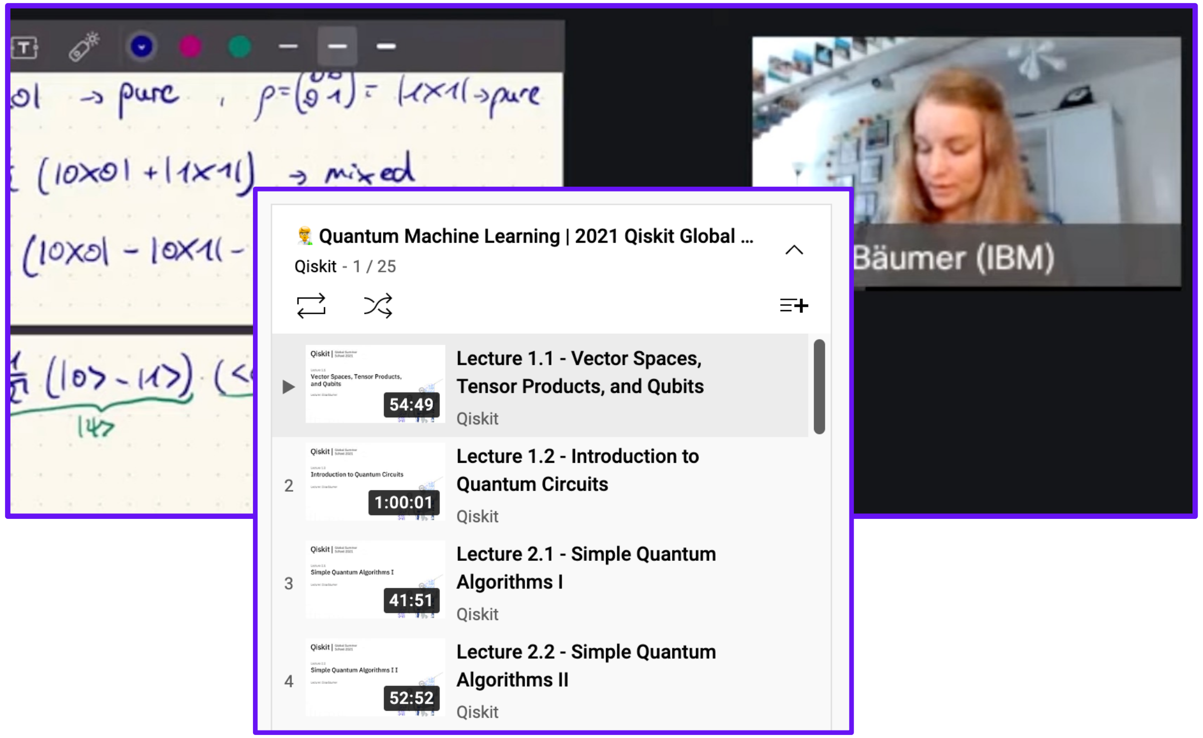
Welcome

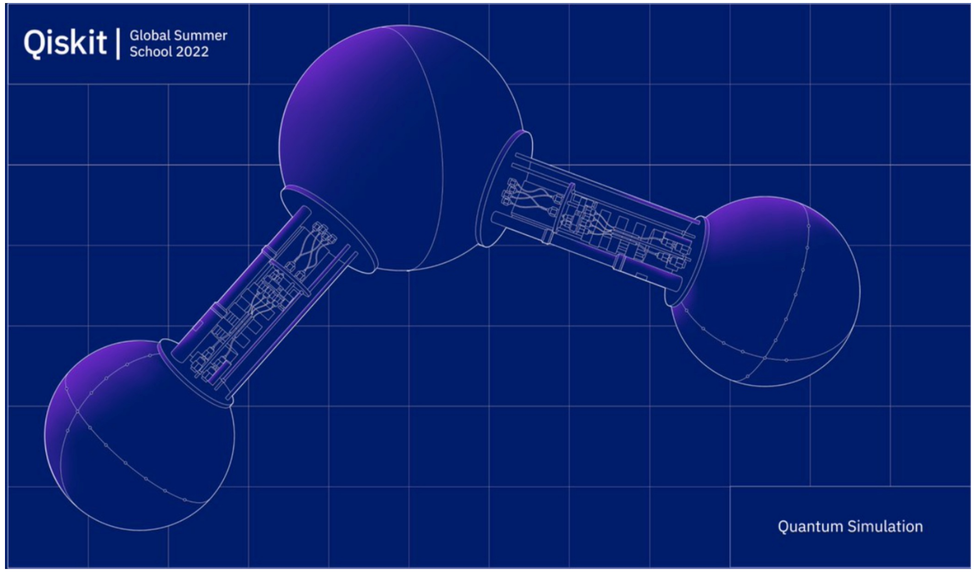
Qiskit Summer School 2022

3rd Annual Qiskit Global Summer School

Qiskit

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





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

Monday

Introduction! What is quantum sim and why should I care.

Dirac notation and quantum facts of life

Tuesday

Mathematics prerequisites

Introduction to quantum circuits

Wednesday

Hamiltonians and time evolution

Thursday

Nature, models, and simulation

Classical methods and limitations, intro to quantum methods

Friday

Introduction to quantum noise and how to deal with it

Week 2

Qiskit

Monday

Introduction to quantum chemistry

Properties, what to measure, how we know if it's correct

Tuesday

Quantum simulation methodology

Second quantization and correlation methods

Wednesday

Static Simulation

Hamiltonian mapping, ansatz selection, VQE

Thursday

Quantum dynamics simulation

Decomposition methods, variational time evolution

Friday

Graduation and expert Q&A panel

Meet the professors



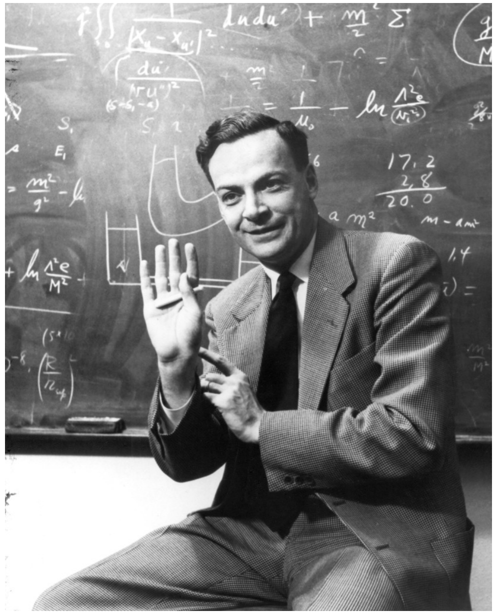




Why quantum simulation?

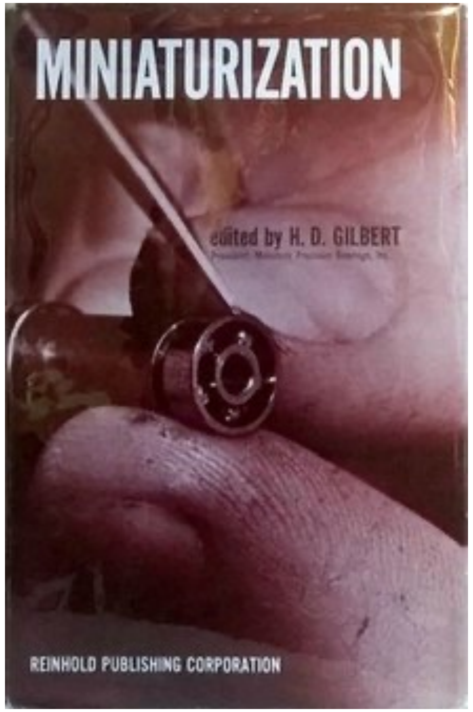
Origins

Qiskit



Richard Feynman, Nobel Laureate and professor of physics

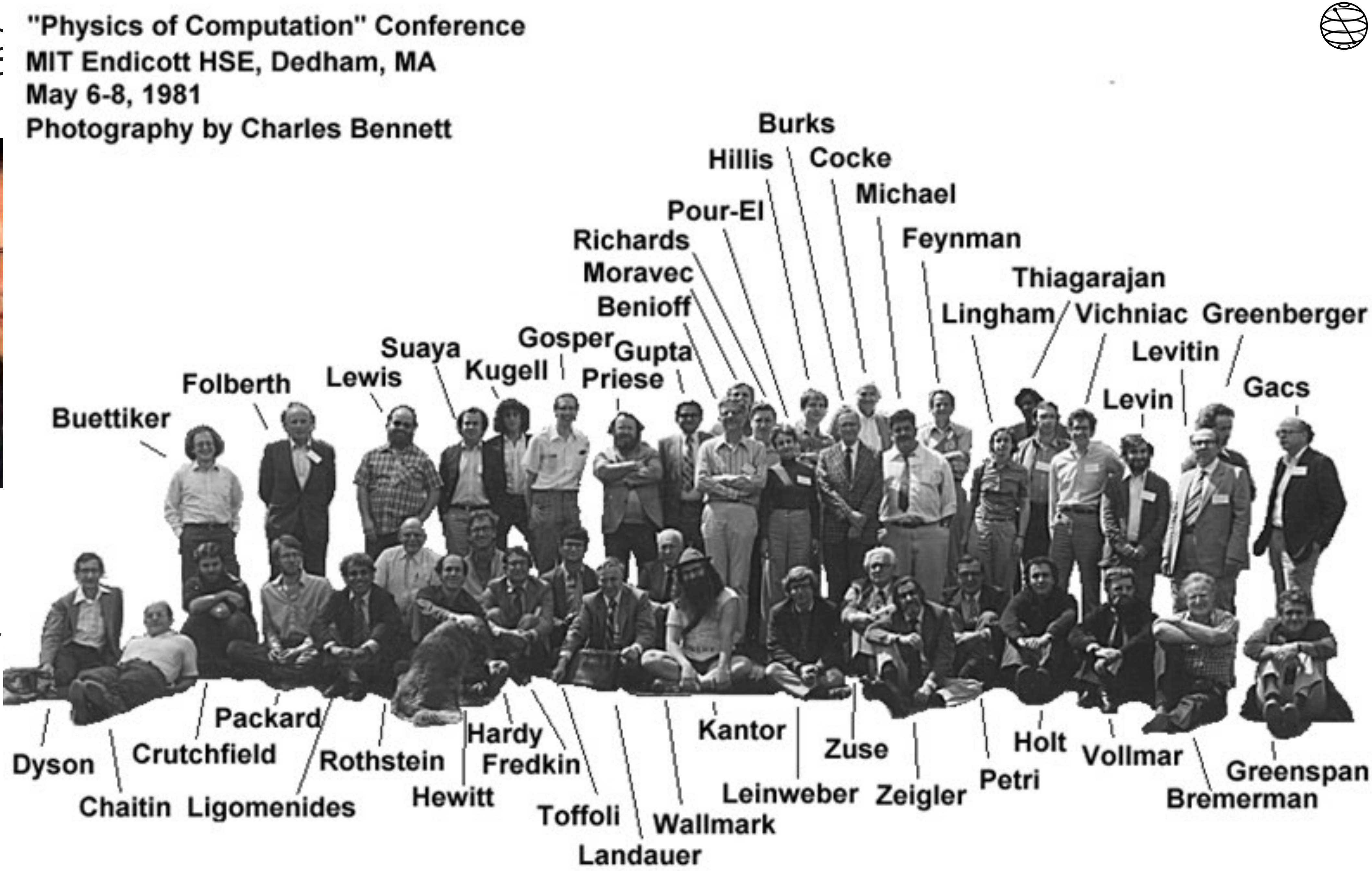
Worked on Manhattan project, authored books, frequent bongo-player



"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

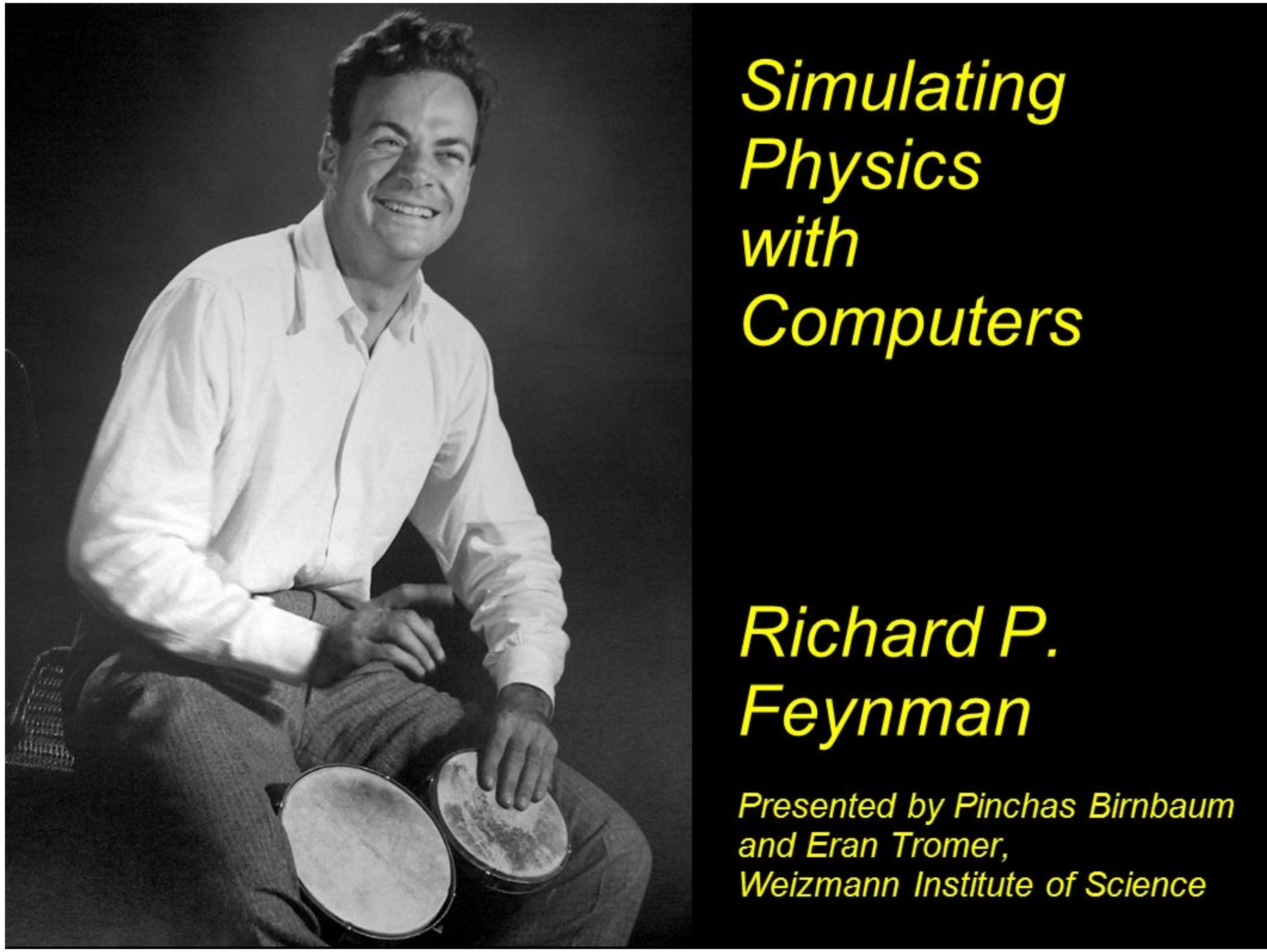


First phy
1981.

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"



What even is a simulation?

- "A computational model that will do exactly the same as nature"

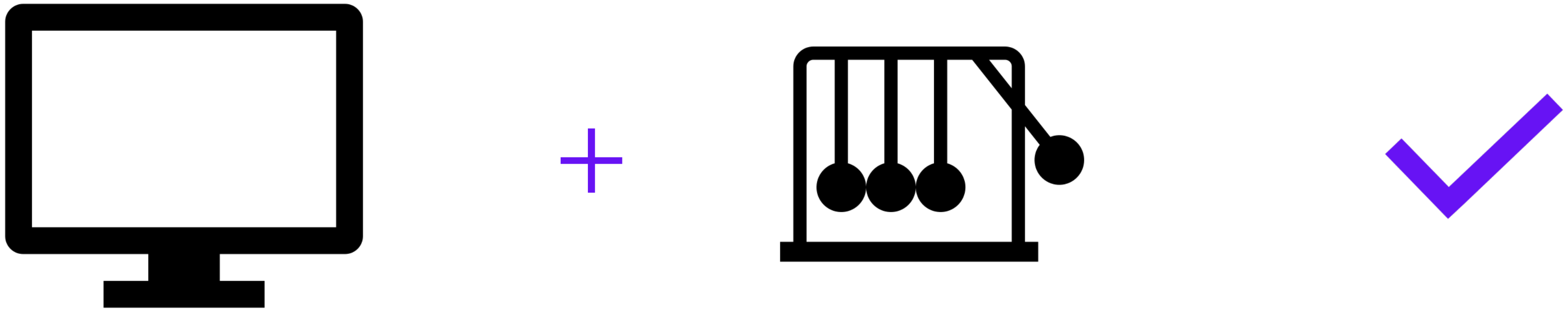
  -Inherently different than numerical methods, which offer only approximate solutions to a system

- 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?

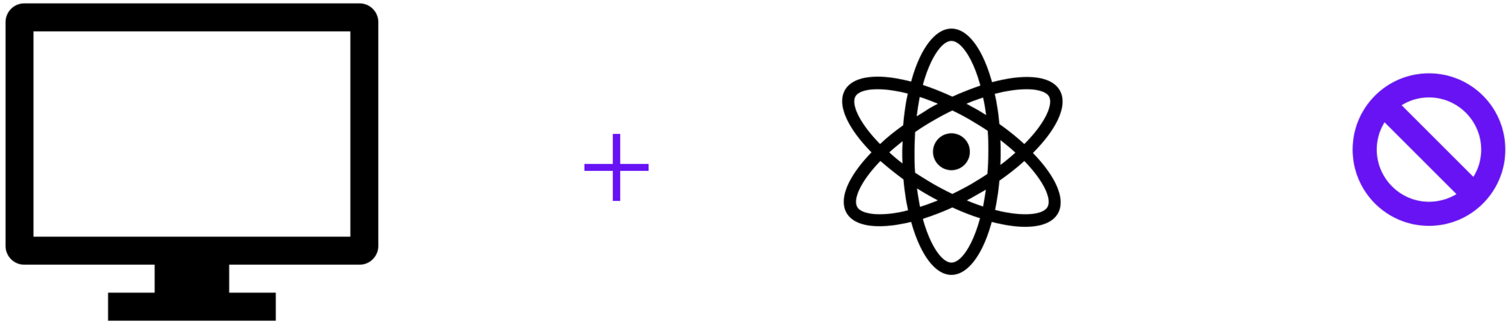
- Time and space may be continuous, but by discretizing nature into sufficiently fine elements, no physics is lost.
- The passage of time is simulated through a causal nature.



Feynman, R.P. Simulating physics with computers. *Int J Theor Phys* **21,** 467–488 (1982).

Can classical computers simulate *quantum* physics?

- Cant 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



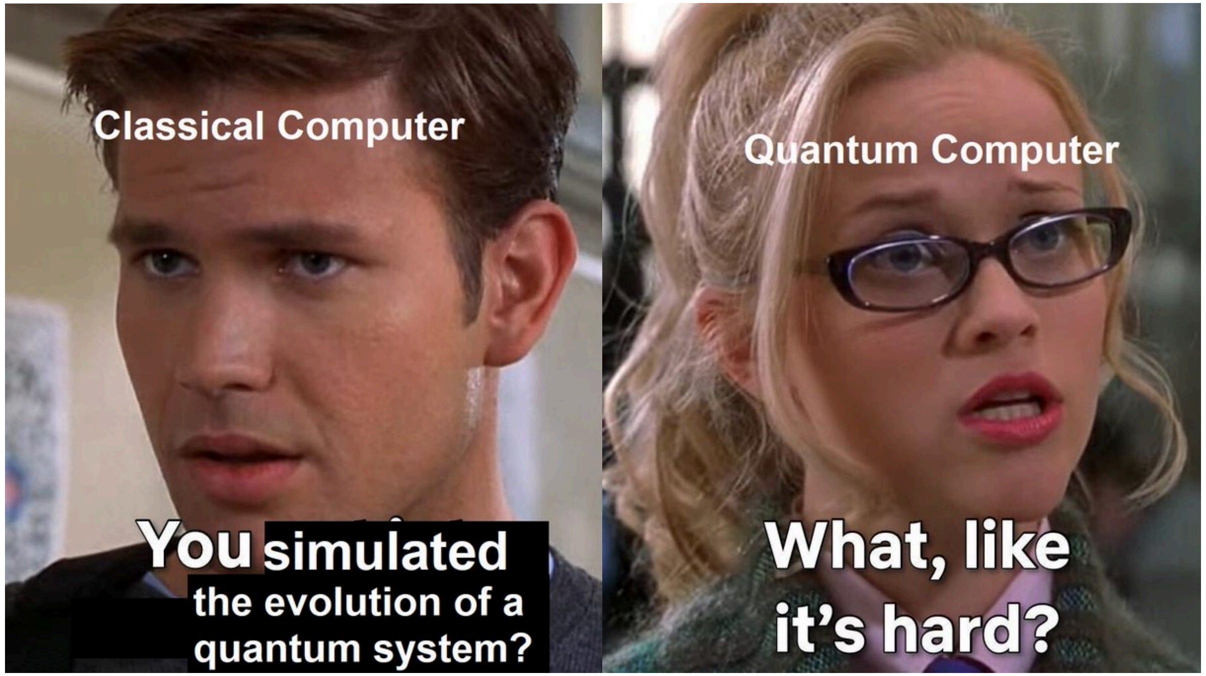
TLDR: ....No

Feynman, R.P. Simulating physics with computers. *Int J Theor Phys* **21,** 467–488 (1982).

Can *quantum* computers simulate *quantum* physics?

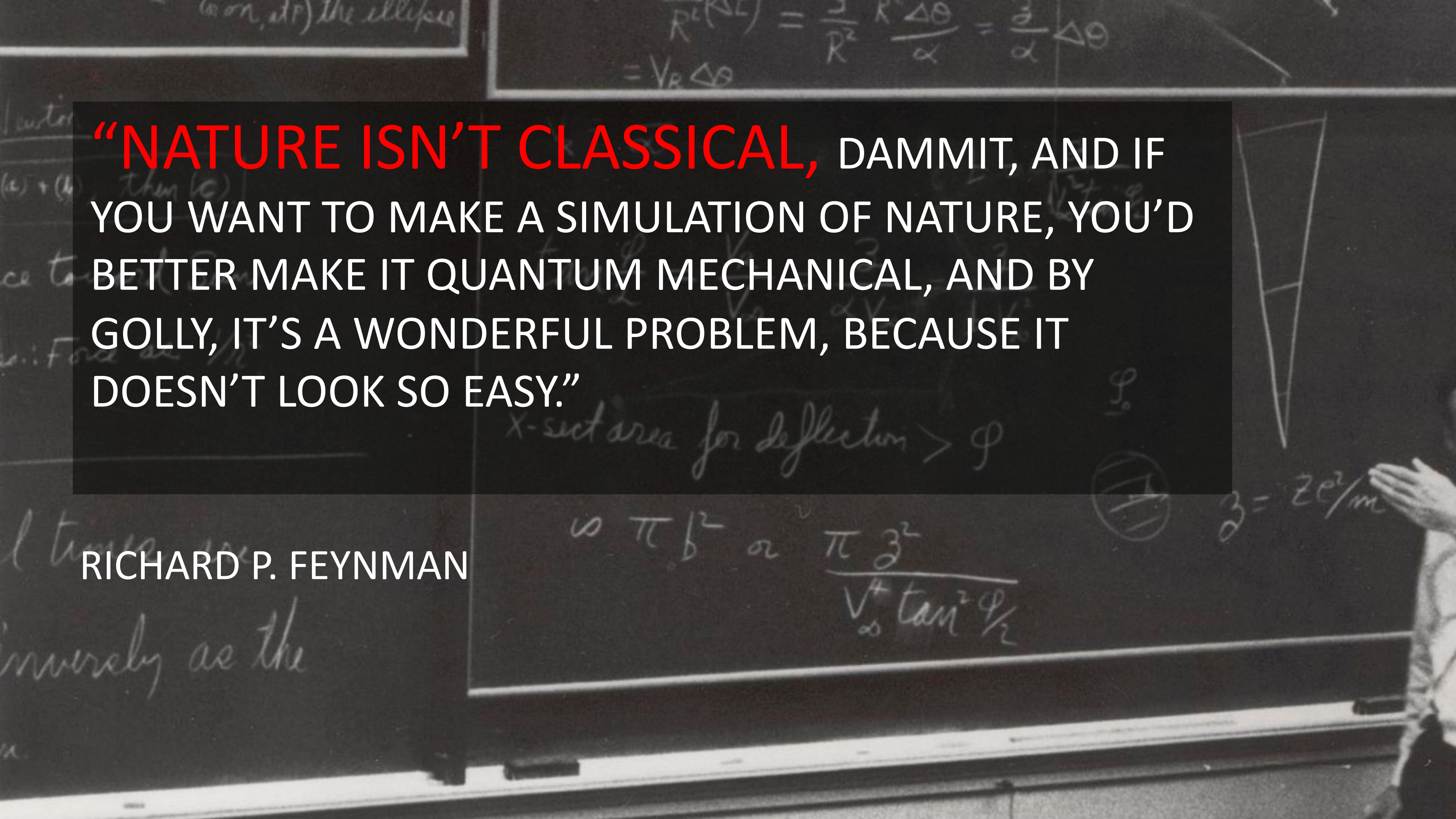
Idea: if quantum physics is too hard for classical computers, build a physical quantum computer that exploits that power.

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)

Feynman, R.P. Simulating physics with computers. *Int J Theor Phys* **21,** 467–488 (1982).



“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

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- 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

Johnson, et al. (2014), Jones et al. (2012)

Entropy 2010, *12*, 2268-2307

State-of-the-art work

Qiskit

ARTICLE OPEN

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

Adam Smith[1,2*], M. S. Kim[1], Frank Pollmann[2] and Johannes Knolle[1]

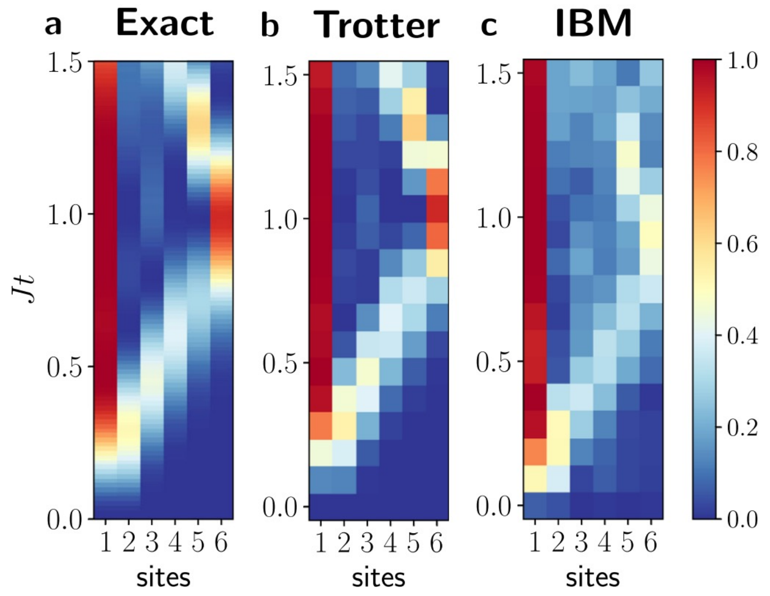
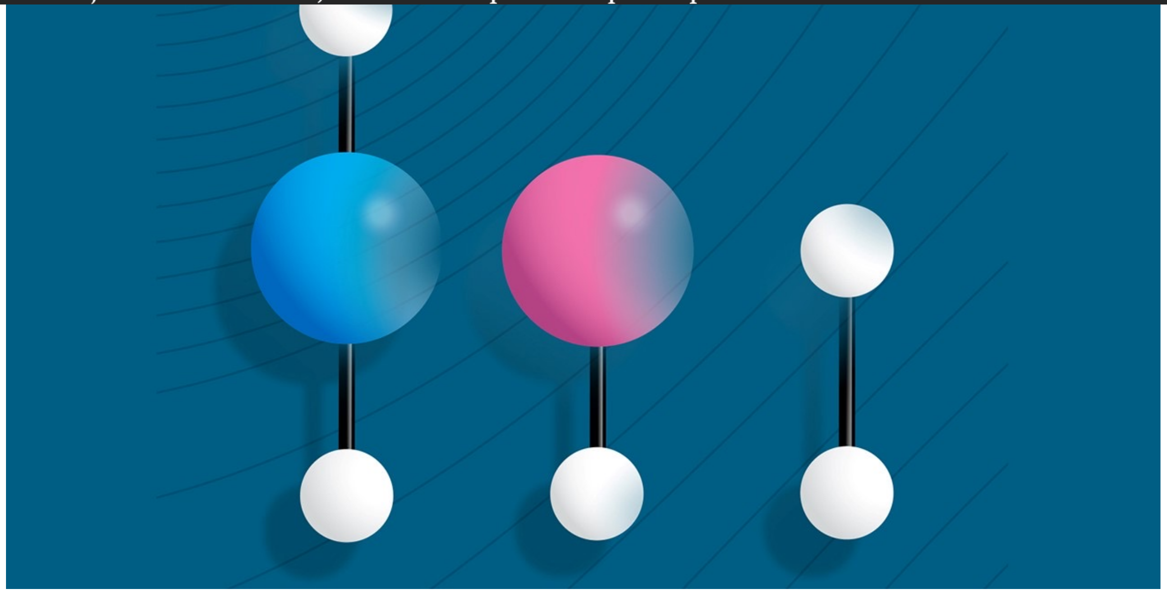


Fig. 4 Results for the connected spin correlator defined in Eq. (6). Data are computed using: **a** exact diagonalization, **b** numerical trotterization, **c** the IBM quantum device. Data are shown for $N = 6, h_j = 0$ and $U = 0$, using a symmetric trotterization, and obtained on 12 March 2019.

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

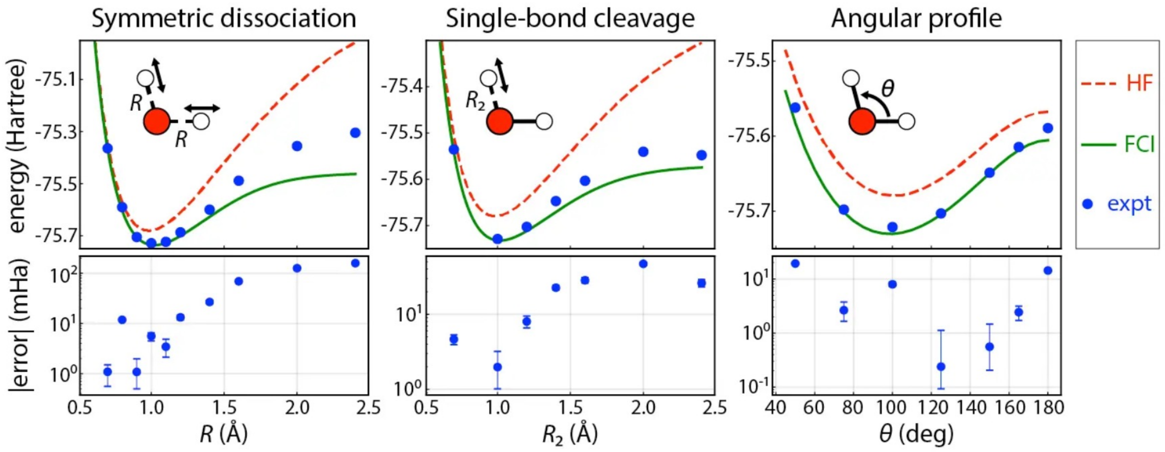


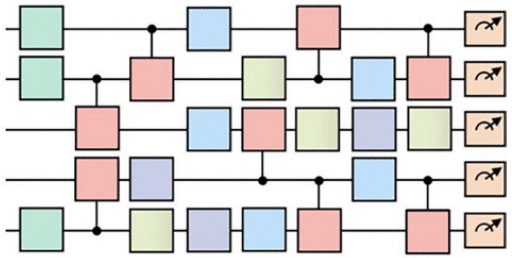
Quantum Chemistry

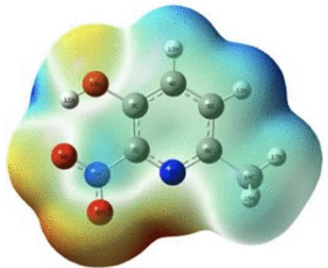
- Studying dynamics and properties of molecular reactions is important to the future study of chemistry

- 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.



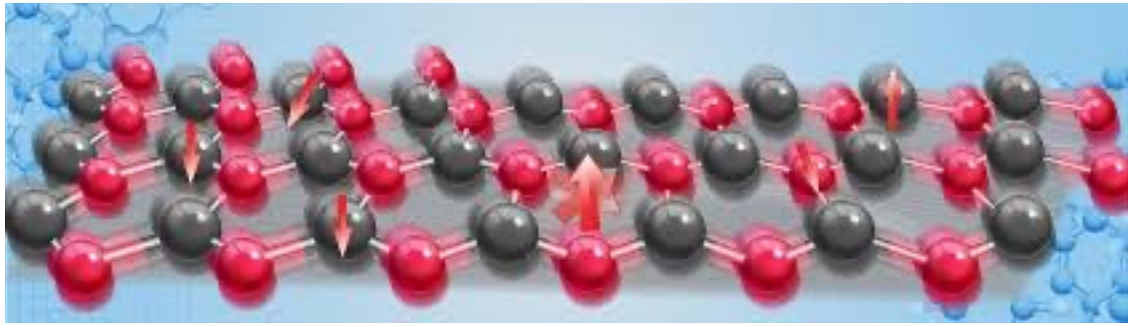




A. Eddins, arXiv (2022), A. Aspuru-Guzik, et al. *Science* (2005), B.Bauer et al. *Chem. Rev.* 2020 (2020)

Future of quantum simulation

Discover new materials?

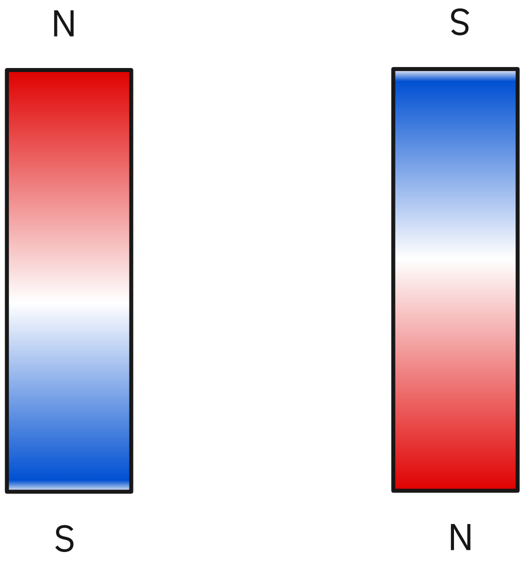


Drug design?

Chemical reactions for battery development?

What’s a quantum computer?

Classical Bit



Encoding information

Qiskit

Color	Coins	Binary
	HHH	000
	HHT	001
	HTH	010
	HTT	011
	THH	100
	THT	101
	TTH	110
	TTT	111

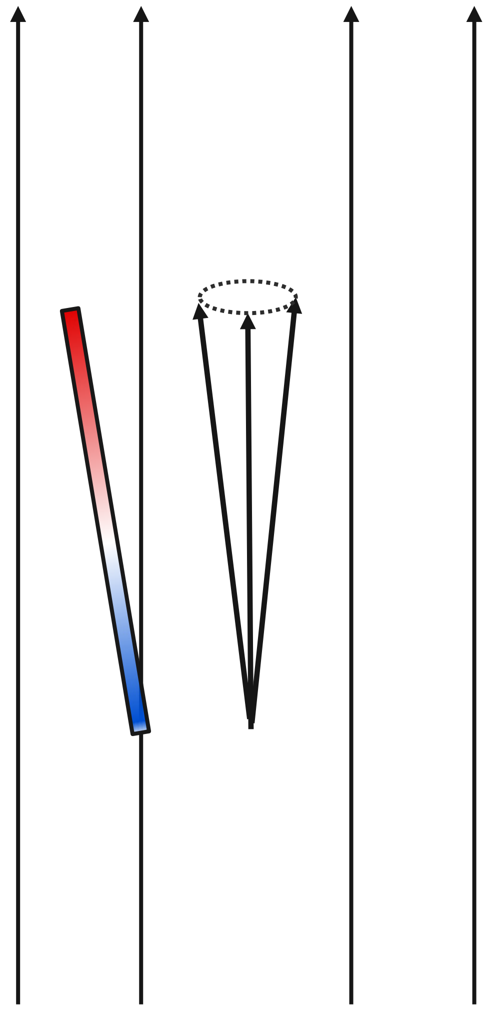
11010

1×2^4 1×2^3 0×2^2 1×2^1 0×2^0

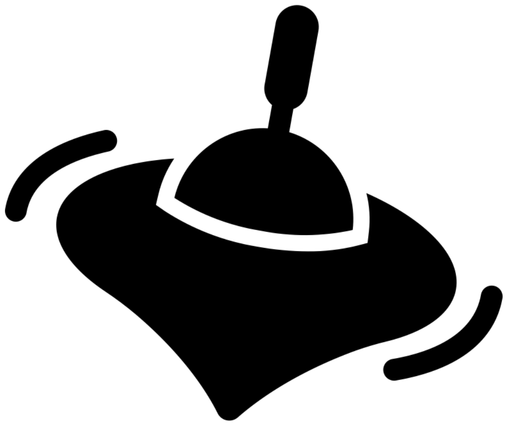
$$= 16 + 8 + 0 + 2 + 0$$

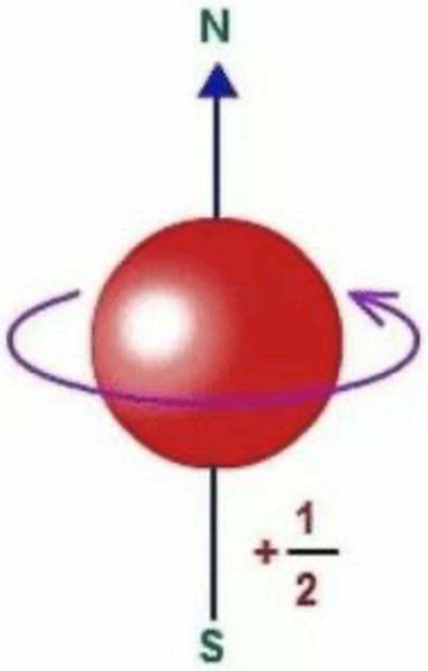
$$= 26$$

Magnetic needle



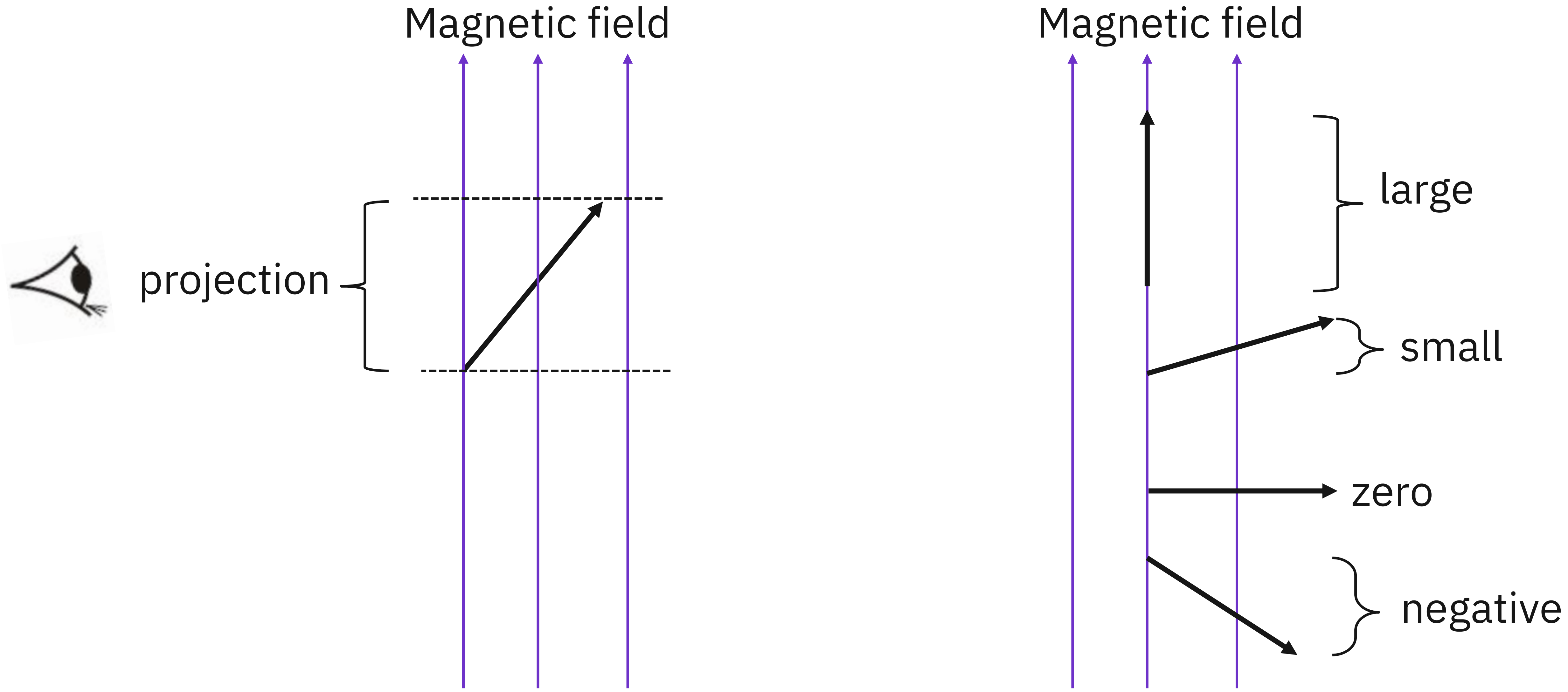
Inhomogeneous field



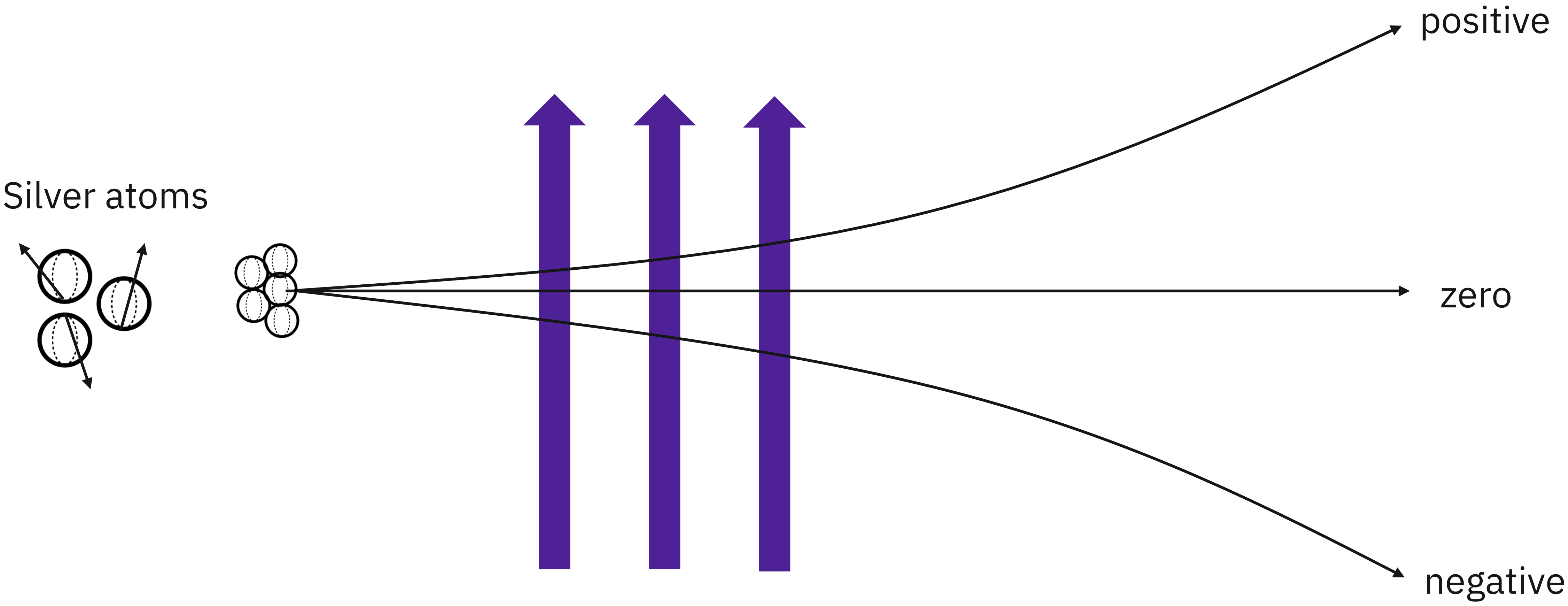


Spin explained: imagine a ball that's rotating…
except it's not a ball and it's not rotating ☺

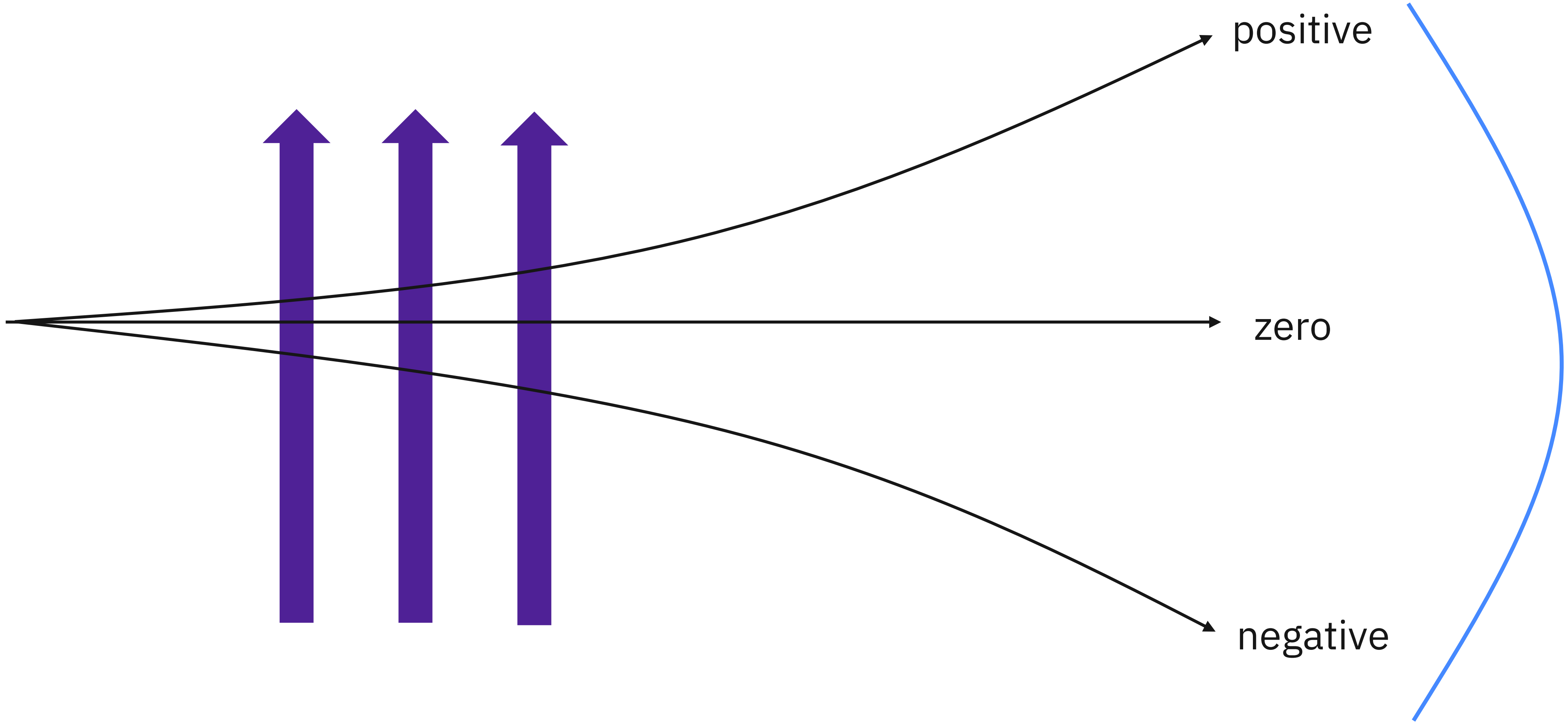
Projections



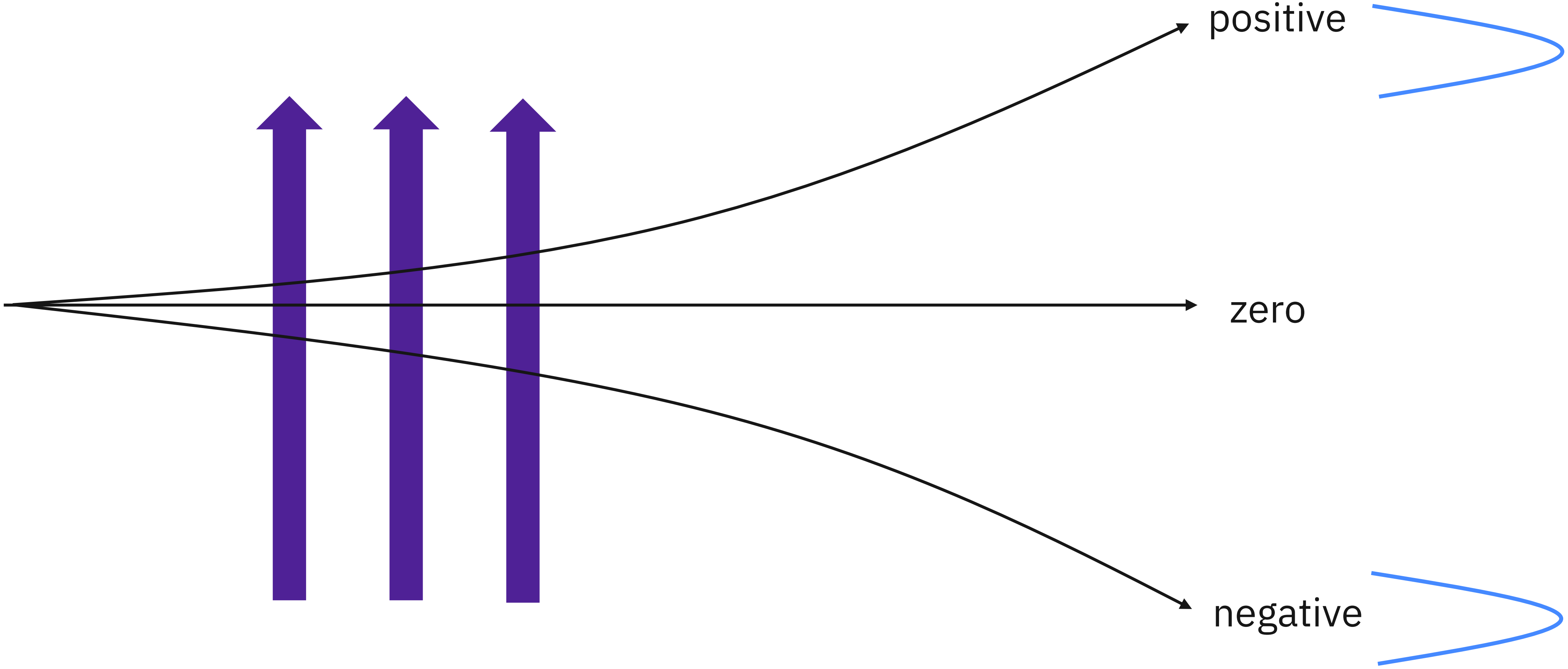
Stern-Gerlach



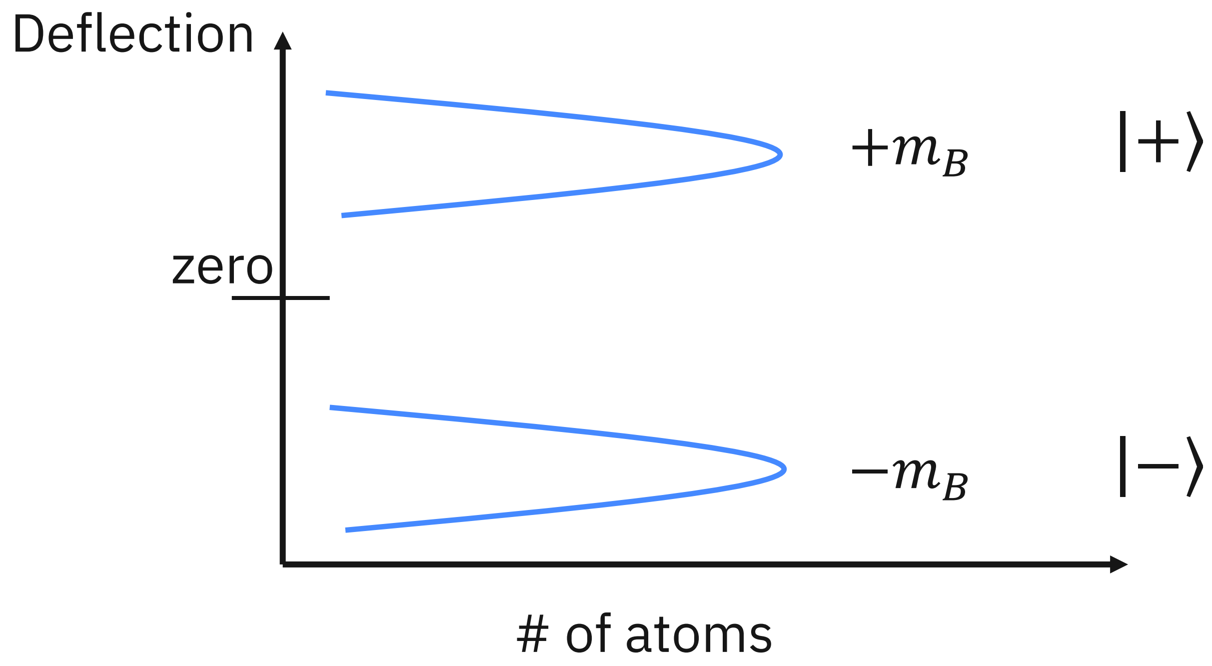
Stern-Gerlach-expected outcome



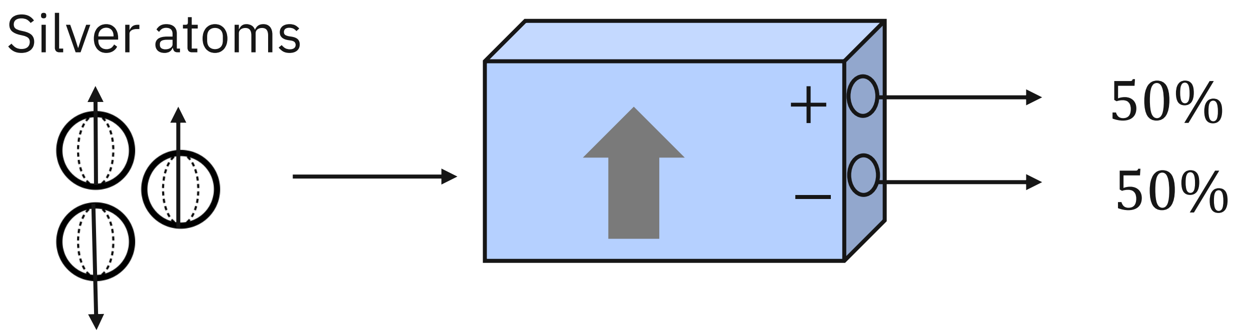
Stern-Gerlach-actual outcome



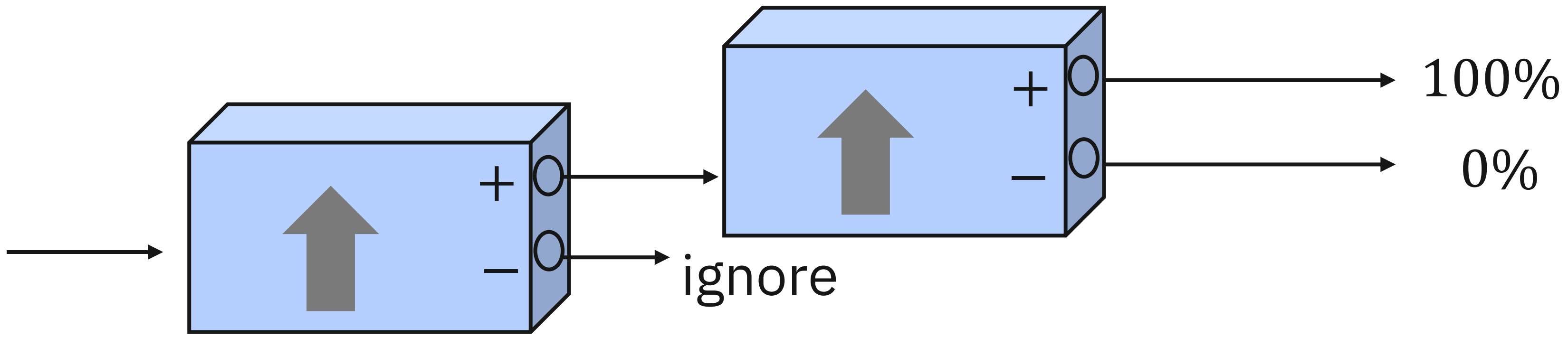
Stern-Gerlach; actual results

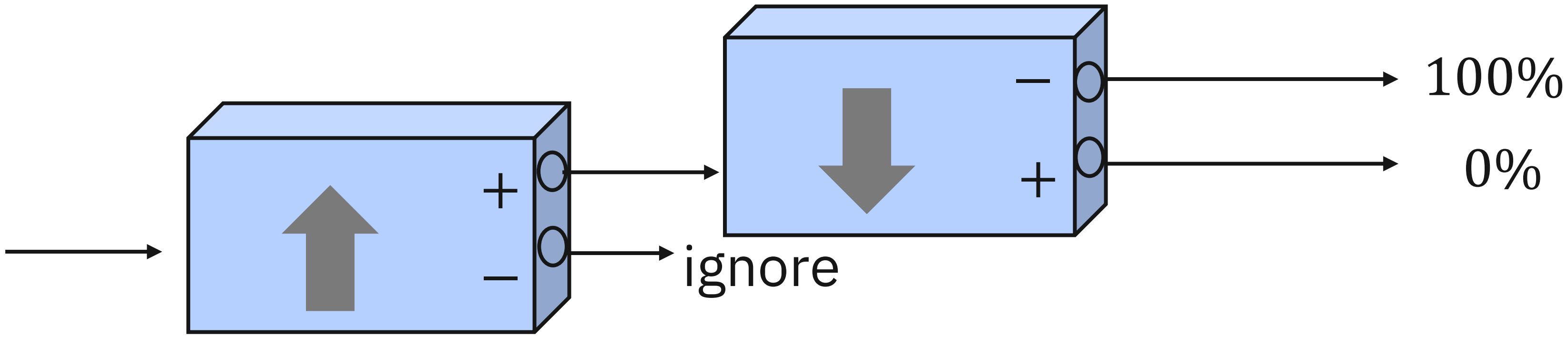


Stern-Gerlach apparatus

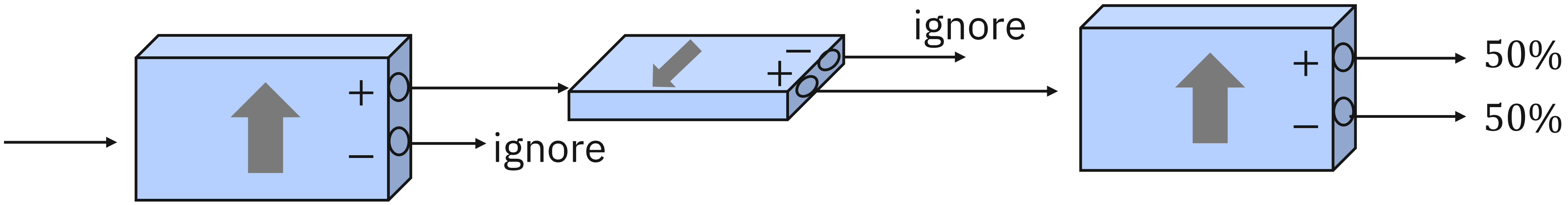


Probabilities with S-G



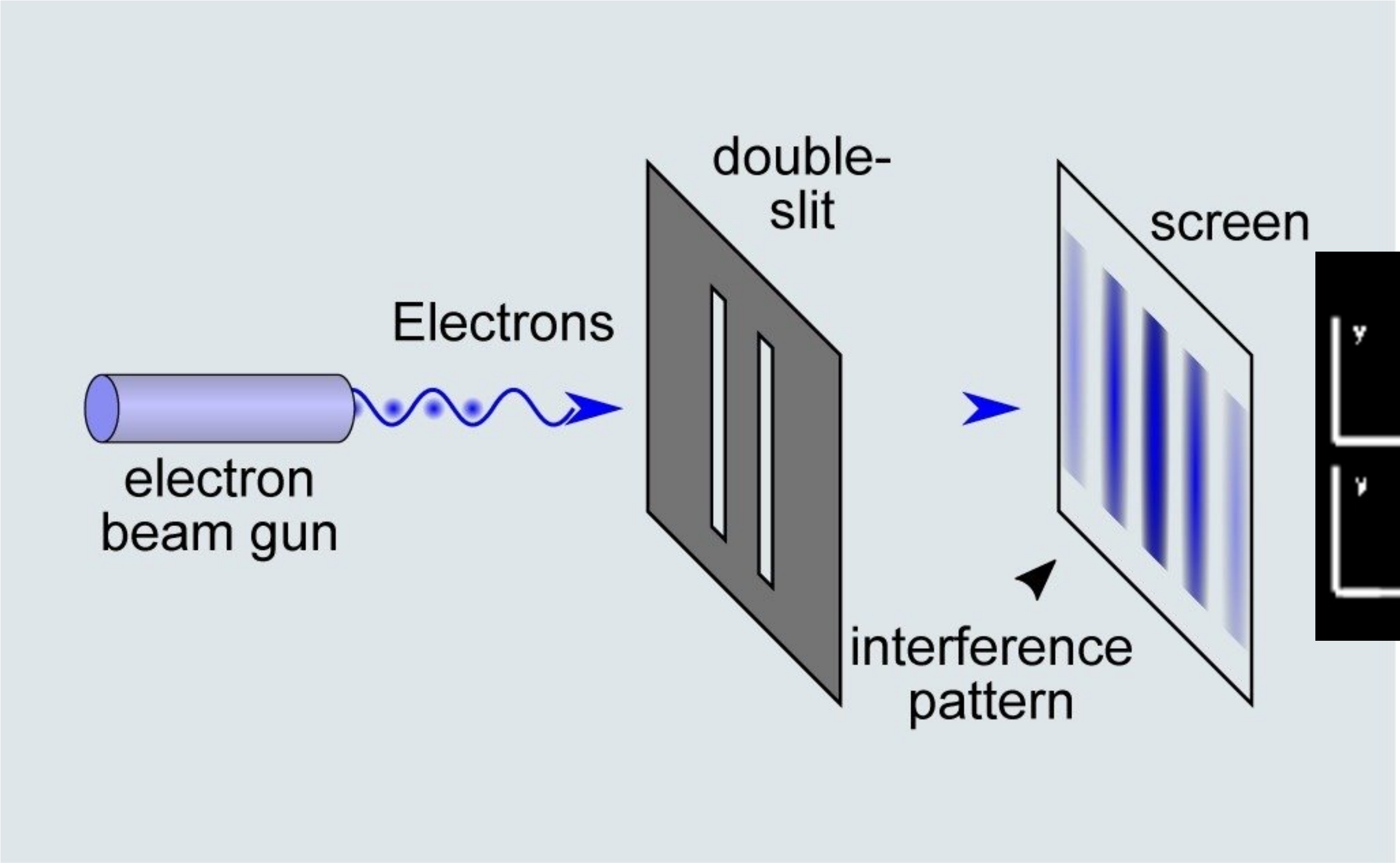


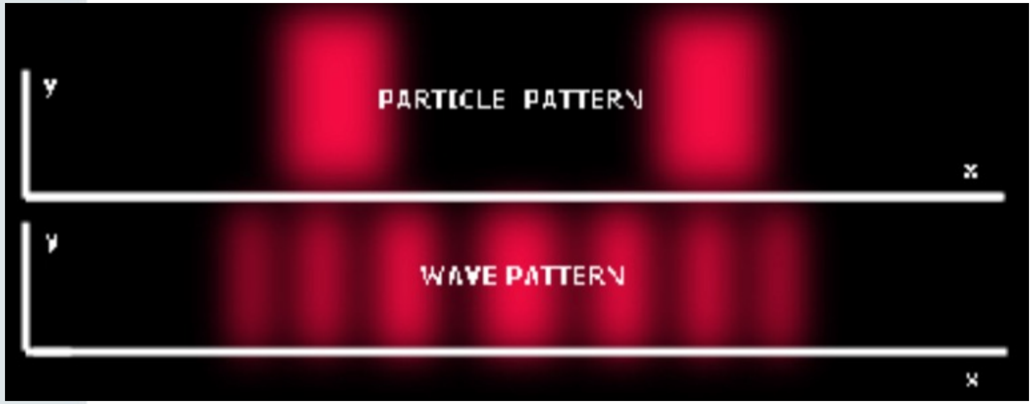
The crucial experiment



Test yourself: What is the distribution at the end?

Measuring the double slit





Universetoday.com

‘’Quantum mechanics forces us to the brink of implausibility …but not beyond’’

What is a superposition??

SOME combination of
$|+\rangle \; AND \; |-\rangle$

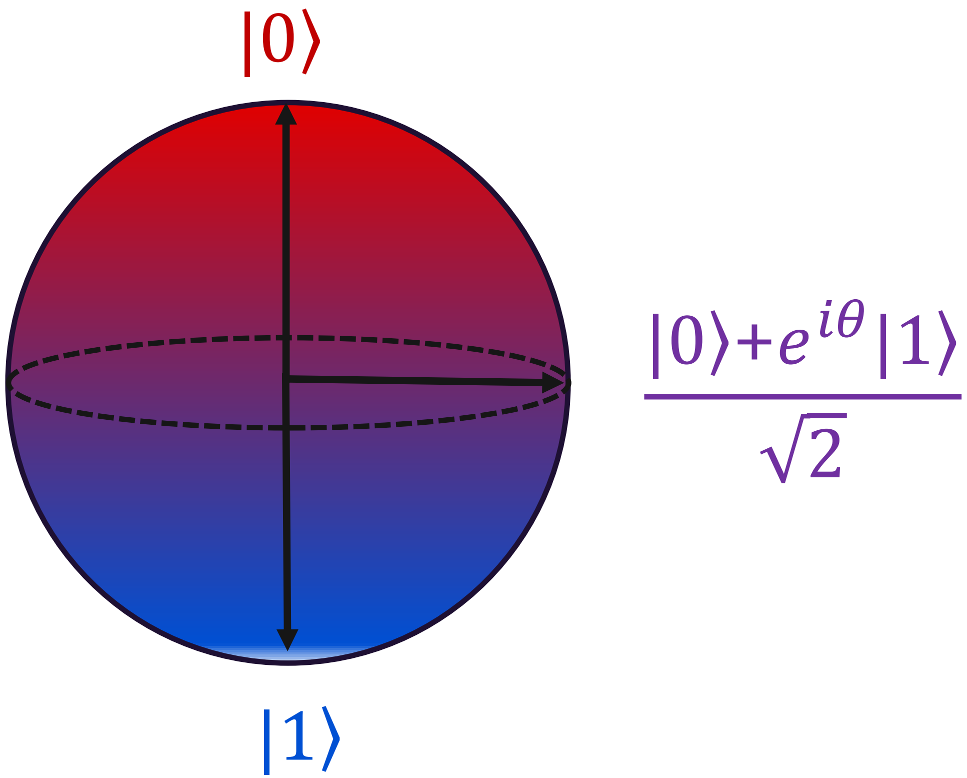
AND NOTHING ELSE

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 *superpostion*, 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)

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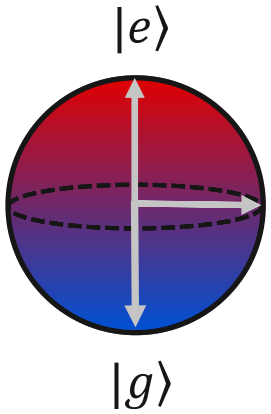
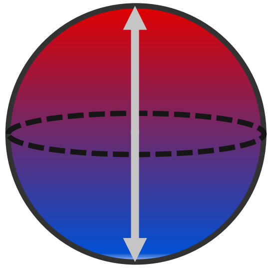
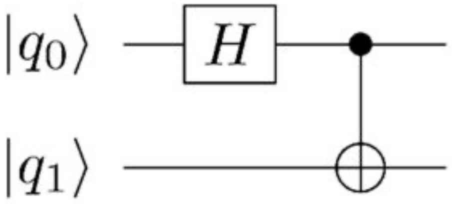
Well-behaved quantum systems



...that we can initialize into a known state

...with relatively-long coherence times





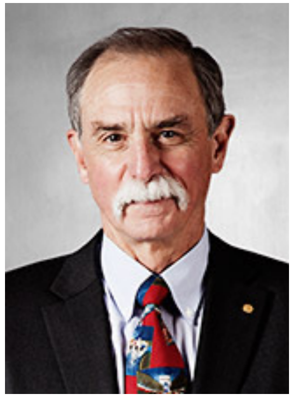
Universal set of quantum gates

...and qubit-specific measurement capability

D. DiVincenzo, arXiv (2020)

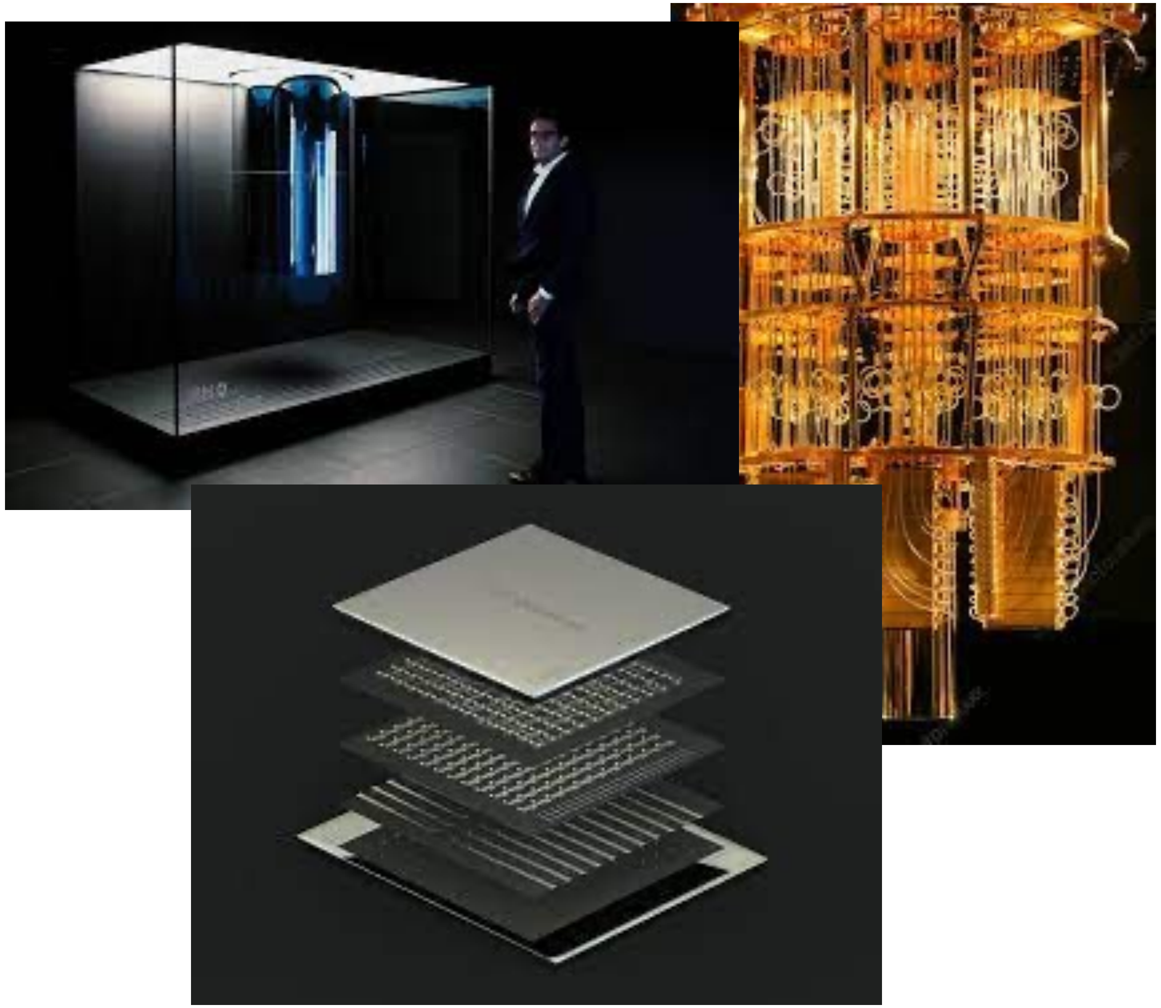
Can we build such systems?

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



Qiskit

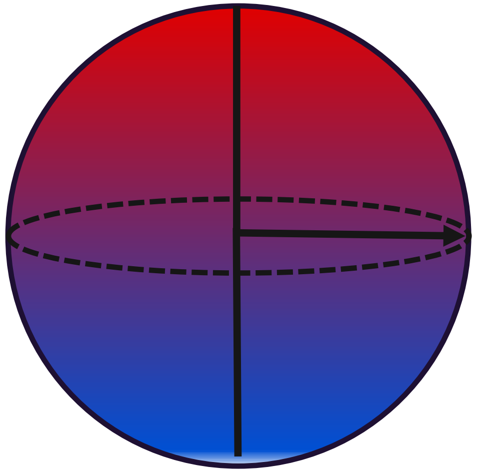
The basics

The Quantum Facts of Life

Superposition

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

$|0\rangle$

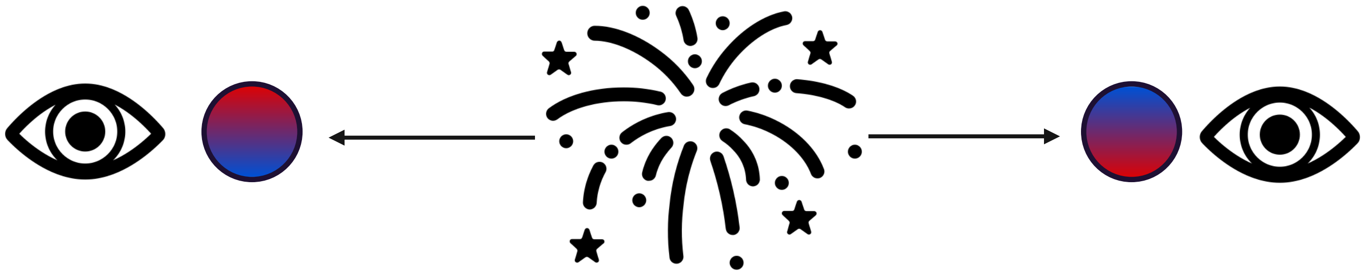


$|1\rangle$

Entanglement

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

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



$|0\rangle$ $|1\rangle$

Quick Review: Complex Numbers

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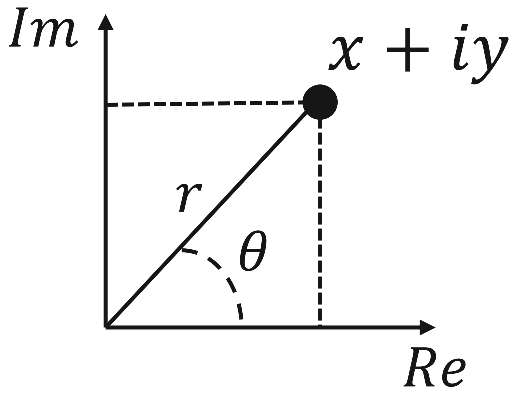
$$z = x + iy$$



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

$$z = re^{i\theta} = r(cos\theta + isin\theta) = \underbrace{rcos\theta}_{x} + \underbrace{rsin\theta}_{y}$$

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

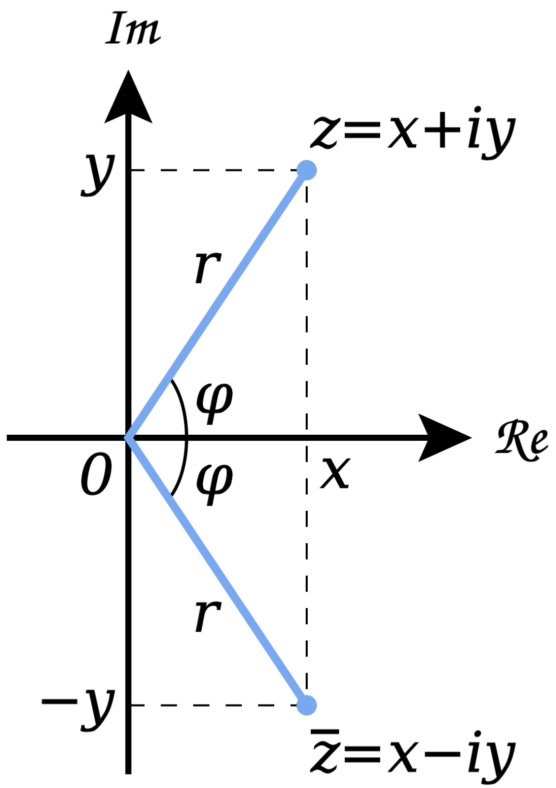
Complex Conjugates + Hermitian Conjugates

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

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

$$\langle\psi|\psi\rangle = 1$$

$$z^* = x - iy$$



$$H = \begin{bmatrix} a & c \\ b & d \end{bmatrix} \longrightarrow H^\dagger = \begin{bmatrix} a^* & b^* \\ c^* & d^* \end{bmatrix}$$

What is a quantum state?

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

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|\psi\rangle^{\dagger} = \langle 0| + \langle 1|$$

$$\begin{pmatrix} 0 & 1 \end{pmatrix} \qquad \qquad \begin{pmatrix} 1 & 0 \end{pmatrix}$$

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

Orthogonality & Inner Products

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

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

$$\langle 0|1\rangle$$

$$\begin{pmatrix} 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$= (0 * 1) + (1 * 0) = 0$$

Tensor Products

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

$$\begin{bmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{bmatrix} \otimes \begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} = \begin{bmatrix} a_{1,1}\begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} & a_{1,2}\begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} \\ a_{2,1}\begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} & a_{2,2}\begin{bmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} a_{1,1}b_{1,1} & a_{1,1}b_{1,2} & a_{1,2}b_{1,1} & a_{1,2}b_{1,2} \\ a_{1,1}b_{2,1} & a_{1,1}b_{2,2} & a_{1,2}b_{2,1} & a_{1,2}b_{2,2} \\ a_{2,1}b_{1,1} & a_{2,1}b_{1,2} & a_{2,2}b_{1,1} & a_{2,2}b_{1,2} \\ a_{2,1}b_{2,1} & a_{2,1}b_{2,2} & a_{2,2}b_{2,1} & a_{2,2}b_{2,2} \end{bmatrix}$$

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

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

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

Tensor Products

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.

Amplitudes

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

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

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

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

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

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

Operators

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

$$\hat{A}\psi = \boxed{a}\boxed{\psi}$$

$^*If\ \psi\ is\ an\ eigenvector\ of\ A$

Eigenvalue Eigenvector

$$\hat{A}\psi = \hat{A}\psi(\mathbf{r}) = \hat{A}\langle \mathbf{r} \mid \psi \rangle = \left\langle \mathbf{r} \middle| \hat{A} \middle| \psi \right\rangle$$

$$a\psi = a\psi(\mathbf{r}) = a\langle \mathbf{r} \mid \psi \rangle = \langle \mathbf{r} \mid a \mid \psi \rangle$$

- 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

Gates

Qiskit

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:

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

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

$$0 * 1 + 1 * 0 = 0$$

$$1 * 1 + 0 * 0 = 1$$

Gates

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

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

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

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

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

Gates must be unitary

Qiskit

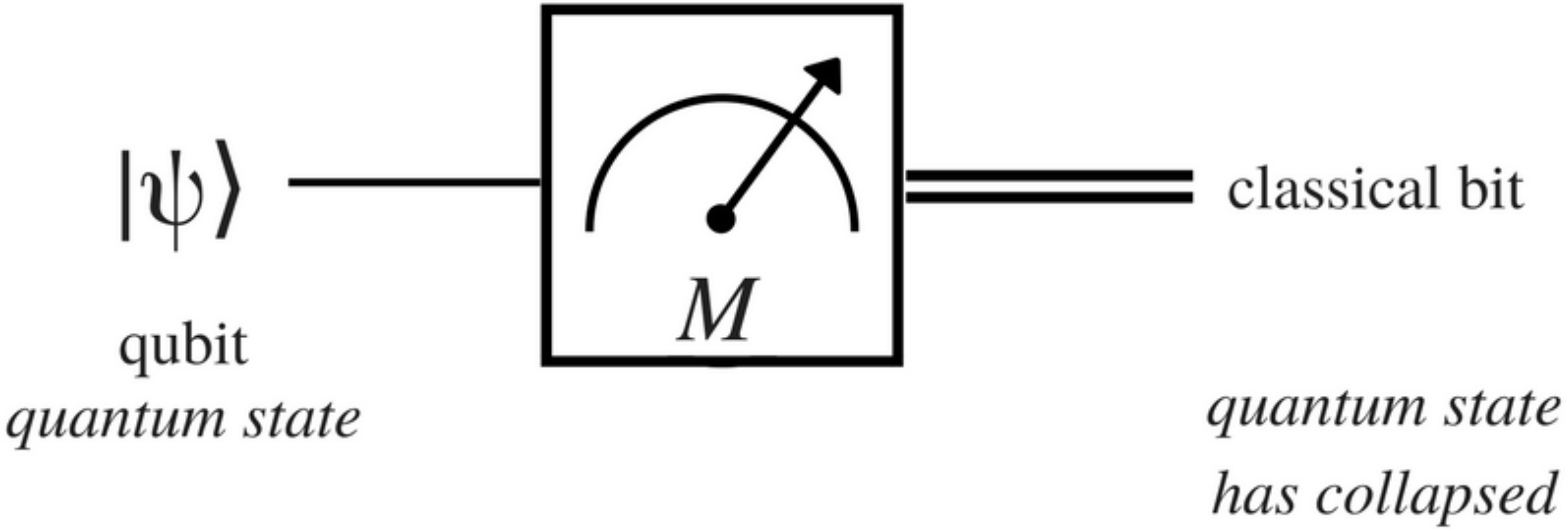
$$U^*U = UU^* = I$$

$I|a\rangle = 1|a\rangle$ *eigenvalue can only be 1

$$I_1 = \begin{bmatrix}1\end{bmatrix},\ I_2 = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix},\ I_3 = \begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix},\ \ldots,\ I_n = \begin{bmatrix}1 & 0 & 0 & \cdots & 0\\ 0 & 1 & 0 & \cdots & 0\\ 0 & 0 & 1 & \cdots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & 0 & \cdots & 1\end{bmatrix}$$

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

Quantum measurement is weird

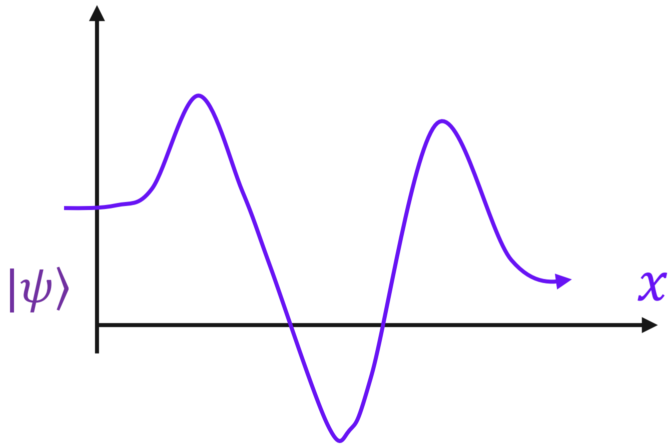


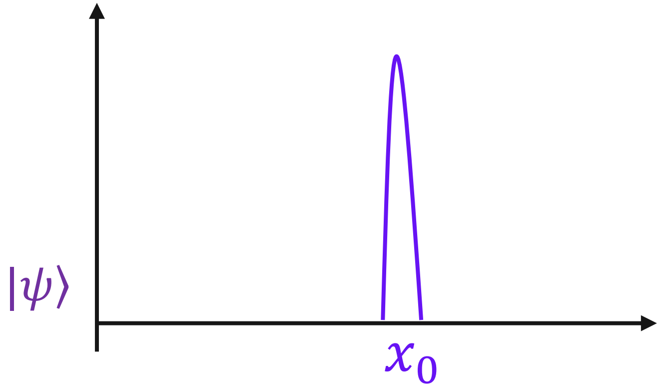
Uncertainty relation:

$$[x, p] = xp - px = i\hbar \qquad \sigma_x \sigma_p \geq \frac{\hbar}{2}.$$

Time Evolution

Qiskit





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

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

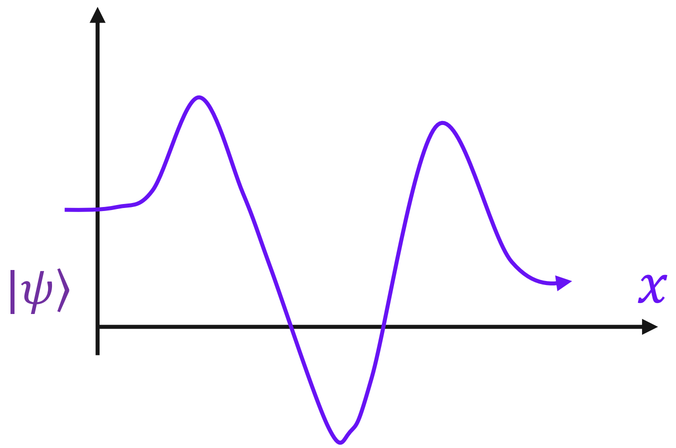
Sometimes it's very challenging. That's where quantum simulation comes in.

3 Stages of Quantum Simulation

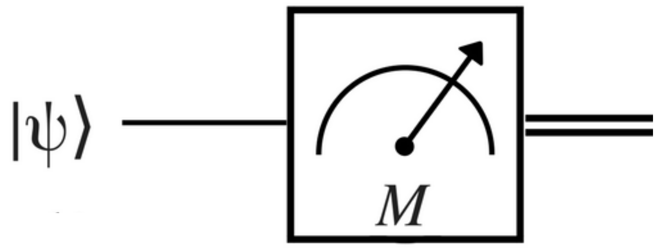
Quantum state preparation

$$|\psi\rangle = |000\rangle$$

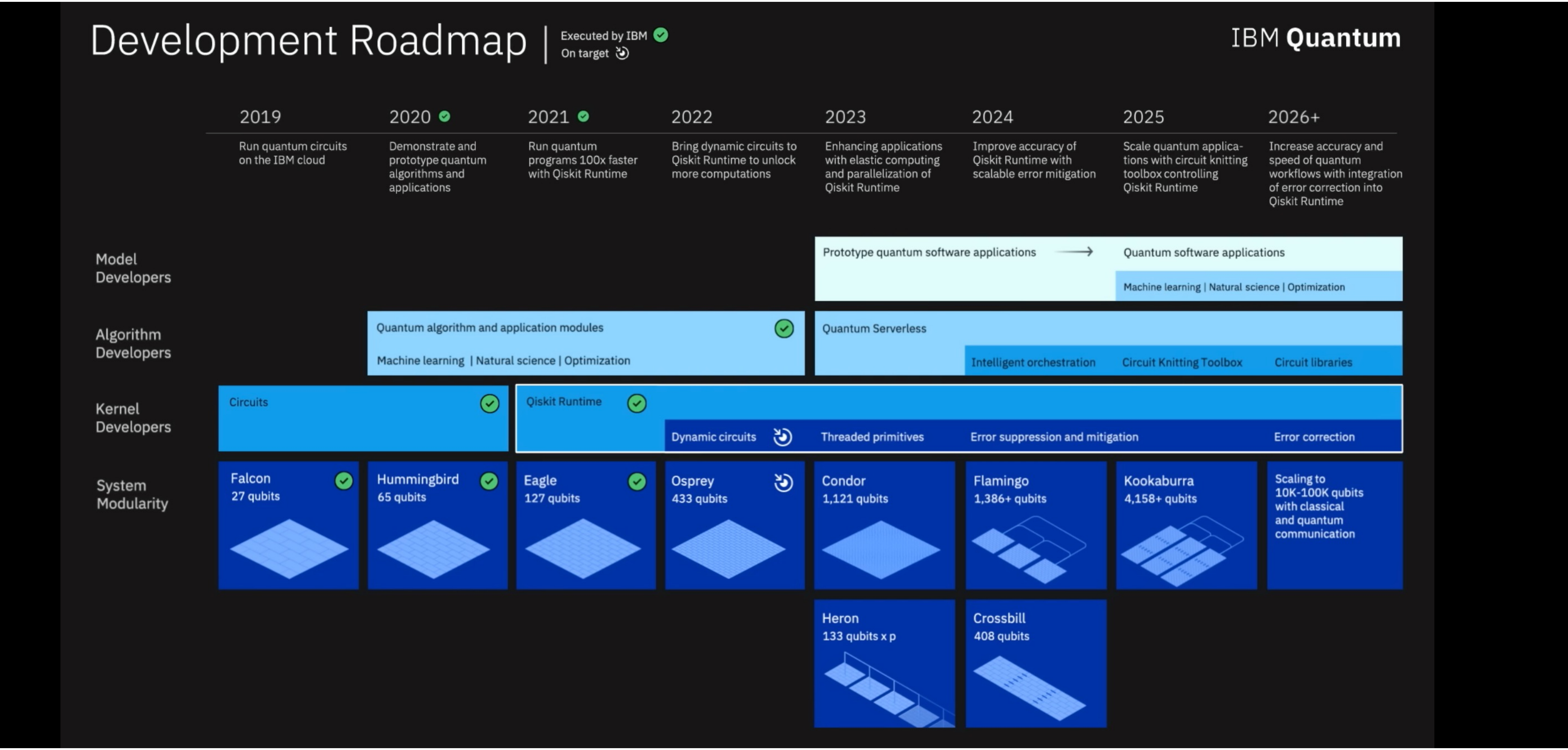
Time Evolution



Measurement



Real world hardware


Development Roadmap
Executed by IBM
On target
IBM Quantum
2019
Run quantum circuits on the IBM cloud
2020
Demonstrate and prototype quantum algorithms and applications
2021
Run quantum programs 100x faster with Qiskit Runtime
2022
Bring dynamic circuits to Qiskit Runtime to unlock more computations
2023
Enhancing applications with elastic computing and parallelization of Qiskit Runtime
2024
Improve accuracy of Qiskit Runtime with scalable error mitigation
2025
Scale quantum applica-tions with circuit knitting toolbox controlling Qiskit Runtime
2026+
Increase accuracy and speed of quantum workflows with integration of error correction into Qiskit Runtime
Model Developers
Prototype quantum software applications
Quantum software applications
Machine learning | Natural science | Optimization
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

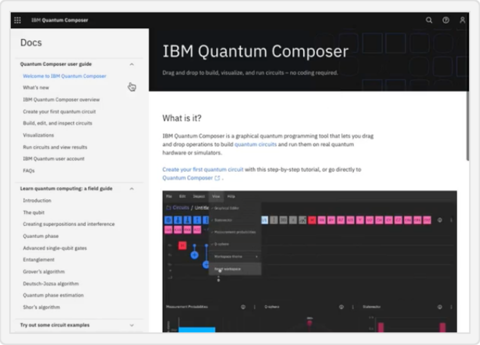
Quantum computing from anywhere

Qiskit

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

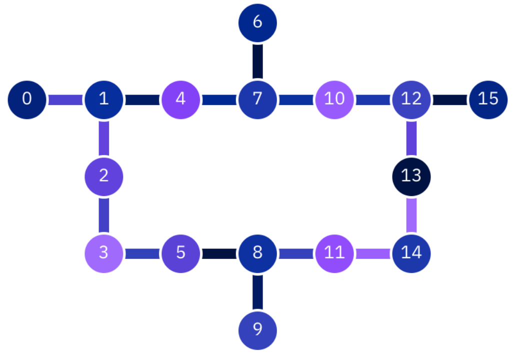
min 5.038 max 5.47

Connection:

CNOT error

Avg 1.333e-2

min 6.804e-3 max 2.293e-2



Types of qubits

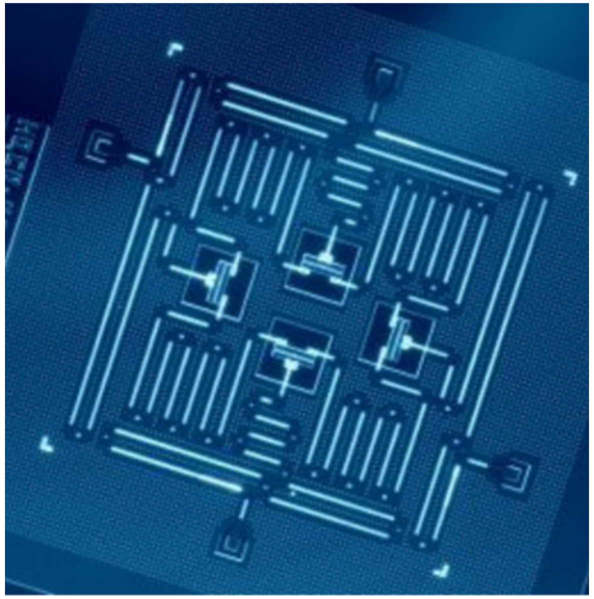
Qiskit

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		

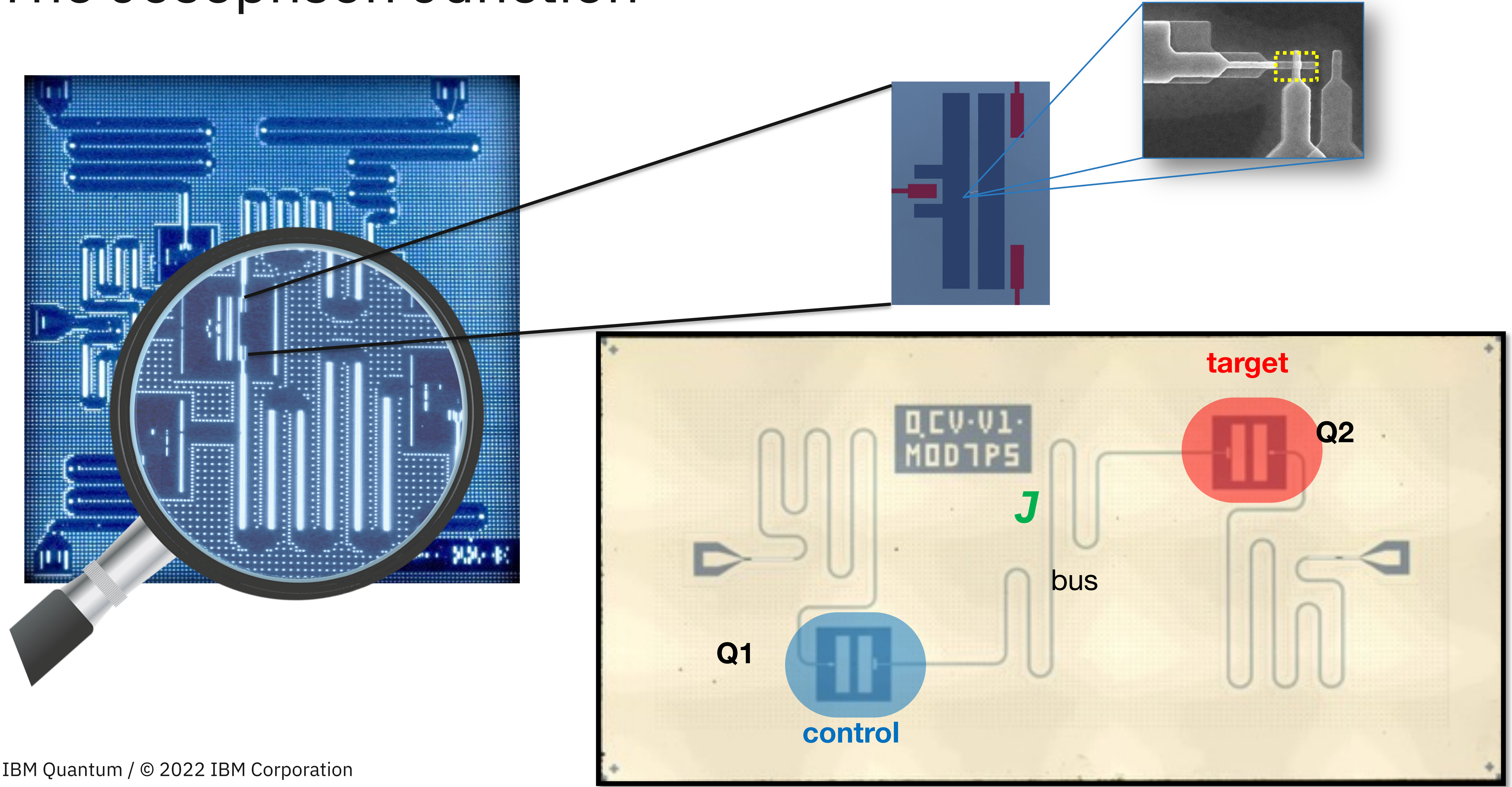
Levylab.com

...we have a favorite.

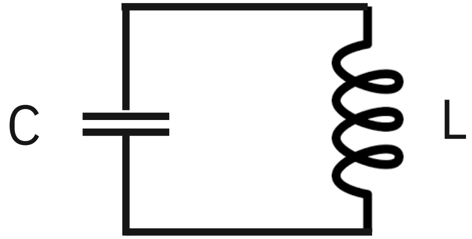


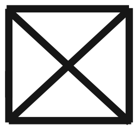
Meet the transmon ☺

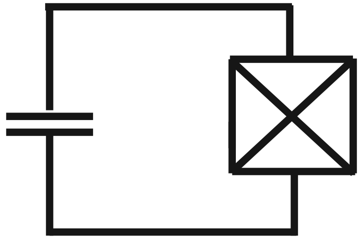
The Josephson Junction

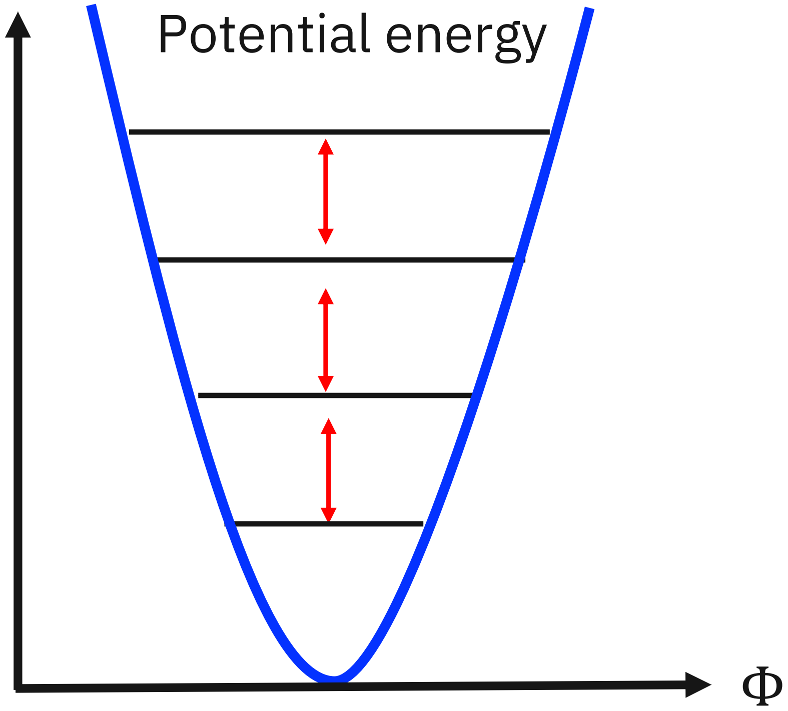


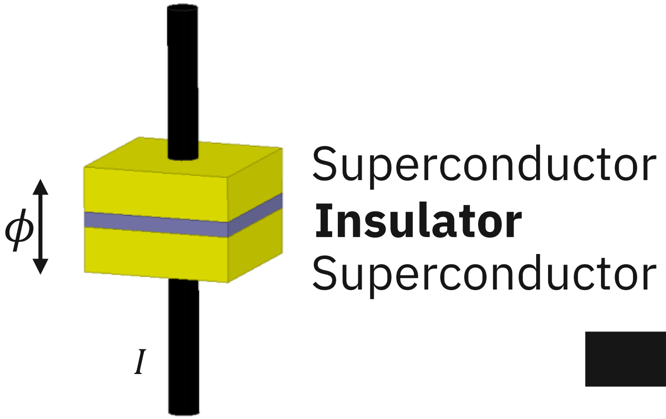
The Josephson Junction





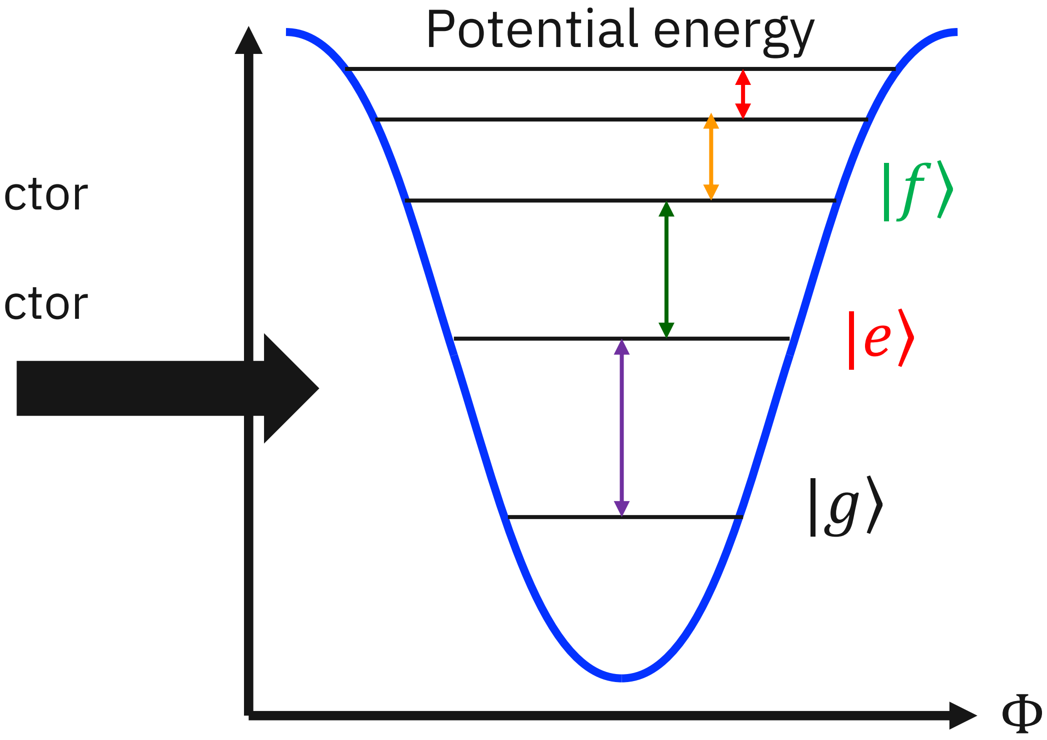




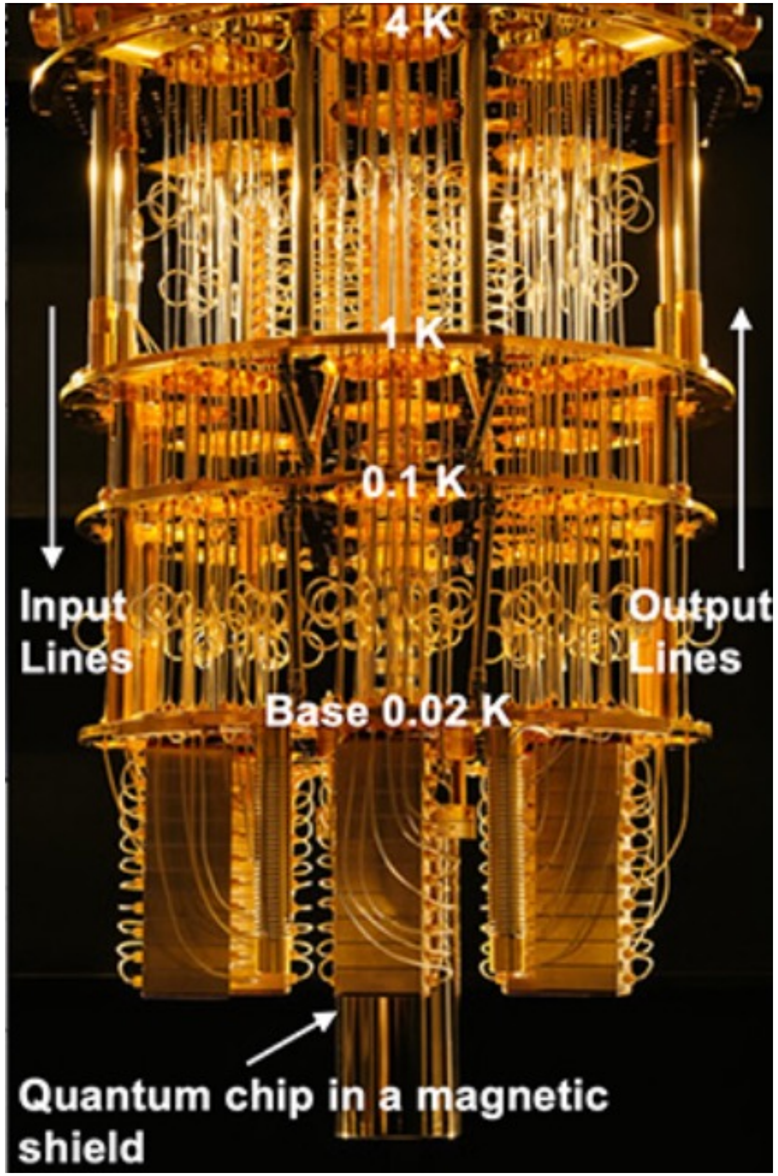


$$I = I_0 \, sin(\phi)$$

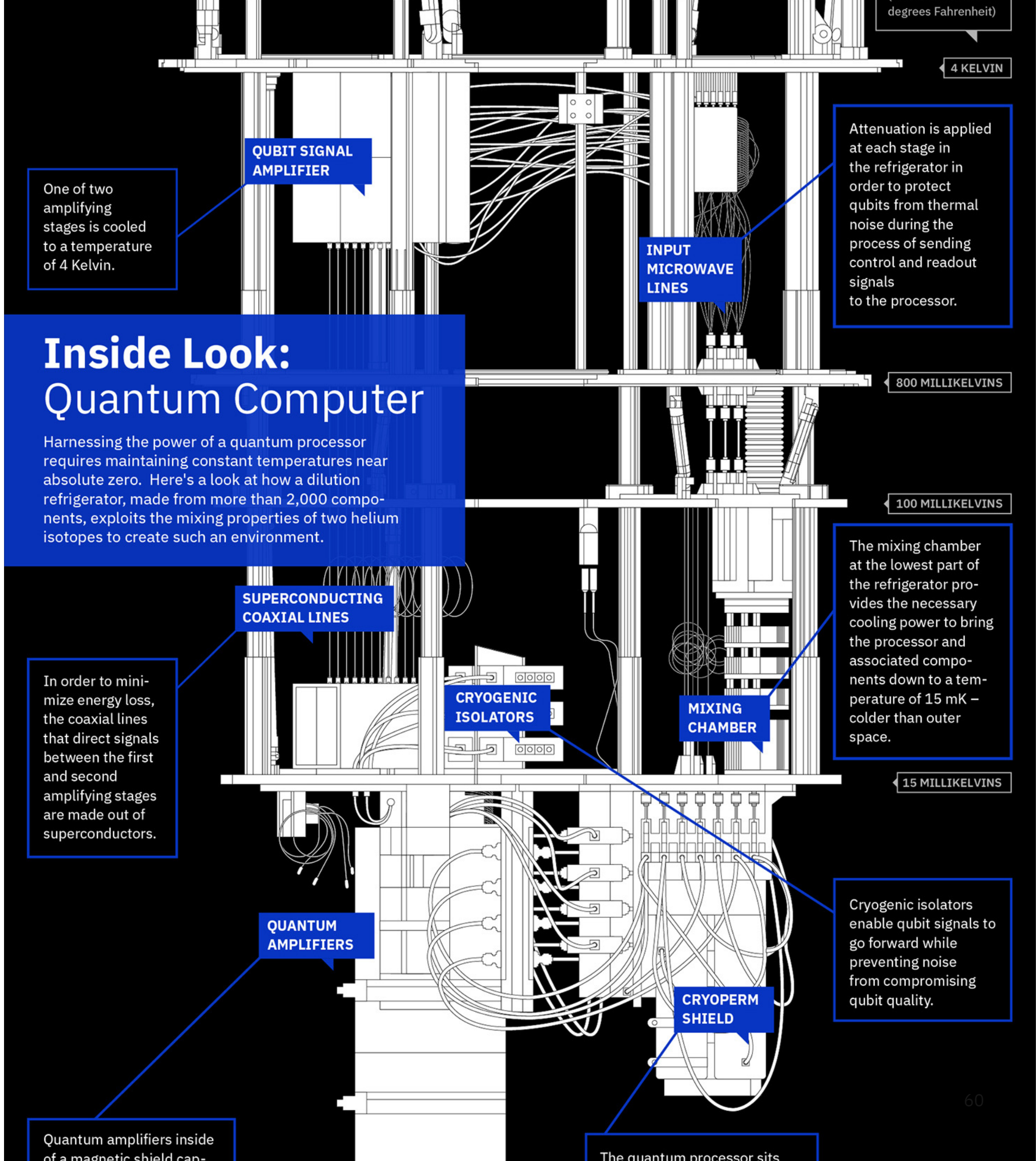
$$\mathrm{E} = E_J cos(\phi)$$



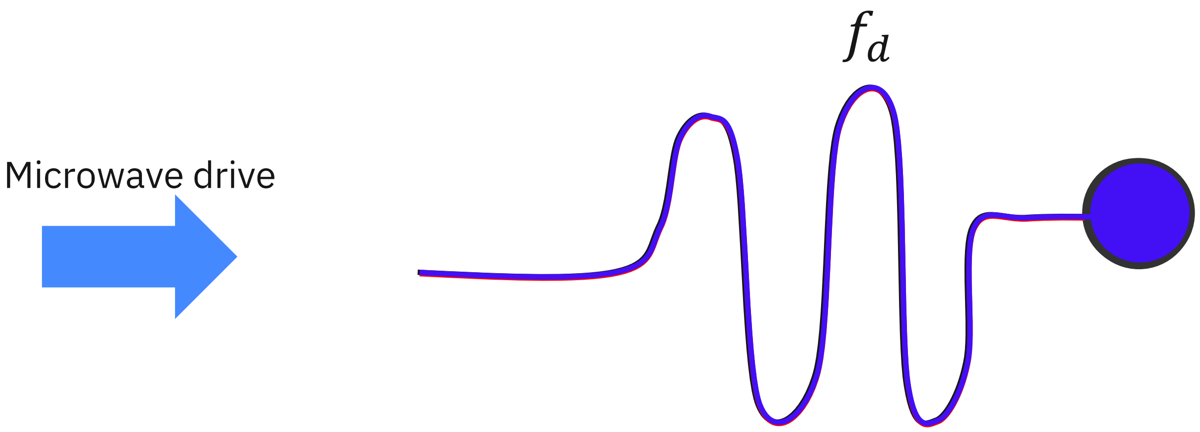
Dilution Refrigeration

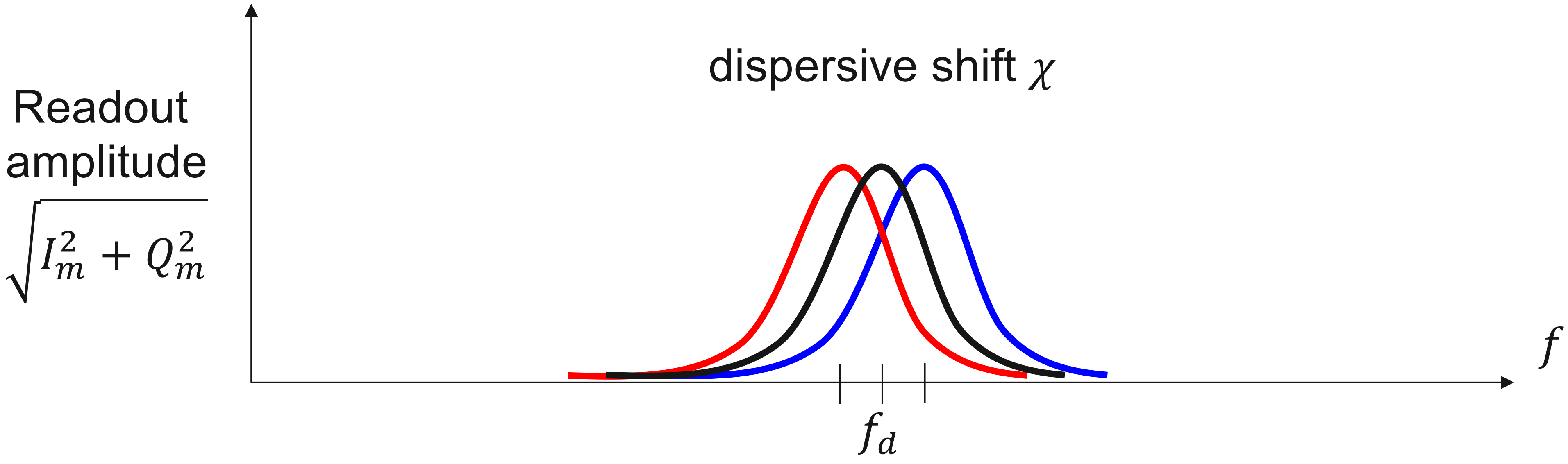


A look inside the dil fridge

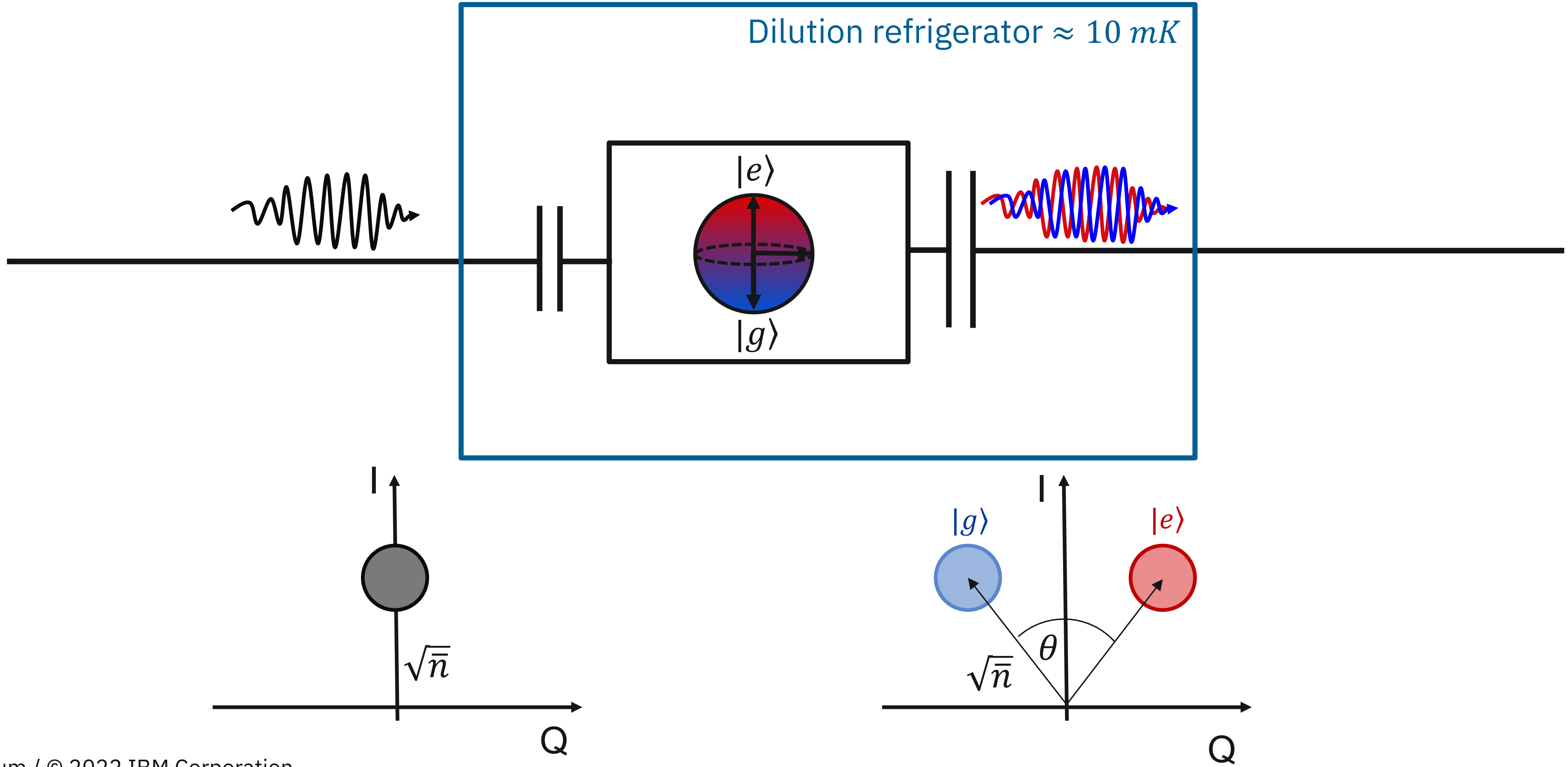


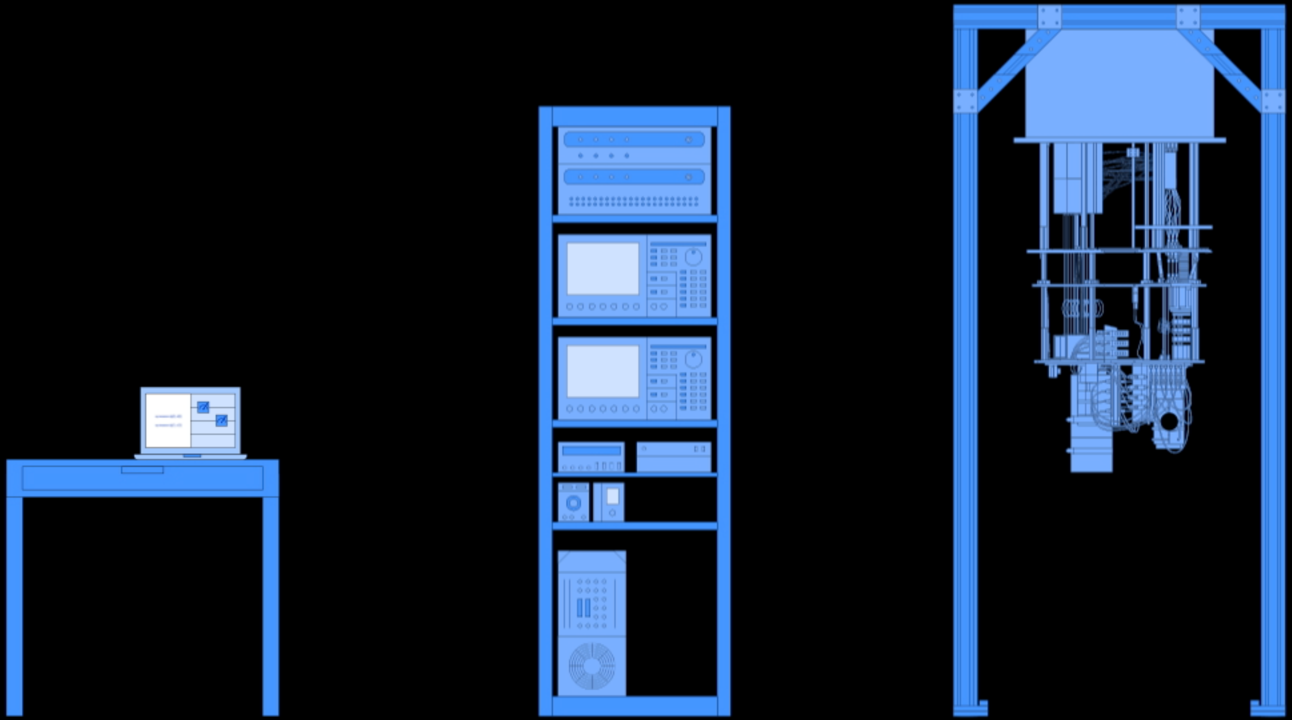
How do we measure a qubit?





Qubit measurement





Summary

Qiskit

Understanding the rules of quantum mechanics is not particularly difficult,**

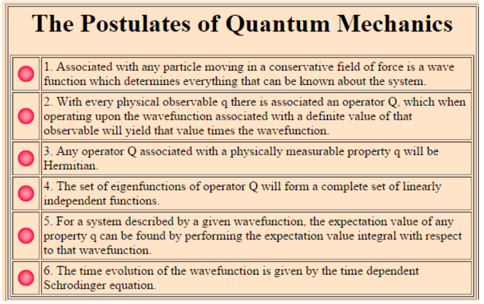
they are simply, unexpected,

the ***applications*** however, are.

Rules of chess

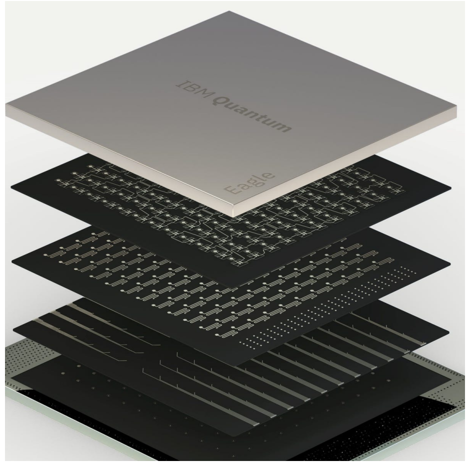
30^{80} possible moves

Rules of quantum



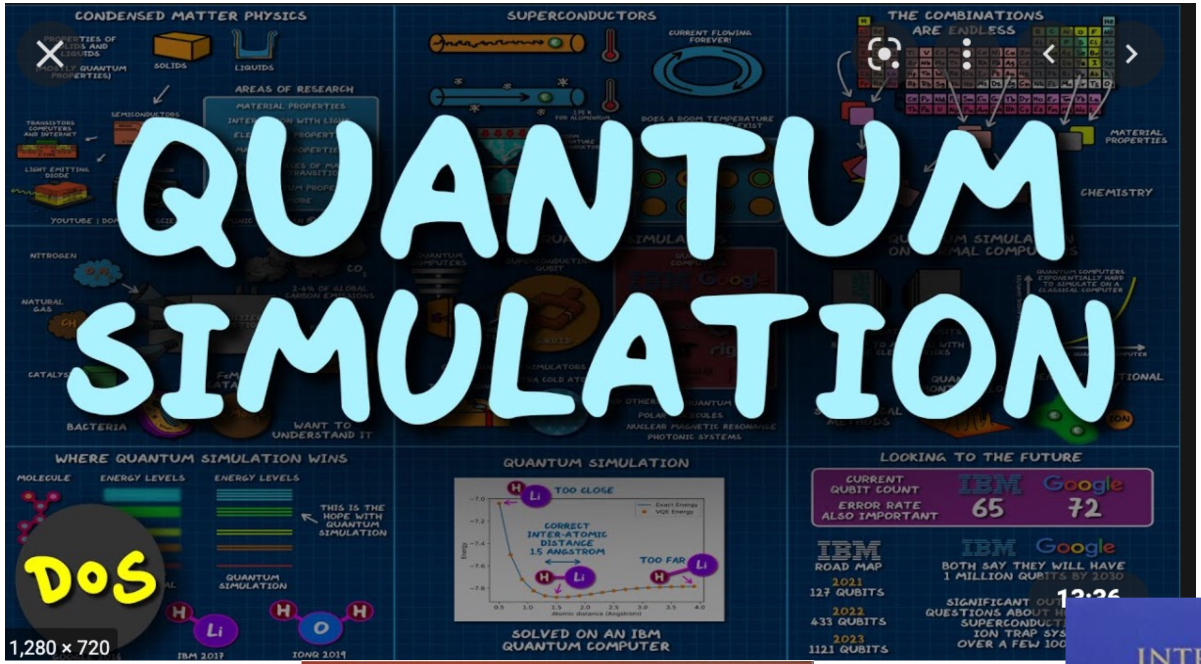
The Postulates of Quantum Mechanics

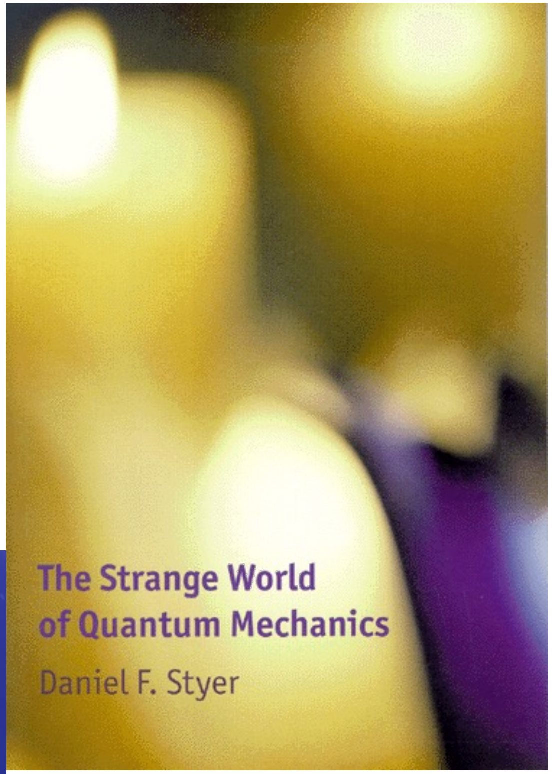
	1. Associated with any particle moving in a conservative field of force is a wave function which determines everything that can be known about the system.
	2. With every physical observable q there is associated an operator Q, which when operating upon the wavefunction associated with a definite value 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 Schrodinger equation.

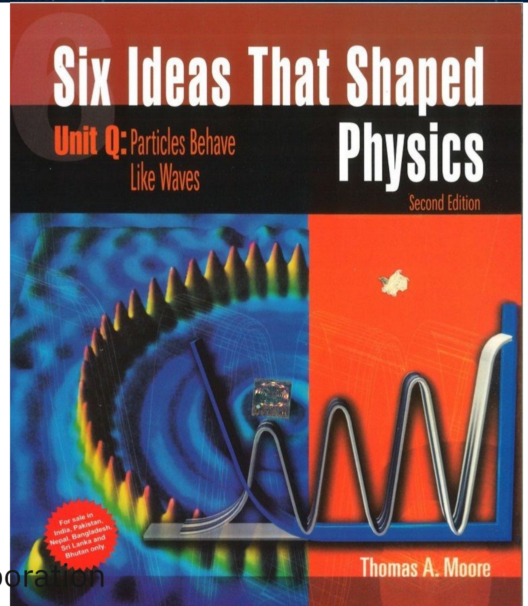


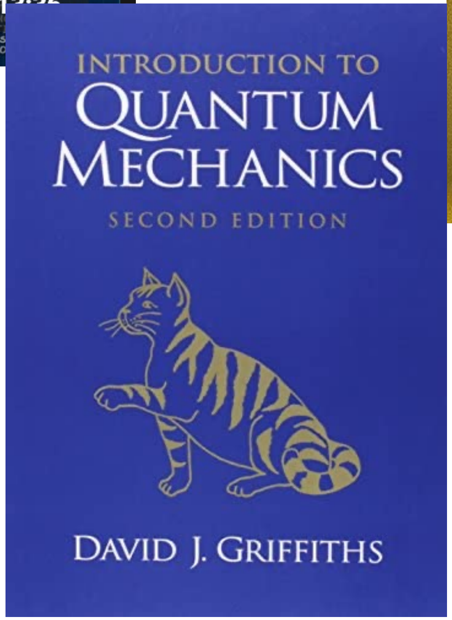
**some people don't agree with me

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