidly evolving

- Grounded in principles like superposition, entanglement, and interference
- Promises exponential speedups for select problems
- We explored core concepts:
  - Qubits, circuits, gates, and measurement
  - Quantum logic, algorithms, and hardware models
  - Key applications: factoring, search, simulation, optimization
- Quantum advantage is still emerging
  - Today's machines are noisy and small
  - Error correction and scalability are the next frontier
- HPC and quantum are deeply connected
  - Both require specialised hardware, remote access, and hybrid workflows
  - CARC provides the tools to explore both worlds