Introduction to IBM Quantum and Qiskit

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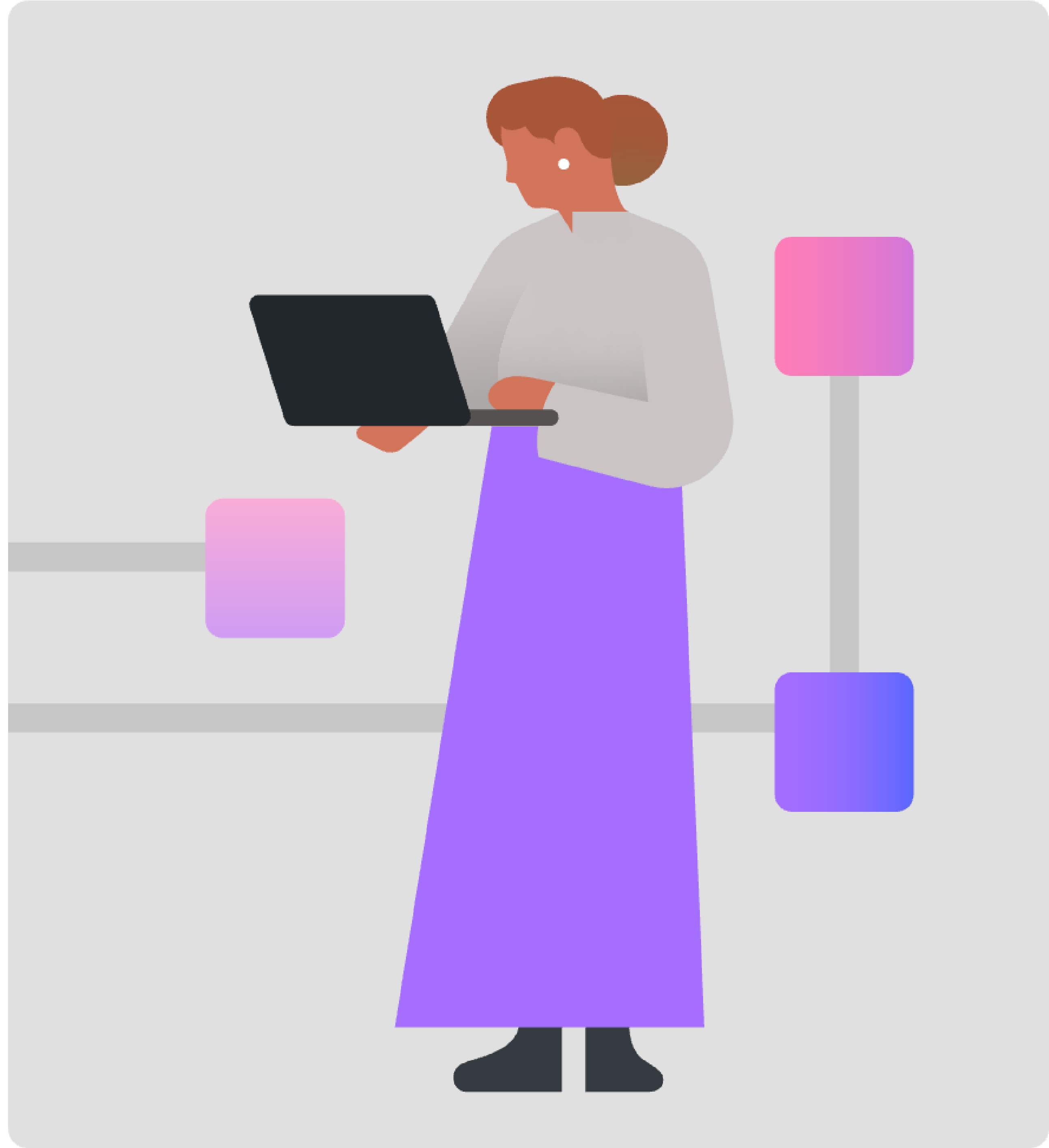
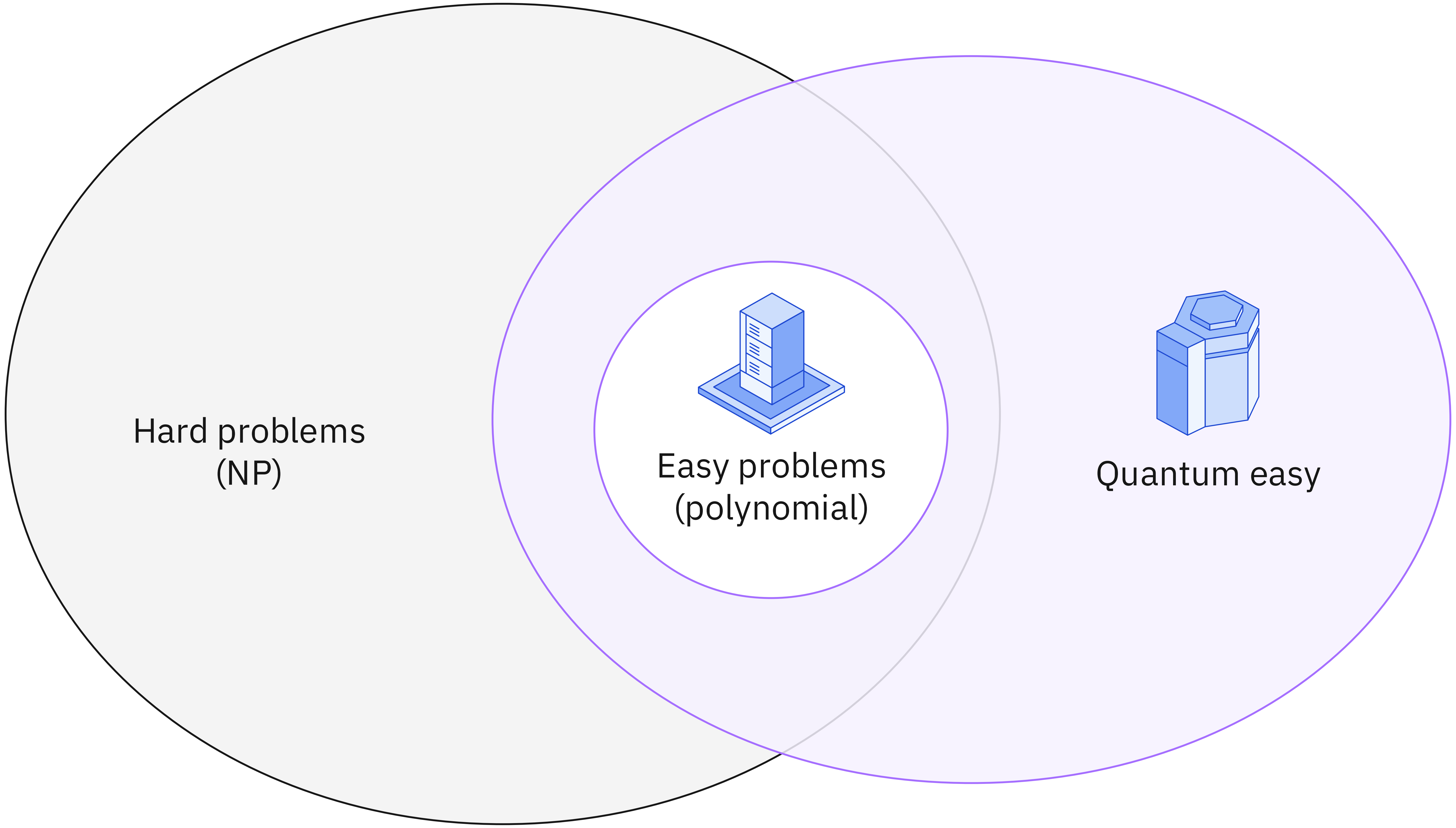
IBM Quantum



Bring useful quantum computing to the world

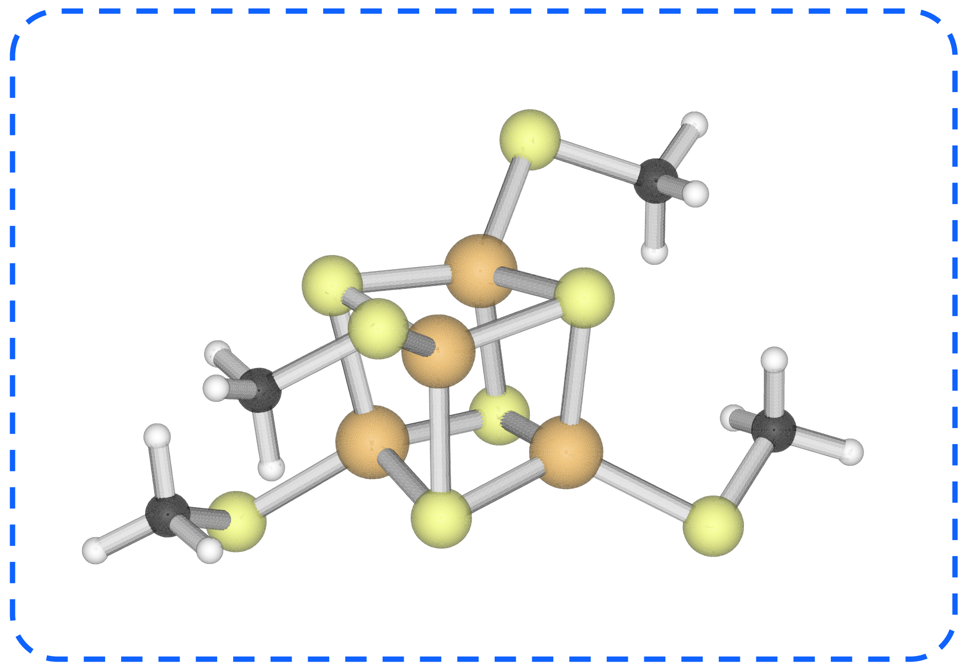
There is a rich seam of problems that cannot be solved by classical and AI supercomputing and never will.

These are the trillion-dollar problems that quantum computing was designed to solve.

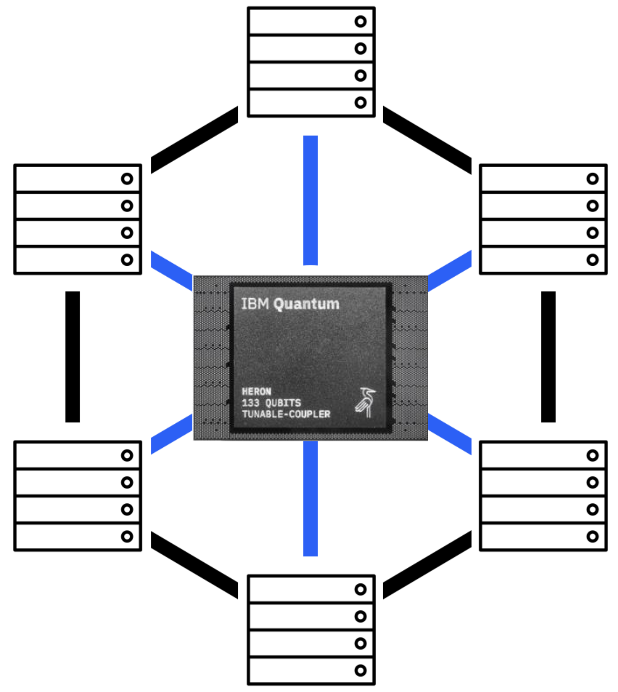


What are these problems?

Modeling molecules, atoms, electrons, and quarks with unprecedented accuracy



[4Fe-4S] using an active space of 54 electrons in 36 orbitals from the TZP-DKH basis set



$$H\Psi = E\Psi$$

Classical exact method	63 PiB of memory[1]
Classical approximate method (DMRG)	8 hours[2,3]
Quantum method (QCSC)	12 min using 77 qubits + 1.5 hours supercomputer time[1]

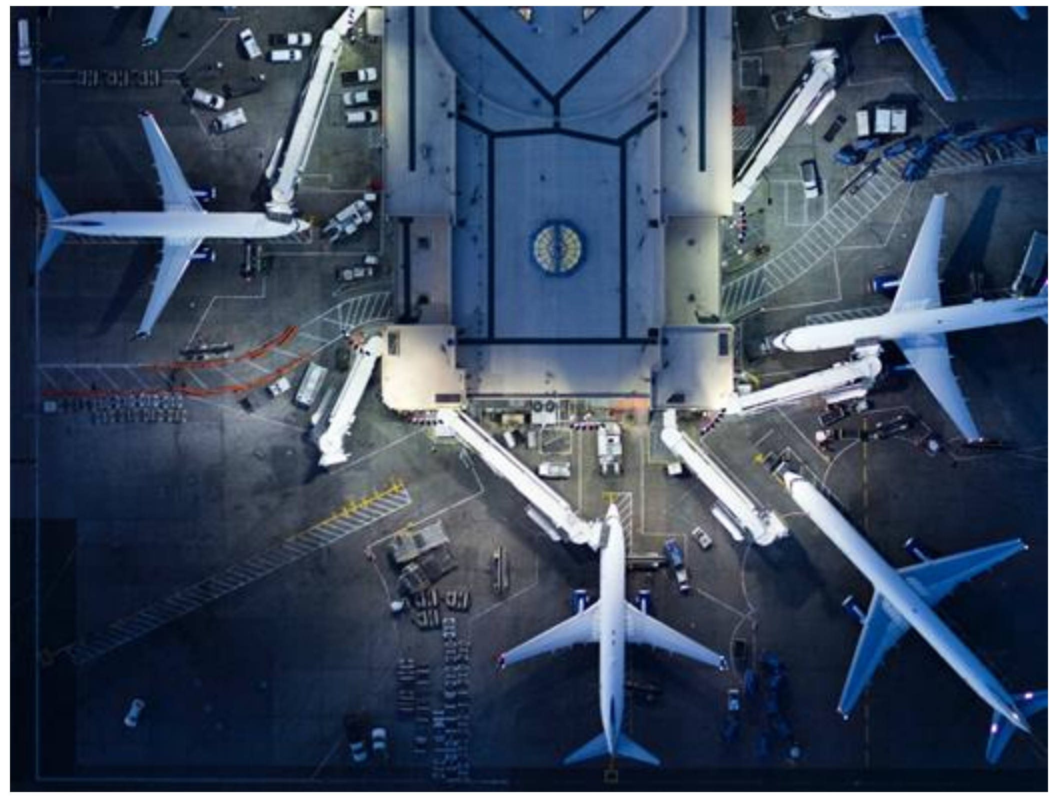
We are already using quantum (Heron, 77 qubits) and HPC (Supercomputer Fugaku) to achieve results comparable with the best classical approximate methods (DMRG) in accuracy and timing

1. Science Advances vol. 11, no. 25 (2025)
2. J. Chem. Theory Comp. 20 (2024): 775–786
3. J. Chem. Phys. 159, 234801 (2023)

What are these problems?

Modeling molecules, atoms, electrons, and quarks with unprecedented accuracy

Developing lighter, longer-lasting batteries for electric vehicles, electronics, and energy grid storage



Designing lighter, stronger materials to allow planes to be more efficient and to need less maintenance

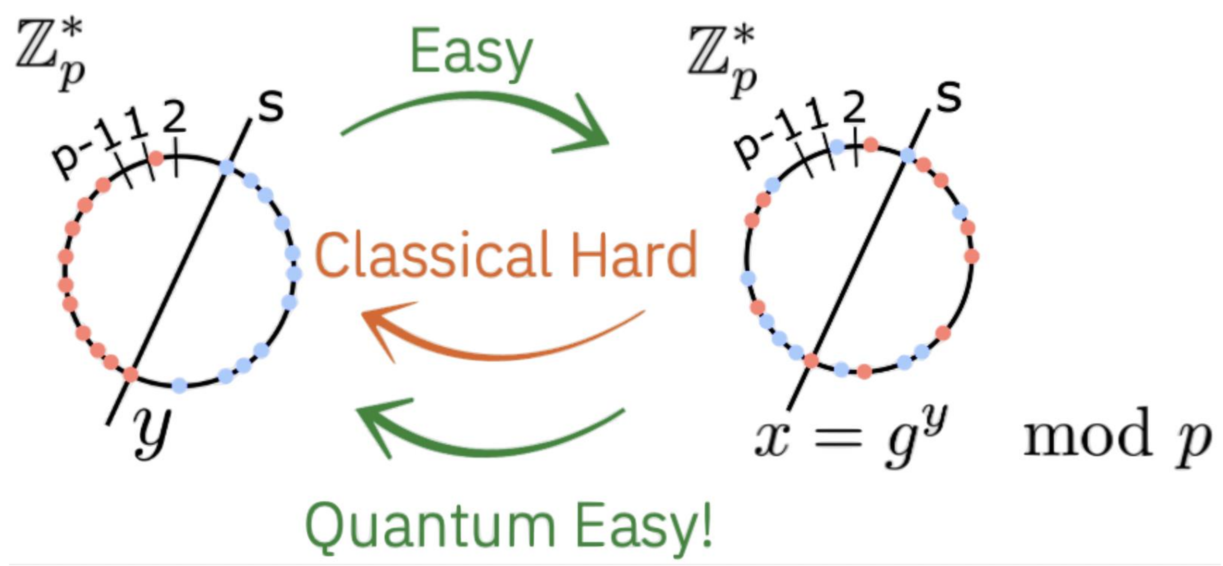
Discovering new classes of antibiotics to counter the emergence of multidrug-resistant bacterial strains

Designing optimal superconductors for MRI, electromobility, and renewable energies

What are these problems?

Solving algebra in [exponential] spaces.
Finding hidden patterns in structured problems.

Groups encode symmetries and transformations of data.



$$f(g\mathbf{b}) = f(g) \qquad \forall\, \mathbf{b} \in B$$

$$\frac{1}{\sqrt{|G|}} \sum_{g \in G} |f(g)\rangle |g\rangle$$

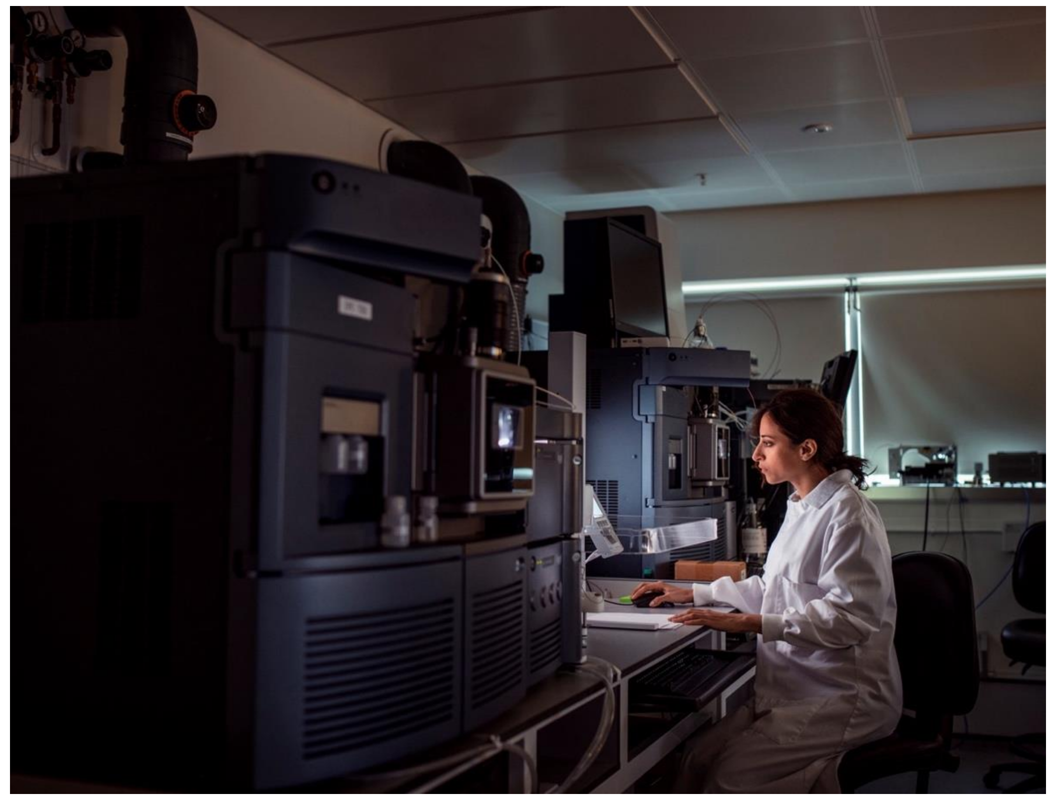
$$= \sqrt{\frac{|B|}{|G|}} \sum_{g_0 \in G/B} |f(g_0)\rangle \frac{1}{\sqrt{|B|}} \sum_{\mathbf{b} \in B} |g_0 \mathbf{b}\rangle$$

Quantum computers speak the mathematics of group theory and work in the large spaces needed to answer difficult computational problems inaccessible to classical methods.

What are these problems?

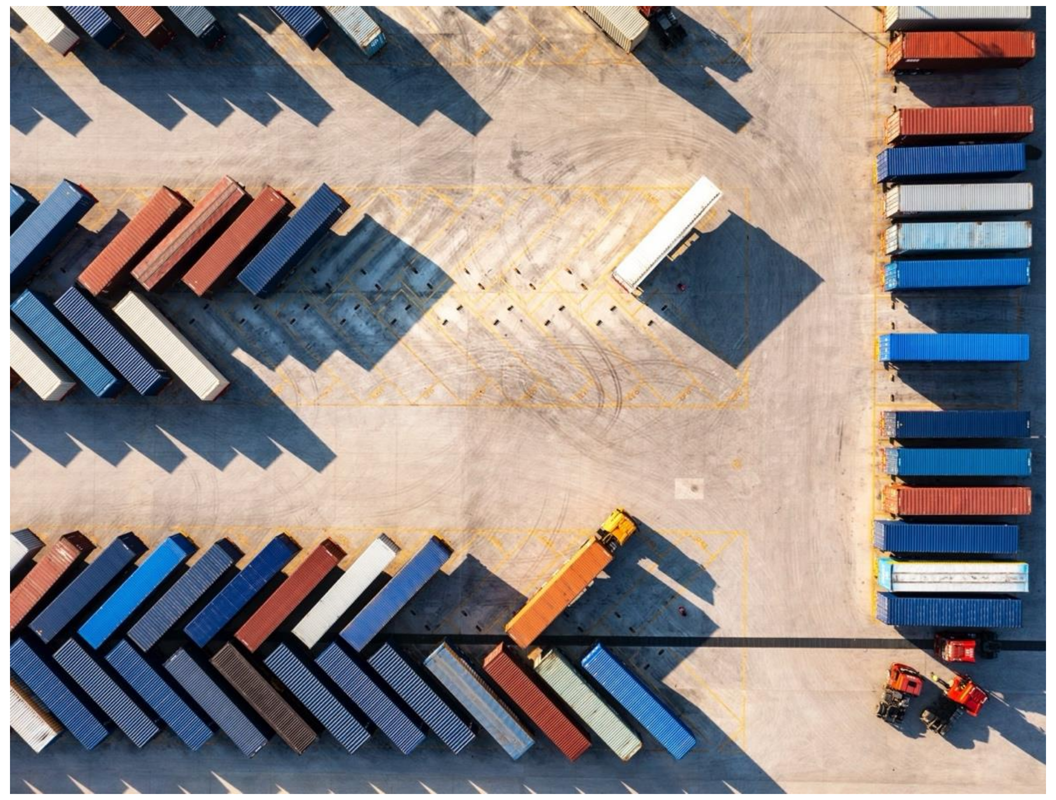
Solving algebra in [exponential] spaces.
Finding hidden patterns in structured problems.

Improving anomaly detection, as for rare events detection and fraud detection



Improving patient outcomes by designing optimal cell-centric therapeutics

Strengthening risk management through better time series and sequence prediction

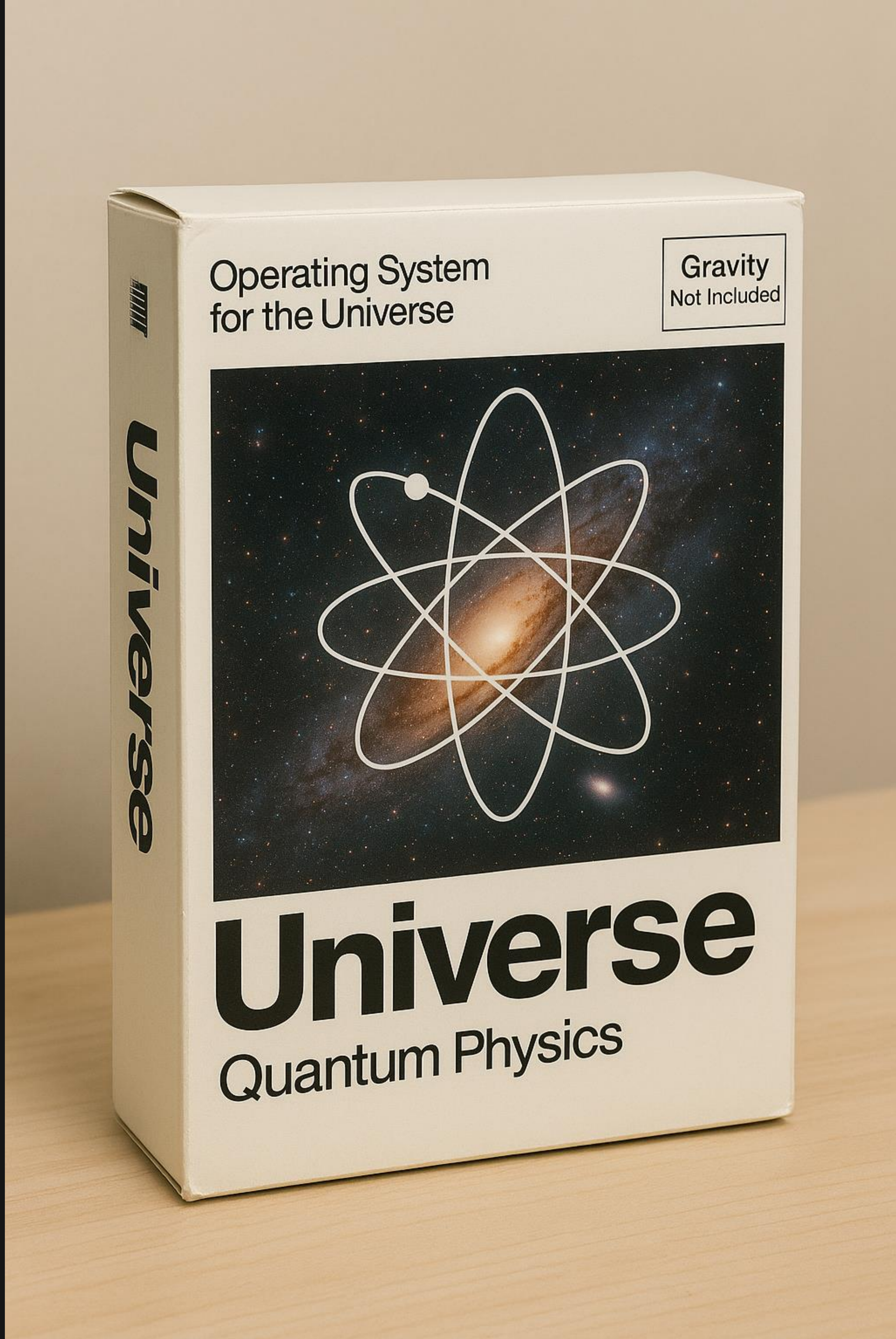


Optimizing vehicle routing and scheduling for large-scale logistics networks

Nature is quantum.

↓

You need quantum to simulate nature.



And we know there are other problems with a structure that quantum can exploit.

↳ So we're also looking for value in problems that are hard classically, like optimization.

State of the technology

Quantum Utility

Gates ⇨ 3K 5K 100M

PRE-UTILITY | ERROR MITIGATION | ERROR CORRECTION

Year ⇨ 2023 2024 2029

All circuits can be brute force run on classical hardware

Only approximate solutions exists and is the regime for exploring quantum advantage

Well in the error correction regime where today’s known quantum algorithms exist


```
for _ in loop:
    qc,matrix,… = do_classical(param)
    A,… = SGESVD(matrix)
    job = sampler.run([qc])
    do_classical(job.result(), A, …)
    …
```

Thesis

The future of computing is mapping all problems to tensors and circuits

What is quantum advantage?

Performing an information processing task more efficiently, cost-effectively, or accurately using quantum computers than is known to be possible with classical computers alone

There are two important nuances to this →

1

We must establish trust in the outputs of a real and noisy quantum device.

A scientific experiment is only as good as confidence in methods.

2

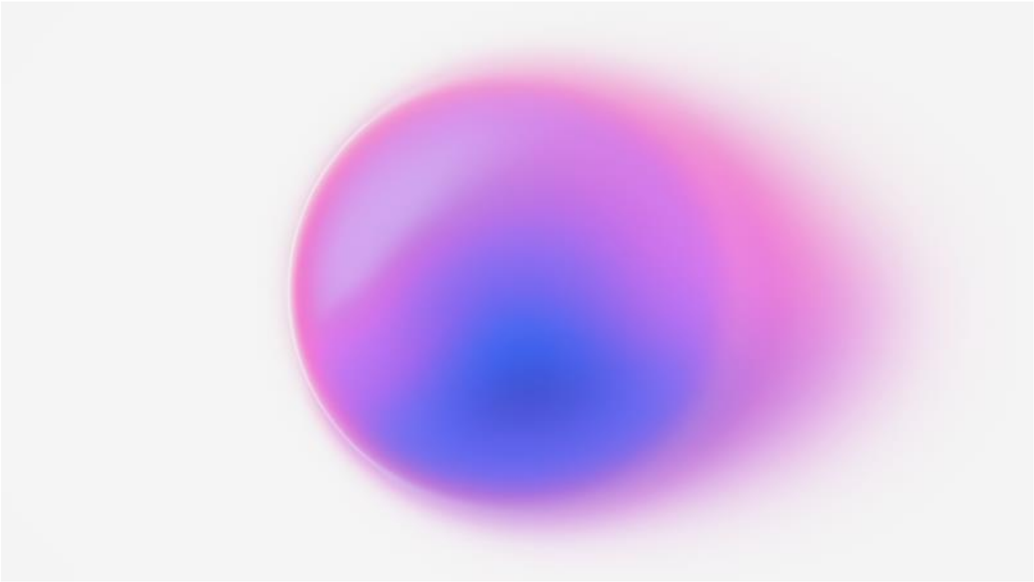
Quantum advantage is not something that will happen at a singular moment in time.

It is a hypothesis that is subject to falsification.

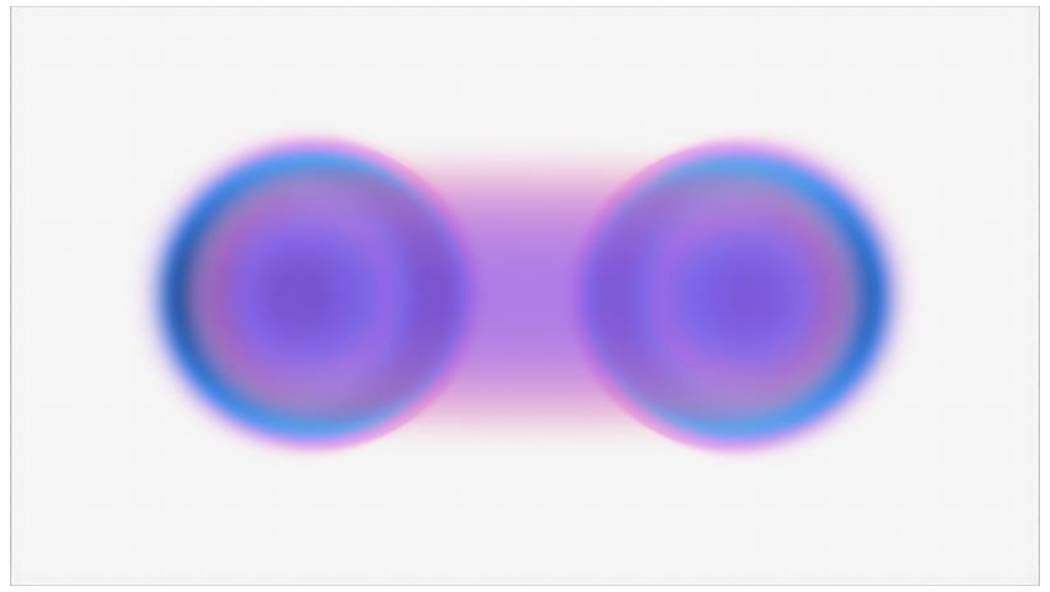
What is quantum computing?

Uniquely quantum

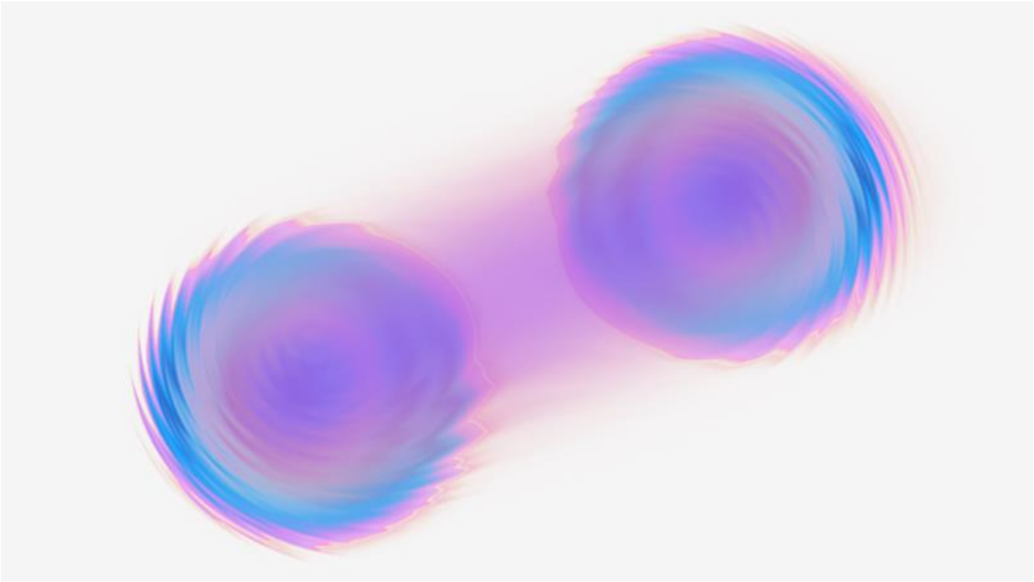
Some problems are classically intractable and will never be solvable with traditional computers



Superposition
A quantum system existing in a complex linear combination of two states until it is measured



Entanglement
Information shared jointly between entangled pairs or groups



Interference
Interaction that affects likelihood of solutions

These Quantum concepts can reduce the number of computational steps required for certain algorithms
&
At a ~100 qubit scale, with sufficient circuit depth and complexity, classical computers can no longer simulate exactly

Moore's law: the number of transistors in a classical integrated circuit doubles about every two years
... but we are approaching the end due to physical limitations

Approaching the physical limit: IBM created the world's first 2 nm node chip in 2021, with transistors as small as 10 silicon atoms

The limit of bits

For decades we've been simplifying nature into 1s and 0s because that was the only way we could manage to create a useful and scalable system of computation.

00100110111001001000100100100110010011100101110
01111100101001000111000100010010100010010010101
01001010101110010011011100100100010010010011001
00111001011100111110010100100011100010001001010
0010010010101010010101011101110011100101011110

The limit of bits

For decades we've been simplifying nature into 1s and 0s because that was the only way we could **manage** to create a useful and scalable system of computation.

But the future isn't just **1**s and **0**s.

0010011011100100100010010010011001001110010111O

0111110010100100011100010001001010001001001010 1

0100101010111001001101110010010001001001001 1001

0011100101110011111001010010001110001000100101 0

0010010010101010010101011101110011100101011110

Bits and classical logic circuits

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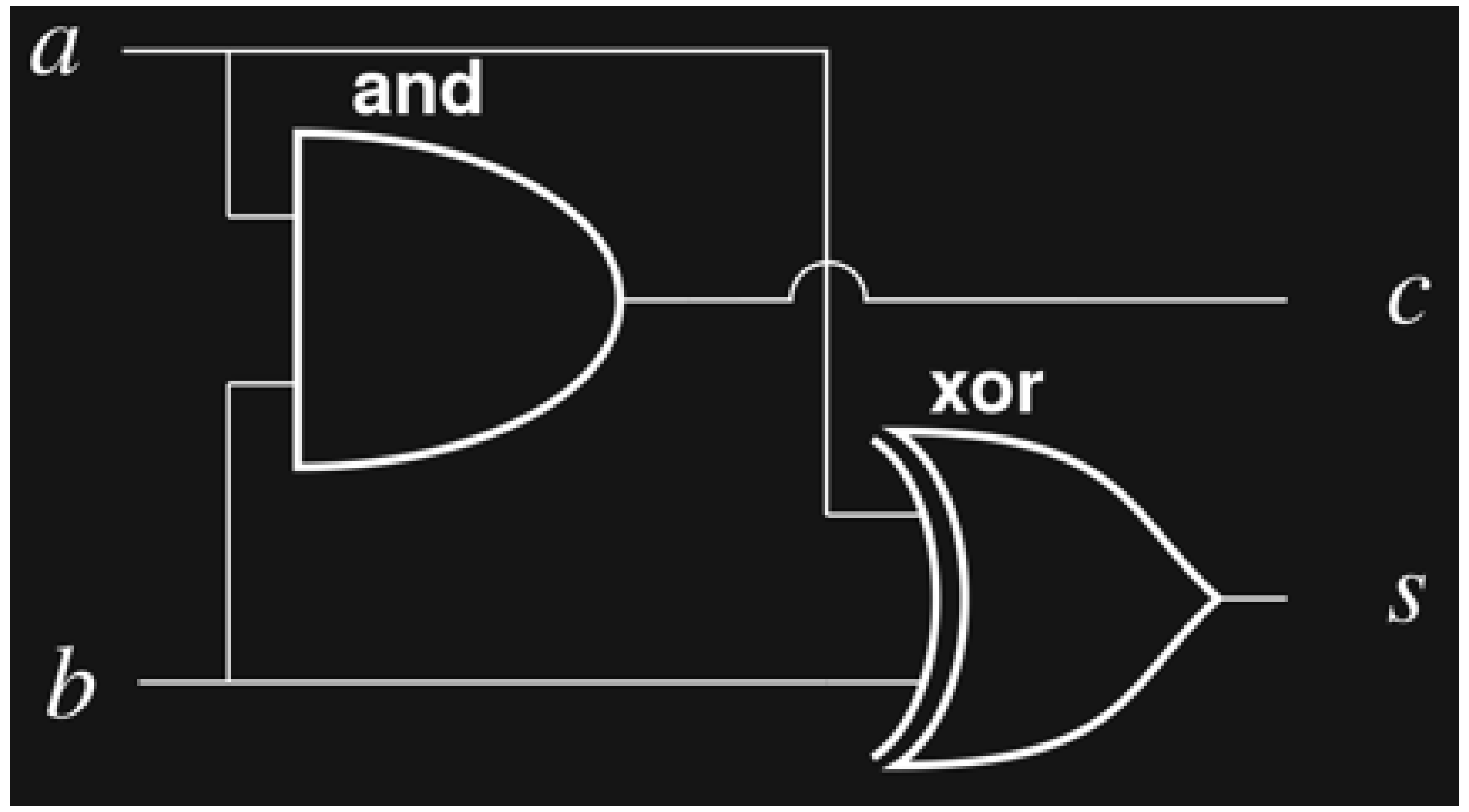
0

•

•

1

A bit is a controllable classical object that is the unit of information



A classical logic circuit is a set of gate operations on bits and is the unit of computation

Quantum bits (qubits) and quantum circuits

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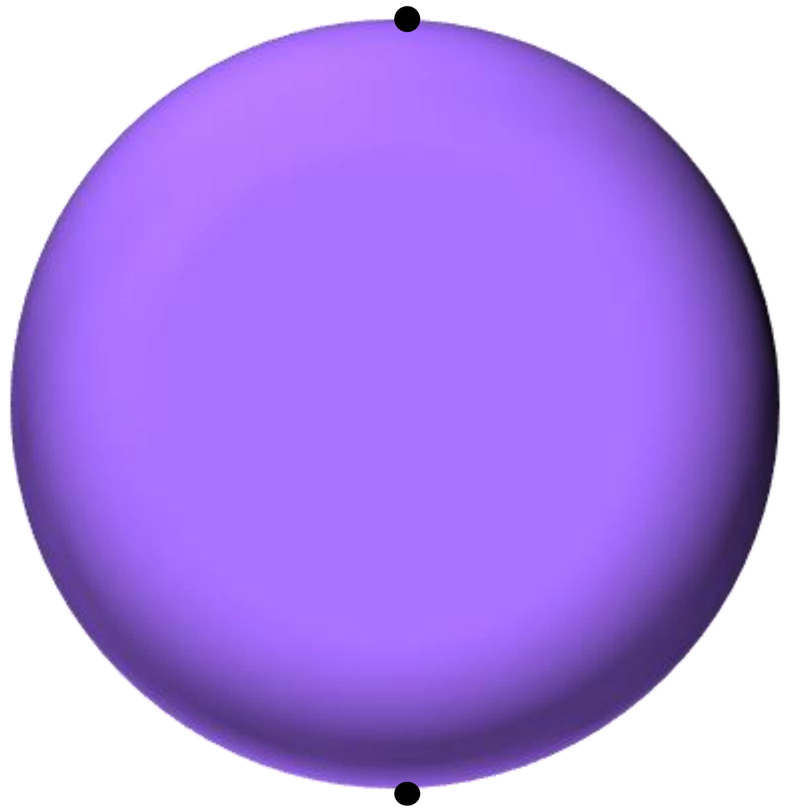
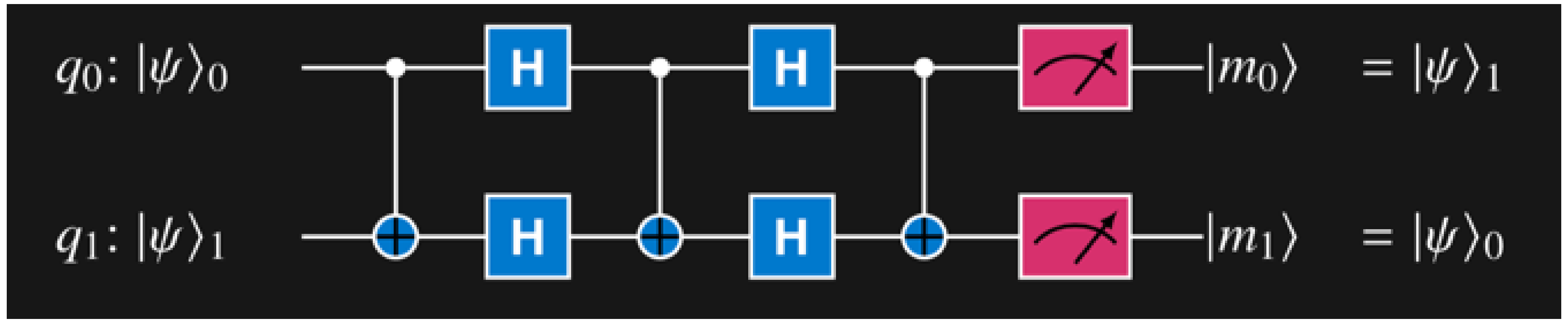
$|0\rangle$



$|1\rangle$

A quantum bit or qubit is a controllable quantum object that is the unit of information



A quantum circuit is a set of quantum gate operations on qubits and is the unit of computation

Bits and qubits

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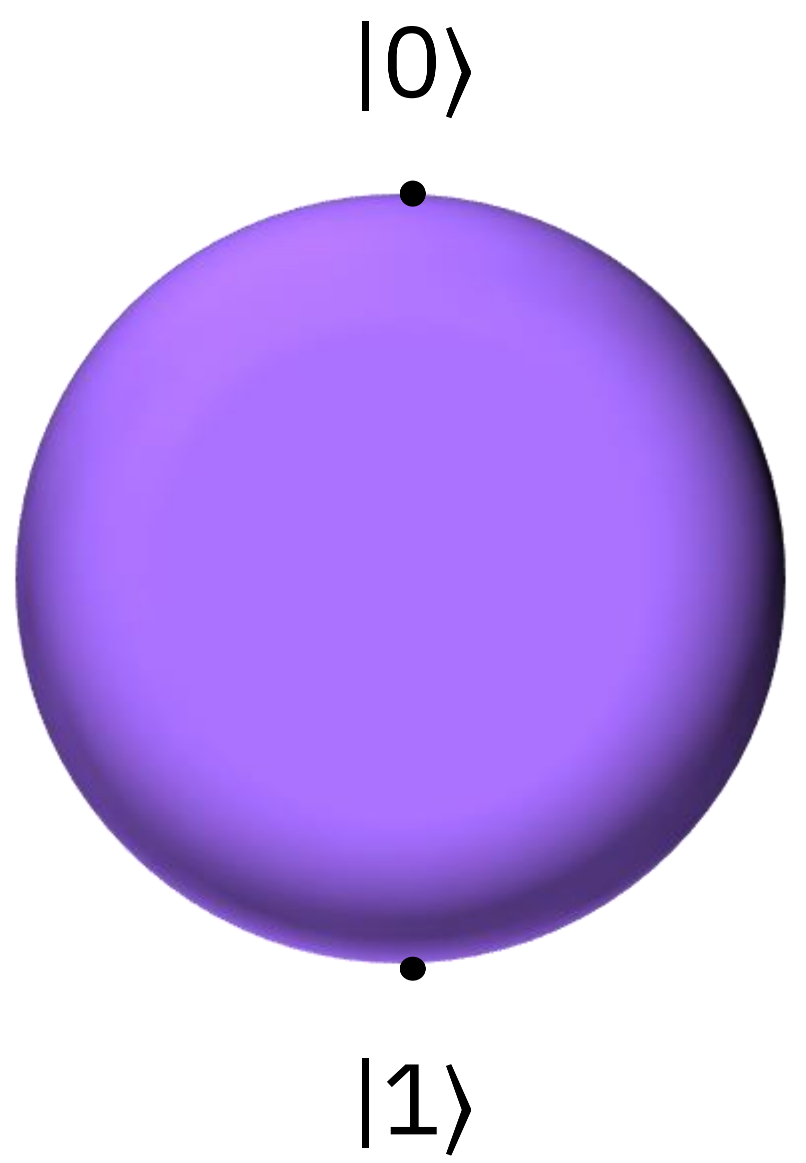

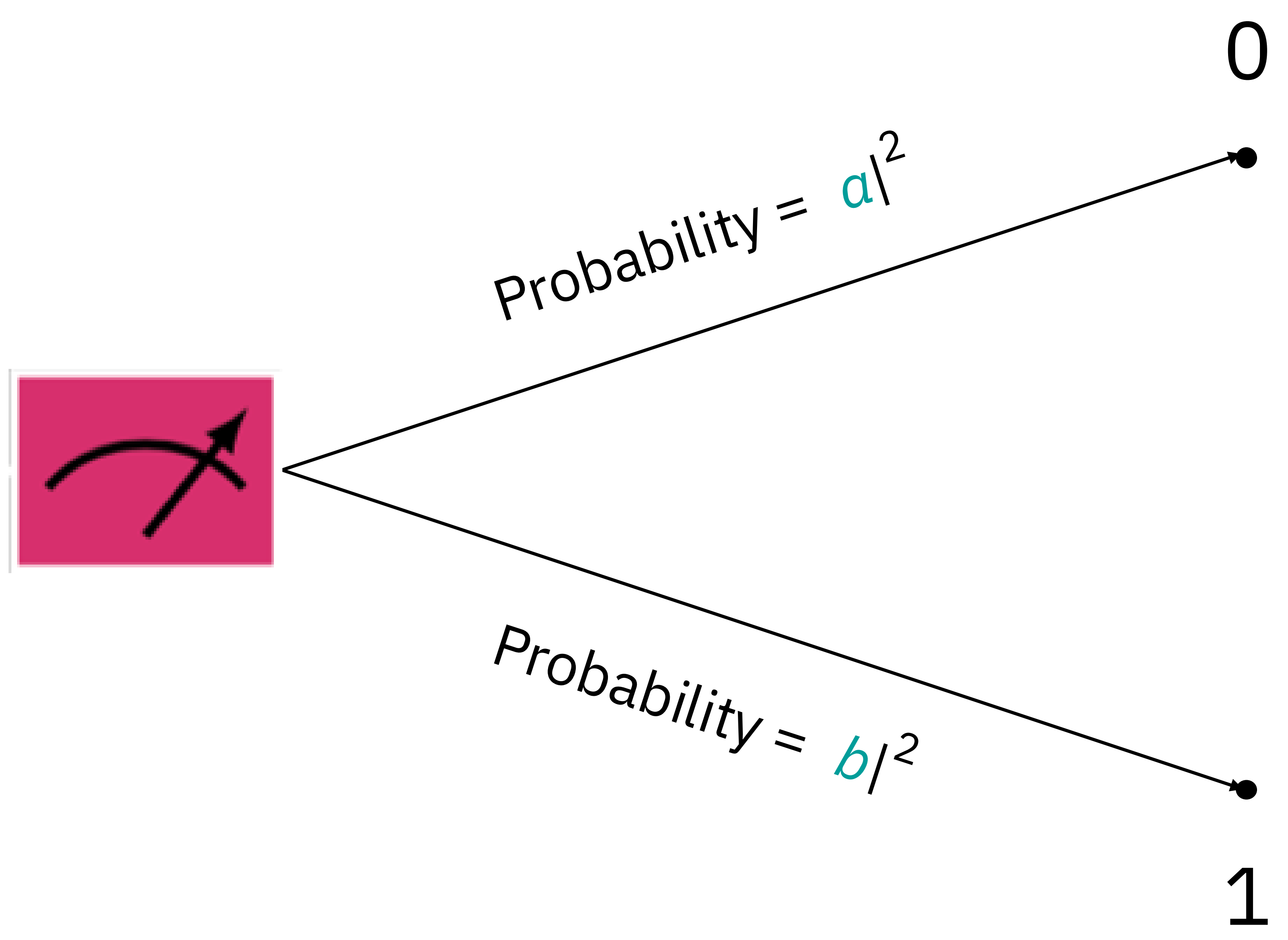

A qubit's state is a combination of $|0\rangle$ and $|1\rangle$:

$$a\,|0\rangle + b\,|1\rangle$$

This means that a single qubit contains two pieces of information.

When we measure a qubit, it becomes **0** or **1** based on probability.

Bits and qubits: the effect of the **X** gate on $|0\rangle$

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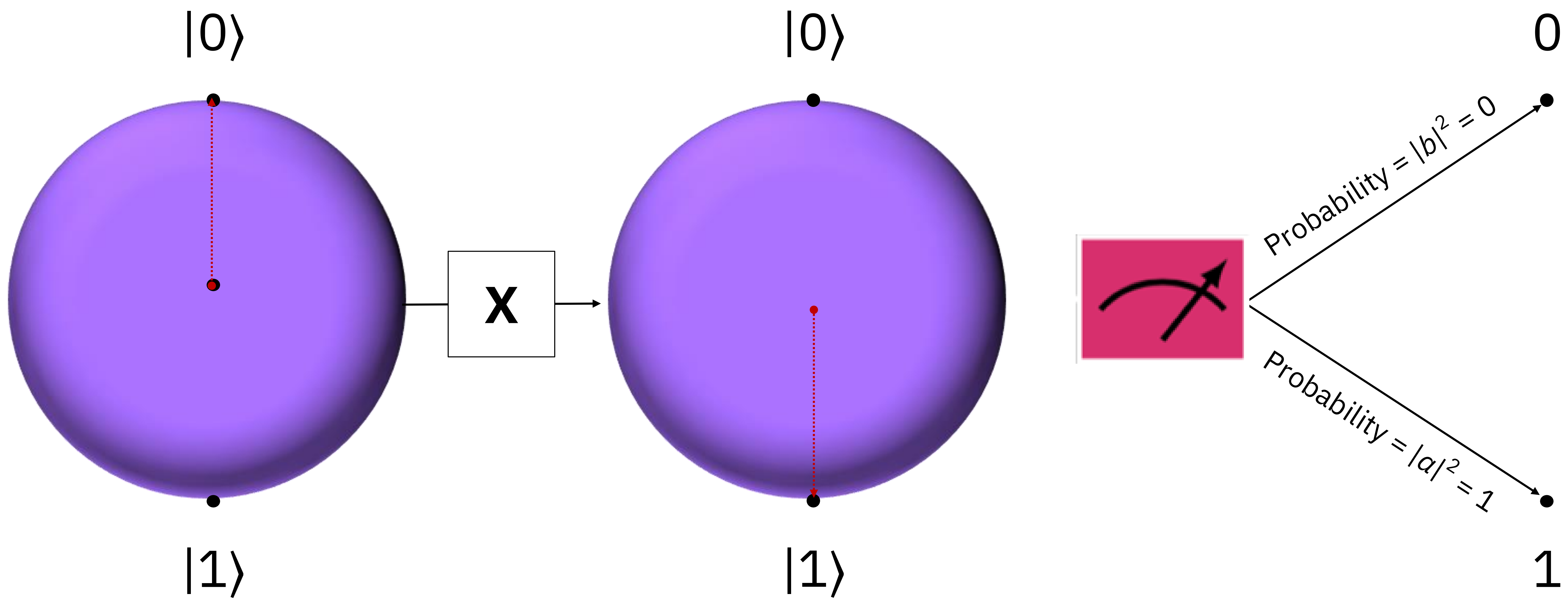


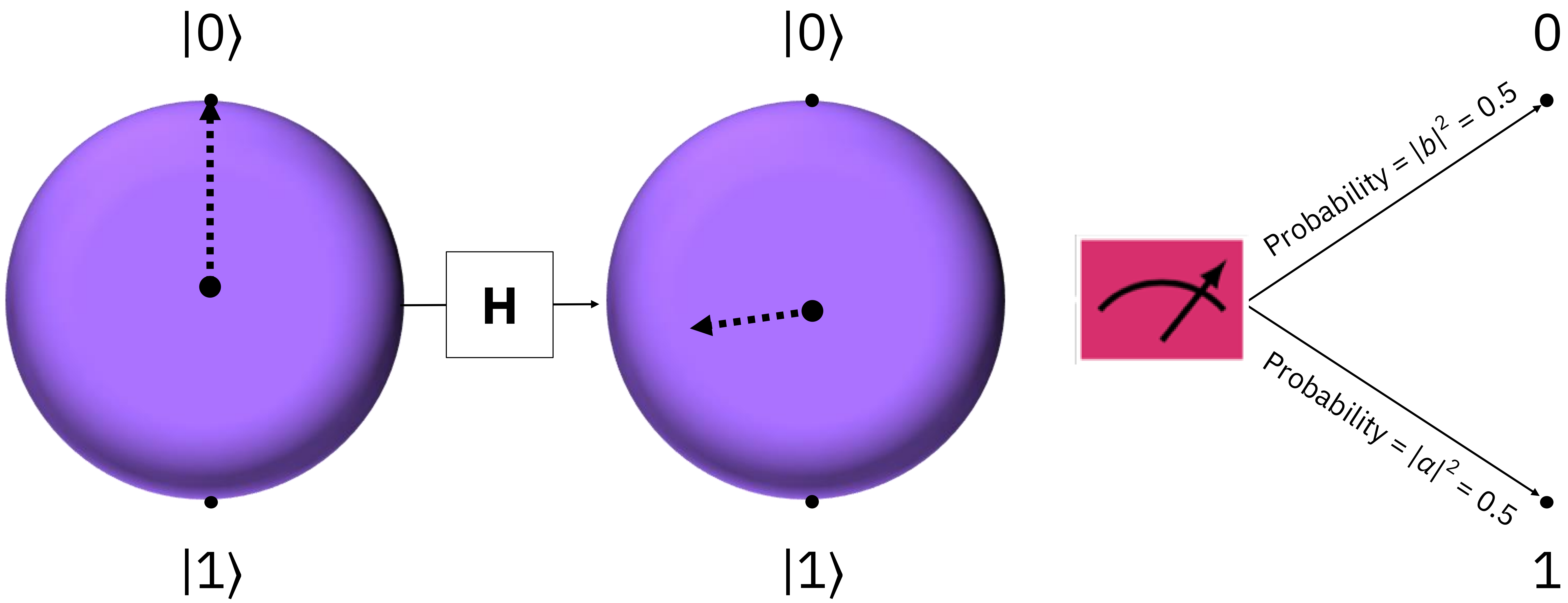
The **X** gate reverses $|0\rangle$ and $|1\rangle$:

$a\,|0\rangle + b\,|1\rangle \;\mapsto\; b\,|0\rangle + a\,|1\rangle$

$a = 1$ and $b = 0$, so $|0\rangle$ is mapped to $|1\rangle$.

When measured, the result is **1** with 100% probability.

Bits and qubits: the effect of the **H** gate on $|0\rangle$



The **H** gate maps $|0\rangle$ via

$$|0\rangle \mapsto (1/\sqrt{2})\,|0\rangle + (1/\sqrt{2})\,|1\rangle = a\,|0\rangle + b\,|1\rangle$$

Since $a = b = 1/\sqrt{2}$, $|a|^2 = |b|^2 = ½$.

When measured, the probability of getting **0** or **1** is the same, 0.5.
Quantum randomness!

Quantum computing uses essential ideas from quantum mechanics

Superposition

$|0\rangle$ and $|1\rangle$ are vectors in the two-dimensional complex vector space $\mathbf{C}^2$:

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

So we can write any vector in $\mathbf{C}^2$ as

$$a\,|0\rangle + b\,|1\rangle$$

We pronounce $|0\rangle$ and $|1\rangle$ as “ket zero” and “ket one.” These are called the *computational basis*.

Quantum computing uses essential ideas from quantum mechanics

Superposition

Superposition is creating a quantum state that is a combination of $|0\rangle$ and $|1\rangle$

$$a\,|0\rangle + b\,|1\rangle$$

where

a and b are complex numbers

$|a|^2 + |b|^2 = 1$

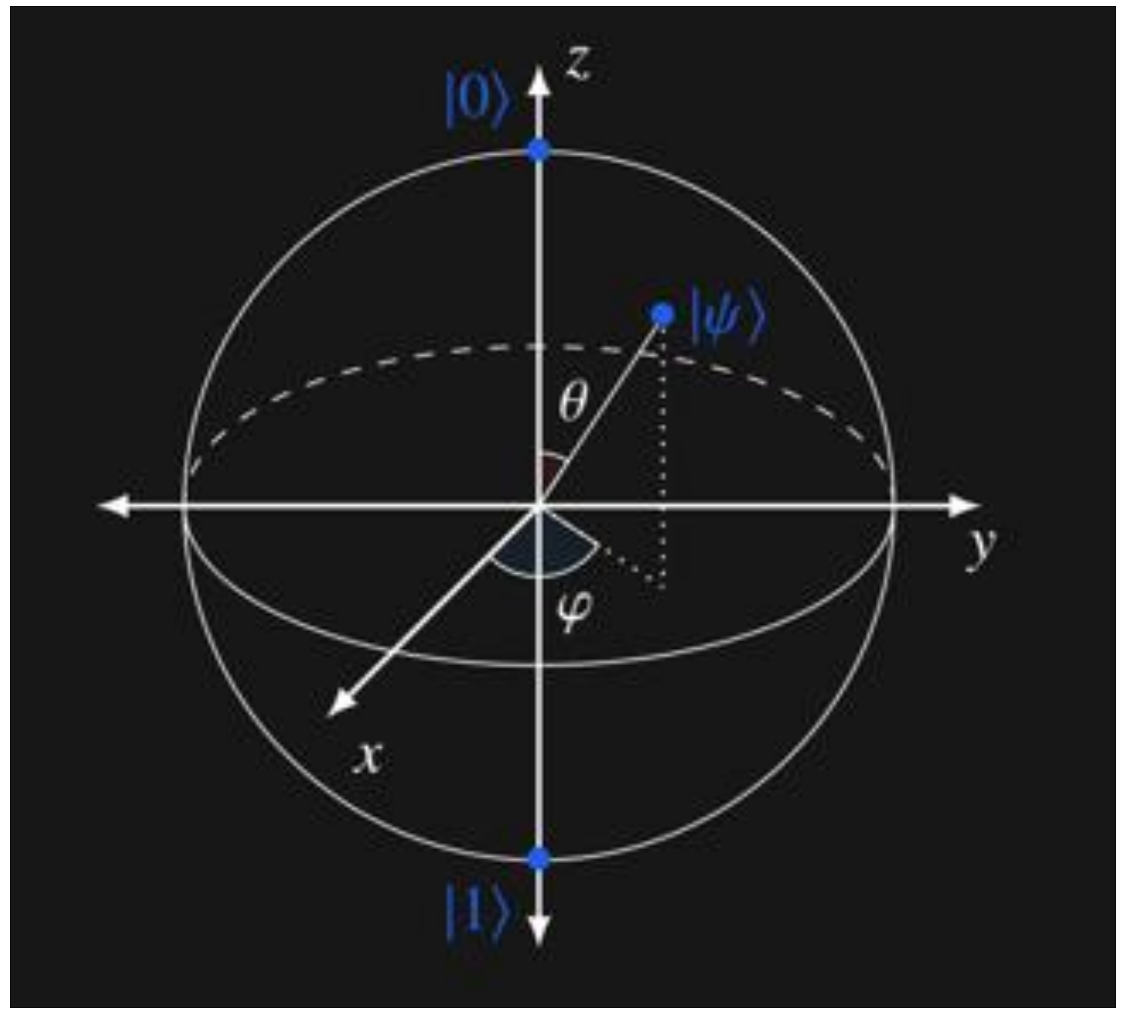
Two quantum states are equivalent if they differ only by a constant multiple u where $|u| = 1$.

This is because

$$|a|^2 + |b|^2 = |au|^2 + |bu|^2 = 1$$

Quantum computing uses essential ideas from quantum mechanics

Superposition



Superposition is creating a quantum state that is a combination of $|0\rangle$ and $|1\rangle$

$$a\,|0\rangle + b\,|1\rangle$$

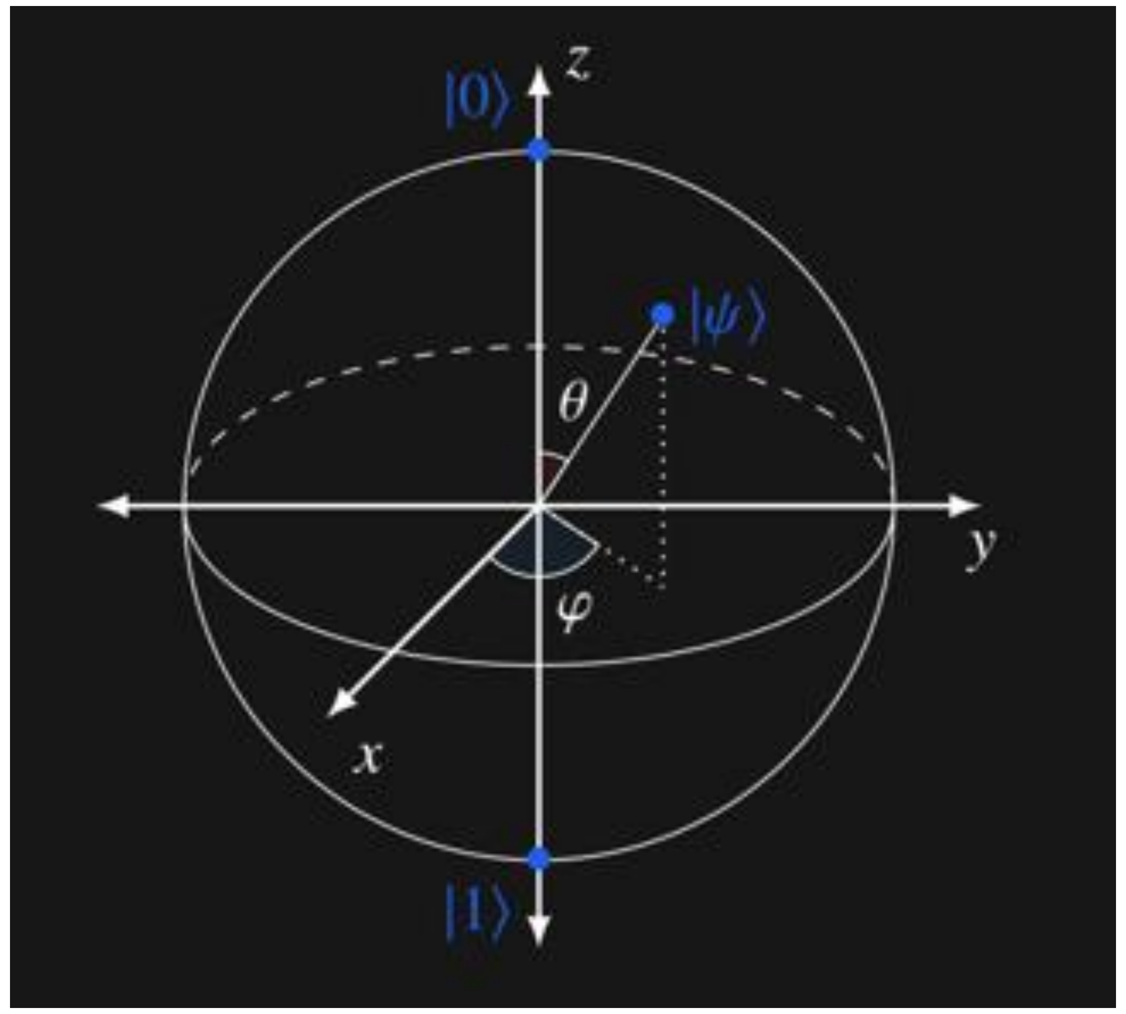
These conditions allow us to map the qubit onto the *Bloch Sphere*.

Note that if a and b are non-zero, then the qubit's state contains both $|0\rangle$ and $|1\rangle$.

This is what people mean when they say that a qubit can be "0 and 1 at the same time."

Quantum computing uses essential ideas from quantum mechanics

Measurement



Measurement is forcing the qubit's state

$$a\,|0\rangle + b\,|1\rangle$$

to $|0\rangle$ or $|1\rangle$ by observing it, where

$|a|^2$ is the probability we will get $|0\rangle$ when we measure

$|b|^2$ is the probability we will get $|1\rangle$ when we measure

For example,

$$\frac{\sqrt{2}}{2}\,|0\rangle + \frac{\sqrt{2}}{2}\,|1\rangle$$

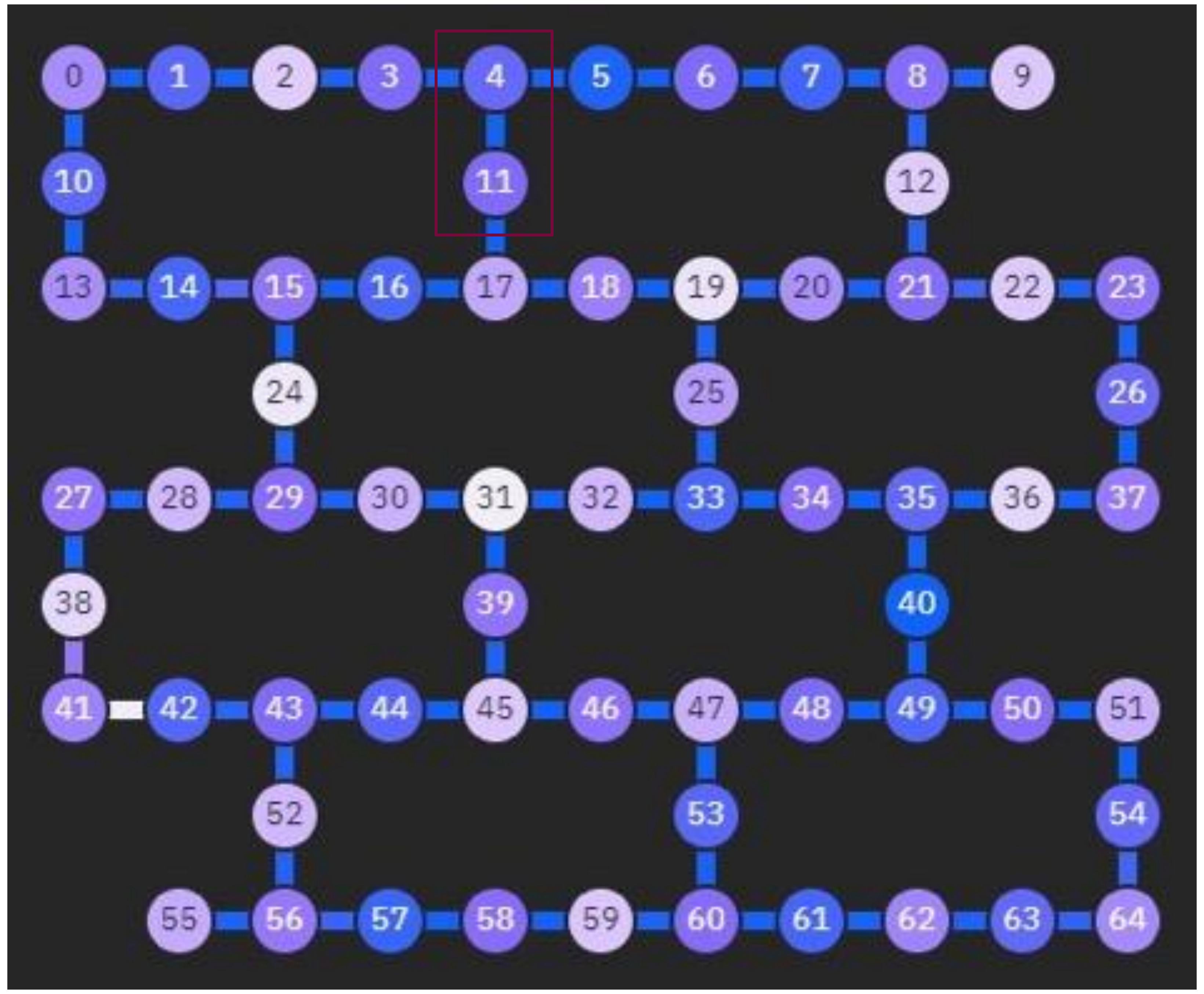
has an equal probability of becoming $|0\rangle$ or $|1\rangle$, and

$$\frac{\sqrt{3}}{2}\,|0\rangle - \frac{1}{2}\,i\,|1\rangle$$

has a 75% chance of becoming $|0\rangle$.

Quantum computing uses essential ideas from quantum mechanics

Entanglement



With two qubits we get combinations like

$$a\,|00\rangle + b\,|01\rangle + c\,|10\rangle + d\,|11\rangle$$

where

$|01\rangle$ means the first qubit is $|0\rangle$ and the second is $|1\rangle$

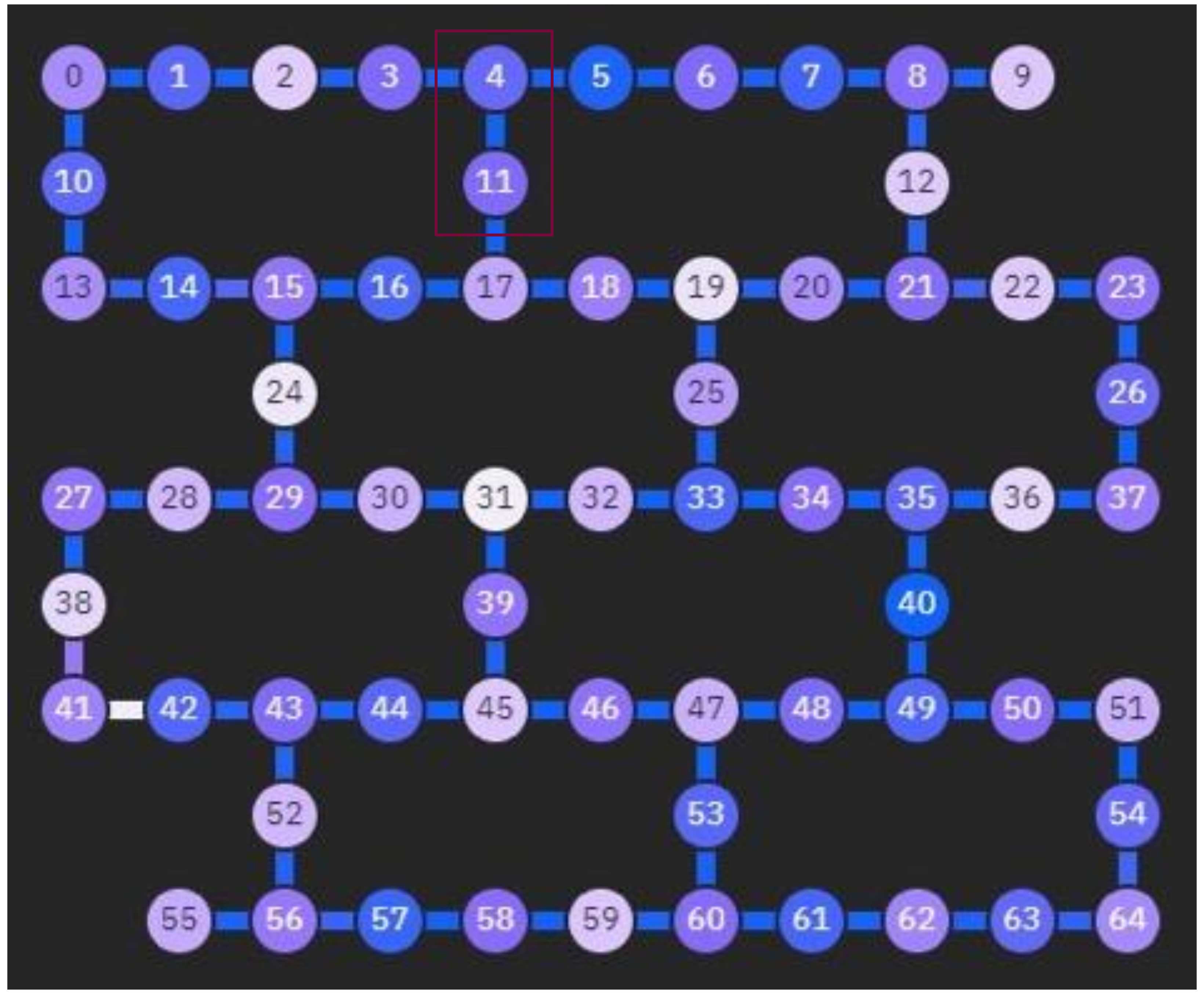
a, b, c, and d are complex numbers and

$$|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1$$

If two or more of the a, b, c, and d are non-zero, and we cannot separate the qubits, they are entangled with perfect correlation and are no longer independent.

Quantum computing uses essential ideas from quantum mechanics

Entanglement



For example,

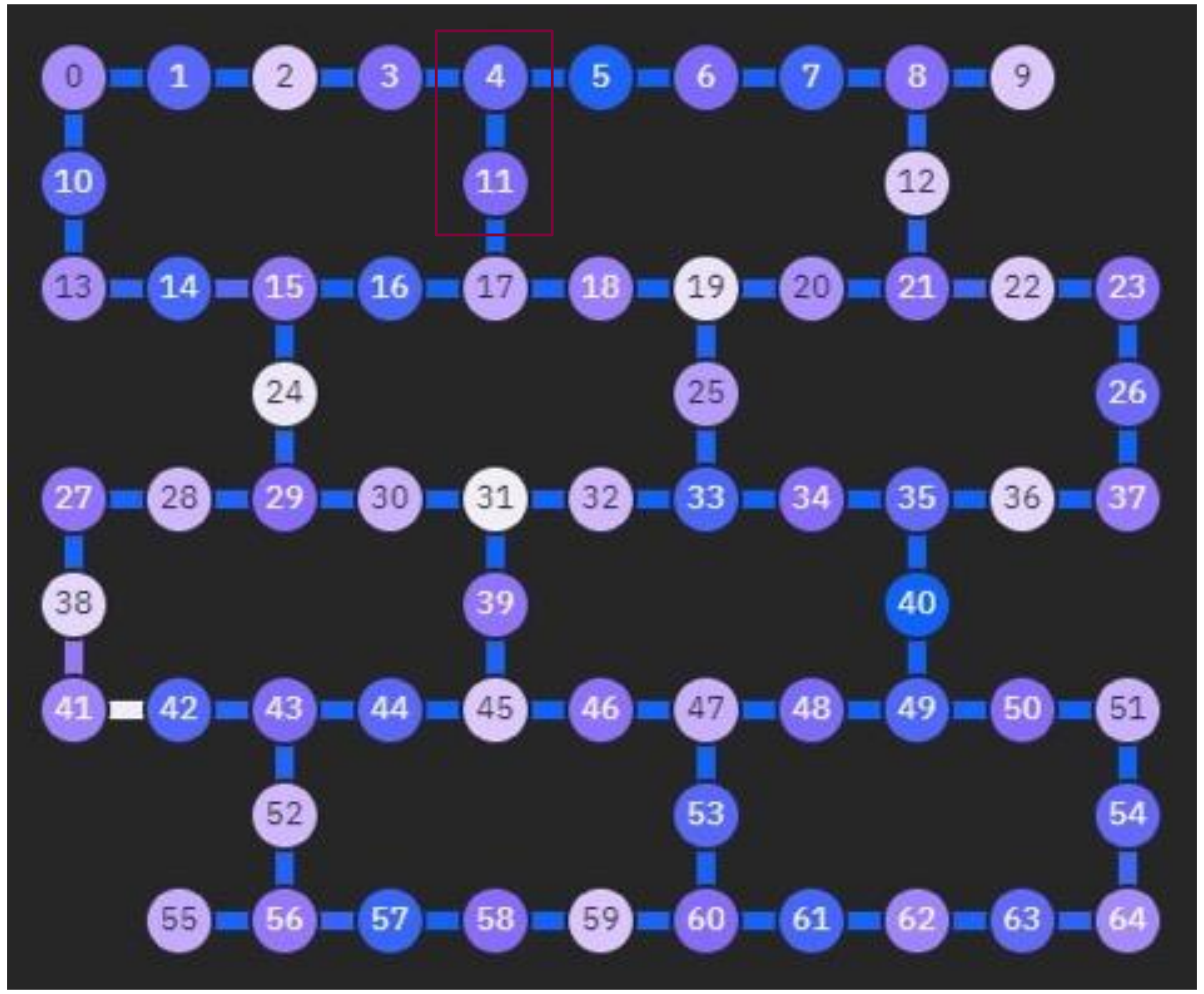
$\frac{\sqrt{2}}{2}|00\rangle + \frac{\sqrt{2}}{2}|01\rangle$ not entangled

$\frac{\sqrt{2}}{2}|01\rangle - \frac{\sqrt{2}}{2}|10\rangle$ entangled

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

Quantum computing uses essential ideas from quantum mechanics

Entanglement



We can write

$$\frac{\sqrt{2}}{2}\,|00\rangle + \frac{\sqrt{2}}{2}|01\rangle$$

as

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

but we cannot write

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

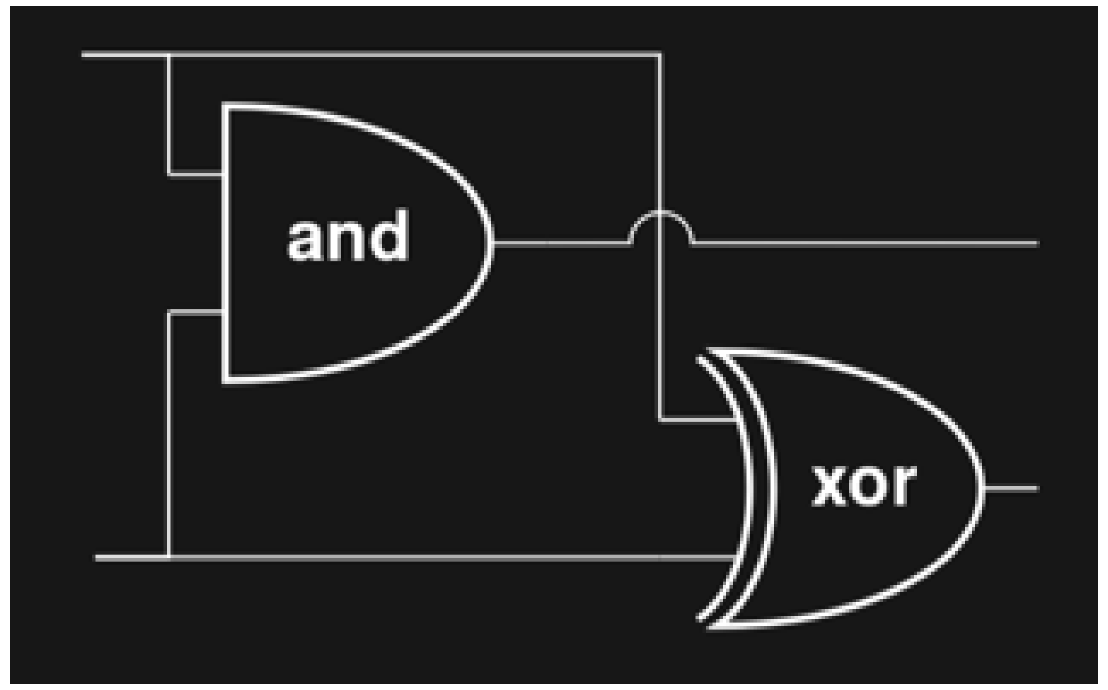
as the “product” of two single qubit states.

They are entangled!

Once you measure the first qubit, the second is uniquely determined.

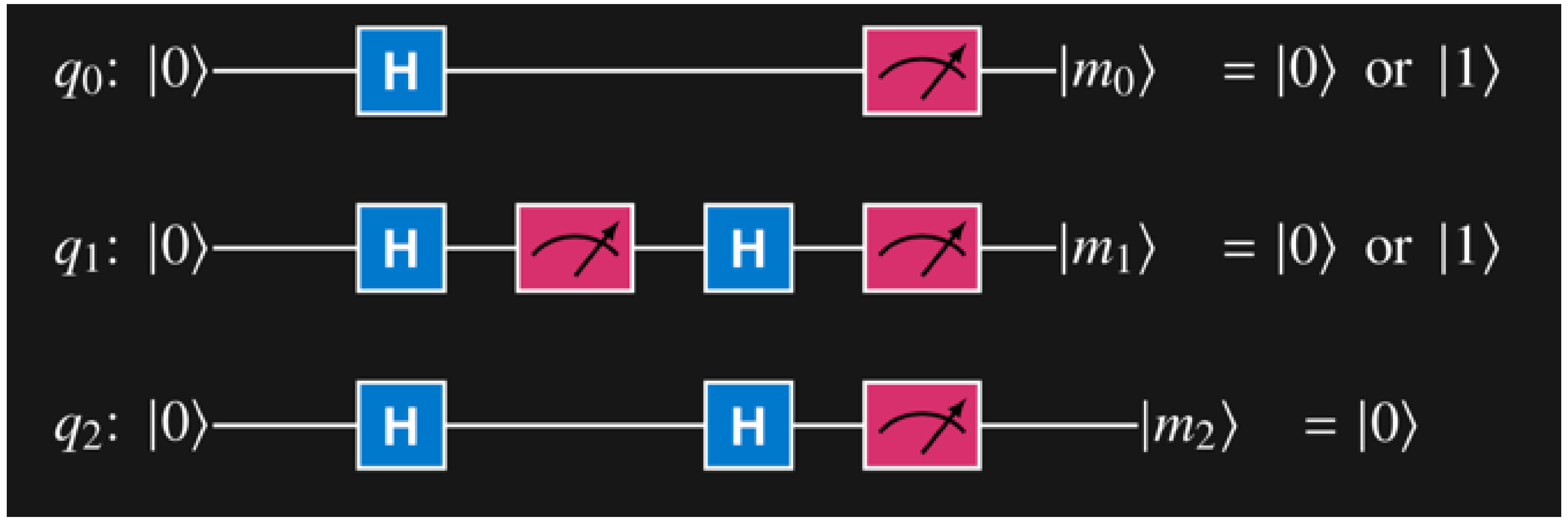
Quantum computing uses essential ideas from quantum mechanics

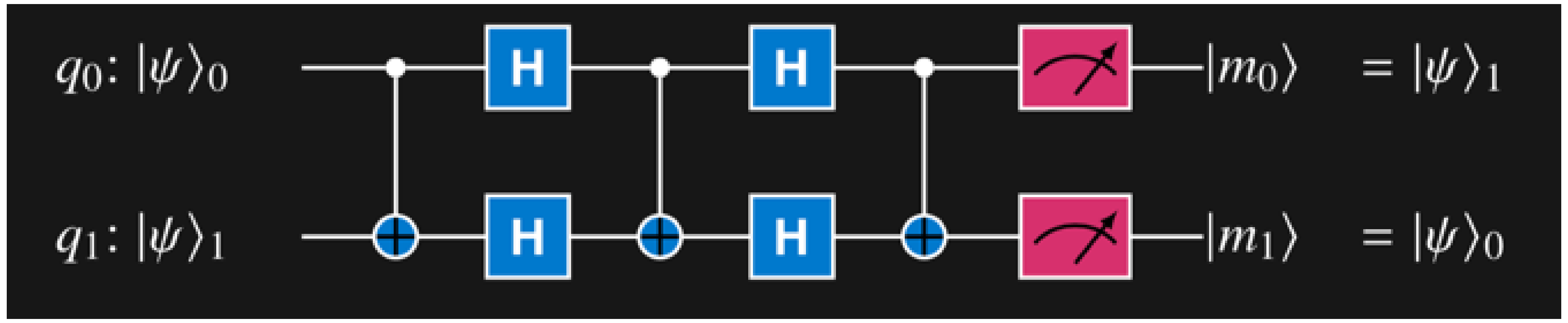
Gates / operations



Classical logical circuits use operations like and, or, not, nand, and xor. We also call these gates.

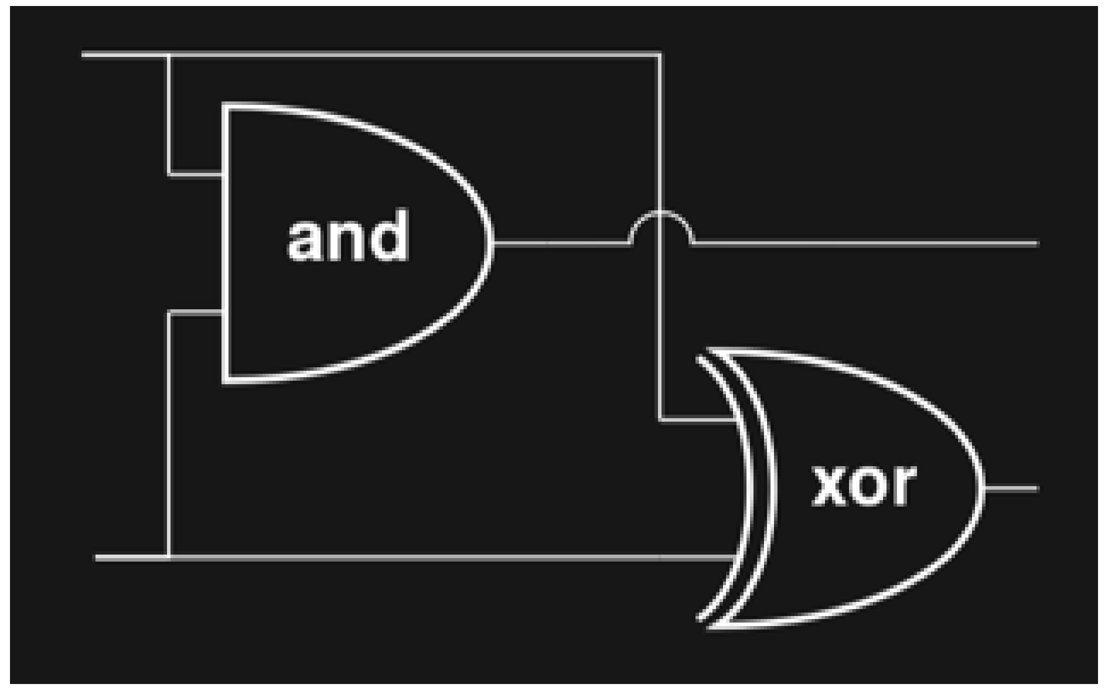
Quantum circuits use reversible gates that change the quantum states of one, two , or more qubits.





Quantum computing uses essential ideas from quantum mechanics

Gates / operations



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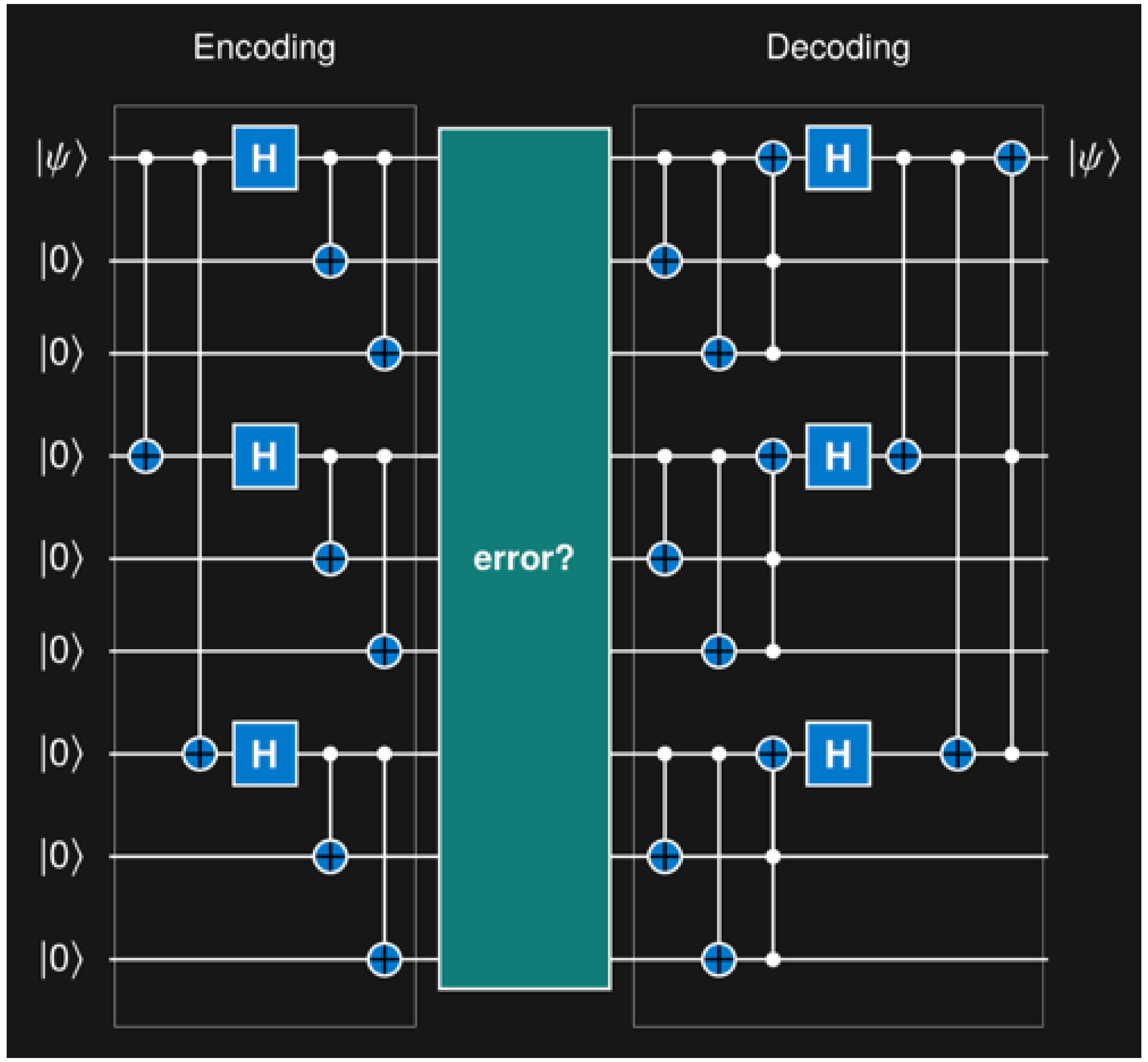
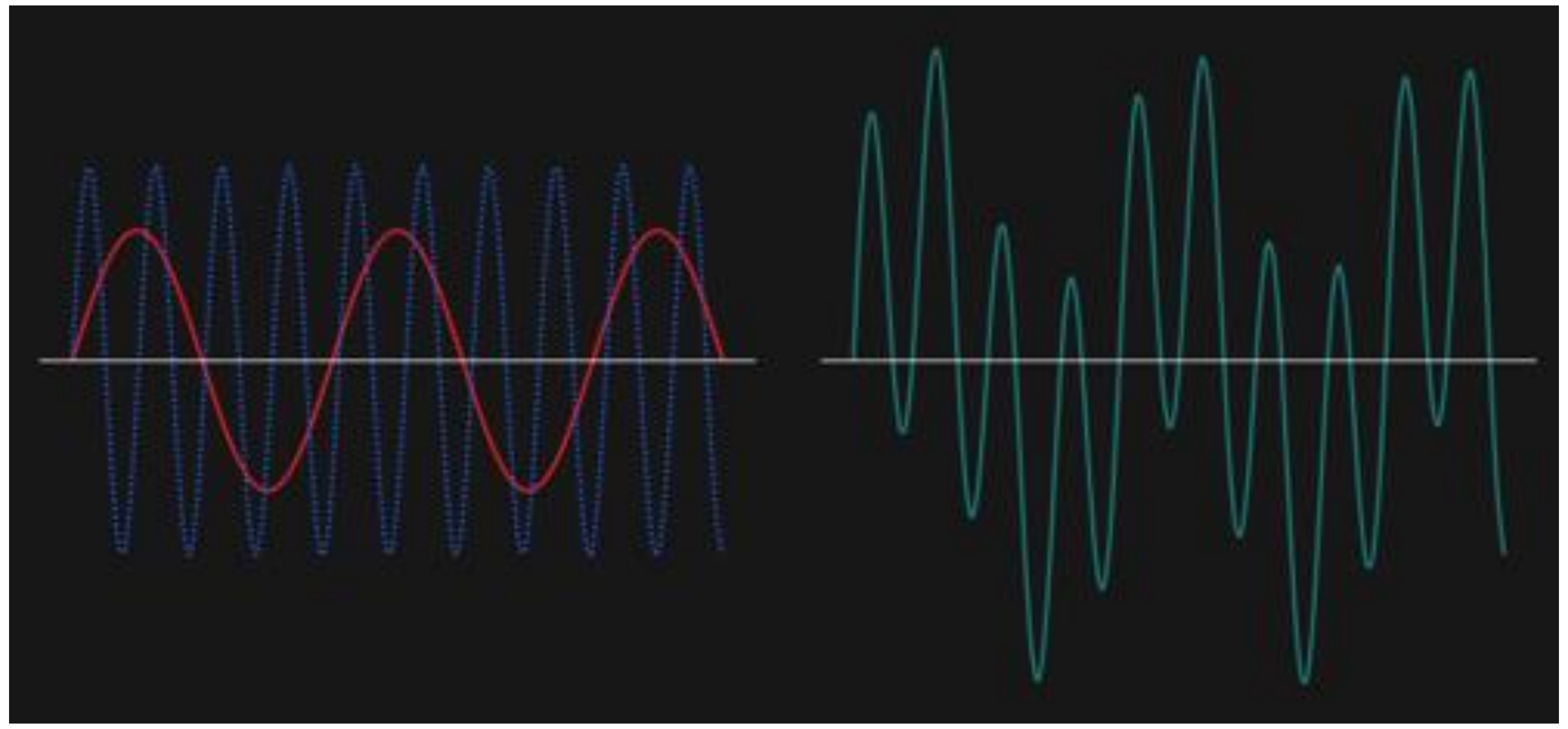
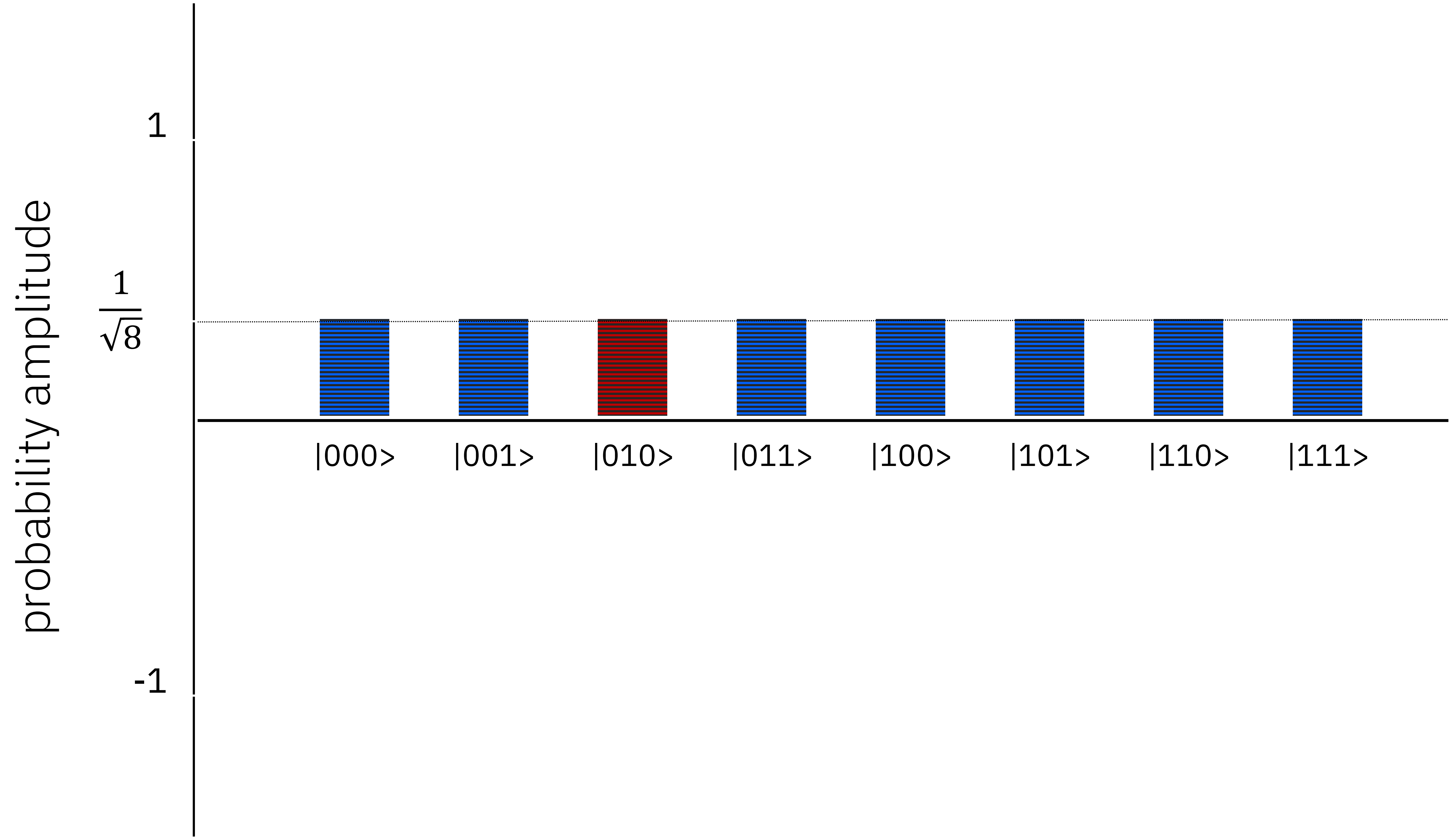


Quantum computing uses essential ideas from quantum mechanics

Interference allows us to increase the probability of getting the right answer and decrease the chance of getting the wrong one.

Interference





Quantum computing uses essential ideas from quantum mechanics

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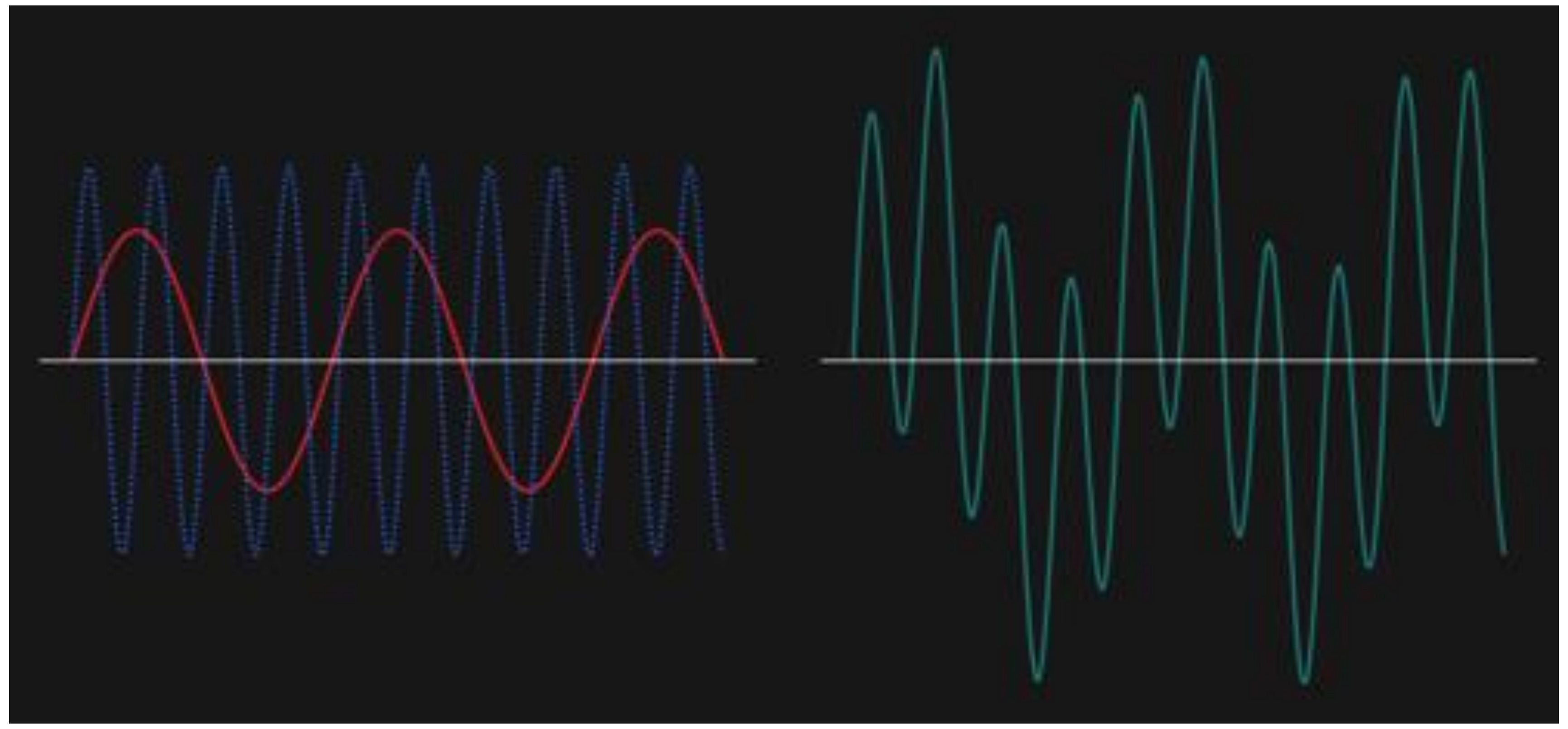
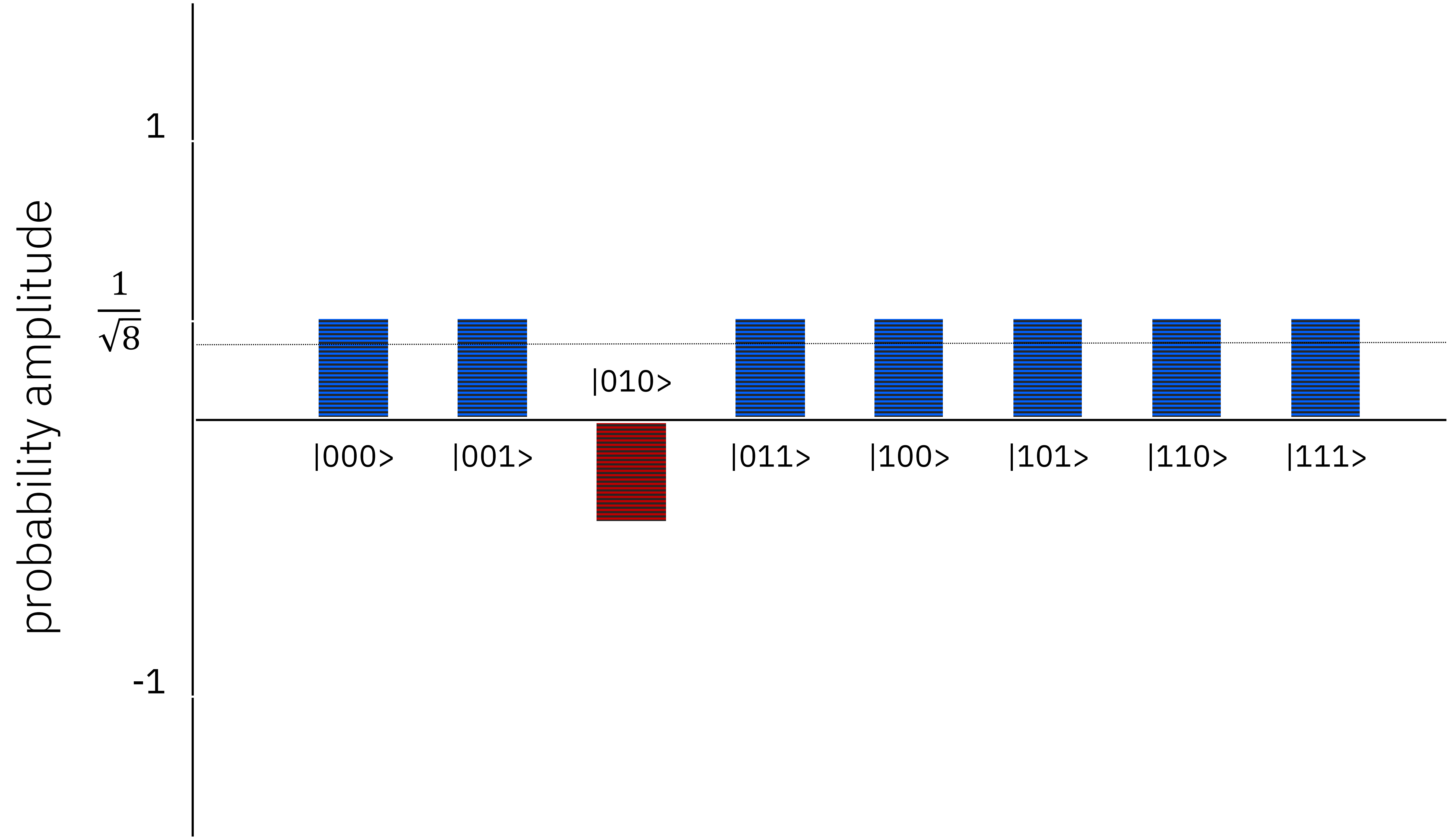
Interference allows us to increase the probability of getting the right answer and decrease the chance of getting the wrong one.





Quantum computing uses essential ideas from quantum mechanics

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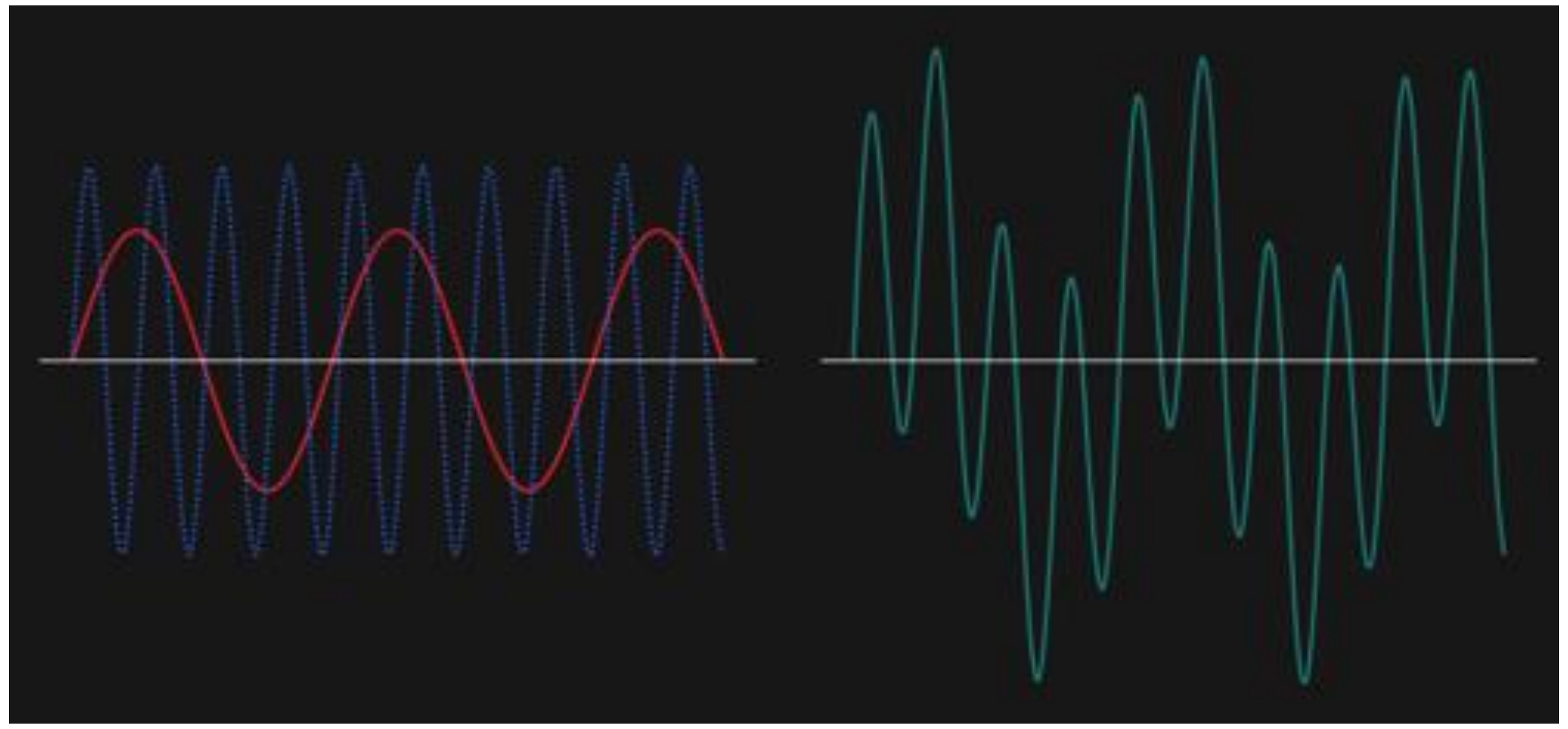
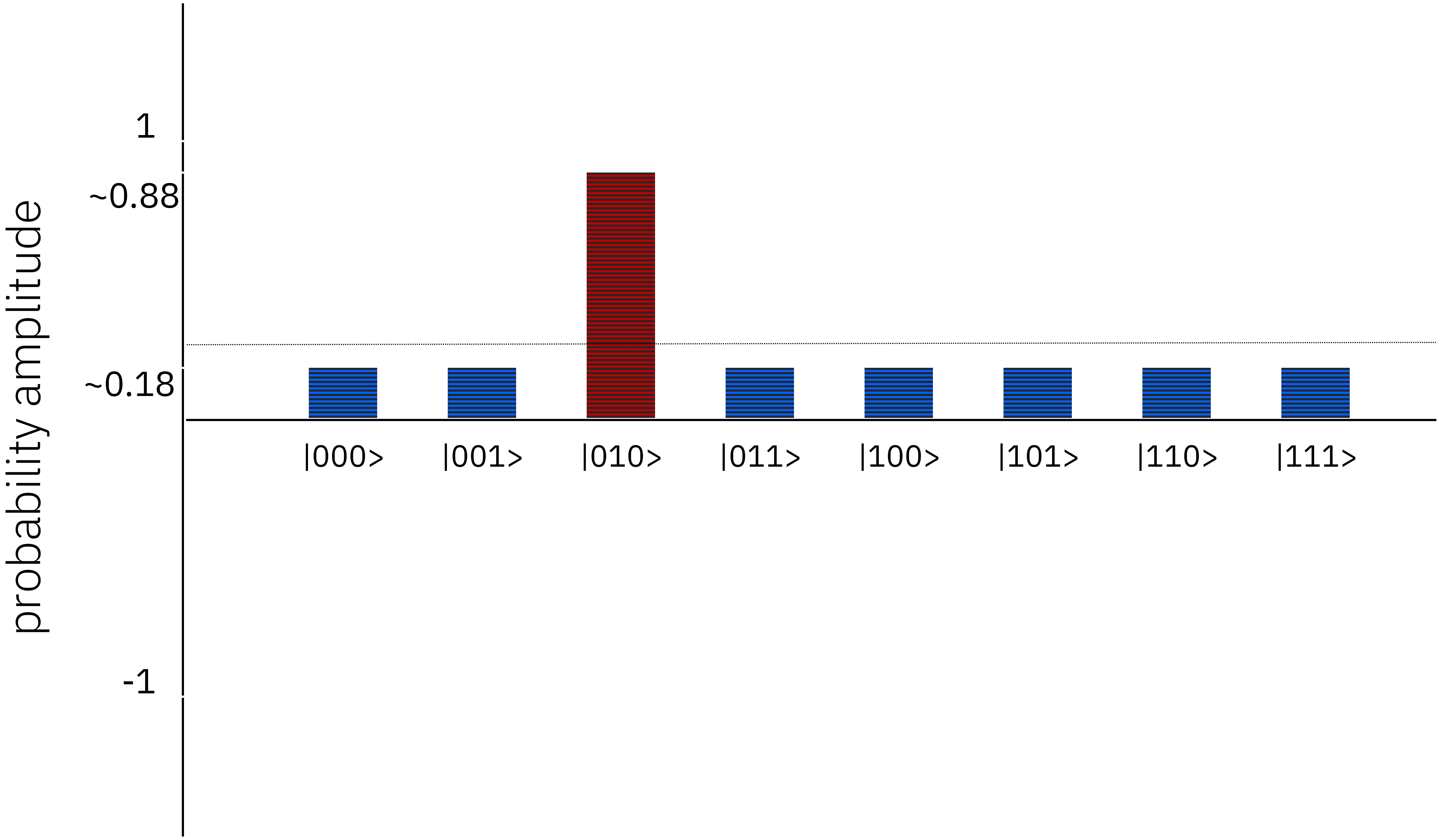
Interference



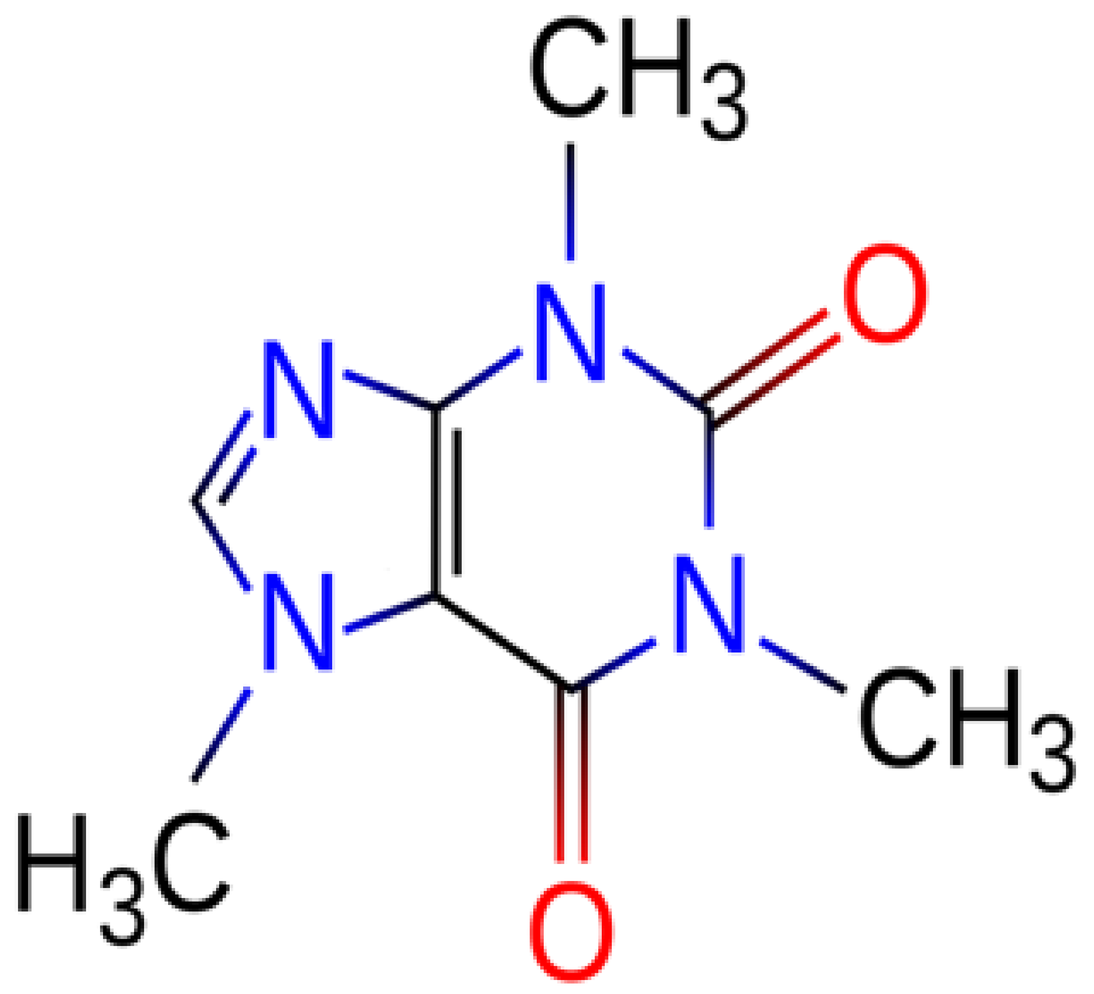


Computing with caffeine

If our best classical computers are so powerful, shouldn't we be able to perfectly simulate molecules and chemical reactions?

This would allow us to accelerate discovery of new compounds and processes for healthcare, materials, alloys, and sustainable energy creation.

Let's consider caffeine …



Computing with caffeine

We would need approximately 10^{48} bits to represent the energy configuration of a single caffeine molecule at a single instant in a classical computer.

This is 1 to 10% of the total number of atoms in the Earth.

10^{48} = 1,000,000,000,000,000,
000,000,000,000,000,000,
000,000,000,000,000

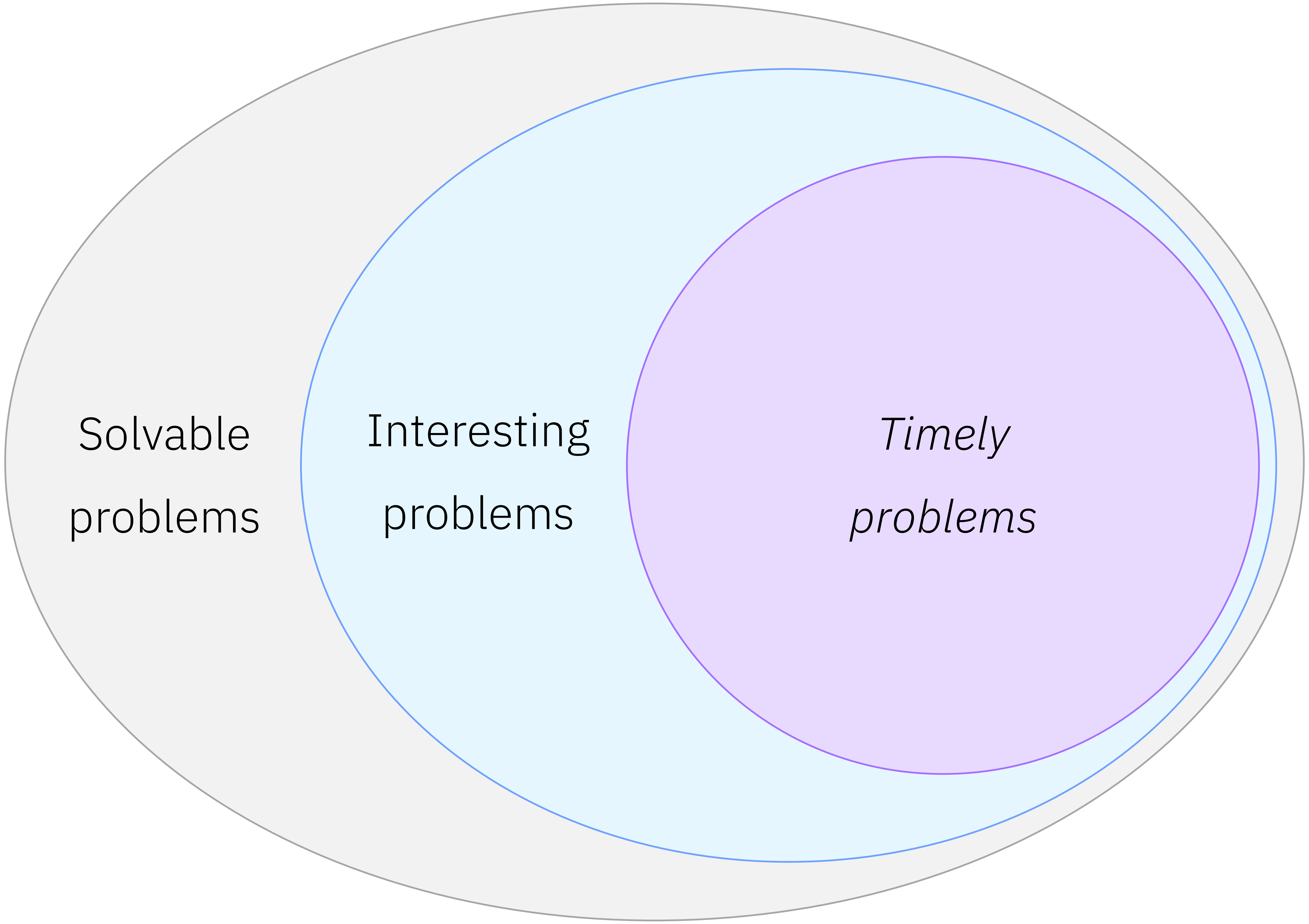
Computing with caffeine

Although it's impossible to completely represent the molecular configuration of caffeine on today's most powerful super computers, we could represent it using 160 logical qubits.

Problem hierarchy

Quantum computers are valuable for solving many different types of problems. However, not all problems are equally relevant.

The success of the field depends on showing value beyond what classical capabilities alone can achieve.



When to use a quantum computer

Easy
Problems

Sweet spot

Very Hard
Problems

**No need
for QC**

Arithmetic
video games

**Need
fault-tolerant QC**

Shor’s Algorithm
Grovers Algorithm

See Quantum Computing in Practice | Which Problems Are Quantum Computers Good For? for additional discussion and insights

Quantum computing is expected to have impact across industries

Example use cases

Nearer Term

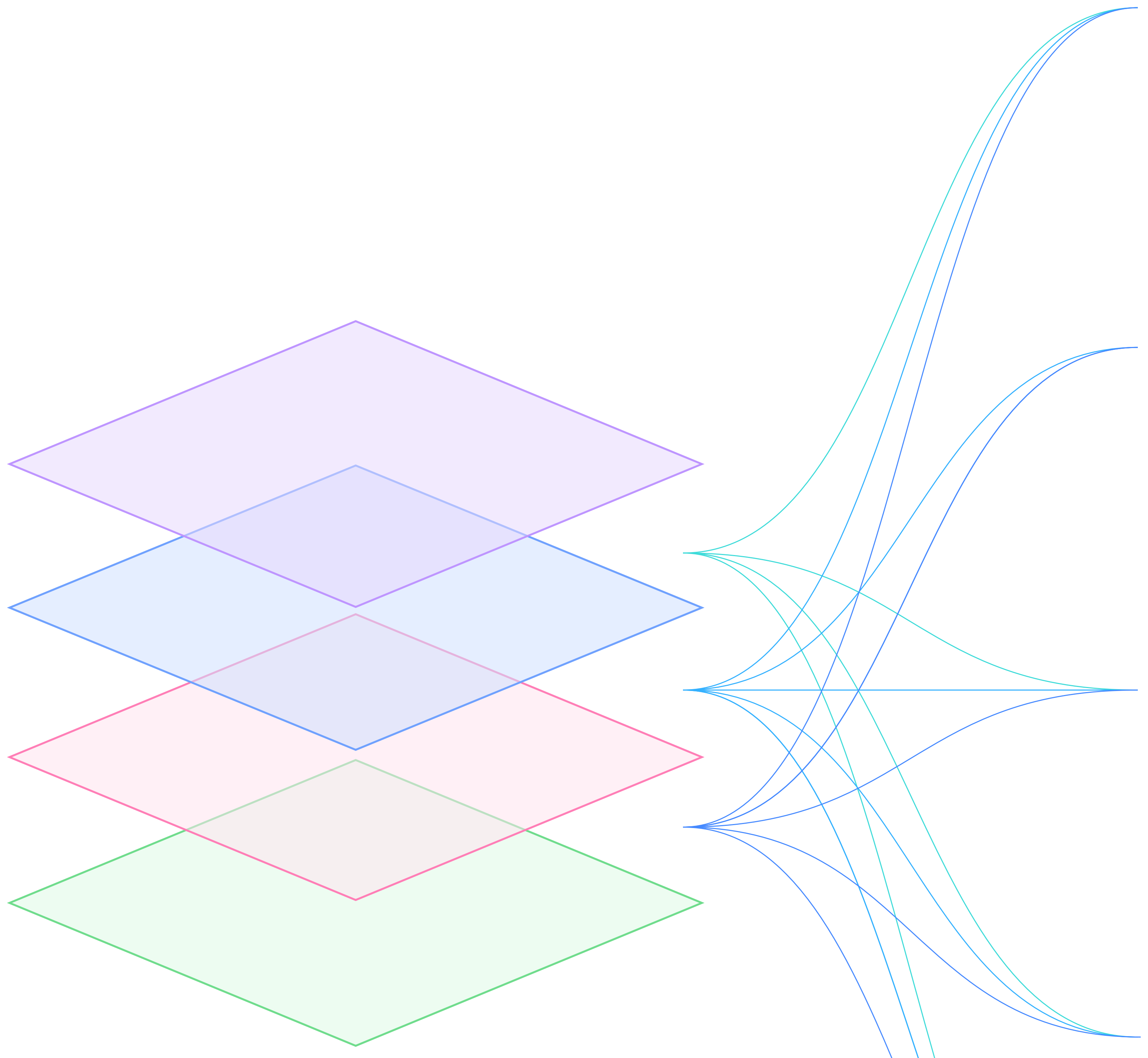
Longer Term

Chemistry & materials

Optimization & Search

Machine Learning/AI

Numerical simulation



Aerospace
- High strength-to-weight materials development
- Wing ply-composite design optimization
- Aircraft computational fluid dynamics

Automotive
- Advanced batteries
- Multi-objective vehicle routing optimization
- Auto design and simulation

Chemicals
- Lower energy fertilizer manufacturing
- Efficient Catalysts
- Accelerated product development

Electronics & semiconductors
- Placement and routing optimization
- Deposition/etch process modeling
- Multi-domain simulation

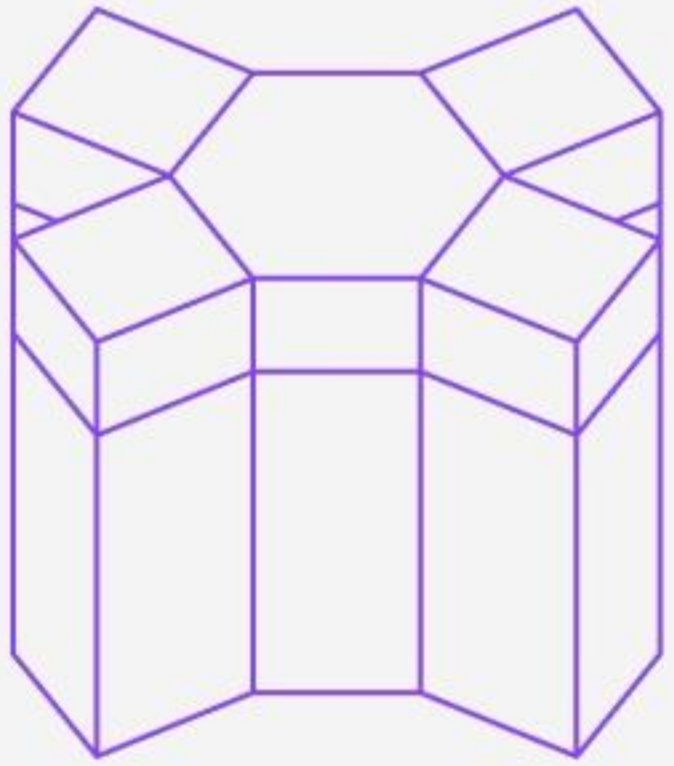
Energy
- Grid management
- Grid optimization with EV's
- Carbon Sequestration

Financial Services
- Portfolio optimization
- Derivatives/options pricing
- Antti-Money laundering

Health Care & Life Sciences
- Drug discovery and drug design optimization
- mRNA & protein structure predictions
- Disease target & biomarker discovery

Qiskit

+



IBM QPUs

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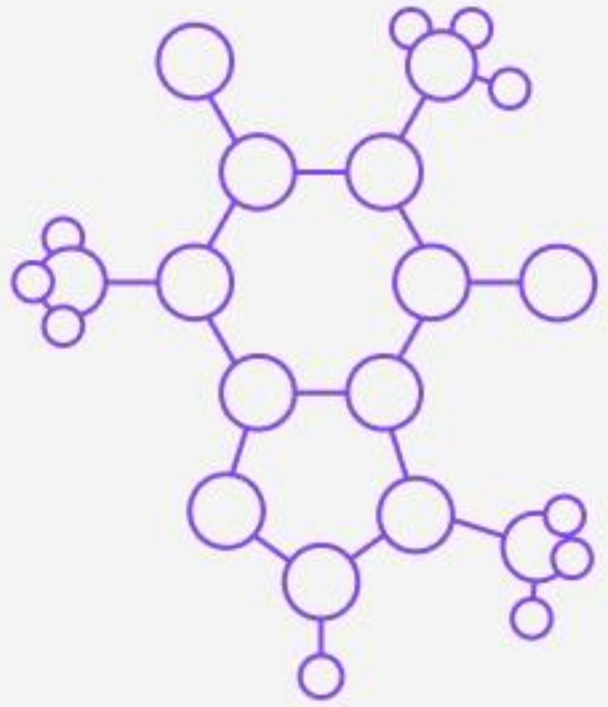
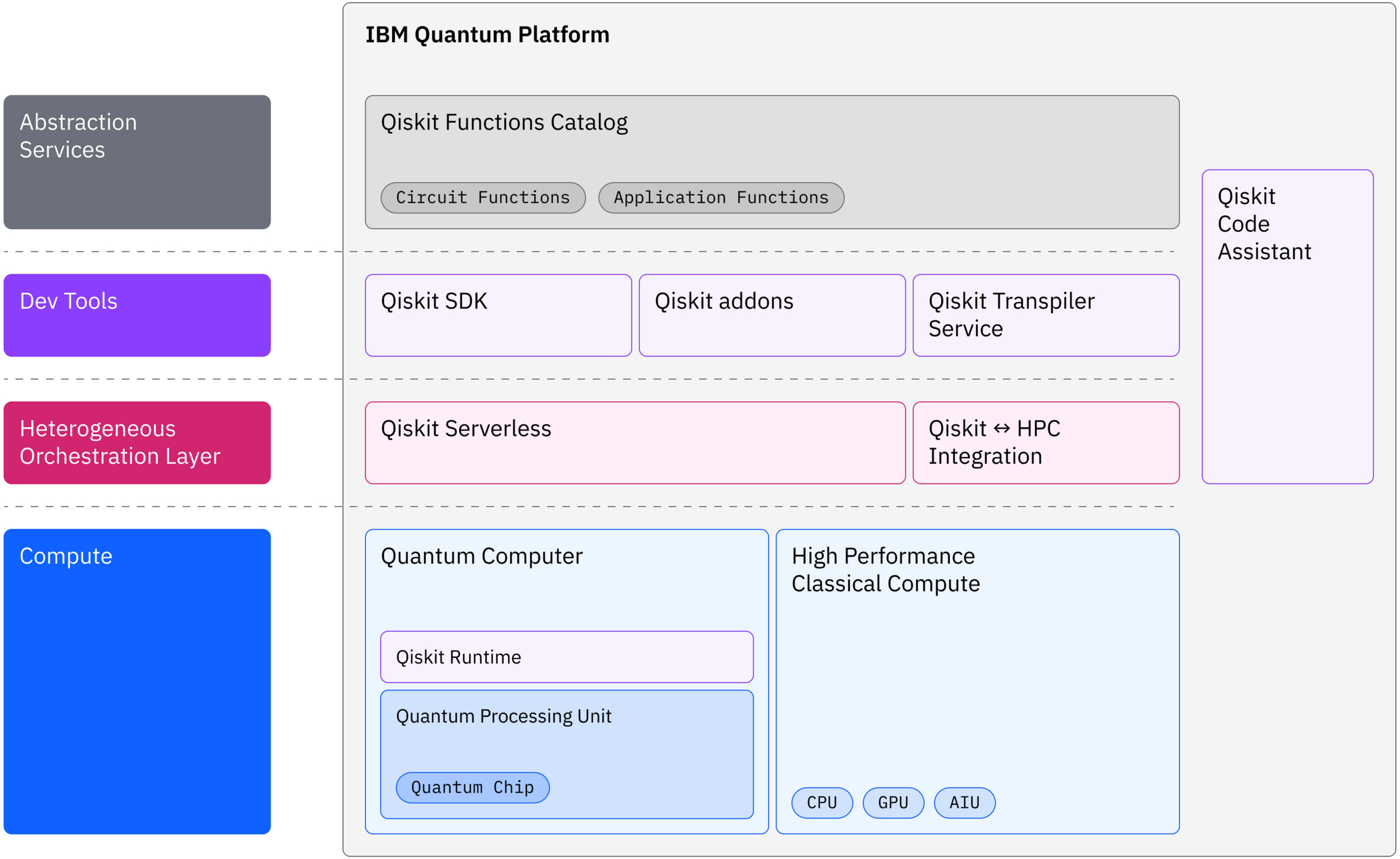


Utility Scale Work

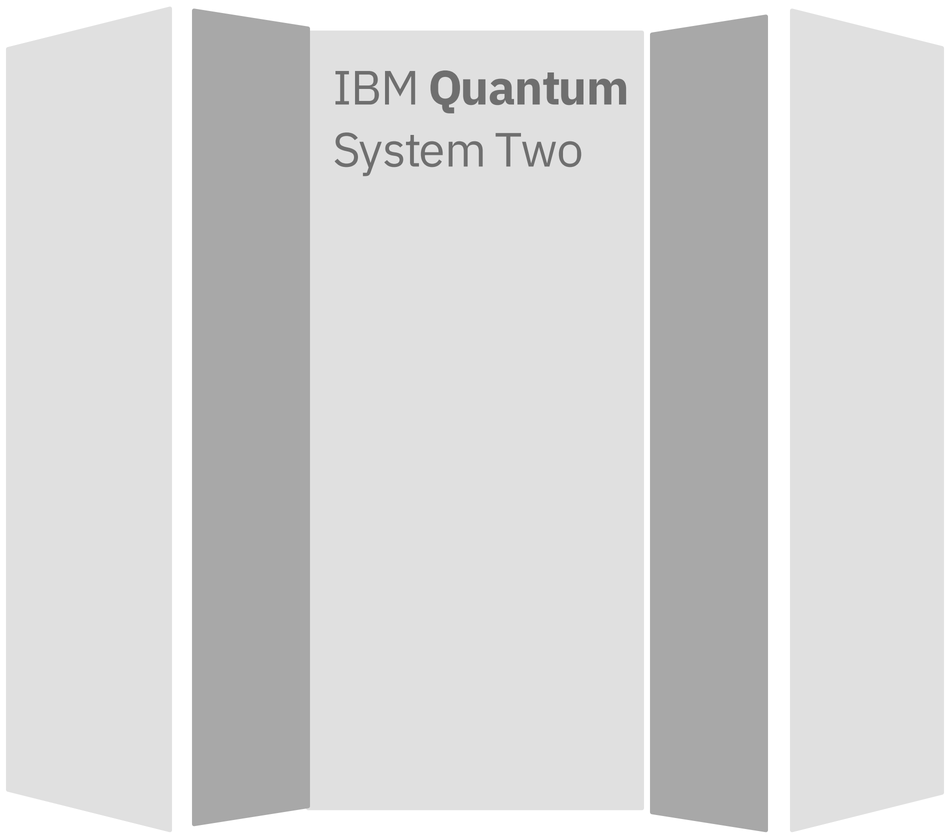
Quantum must be performant

Quantum must be easy-to-use


Abstraction Services
Dev Tools
Heterogeneous Orchestration Layer
Compute
IBM Quantum Platform
Qiskit Functions Catalog
Circuit Functions
Application Functions
Qiskit Code Assistant
Qiskit SDK
Qiskit addons
Qiskit Transpiler Service
Qiskit Serverless
Qiskit ↔ HPC Integration
Quantum Computer
Qiskit Runtime
Quantum Processing Unit
Quantum Chip
High Performance Classical Compute
CPU
GPU
AIU

It’s simple…

If it needs a circuit, it needs Qiskit



Quantum Software
(powered by Qiskit Addons and Qiskit Functions)

+

Qiskit

+

QPUs

=

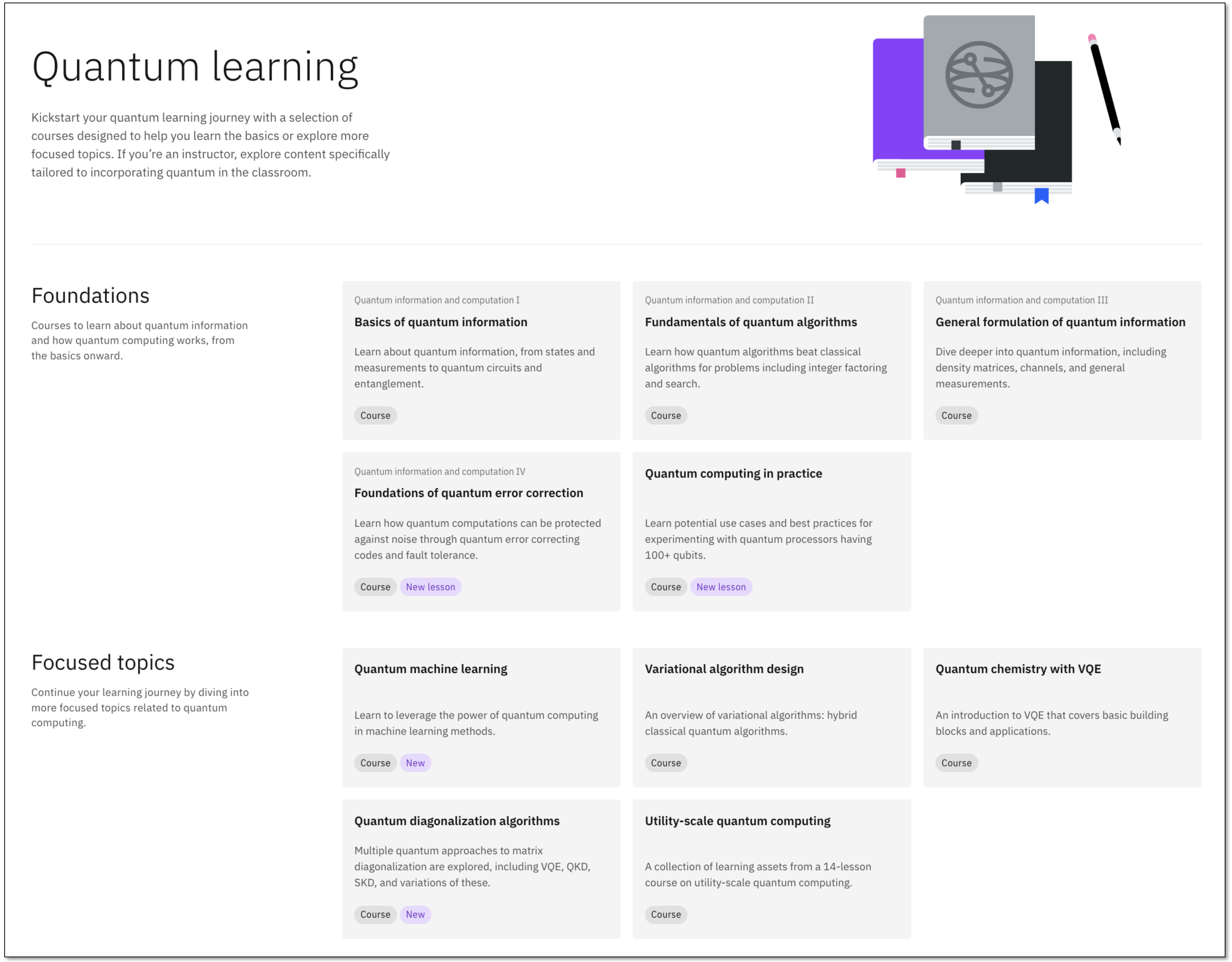
Useful Work

The IBM Quantum platform unlocks research with quantum

IBM Quantum Learning

Learn the basics of quantum computing and how to solve real-world problems with IBM Quantum services and systems

Courses, tutorials, and educational resources by leading quantum experts.



Quantum learning

Kickstart your quantum learning journey with a selection of courses designed to help you learn the basics or explore more focused topics. If you're an instructor, explore content specifically tailored to incorporating quantum in the classroom.

Foundations

Courses to learn about quantum information and how quantum computing works, from the basics onward.

Quantum information and computation I
Basics of quantum information
Learn about quantum information, from states and measurements to quantum circuits and entanglement.
Course

Quantum information and computation II
Fundamentals of quantum algorithms
Learn how quantum algorithms beat classical algorithms for problems including integer factoring and search.
Course

Quantum information and computation III
General formulation of quantum information
Dive deeper into quantum information, including density matrices, channels, and general measurements.
Course

Quantum information and computation IV
Foundations of quantum error correction
Learn how quantum computations can be protected against noise through quantum error correcting codes and fault tolerance.
Course New lesson

Quantum computing in practice
Learn potential use cases and best practices for experimenting with quantum processors having 100+ qubits.
Course New lesson

Focused topics

Continue your learning journey by diving into more focused topics related to quantum computing.

Quantum machine learning
Learn to leverage the power of quantum computing in machine learning methods.
Course New

Variational algorithm design
An overview of variational algorithms: hybrid classical quantum algorithms.
Course

Quantum chemistry with VQE
An introduction to VQE that covers basic building blocks and applications.
Course

Quantum diagonalization algorithms
Multiple quantum approaches to matrix diagonalization are explored, including VQE, QKD, SKD, and variations of these.
Course New

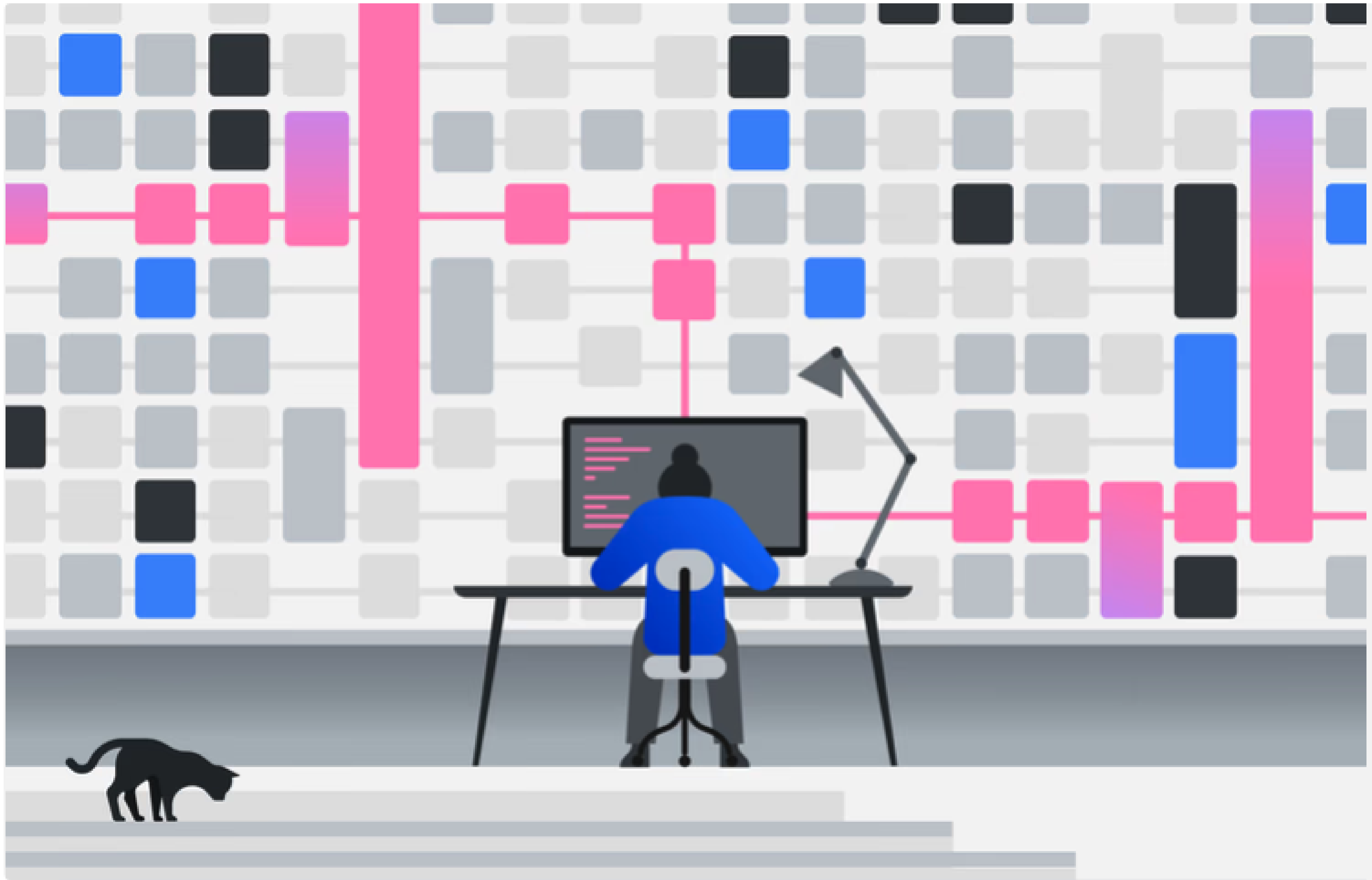
Utility-scale quantum computing
A collection of learning assets from a 14-lesson course on utility-scale quantum computing.
Course

IBM Quantum Learning

Learn the basics of quantum computing, and how to use IBM Quantum services and systems to solve real-world problems.

IBM Quantum Challenge 2024 starts June 5th

Register today →



Quantum Computing in Practice

New Video

Learn about realistic potential use cases for quantum computing and best practices for experimenting with quantum processors having 100 or more qubits.

Lessons
2

Your progress
N/A

Start course →

IBM Quantum community

IBM Quantum Learning

An online platform for learning the basics of quantum computing, and how to use IBM Quantum services and systems to solve real-world problems.

Qiskit Advocates

A global program that provides support to individuals who actively contribute to the Qiskit community. There are hundreds of Qiskit advocates representing many countries who contribute to the Qiskit community.

Qiskit Global Summer School

An annual event featuring online lectures delivered by various IBM Quantum experts, as well as live Q&A sessions.

Qiskit YouTube channel

The Qiskit YouTube channel hosts hundreds of useful videos on quantum computing.

Qiskit Developer Certification

The world's first ever developer certification for programming a quantum computer, setting the benchmark for quantum developer skills.

IBM Quantum Summer Internship Program

Work across the entire IBM Quantum team, from programming to materials research, on real projects that matter.

Applications open in the fall and continue through winter for different roles globally.

IBM Quantum interns, class of 2025

IBM **Quantum**