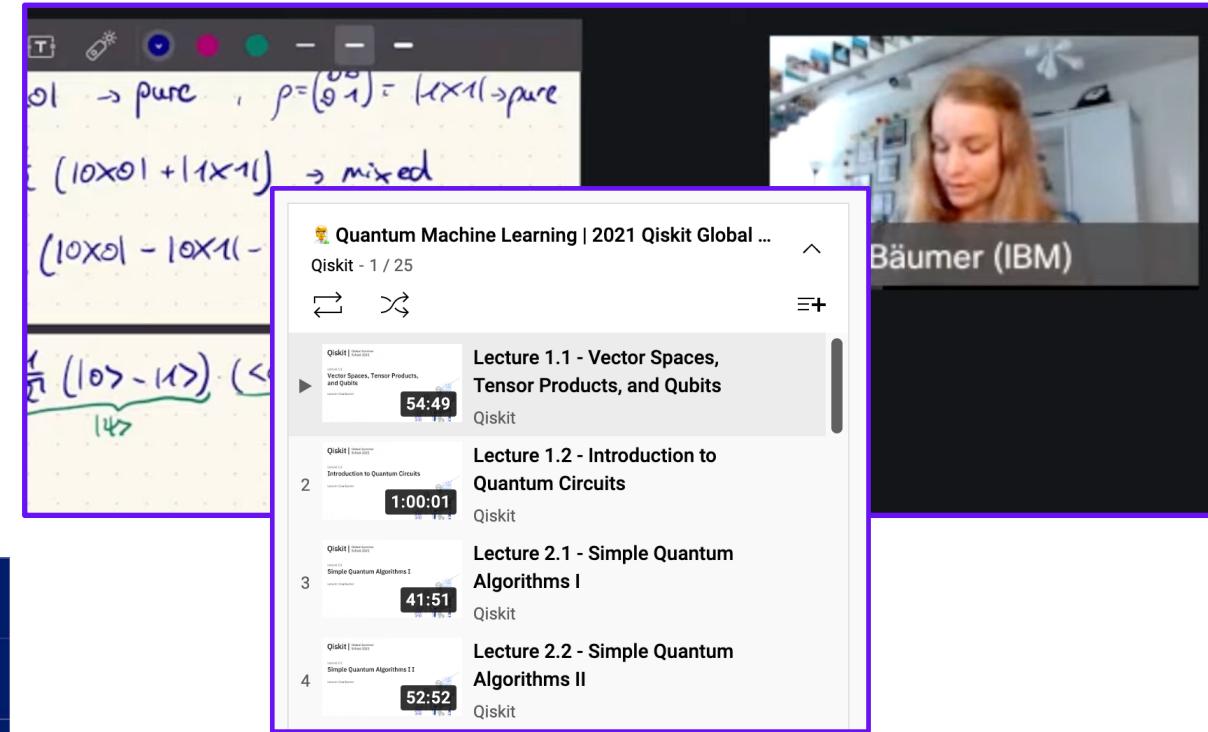
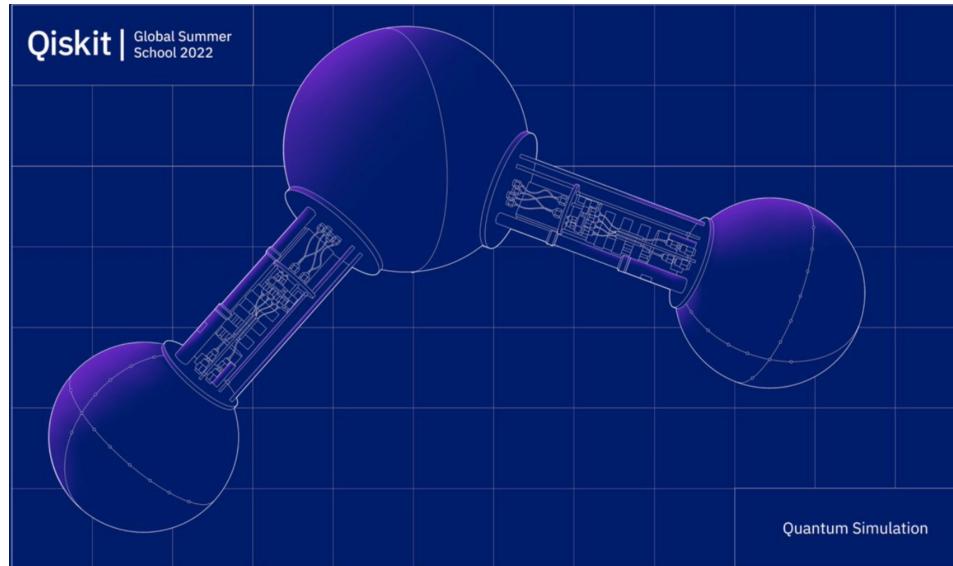


Welcome

Qiskit Summer School 2022

3rd Annual Qiskit Global Summer School

Previous years focused on a general introduction to quantum computing and quantum machine learning



ol \rightarrow pure , $\rho = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = 1 \times 1 \rightarrow$ pure

$(1 \times 0 + 1 \times 1) \rightarrow$ mixed

$(1 \times 0) - 1 \times 1 -$

$\frac{1}{2} (|0\rangle - |1\rangle) (\langle 0| + \langle 1|)$

Quantum Machine Learning | 2021 Qiskit Global ...
Qiskit - 1 / 25

Lecture 1.1 - Vector Spaces, Tensor Products, and Qubits
Qiskit

54:49

Lecture 1.2 - Introduction to Quantum Circuits
Qiskit

1:00:01

Lecture 2.1 - Simple Quantum Algorithms I
Qiskit

41:51

Lecture 2.2 - Simple Quantum Algorithms II
Qiskit

52:52

Bäumer (IBM)

This year, our topic is quantum simulation + quantum chemistry applications

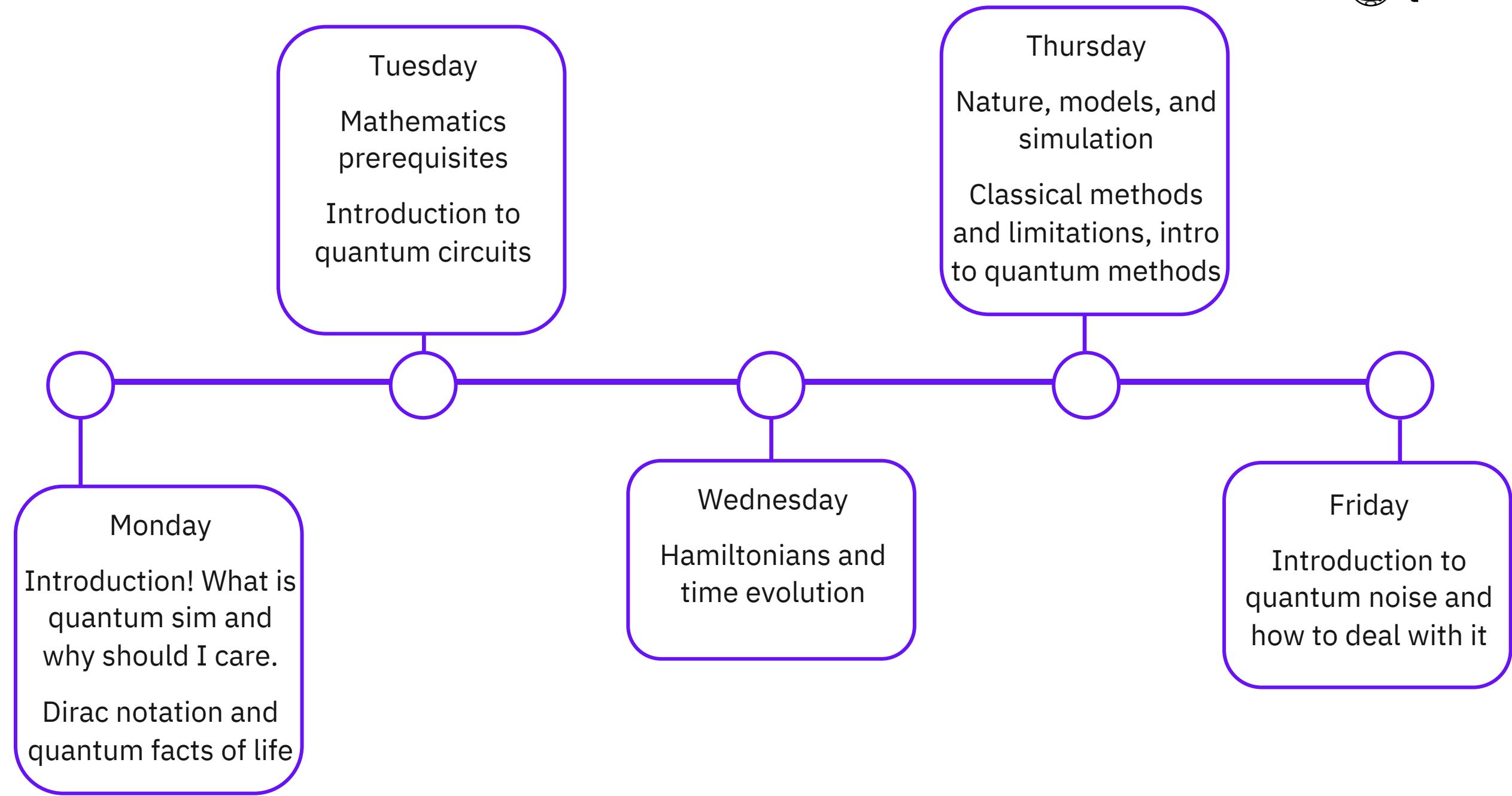
Introduction



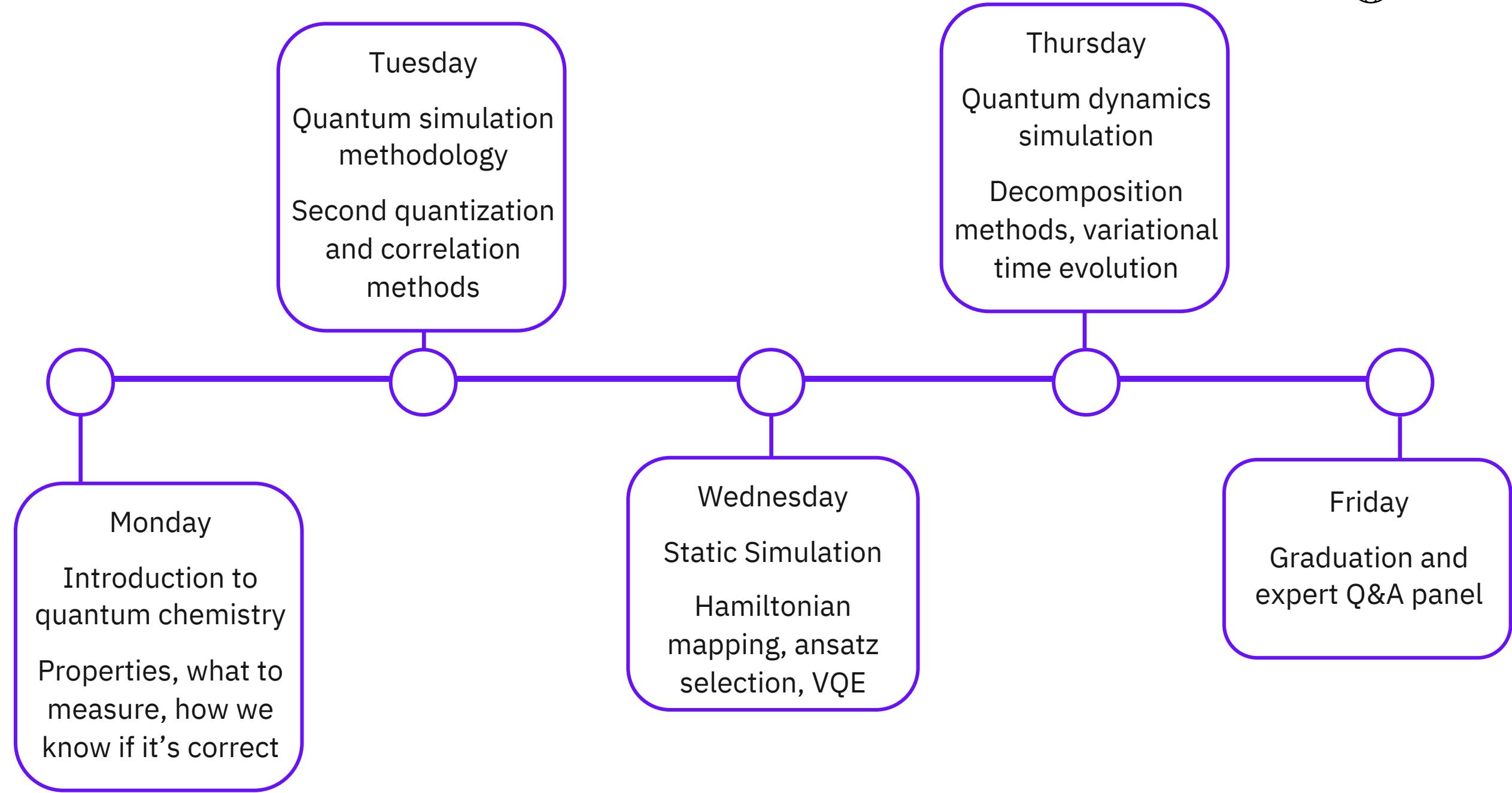
- North American Lead for Qiskit Education/Research
- Completed PhD in physics in 2020 from the University of Pittsburgh, studied experimental quantum measurement
- Joined IBM in 2020
- Equally interested in working with both students and researchers to push the boundaries of their education and research outcomes
- Never attempted quantum simulation experiments until last year!



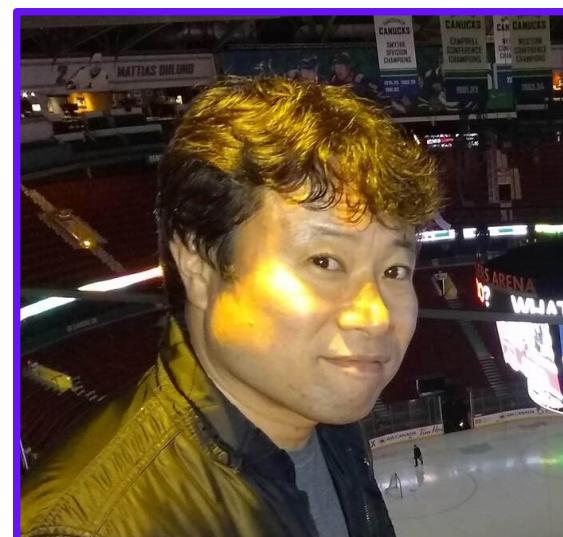
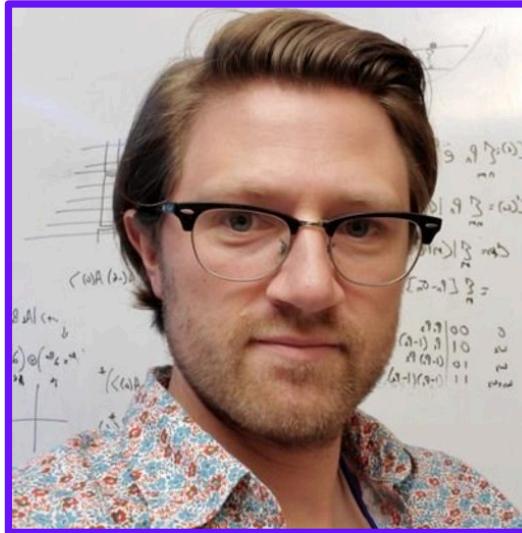
Outline for rest of week



Week 2

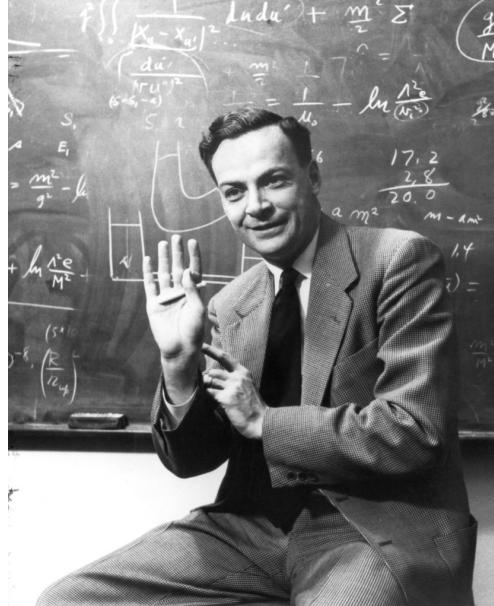


Meet the professors



Why quantum simulation?

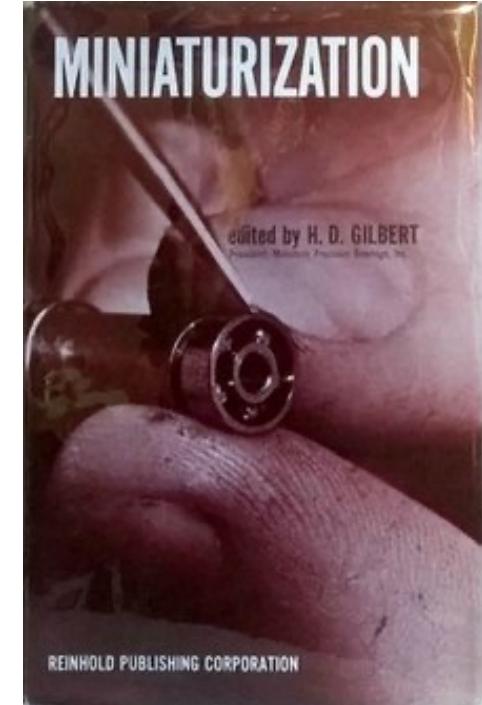
Origins



Richard Feynman, Nobel Laureate and professor of physics

Worked on Manhattan project, authored books, frequent bongo-player

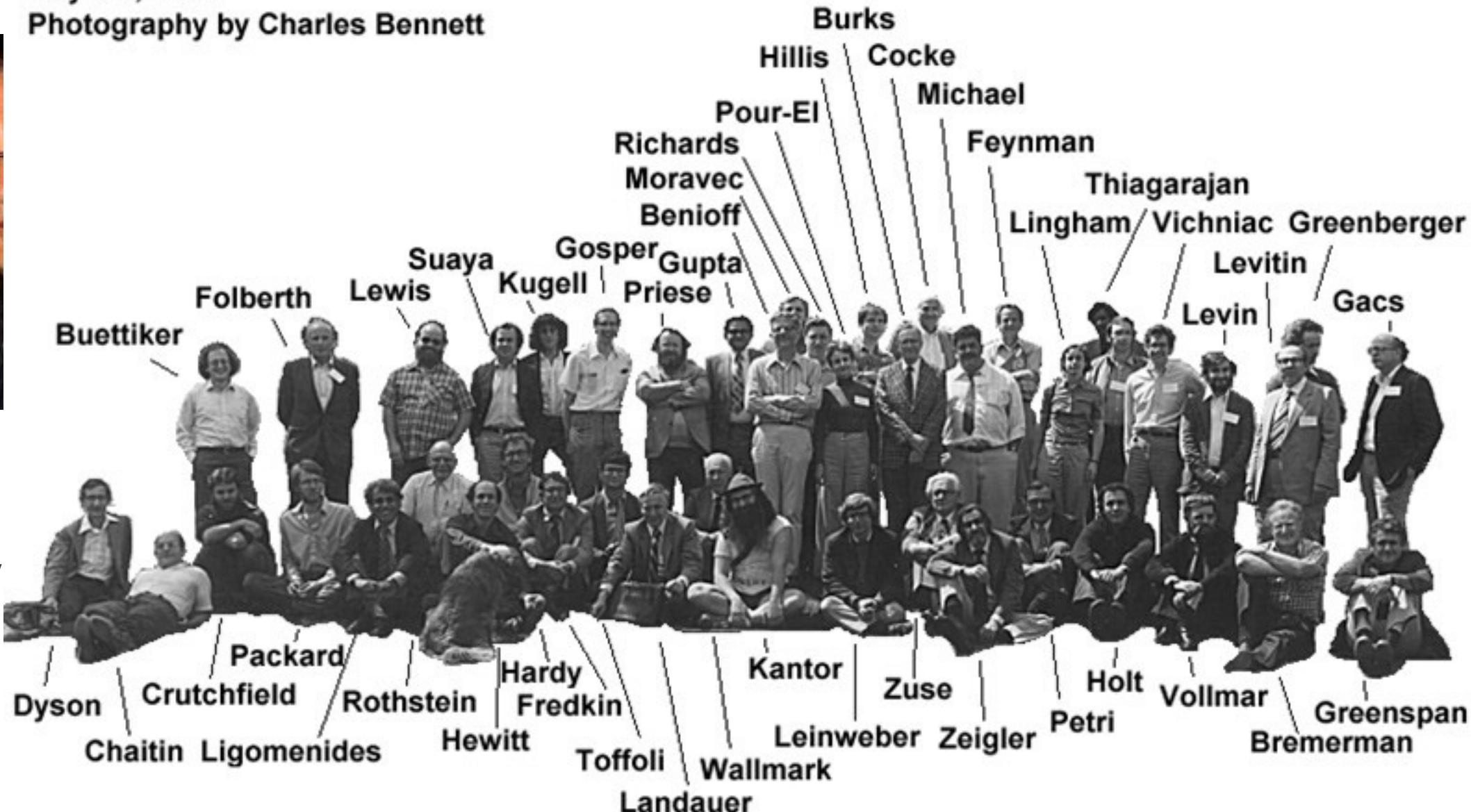
“There’s plenty of room at the bottom” speech given at Caltech in 1959 was an invitation to join a new field of physics.



“It would be in principle possible (I think) for a physicist to synthesize any chemical substance that the chemist writes down...put the atoms down where the chemist says, and so you make your substance.”

Orig

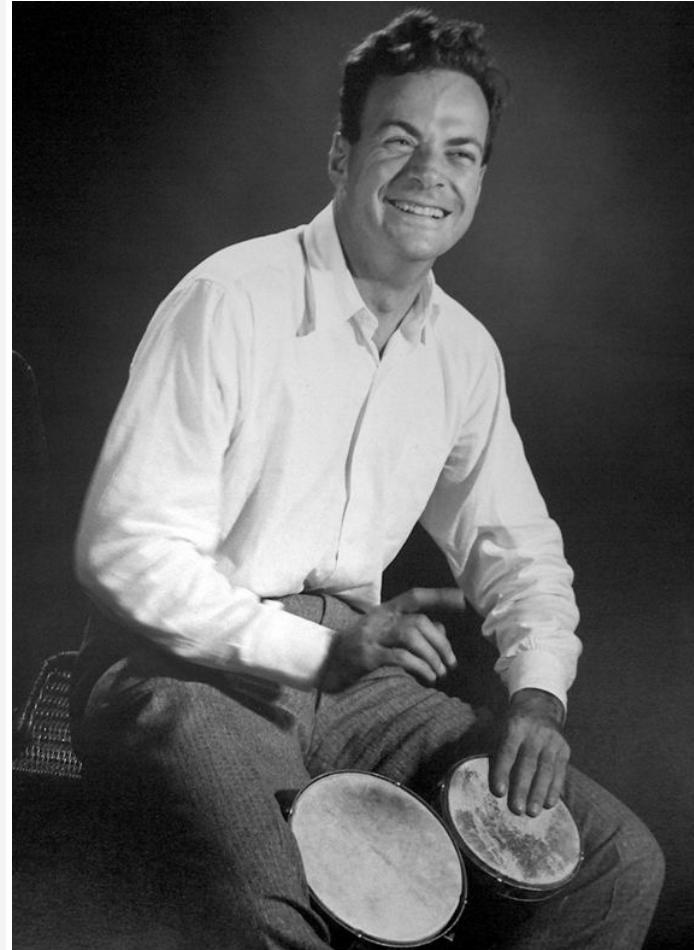
"Physics of Computation" Conference
MIT Endicott HSE, Dedham, MA
May 6-8, 1981
Photography by Charles Bennett



Simulating physics with Computers

- Inherently important to use what we learn in the physics lab in *other* subjects
- Simulation provides key bridge between theory and experiment
- Identify deficiencies in theory and develop new interpretations
- Computations will lead to scientific breakthroughs

“Can you do it with a new kind of computer — a quantum computer? Now it turns out, as far as I can tell, that you can simulate this with a quantum system, with quantum computer elements. It’s not a Turing machine, but a machine of a different kind”



*Simulating
Physics
with
Computers*

*Richard P.
Feynman*

*Presented by Pinchas Birnbaum
and Eran Tromer,
Weizmann Institute of Science*

What even is a simulation?

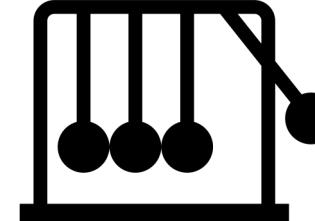
- “A computational model that will do exactly the same as nature”
 - Inherently different than numerical methods, which offer only approximate solutions to a system
- The computational elements required for the simulation must be proportional to the space-time volume of the physical system
- No long travel distances for communication paths

Can classical computers simulate classical physics?

- Time and space may be continuous, but by discretizing nature into sufficiently fine elements, no physics is lost.
- The passage of time is simulated through a causal nature.

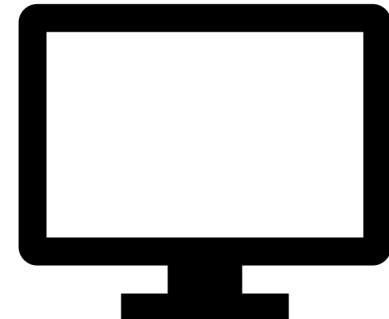


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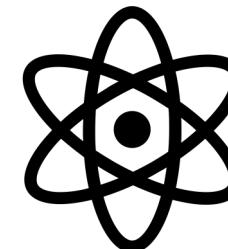


Can classical computers simulate quantum physics?

- Can't compute probabilistic configurations of a probabilistic theory
- To configure a problem with R particles at N points in space would require N^R probabilities. This is too large for a computer of order $O(N)$
- Hidden variable theory: quantum probability cannot be simulated on classical machine



+

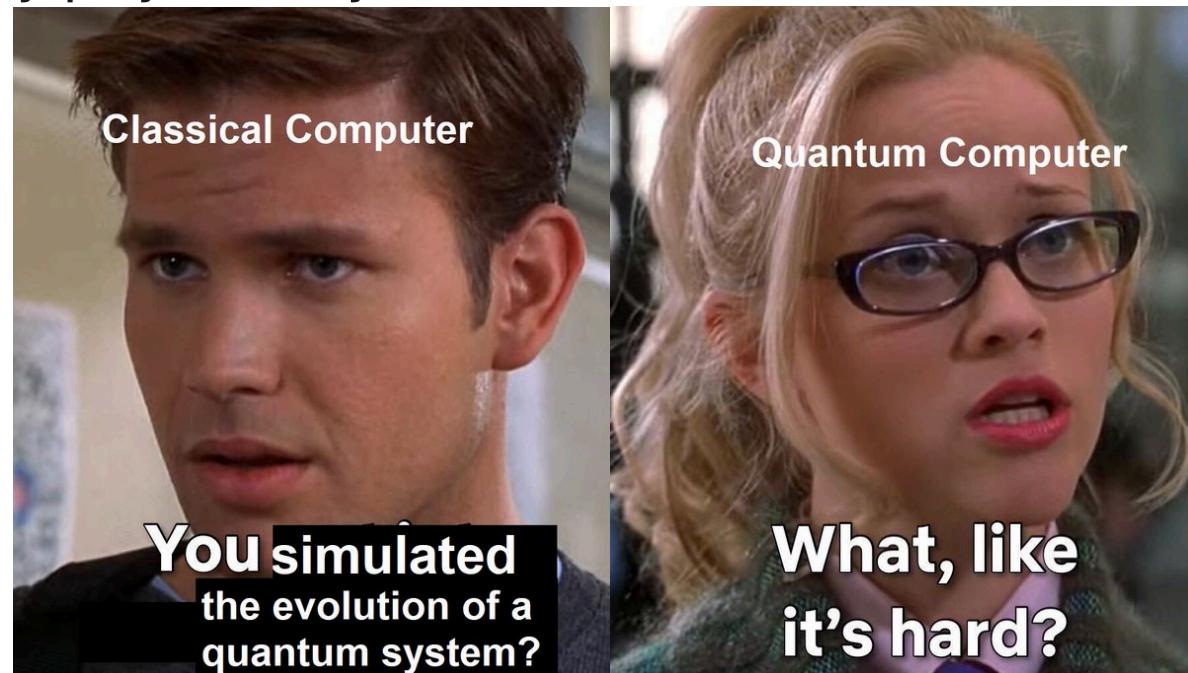


TLDR:No

Can quantum computers simulate quantum physics?

Idea: if quantum physics is too hard for classical computers, build a physical quantum computer that exploits that power.

Conjecture: There is a universal quantum simulator, which is physically realizable, that can simulate any physical system.



[1] Quantum Computing Memes for QMA-Complete Teens, Harvard Law & Meme Review (2021)

**"NATURE ISN'T CLASSICAL, DAMMIT, AND IF
YOU WANT TO MAKE A SIMULATION OF NATURE, YOU'D
BETTER MAKE IT QUANTUM MECHANICAL, AND BY
GOLLY, IT'S A WONDERFUL PROBLEM, BECAUSE IT
DOESN'T LOOK SO EASY."**

RICHARD P. FEYNMAN

The necessity of quantum simulation

- A system with >60 qubits cannot be simulated with a classical computer
- A moderately sized quantum processor (~100 qubits) could outperform supercomputers for exact solutions
- Quantum sim is expected to be crucial for large network (e.g. lattice) models, featuring Fermions or frustration and strong entanglement (phase-transitions)
- Quantum sim will allow probing into reactions and situations that cannot be done in the lab

State-of-the-art work

ARTICLE OPEN

Simulating quantum many-body dynamics on a current digital quantum computer

Adam Smith^{1,2*}, M. S. Kim¹, Frank Pollmann² and Johannes Knolle¹

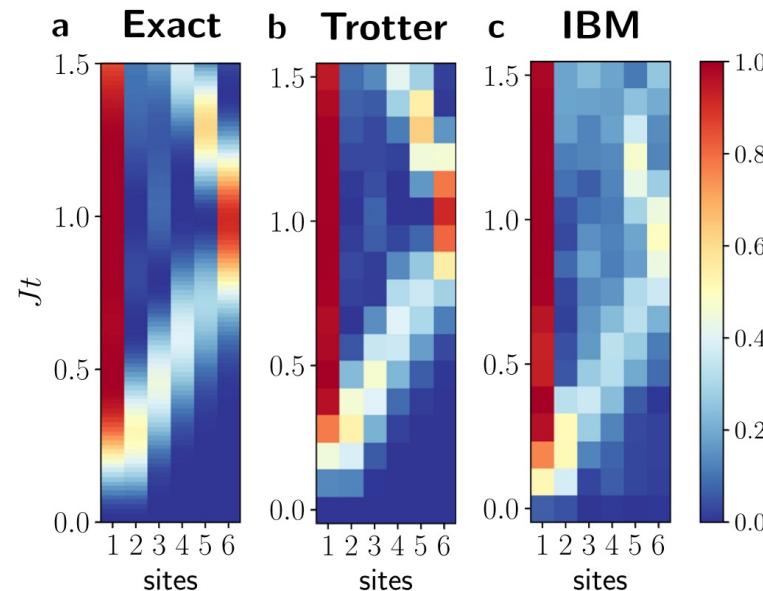
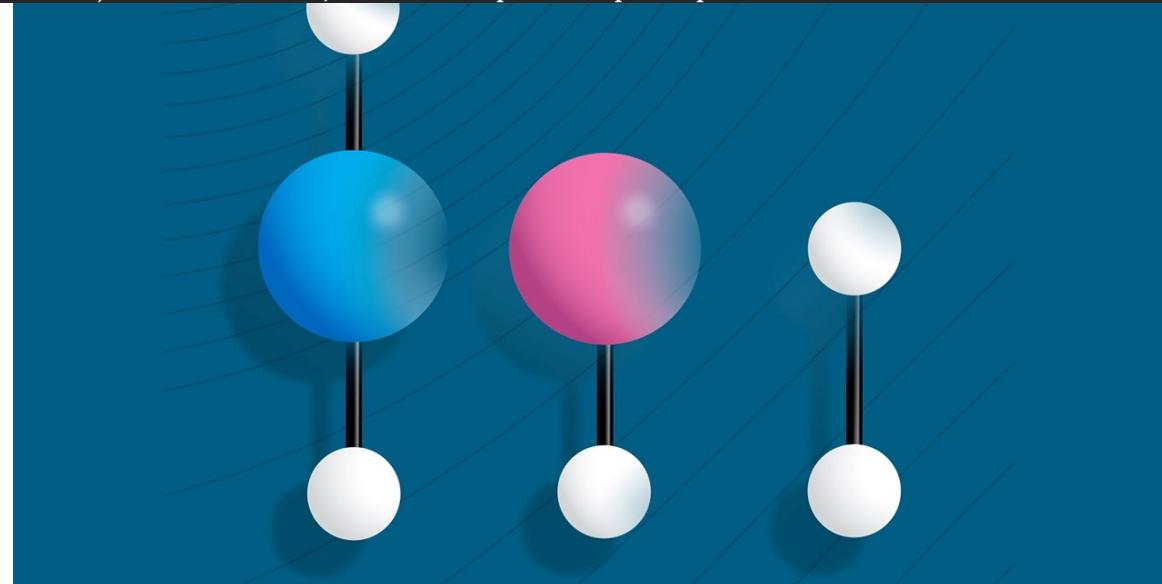


Fig. 4 Results for the connected spin correlator defined in Eq. (6). Data are computed using: **a** exact diagonalization, **b** numerical trotterization, **c** the IBM quantum device. Data are shown for $N = 6$, $h_j = 0$ and $U = 0$, using a symmetric trotterization, and obtained on 12 March 2019.

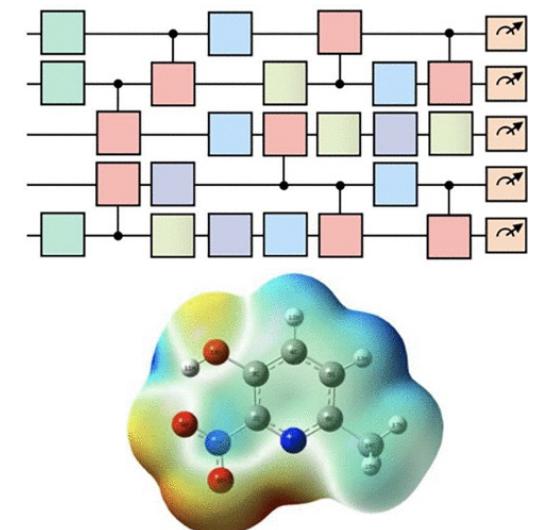
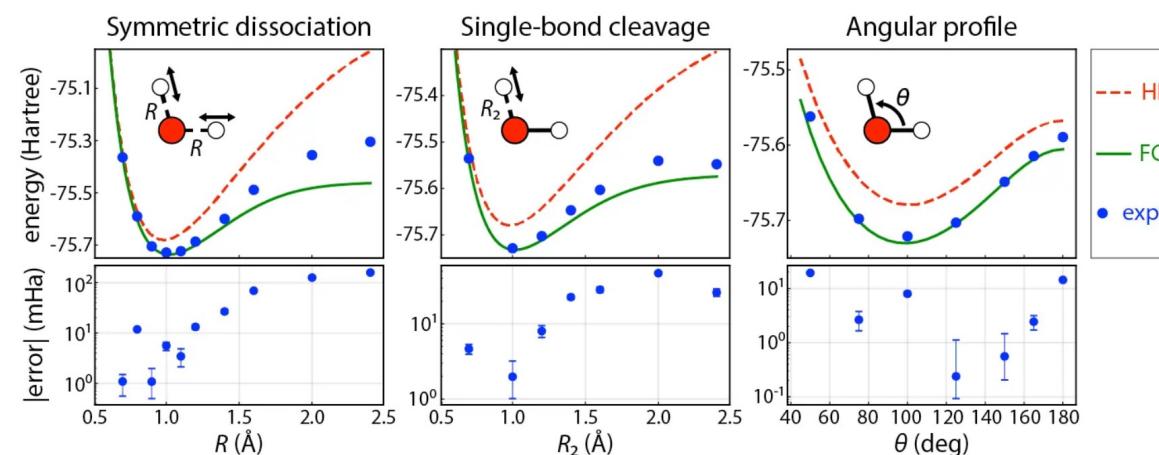
Quantum computer simulates largest molecule yet, sparking hope of future drug discoveries

Beryllium hydride has just three atoms, but it's the proof of principle that counts



Quantum Chemistry

- Studying dynamics and properties of molecular reactions is important to the future study of chemistry
- Quantum effects are important at the level of molecular reactions, but exact calculations are beyond the capabilities of classical computation, except for the smallest molecules.
- It has been demonstrated that a quantum computer can obtain molecular energies to a degree of precision greater than what's required by chemists for understanding reaction dynamics, and better than standard classical methods.



Future of quantum simulation

Discover new materials?



Drug design?



Chemical reactions for battery development?



What's a quantum computer?

Classical Bit

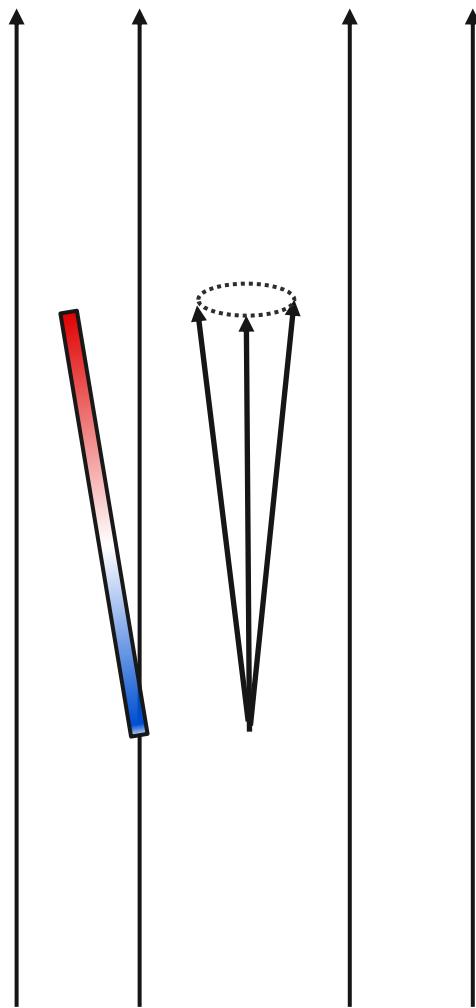


Encoding information

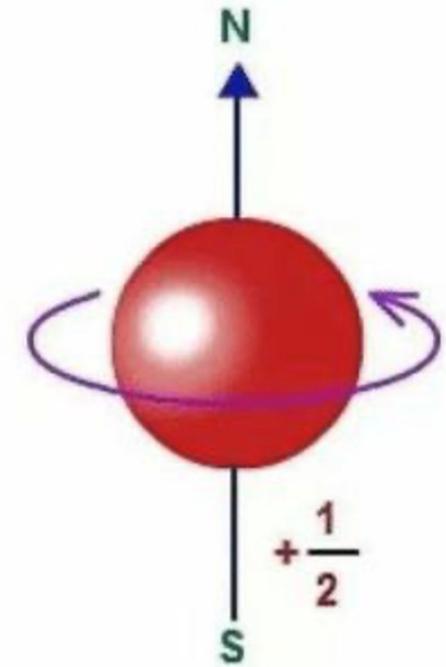
Color	Coins	Binary
Red	HHH	000
Yellow	HHT	001
Yellow	HTH	010
Green	HTT	011
Cyan	THH	100
Purple	THT	101
Purple	TTH	110
Magenta	TTT	111

$$\begin{array}{r} 11010 \\ \swarrow \quad \searrow \quad | \\ 1 \times 2^4 \quad 0 \times 2^2 \quad 0 \times 2^0 \\ \downarrow \quad \downarrow \quad \downarrow \\ 1 \times 2^3 \quad \quad \quad 1 \times 2^1 \\ = 16 + 8 + 0 + 2 + 0 \\ = 26 \end{array}$$

Magnetic needle

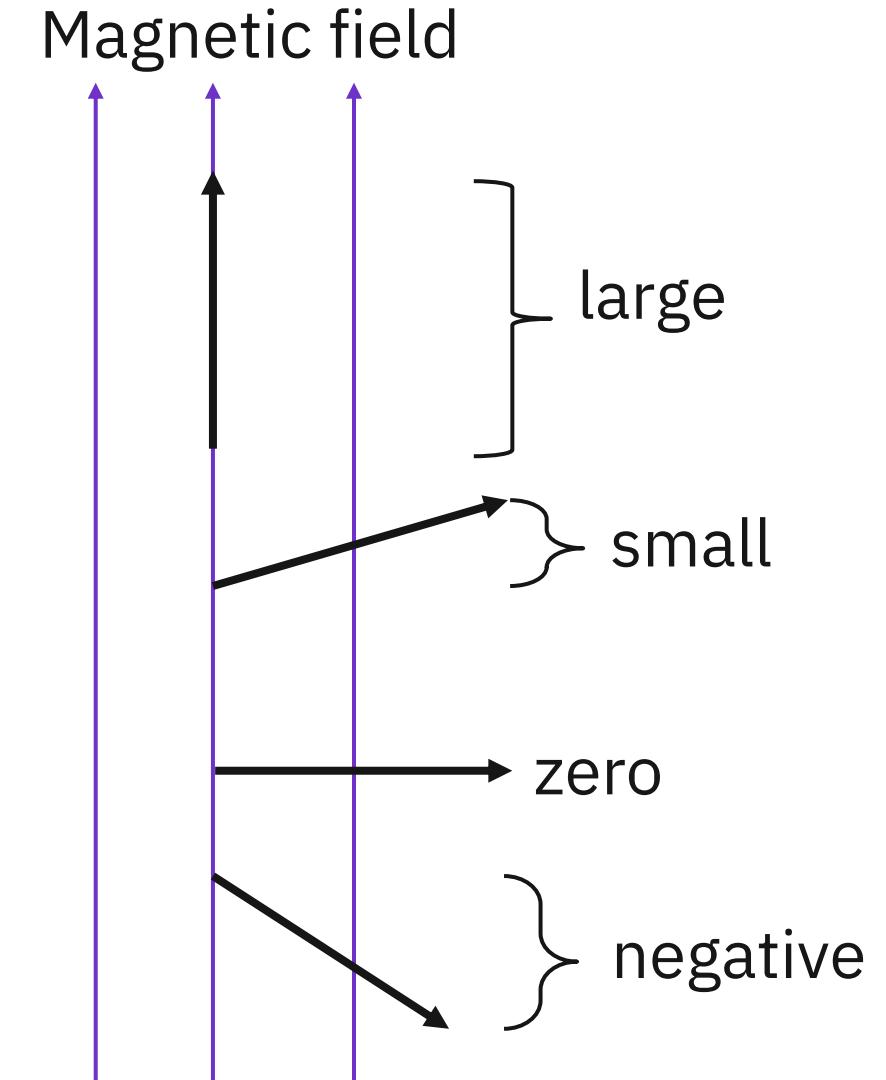
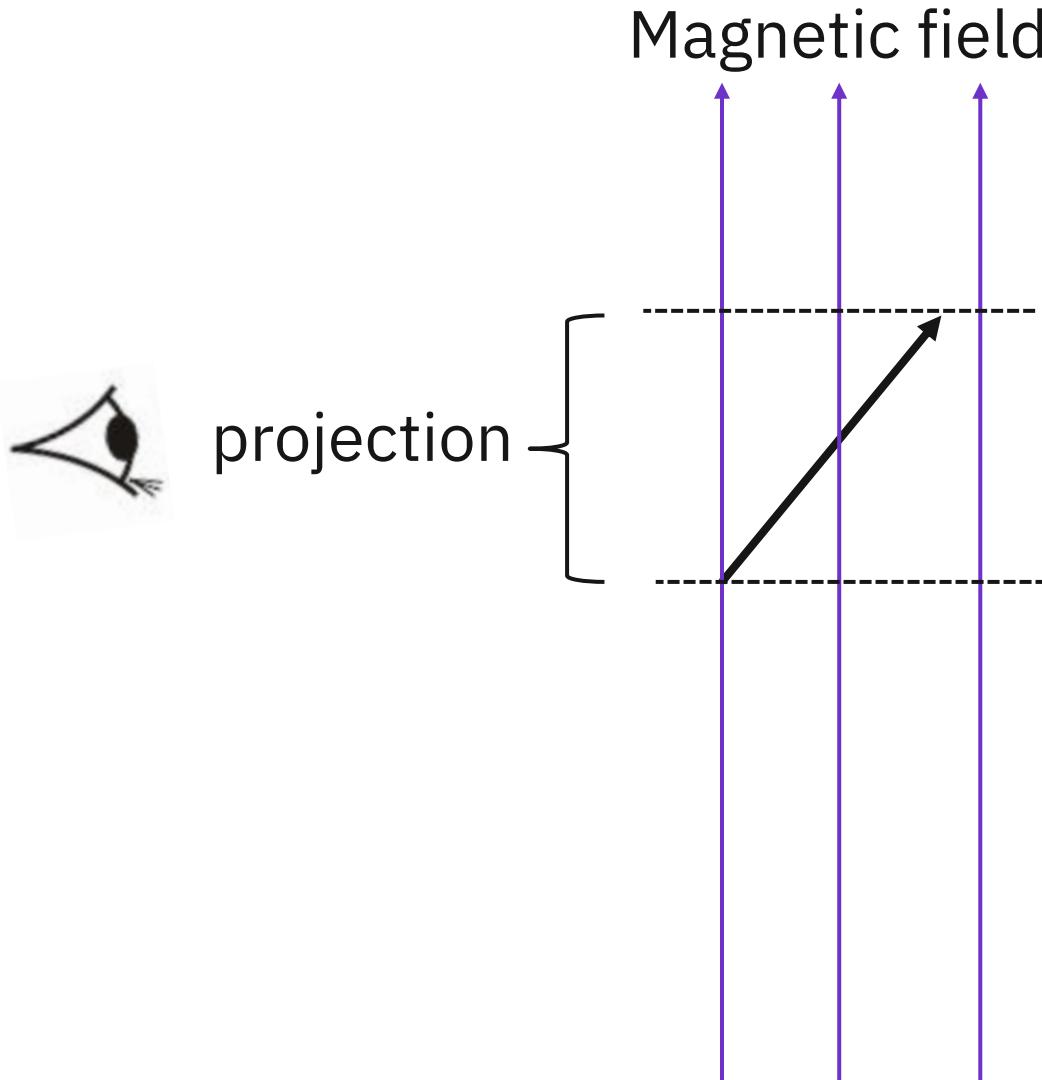


Inhomogeneous field

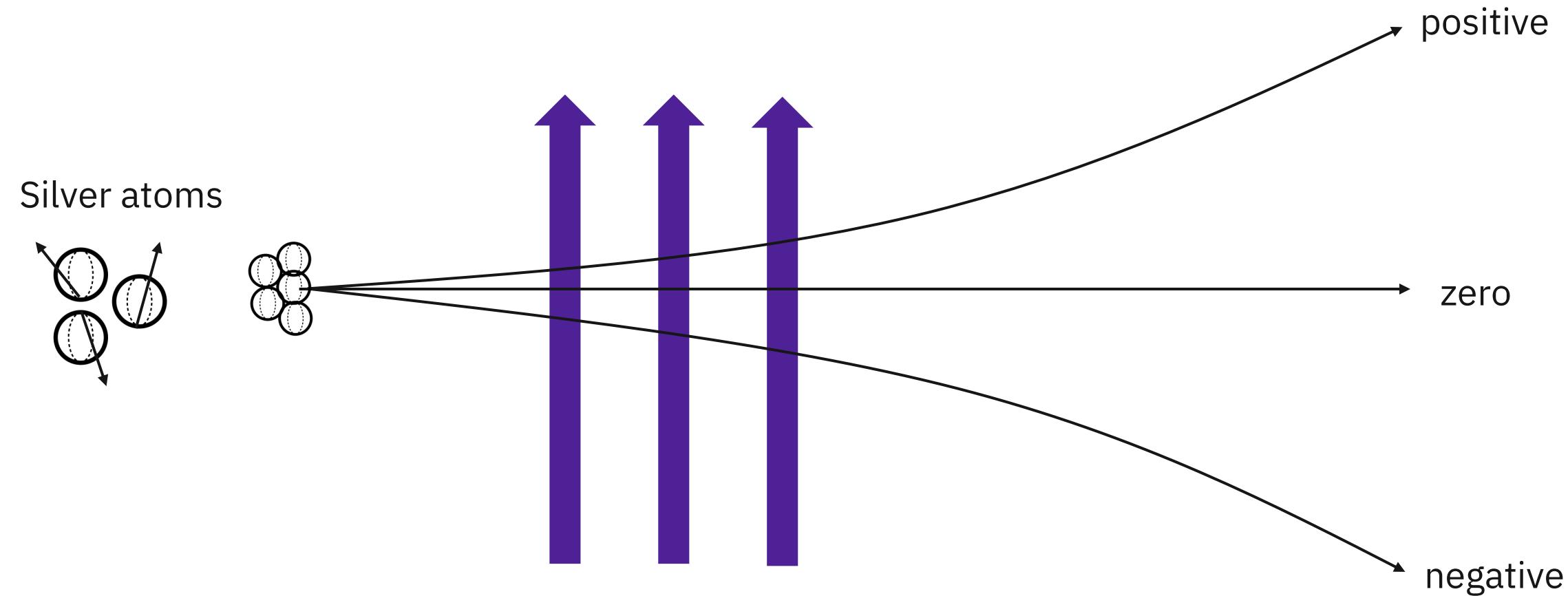


Spin explained: imagine a ball that's rotating...
except it's not a ball and it's not rotating ☺

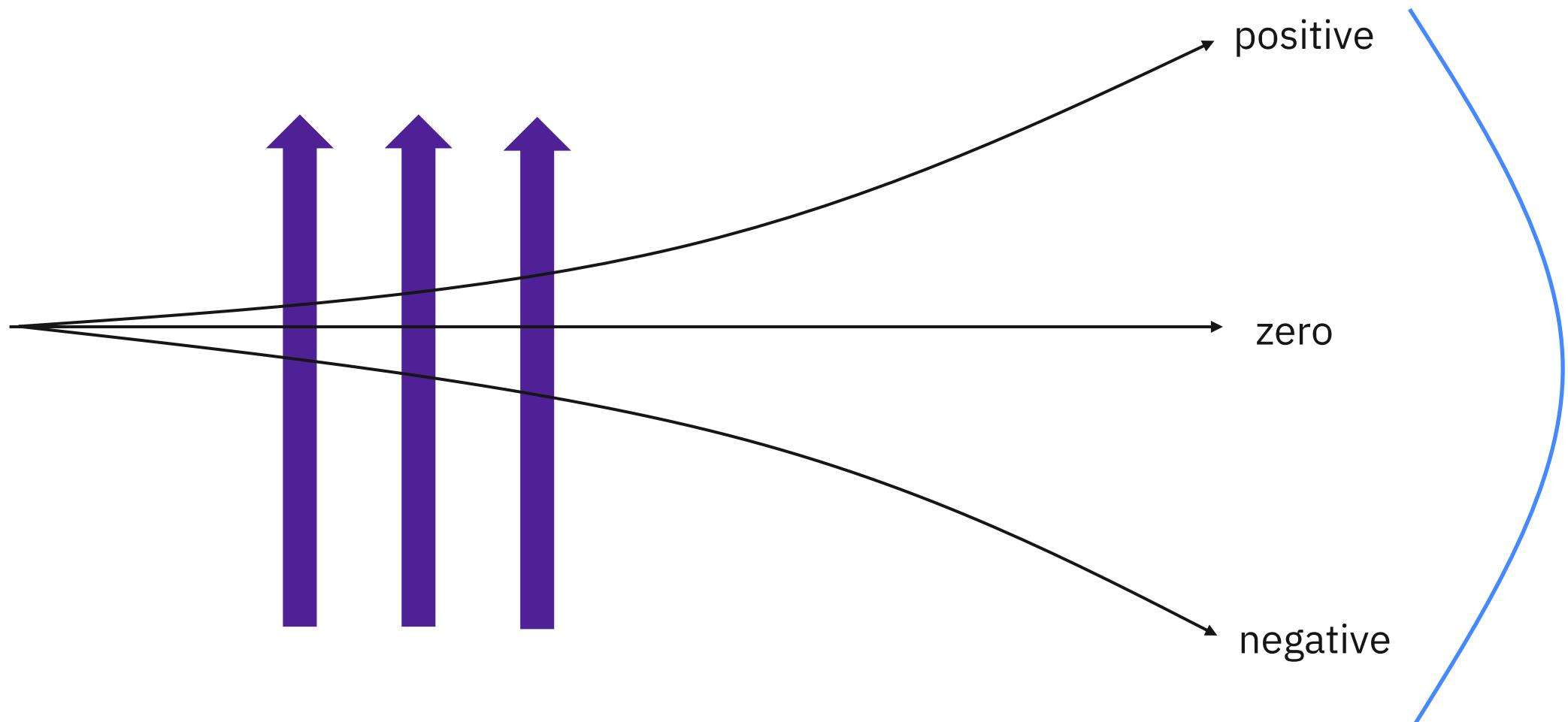
Projections



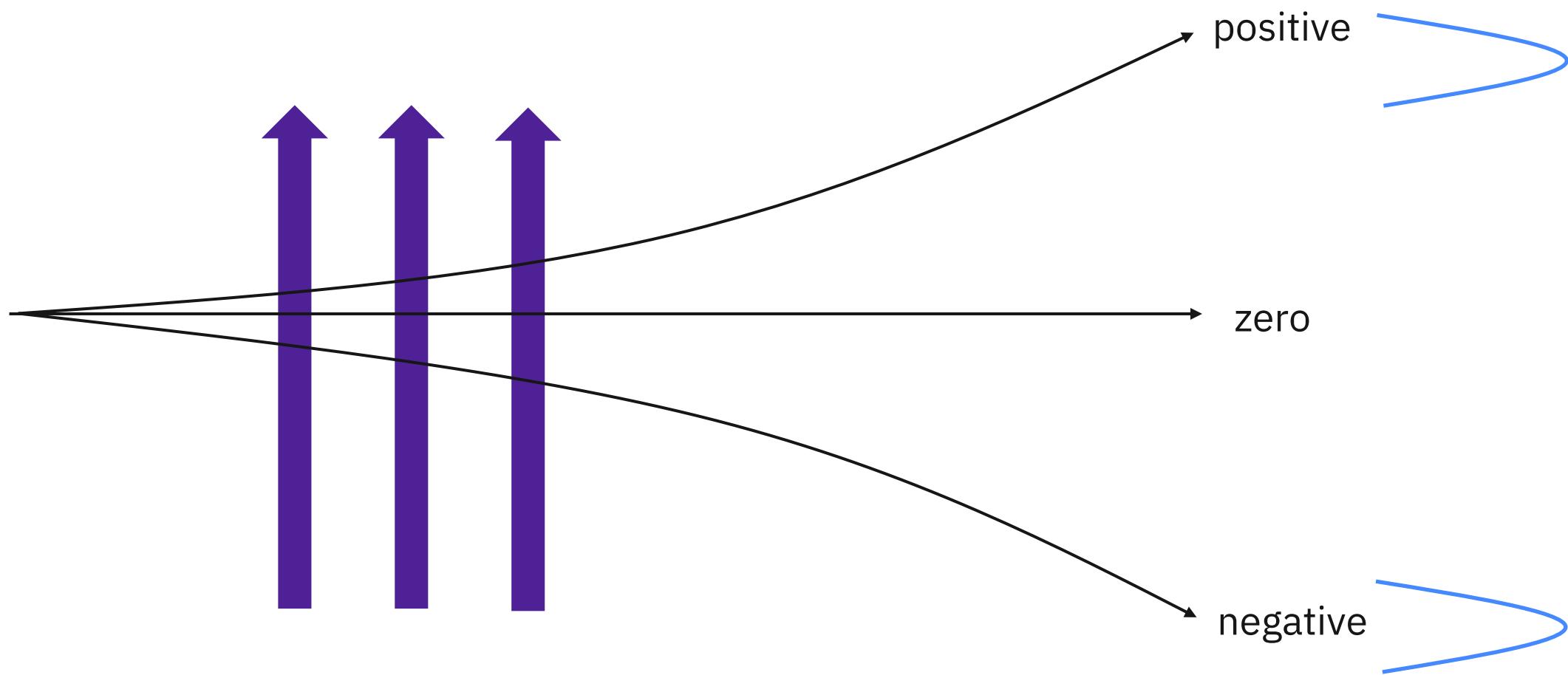
Stern-Gerlach



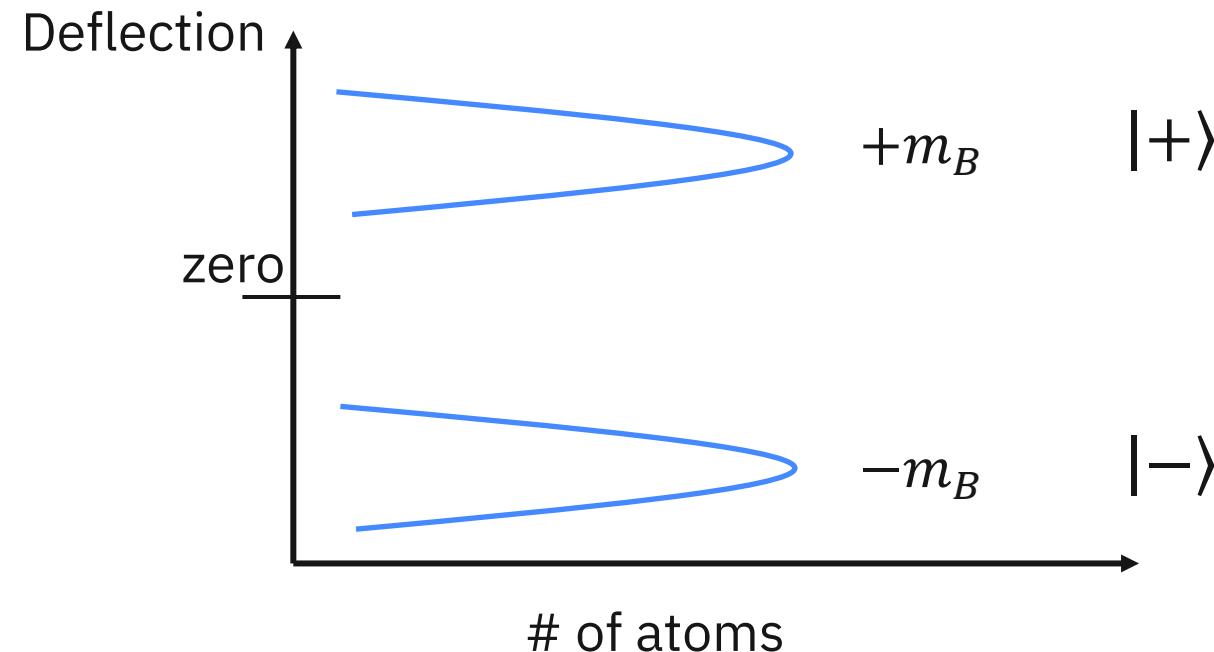
Stern-Gerlach-expected outcome



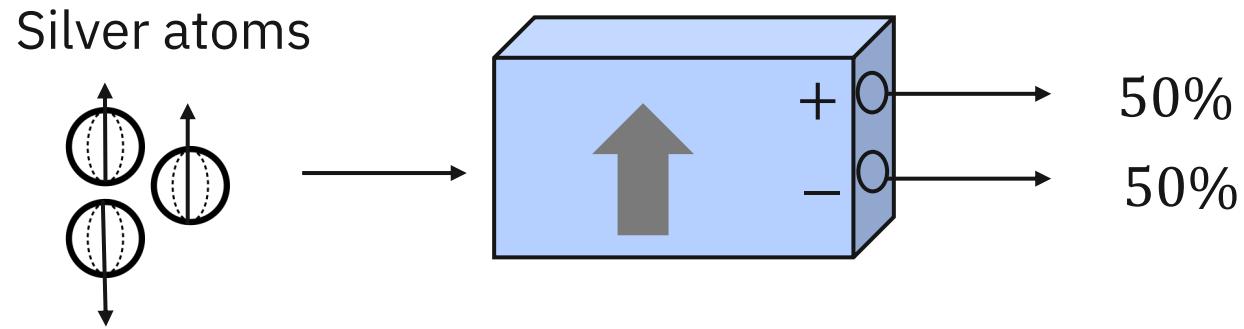
Stern-Gerlach-actual outcome



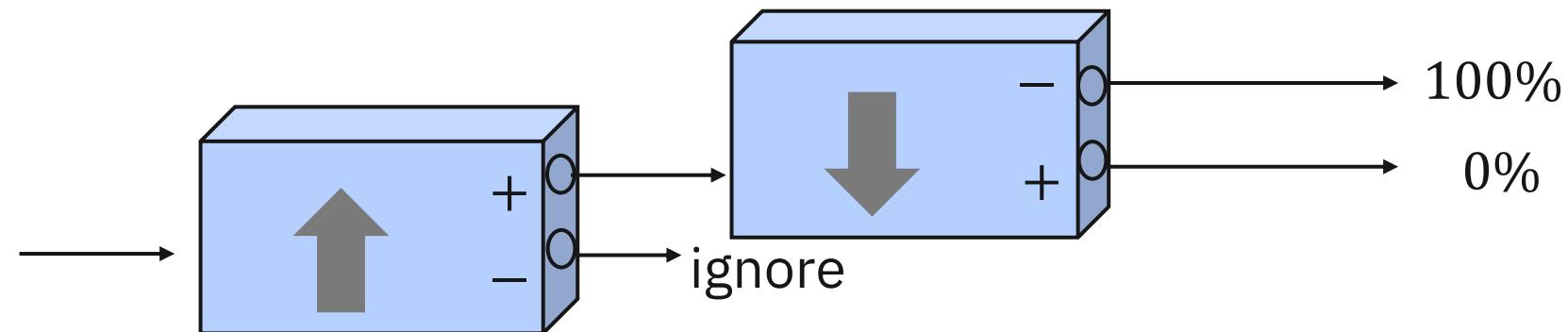
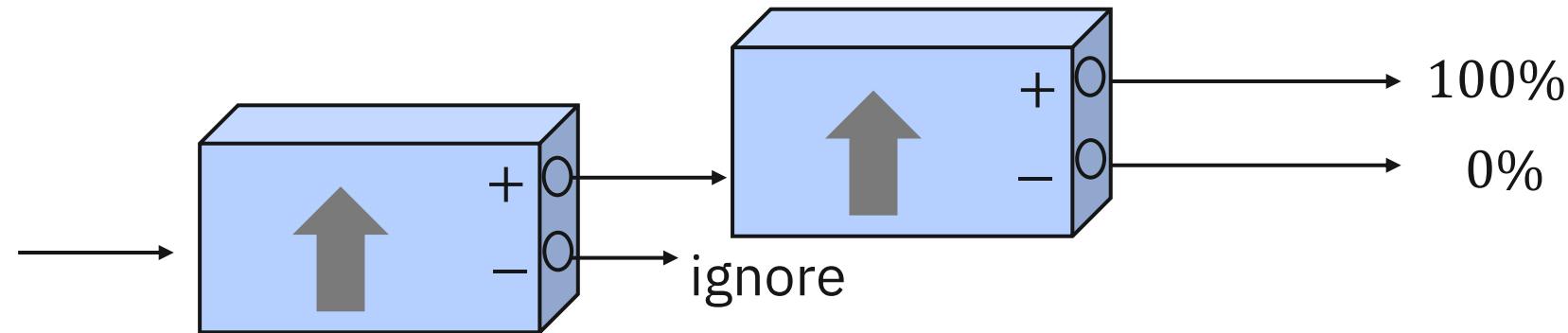
Stern-Gerlach; actual results



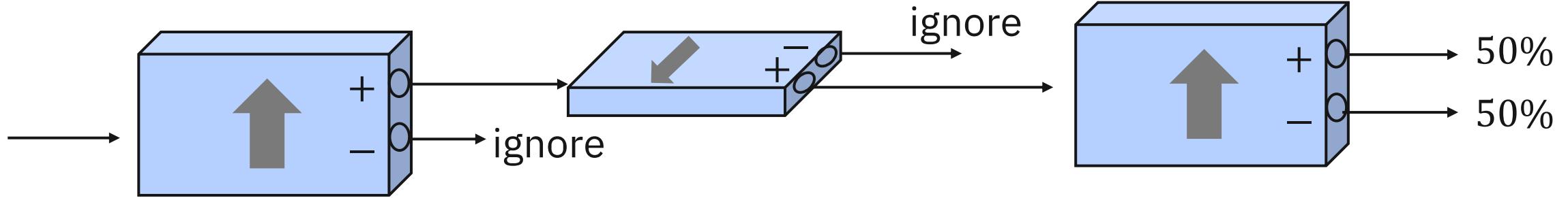
Stern-Gerlach apparatus



Probabilities with S-G

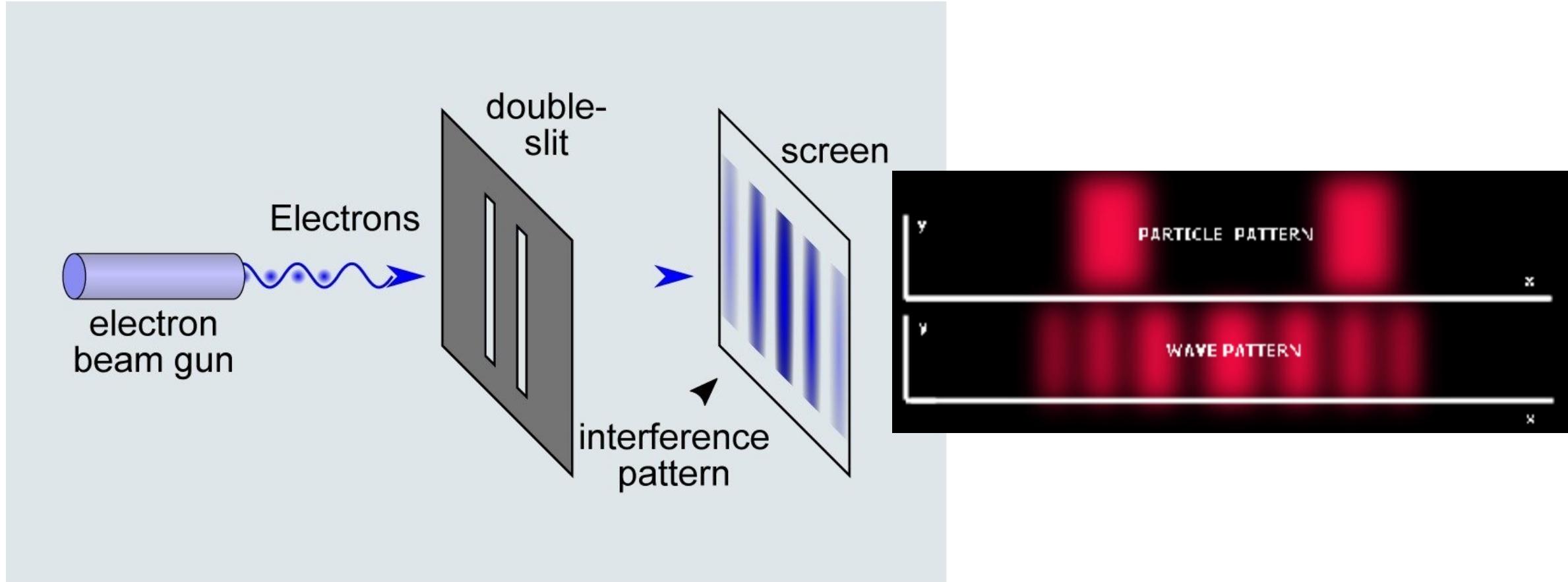


The crucial experiment



Test yourself: What is the distribution at the end?

Measuring the double slit



“Quantum mechanics forces us to the brink of implausibility
...but not beyond”

What is a superposition??

SOME combination of

$|+\rangle$ AND $|-\rangle$

AND NOTHING ELSE

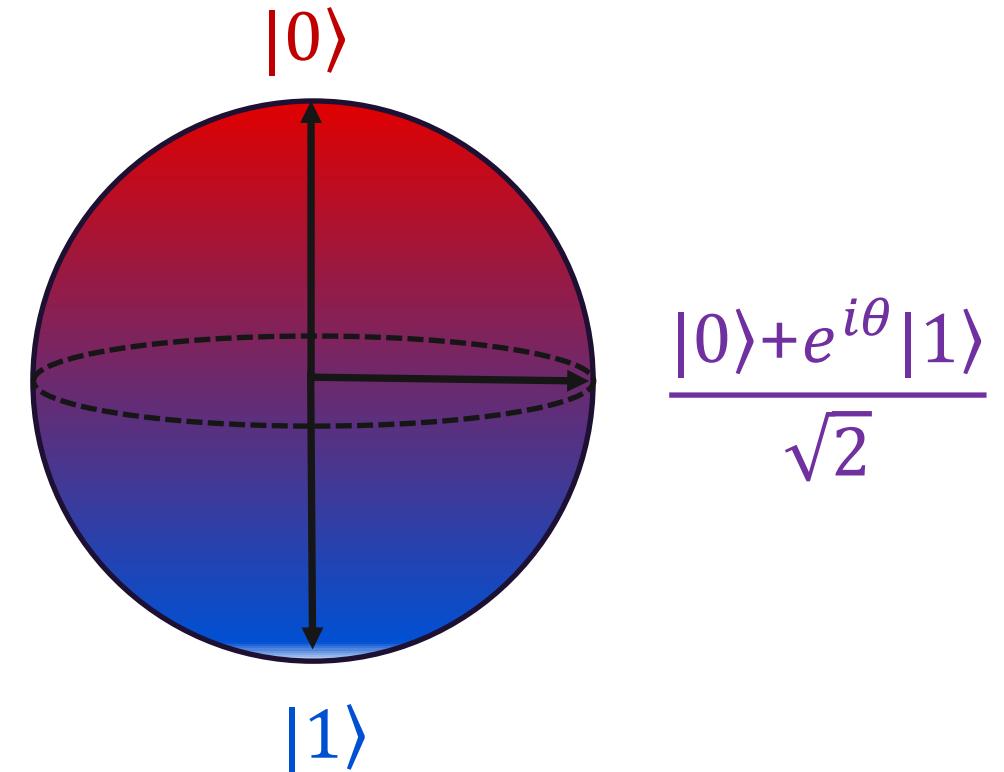
We can write this strange state as:

$$\psi = |+\rangle \mp |-\rangle$$

Conclusions and qubits

WHAT MUST BE TRUE

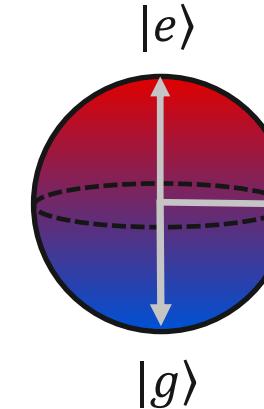
- Single particles can exist in states of *superposition*, which combines multiple measurable states with certain probabilities associated with them
- Single particles can interfere *with themselves* due to this nature
- Upon measurement, *only* these definite states can be observed and the outcome is *probabilistic*, not determinate



How do we build a quantum computer? (DiVincenzo Criteria)

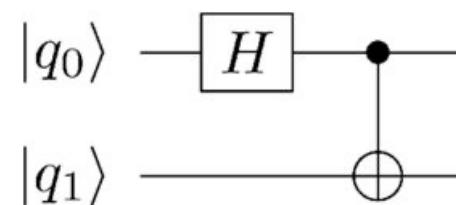
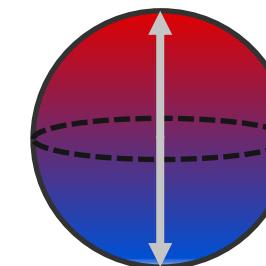


Well-behaved quantum systems



...that we can initialize into a known state

...with relatively-long coherence times

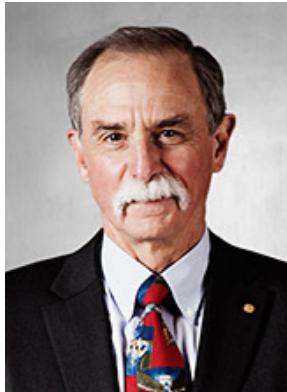


Universal set of quantum gates

...and qubit-specific measurement capability

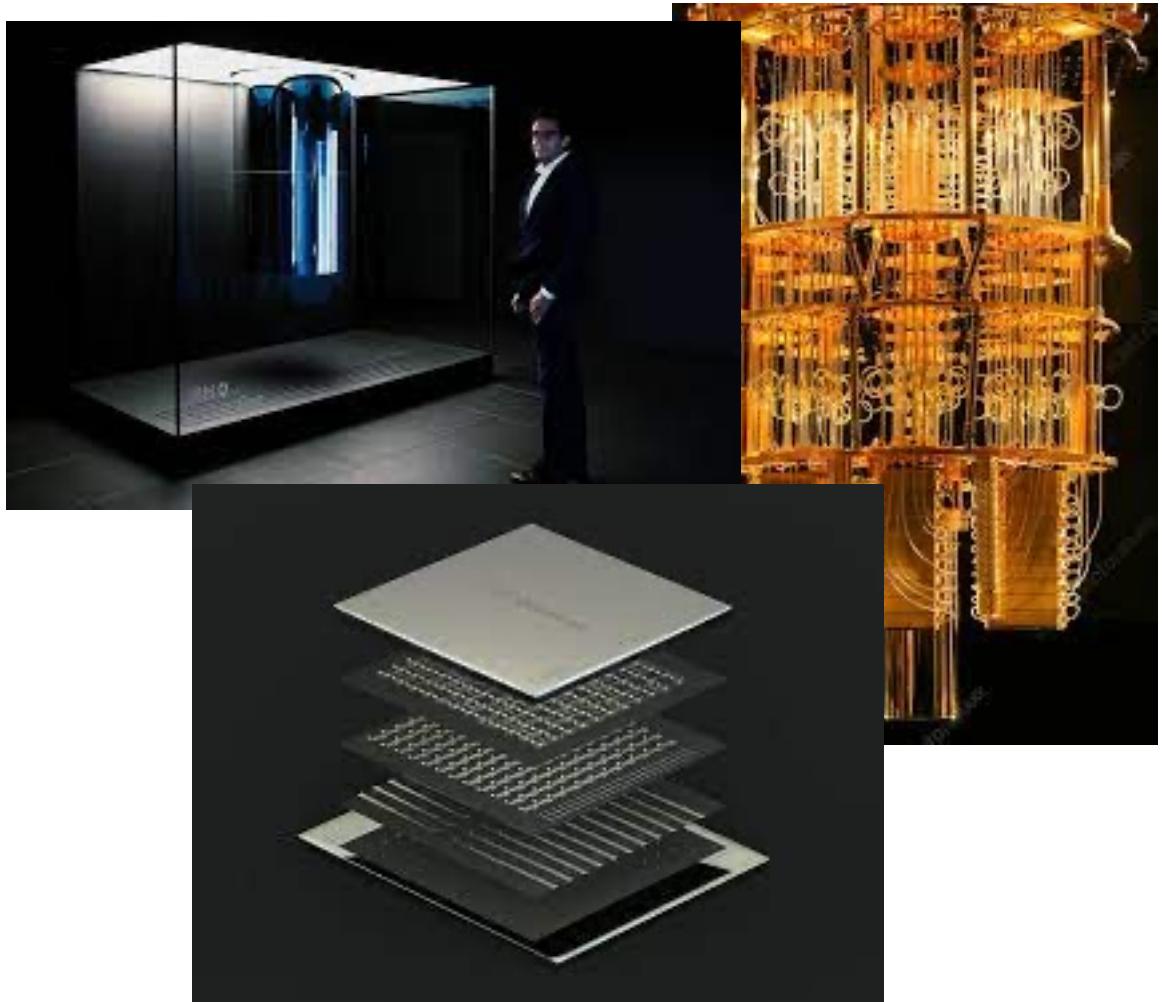
Can we build such systems?

2012



The Nobel Prize in Physics 2012 was awarded jointly to Serge Haroche and David J. Wineland *"for ground-breaking experimental methods that enable measuring and manipulation of individual quantum systems"*

2022

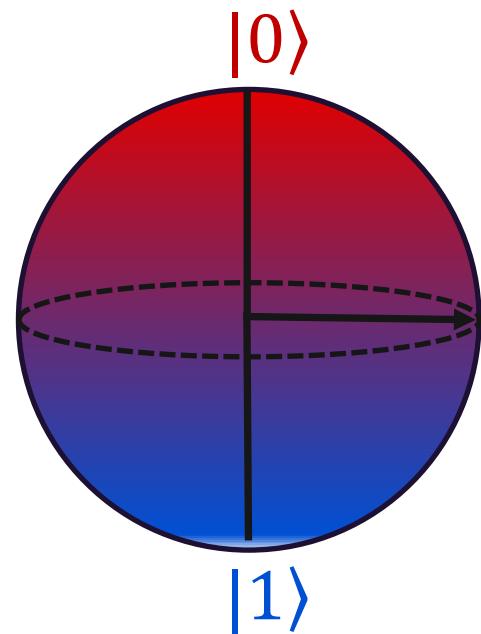


The basics

The Quantum Facts of Life

Superposition

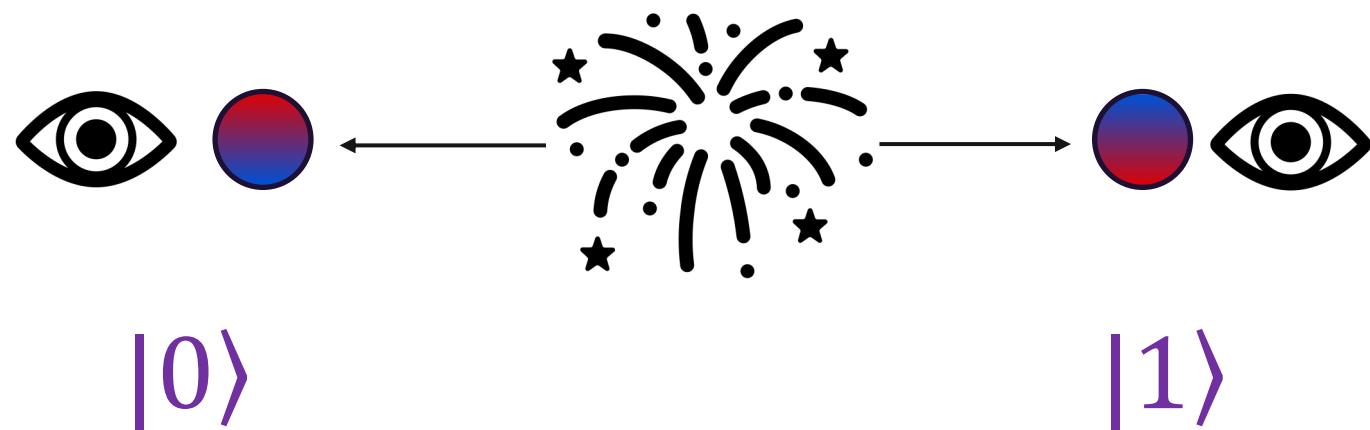
$$\psi = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$



Entanglement

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

Side note: $|01\rangle$ is just another way of writing a tensor product \otimes

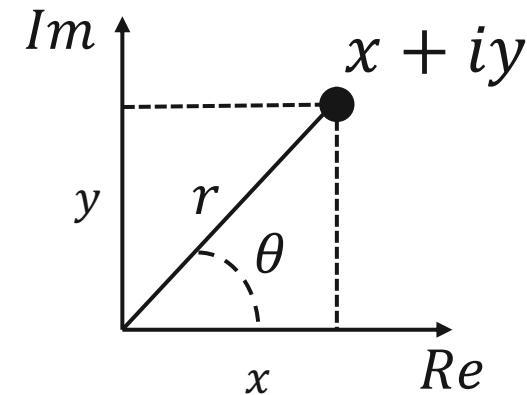


Quick Review: Complex Numbers



$$z = x + iy$$

$$i = \sqrt{-1}$$



$$e^{i\theta} = \cos\theta + i\sin\theta$$

$$z = re^{i\theta} = r(\cos\theta + i\sin\theta) = r\underbrace{\cos\theta}_x + i\underbrace{r\sin\theta}_y$$

$$x^2 + y^2 = r^2\cos^2\theta + r^2\sin^2\theta = r^2(\cos^2\theta + \sin^2\theta) = r^2$$

Complex Conjugates + Hermitian Conjugates

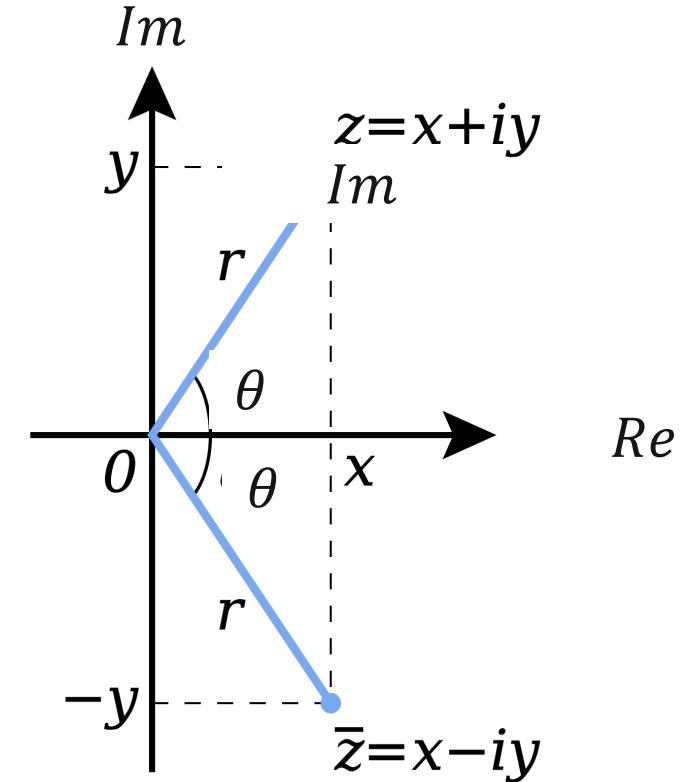
$$z^* = x - iy = re^{-i\theta}$$

Norm squared: $|z|^2 = z^*z = r^2$

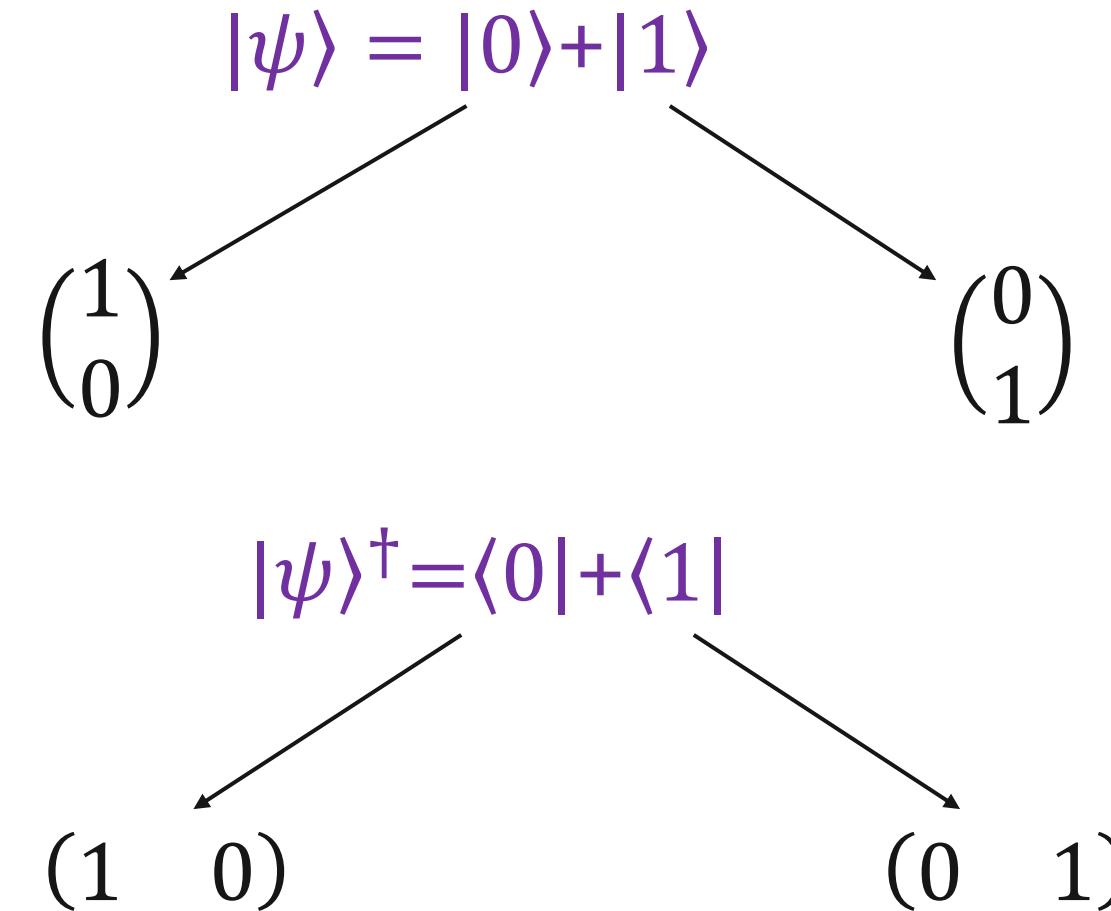
$$|\psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

$$|\psi\rangle^\dagger = \langle\psi| = (a \quad b)$$

$$H = \begin{bmatrix} a & c \\ b & d \end{bmatrix} \quad \xrightarrow{\text{blue arrow}} \quad H^\dagger = \begin{bmatrix} a^* & b^* \\ c^* & d^* \end{bmatrix}$$



What is a quantum state?



All quantum computations and quantum states live in a vector space we call the Hilbert space, where $H = \mathbb{C}^{2^n}$

$$\langle \alpha | \beta \rangle = \langle \beta | \alpha \rangle^* = a_1^* b_1 + a_2^* b_2 + \cdots + a_n^* b_n$$

Test yourself: What is the inner product of the 0 and 1 qubit state?

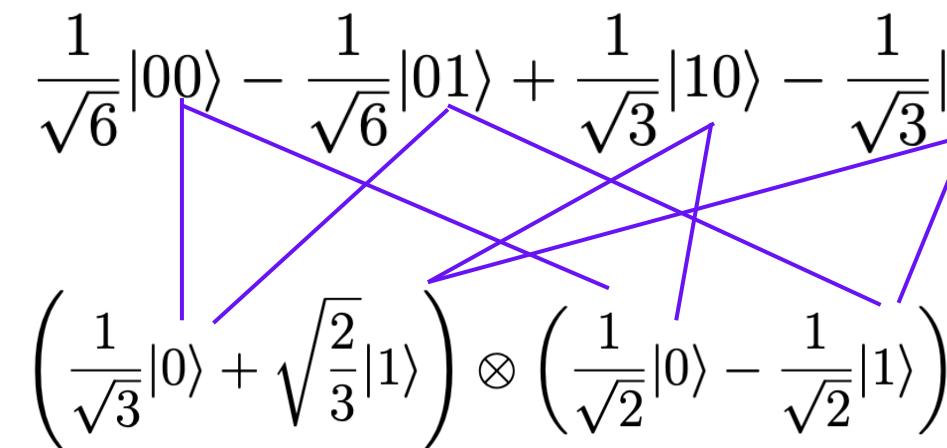
$$\begin{aligned} & \langle 0 | 1 \rangle \\ & (1 \quad 0) \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ & = (1 * 0) + (0 * 1) = 0 \end{aligned}$$

$$|a\rangle \otimes |b\rangle = |ab\rangle$$

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \otimes \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} a_1 \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \\ a_2 \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} a_1 b_1 \\ a_1 b_2 \\ a_2 b_1 \\ a_2 b_2 \end{pmatrix}$$

Test yourself: How would you rewrite the following two qubit state as a tensor product?

$$\frac{1}{\sqrt{6}}|00\rangle - \frac{1}{\sqrt{6}}|01\rangle + \frac{1}{\sqrt{3}}|10\rangle - \frac{1}{\sqrt{3}}|11\rangle$$

$$\left(\frac{1}{\sqrt{3}}|0\rangle + \sqrt{\frac{2}{3}}|1\rangle \right) \otimes \left(\frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle \right)$$


Now try to separate this state into a tensor product:

$$\frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$$

Having some trouble?

That's because it's impossible. This is an example of two entangled qubits which cannot be described by their individual parts alone.

Quantum states are normalized, and probability is calculated by the norm squared of the amplitudes

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

$$\langle\psi|\psi\rangle = \left(\frac{1}{\sqrt{2}}(\langle 0| + \langle 1|)\right) \left(\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\right) = \frac{1}{2}\langle 0|0\rangle + \frac{1}{2}\langle 1|1\rangle = 1$$

Test yourself: What is the probability of measuring $|1\rangle$ from the quantum state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{i\pi/6}|1\rangle) ?$$

$$\left| \frac{e^{i\pi/6}}{\sqrt{2}} \right|^2 = \frac{e^{i\pi/6}}{\sqrt{2}} \frac{e^{-i\pi/6}}{\sqrt{2}} = \frac{e^0}{2} = \frac{1}{2}$$

$$\hat{A} = \hat{A}^\dagger$$

$$A|\psi\rangle = \boxed{a} |\psi\rangle$$

Eigenvalue Eigenvector

*If $|\psi\rangle$ is an eigenvector of A

- Quantum observables are Hermitian operators
- They all have real eigenvalues
- Eigenvectors with different eigenvalues are orthogonal
- Eigenvectors of an operator form a complete orthonormal basis

Quantum gates are linear maps:

$$U(\alpha|0\rangle + \beta|1\rangle) = \alpha U|0\rangle + \beta U|1\rangle$$

*Total probability must remain equal to 1.

Gates are represented by matrices:

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = |0\rangle\langle 1| + |1\rangle\langle 0|$$

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

Diagram illustrating the matrix multiplication $X|0\rangle$. The vector $|0\rangle$ is $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$. The matrix X is $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. The result is $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$, which is $|1\rangle$. The calculation is shown as $0 * 1 + 1 * 0 = 0$ (blue) and $1 * 1 + 0 * 0 = 1$ (pink).

Test yourself: What is the effect of the Hadamard gate on the $|0\rangle$ and $|1\rangle$ states ?

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

$$H|0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\frac{1}{\sqrt{2}}(1 * 1 + 1 * 0) = \frac{1}{\sqrt{2}} \quad \frac{1}{\sqrt{2}}(1 * 1 - 1 * 0) = \frac{1}{\sqrt{2}}$$

$$= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} |0\rangle + \frac{1}{\sqrt{2}} |1\rangle$$

Gates must be unitary



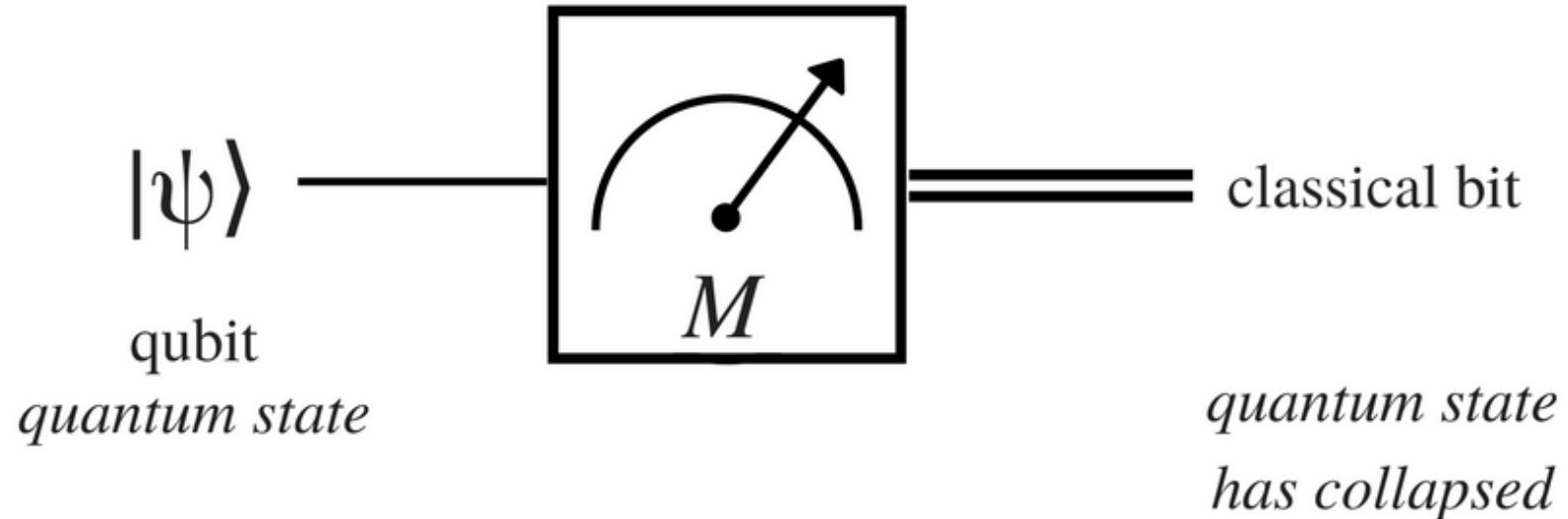
$$U^\dagger U = UU^\dagger = I$$

$$I|a\rangle = 1|a\rangle \quad \text{*eigenvalue can only be 1}$$

$$I_1 = [1], \quad I_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad I_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \dots, \quad I_n = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

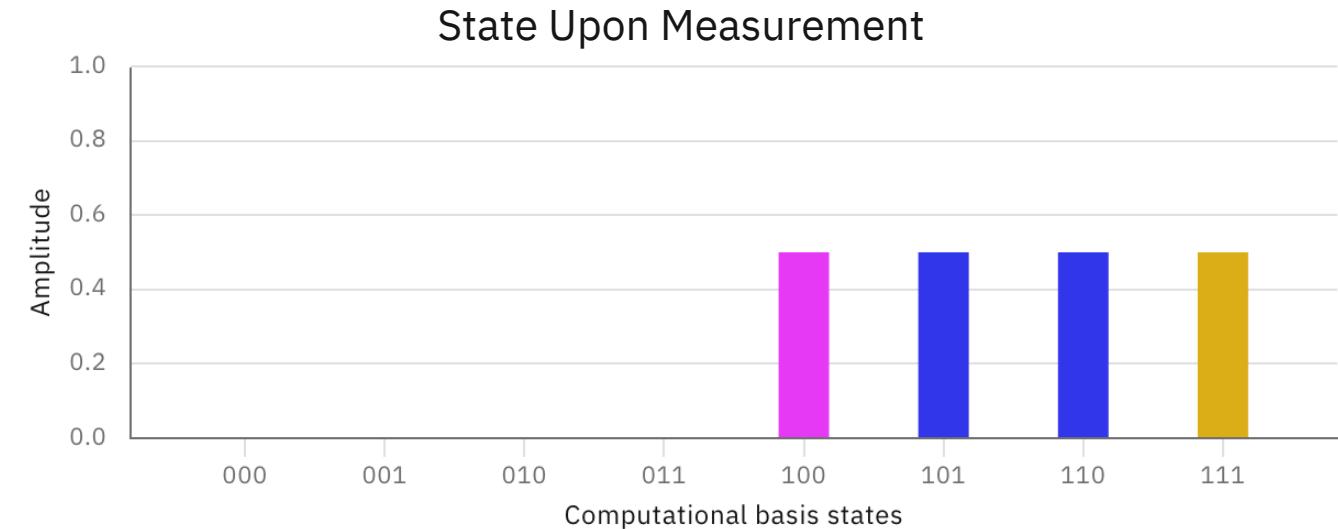
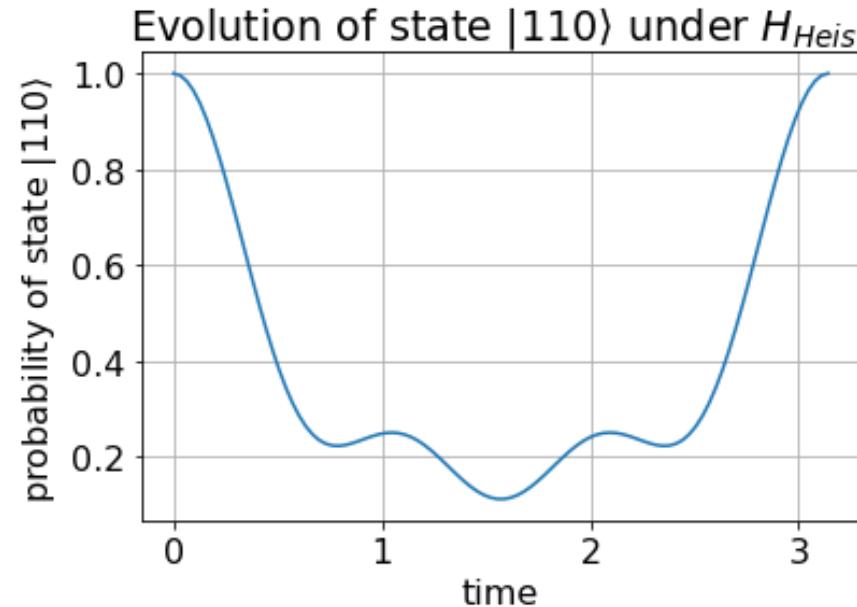
$$X^*X = XX^* = I^2 = I$$

Quantum measurement is weird



$$[\sigma_z, \sigma_x] \neq 0$$

Time Evolution



What happens if we wait to measure, and let $|\psi\rangle$ evolve naturally?

Finding $|\psi(t)\rangle$ is the name of the game.

Sometimes it's very challenging. That's where quantum simulation comes in.

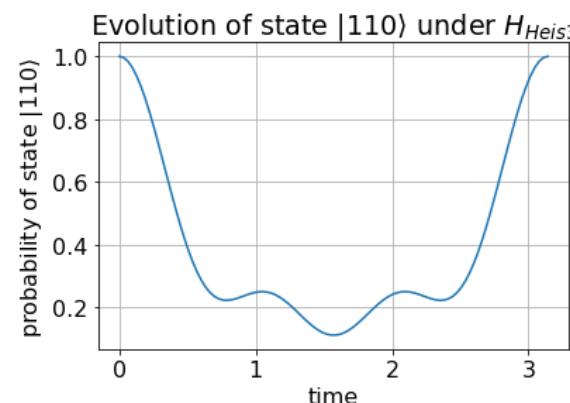
3 Stages of Quantum Simulation



Quantum state preparation

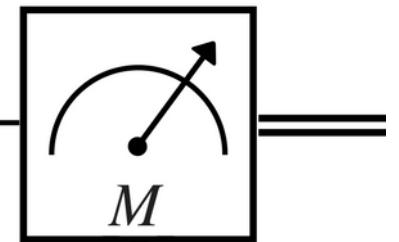
$$|\psi\rangle = |110\rangle$$

Time Evolution



Measurement

$$|\psi(t)\rangle$$



Real world hardware

Development Roadmap |

Executed by IBM ✓
On target ✅

IBM Quantum

	2019	2020 ✓	2021 ✓	2022	2023	2024	2025	2026+
	Run quantum circuits on the IBM cloud	Demonstrate and prototype quantum algorithms and applications	Run quantum programs 100x faster with Qiskit Runtime	Bring dynamic circuits to Qiskit Runtime to unlock more computations	Enhancing applications with elastic computing and parallelization of Qiskit Runtime	Improve accuracy of Qiskit Runtime with scalable error mitigation	Scale quantum applications with circuit knitting toolbox controlling Qiskit Runtime	Increase accuracy and speed of quantum workflows with integration of error correction into Qiskit Runtime
Model Developers					Prototype quantum software applications →	Quantum software applications		
Algorithm Developers		Quantum algorithm and application modules ✓	Machine learning Natural science Optimization		Quantum Serverless	Intelligent orchestration	Circuit Knitting Toolbox	Circuit libraries
Kernel Developers	Circuits ✓	Qiskit Runtime ✓		Dynamic circuits ⚡ Threaded primitives	Error suppression and mitigation		Error correction	
System Modularity	Falcon 27 qubits ✓	Hummingbird 65 qubits ✓	Eagle 127 qubits ✓	Osprey 433 qubits ⚡	Condor 1,121 qubits	Flamingo 1,386+ qubits	Kookaburra 4,158+ qubits	Scaling to 10K-100K qubits with classical and quantum communication
				Heron 133 qubits x p	Crossbill 408 qubits			

Quantum computing from anywhere

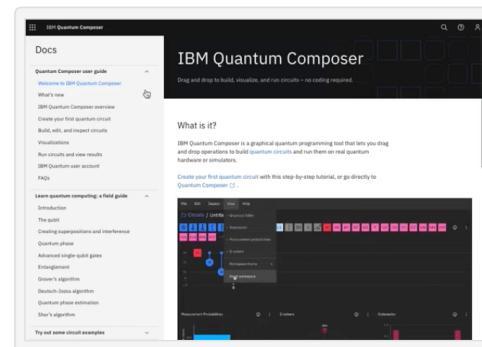


IBM Quantum



Real quantum computers. Right at your fingertips.

IBM offers cloud access to the most advanced quantum computers available.
Learn, develop, and run programs with our quantum applications and systems.



Learn quantum computing

Learn quantum programming and how to use our tools
step-by-step tutorials and guides.

[Explore the docs](#)

ibmq_guadalupe

16 Qubits	Status: Online	Avg. CNOT Error: 1.333e-2
32 QV	Total pending jobs: 14 jobs	Avg. Readout Error: 2.867e-2
2.4K CLOPS	Processor type ⓘ: Falcon r4P	Avg. T1: 83.83 us
	Version: 1.3.24	Avg. T2: 96.75 us
	Basis gates: CX, ID, RZ, SX, X	Providers with access: 1 Providers ↓
	Your usage: 0 jobs	Supports Qiskit Runtime: Yes

Your upcoming reservations 0

Calibration data

Last calibrated: about 15 hours ago

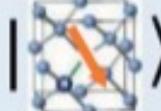
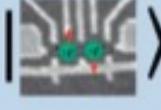
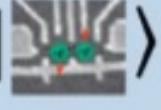
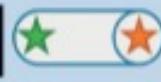
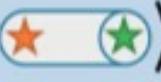
Map view Graph view Table view

Qubit: Frequency (GHz) Avg 5.246 min 5.038 max 5.47

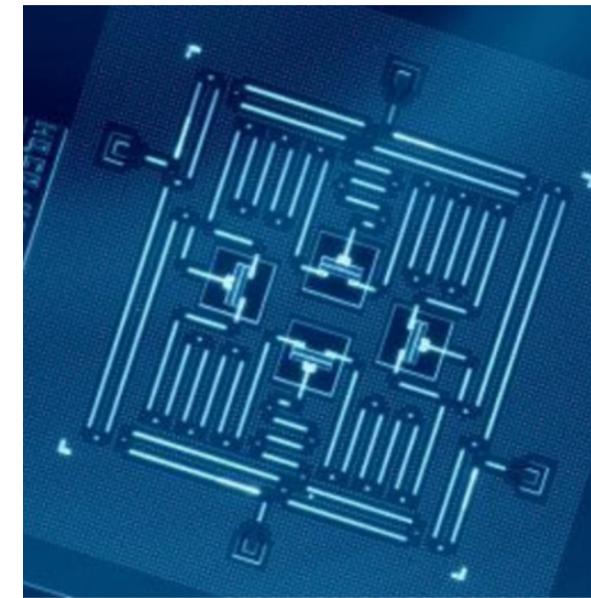
Connection: CNOT error Avg 1.333e-2 min 6.804e-3 max 2.293e-2

Types of qubits

While there are many physical realization of qubits....

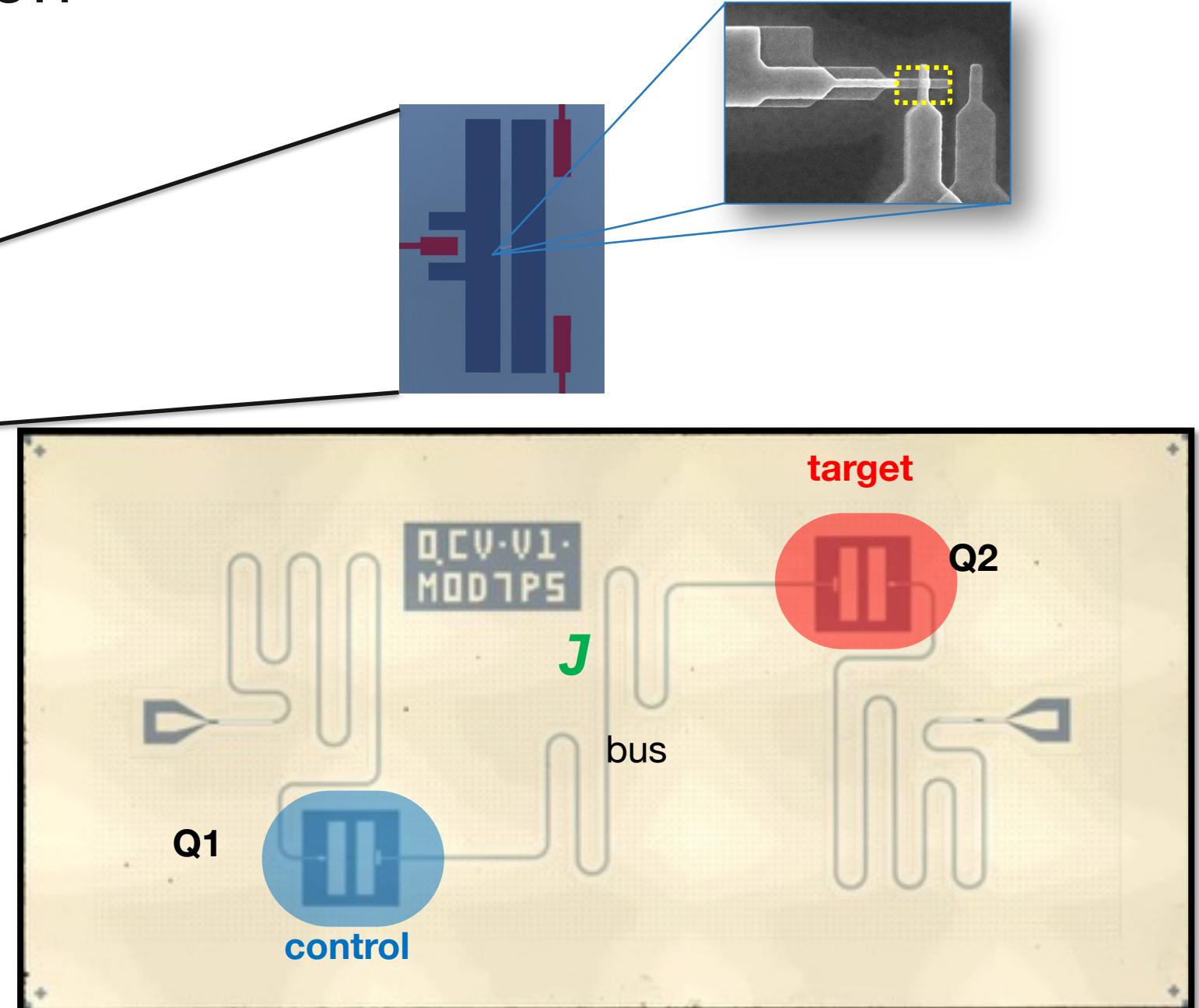
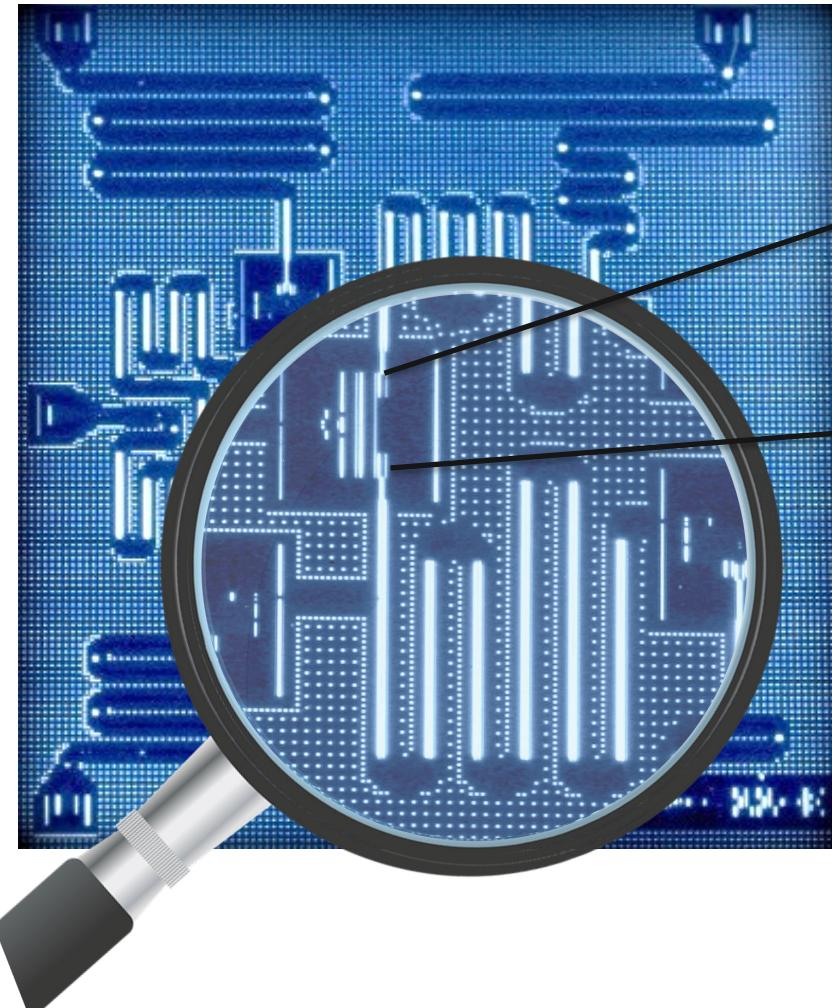
Material System	$ 0\rangle$	$ 1\rangle$
Ion traps		
Defects in solids		
Semiconductor quantum dot		
Superconducting		
Topological nanowire		

...we have a favorite.

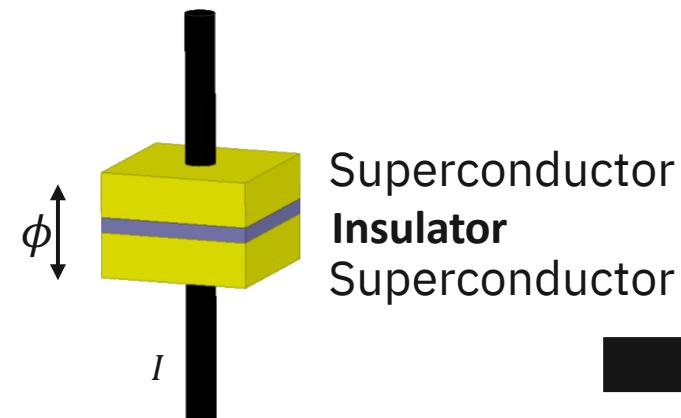
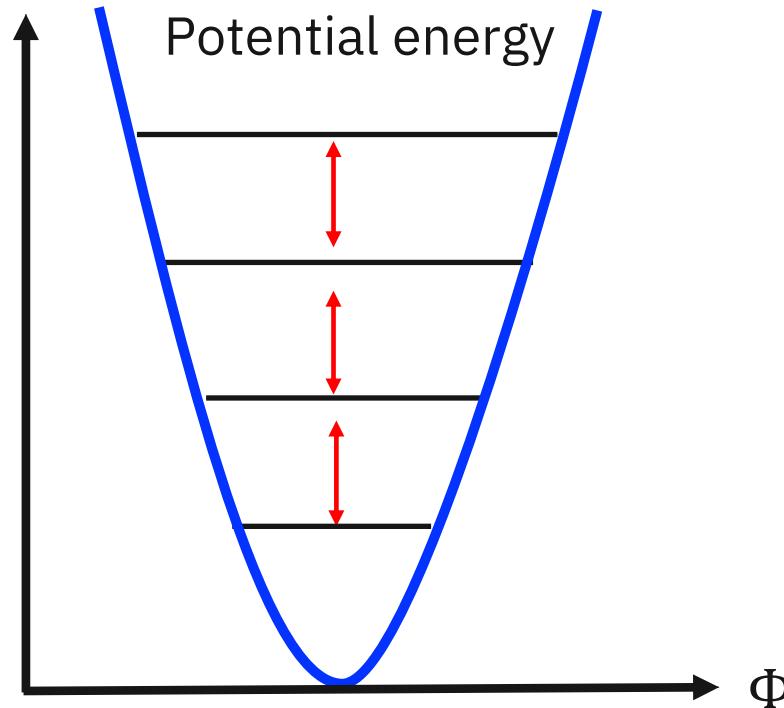
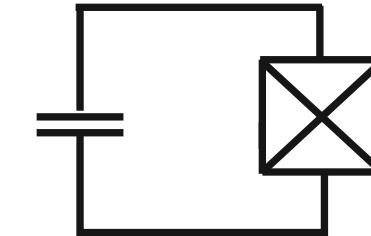
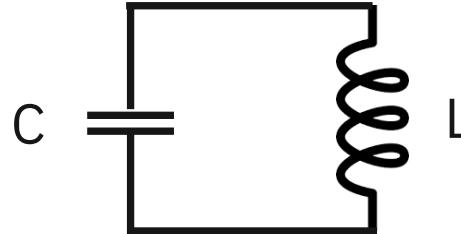


Meet the transmon ☺

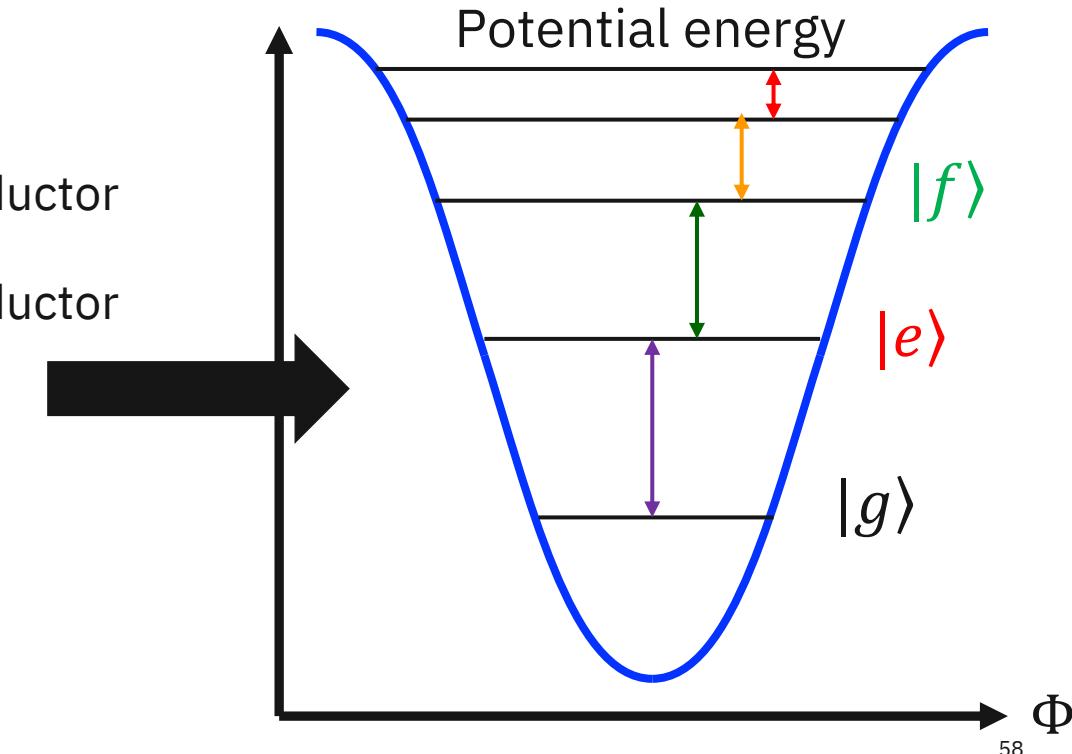
The Josephson Junction



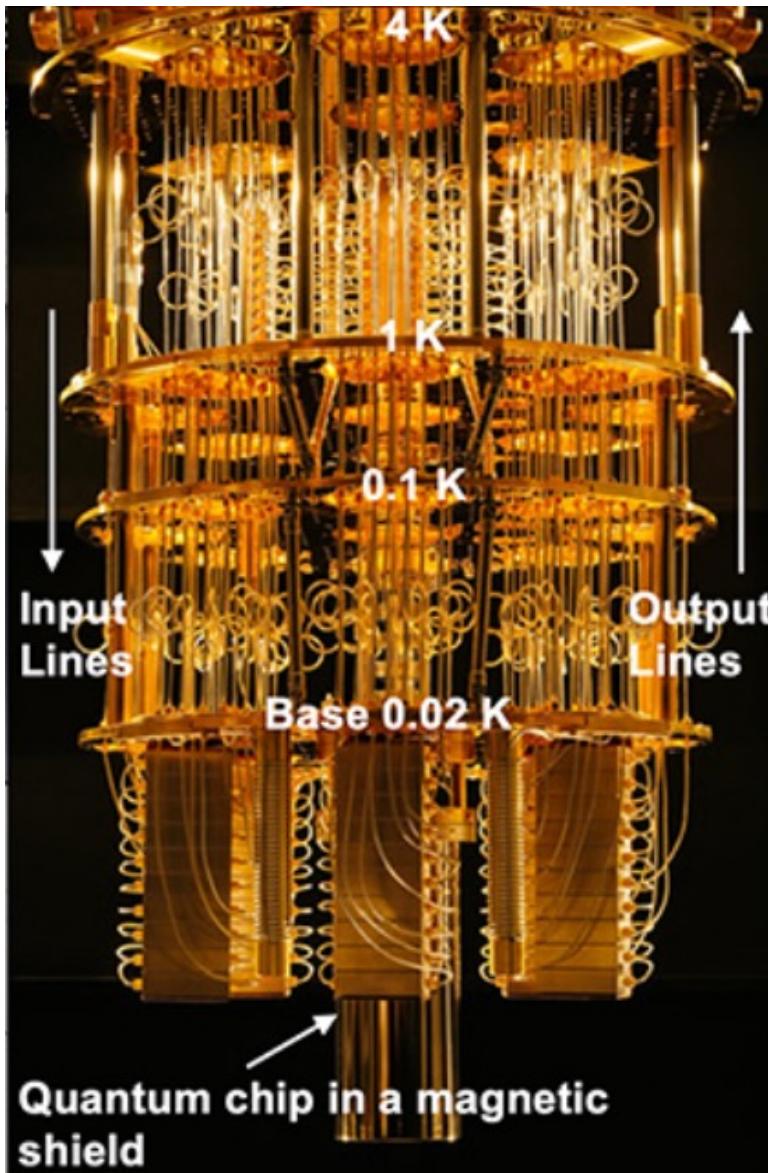
The Josephson Junction



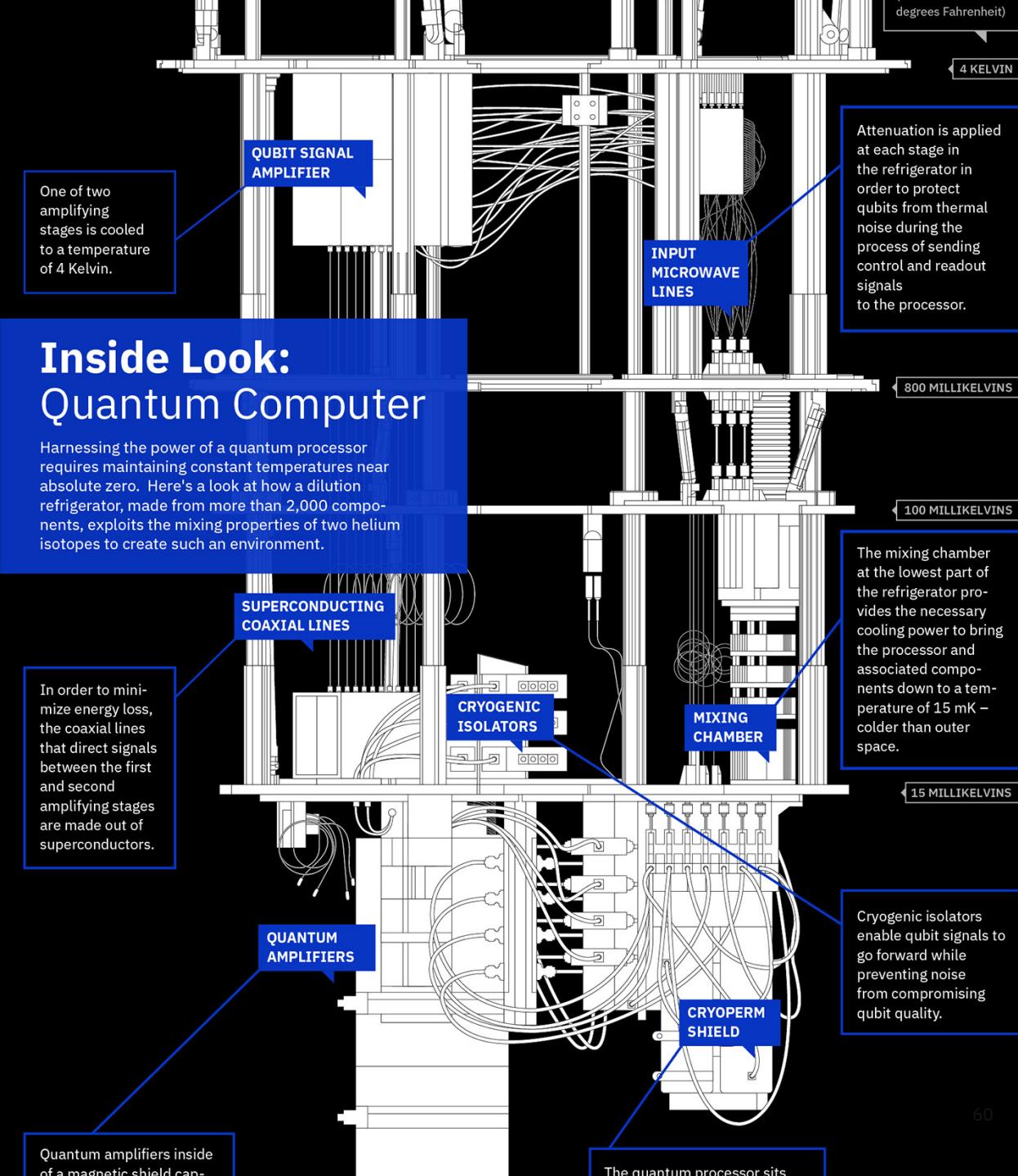
$$I = I_0 \sin(\phi)$$
$$E = E_J \cos(\phi)$$



Dilution Refrigeration



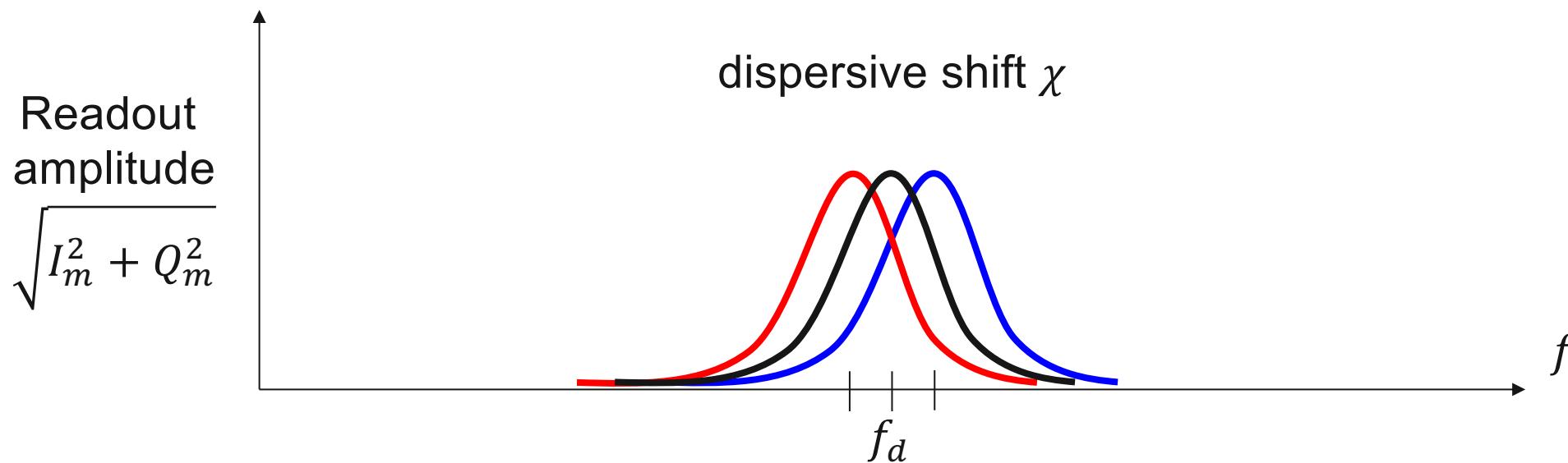
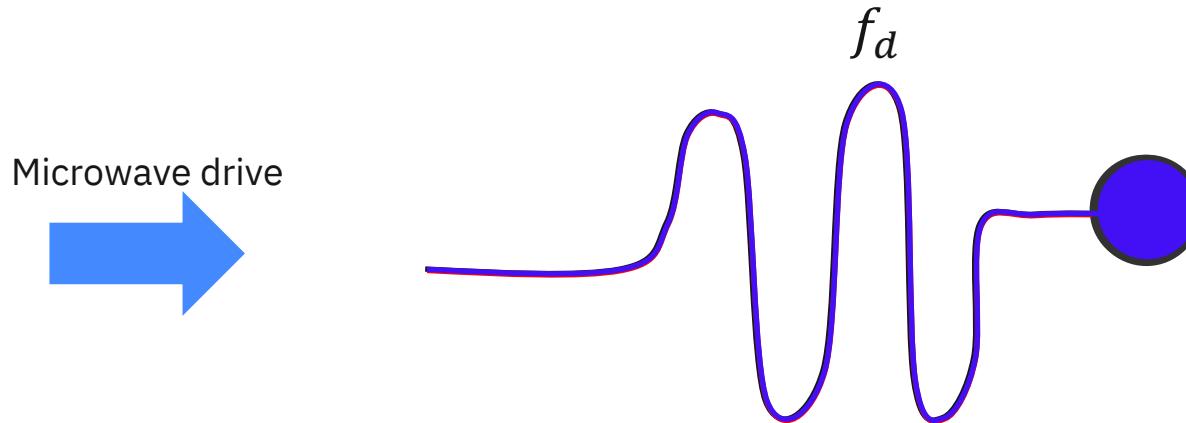
A look inside the dil fridge



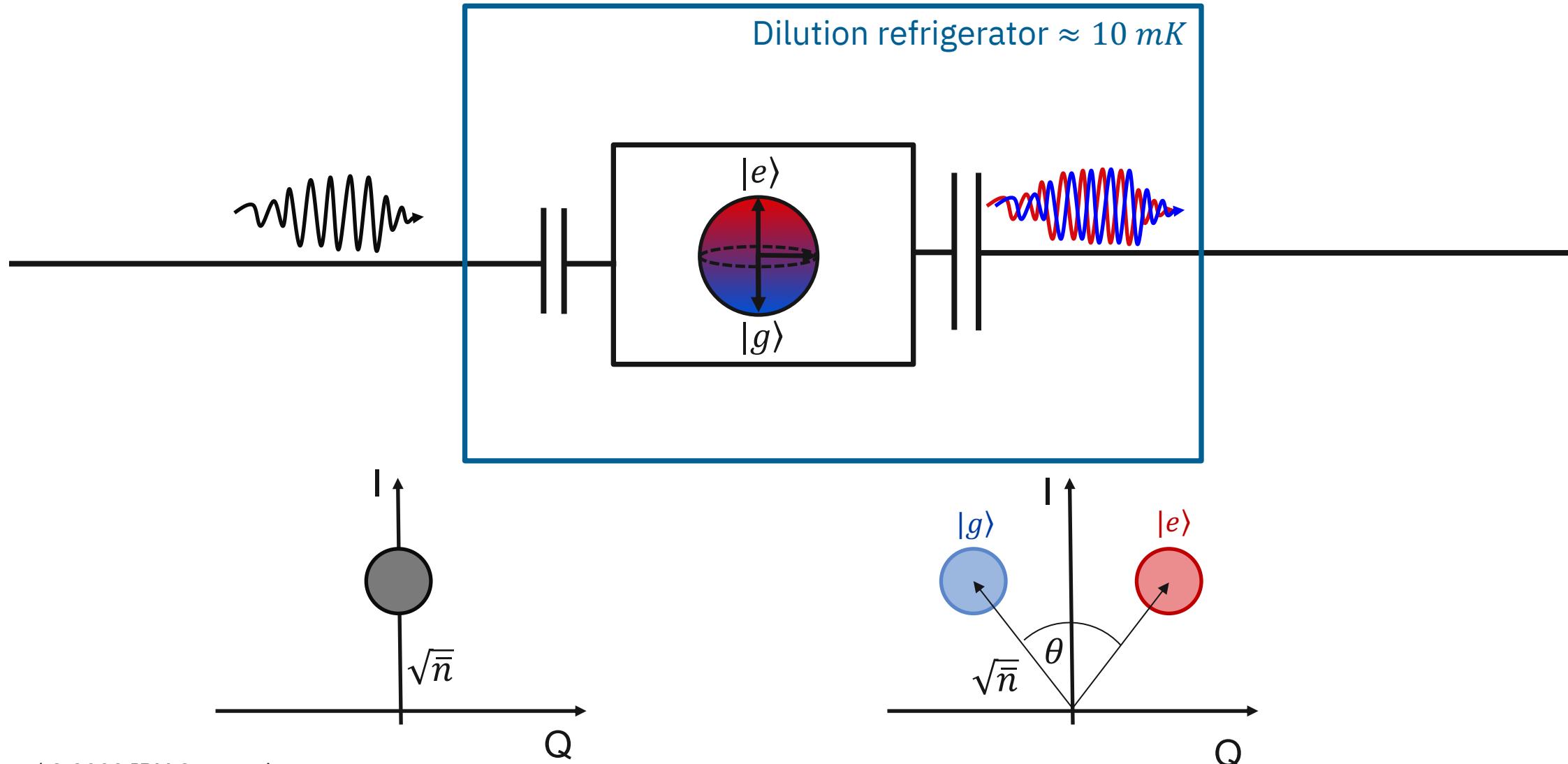
Inside Look: Quantum Computer

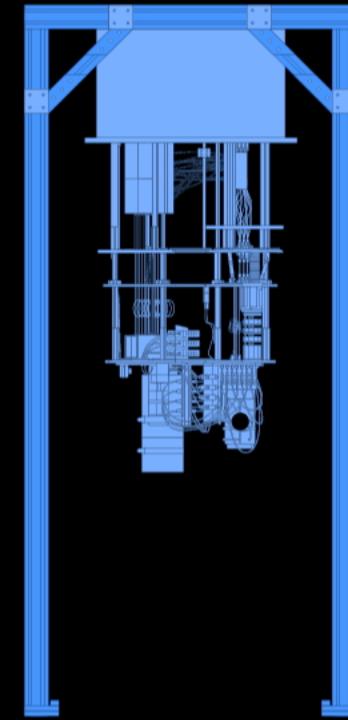
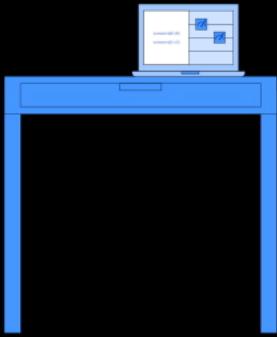
Harnessing the power of a quantum processor requires maintaining constant temperatures near absolute zero. Here's a look at how a dilution refrigerator, made from more than 2,000 components, exploits the mixing properties of two helium isotopes to create such an environment.

How do we measure a qubit?



Qubit measurement





Summary

Understanding the rules of quantum mechanics is not particularly difficult, **
 they are simply, unexpected,
 the ***applications*** however, are.

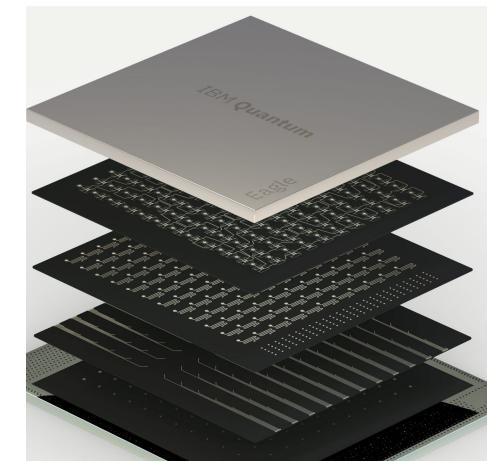
Rules of chess



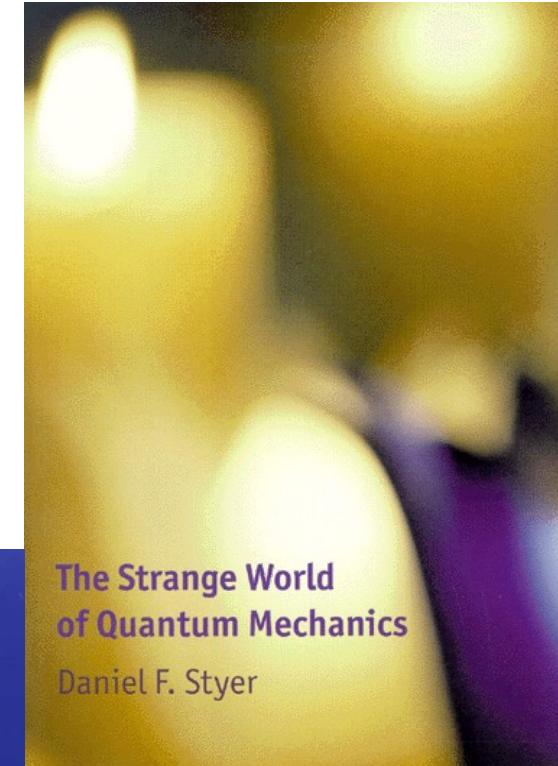
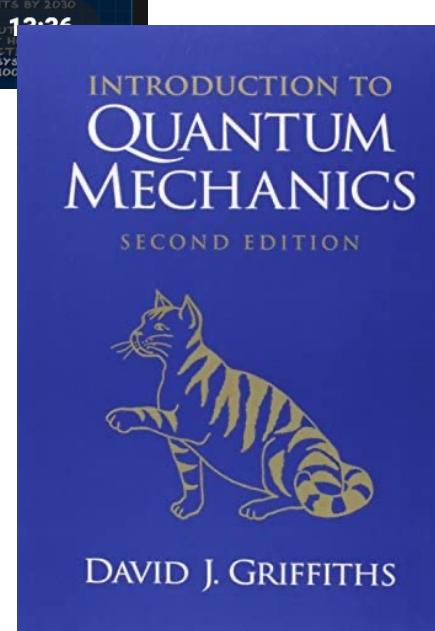
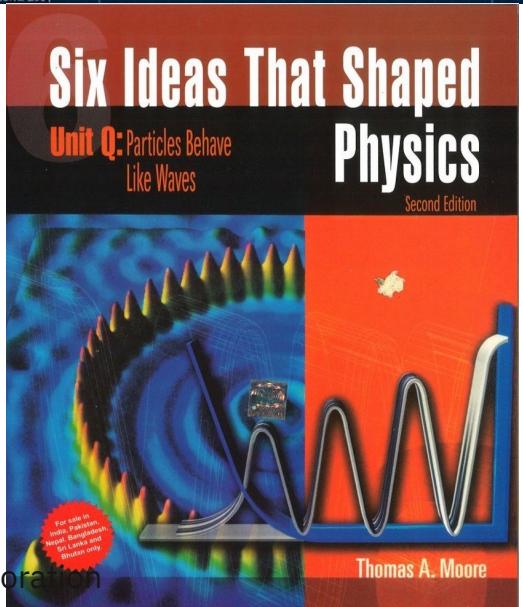
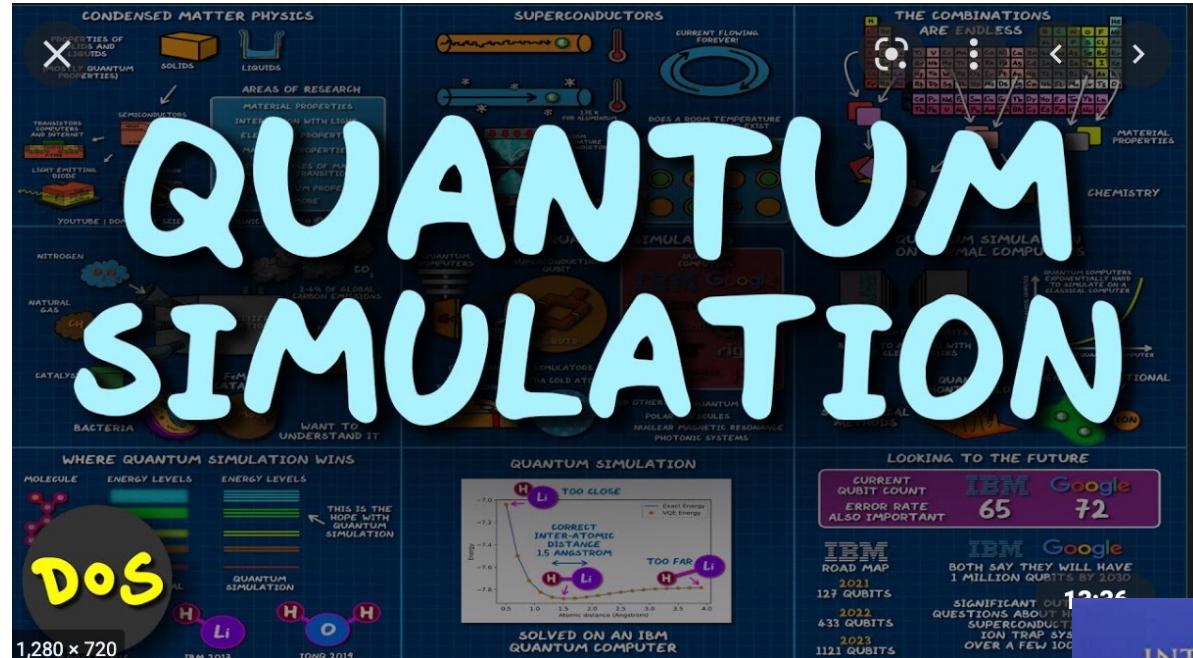
30^{80} possible moves

Rules of quantum

The Postulates of Quantum Mechanics	
1.	Associated with any particle moving in a conservative field of force is a wave function which determines everything that can be known about the system.
2.	With every physical observable q there is associated an operator Q , which when operating upon the wavefunction associated with a definite value of that observable will yield that value times the wavefunction.
3.	Any operator Q associated with a physically measurable property q will be Hermitian.
4.	The set of eigenfunctions of operator Q will form a complete set of linearly independent functions.
5.	For a system described by a given wavefunction, the expectation value of any property q can be found by performing the expectation value integral with respect to that wavefunction.
6.	The time evolution of the wavefunction is given by the time dependent Schrödinger equation.



Additional resources:



Questions?

“Feynman was on the right track when he suggested using quantum computers to solve problems in quantum physics and chemistry. That is still the most important application we can clearly foresee, and there is plenty of opportunity to flesh out our ideas about how quantum computers can best be used to advance science.” – John Preskill