Introduction to IBM Quantum and Qiskit

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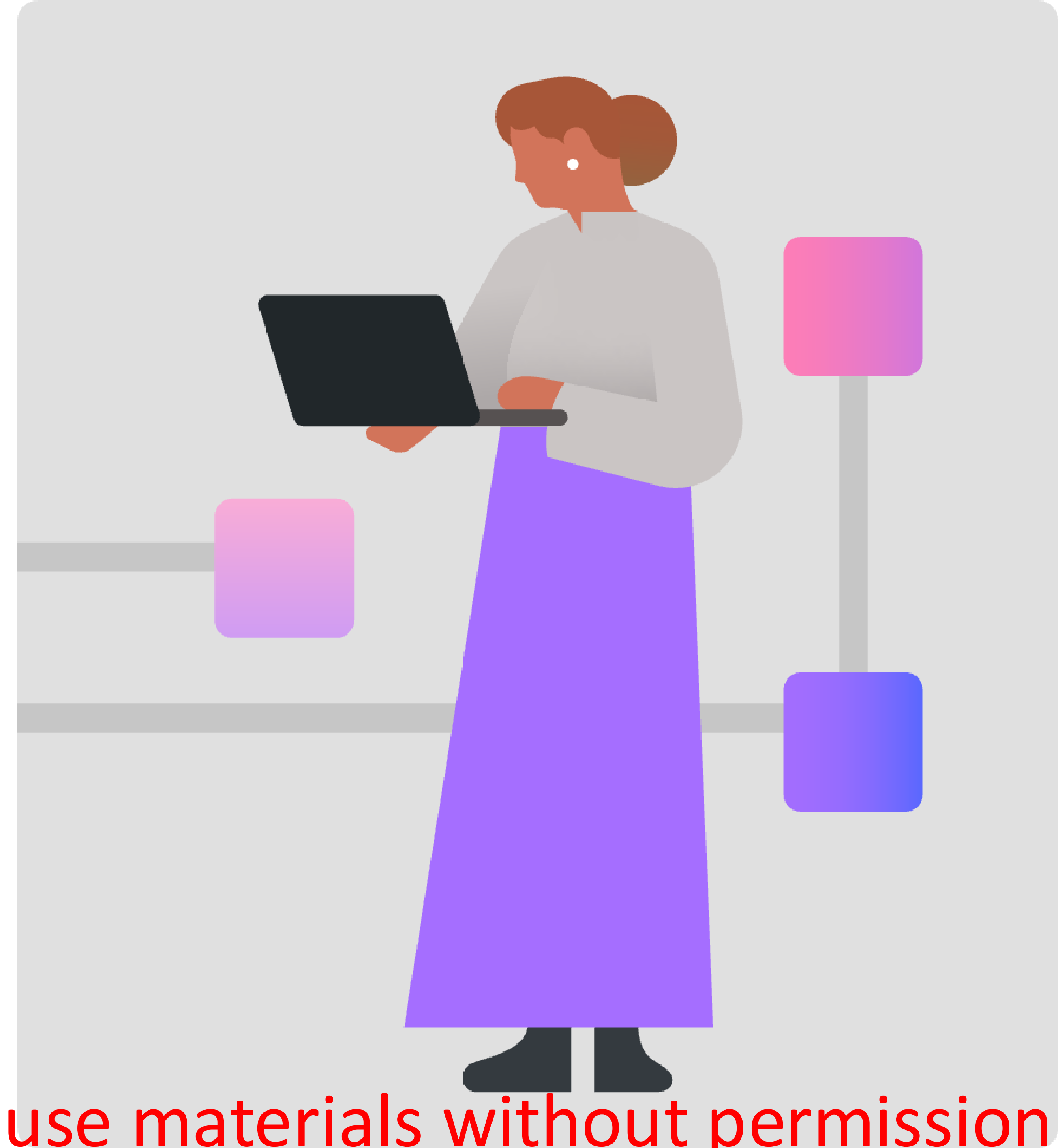
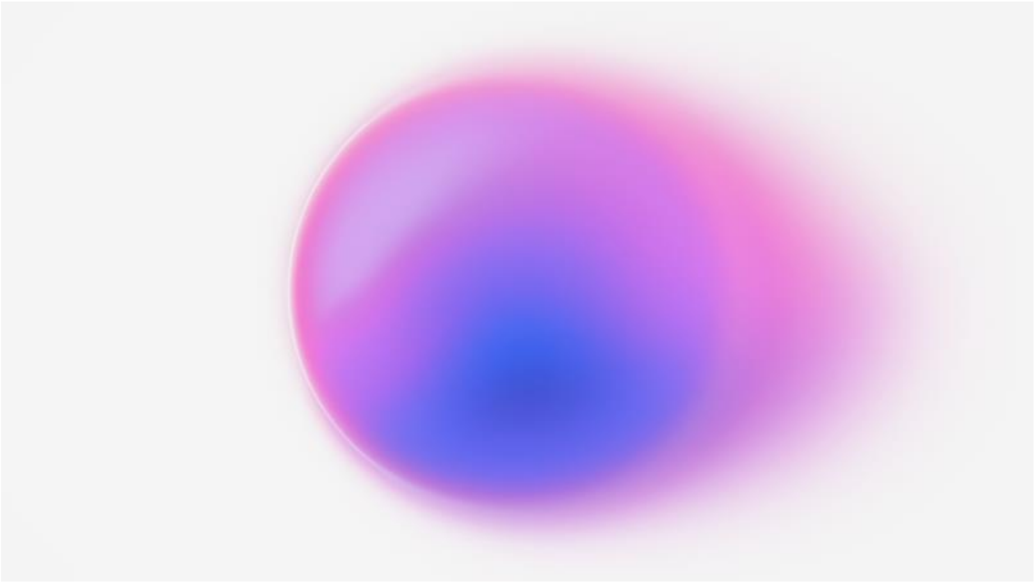
Global Strategic Research Development Lead`
IBM Quantum



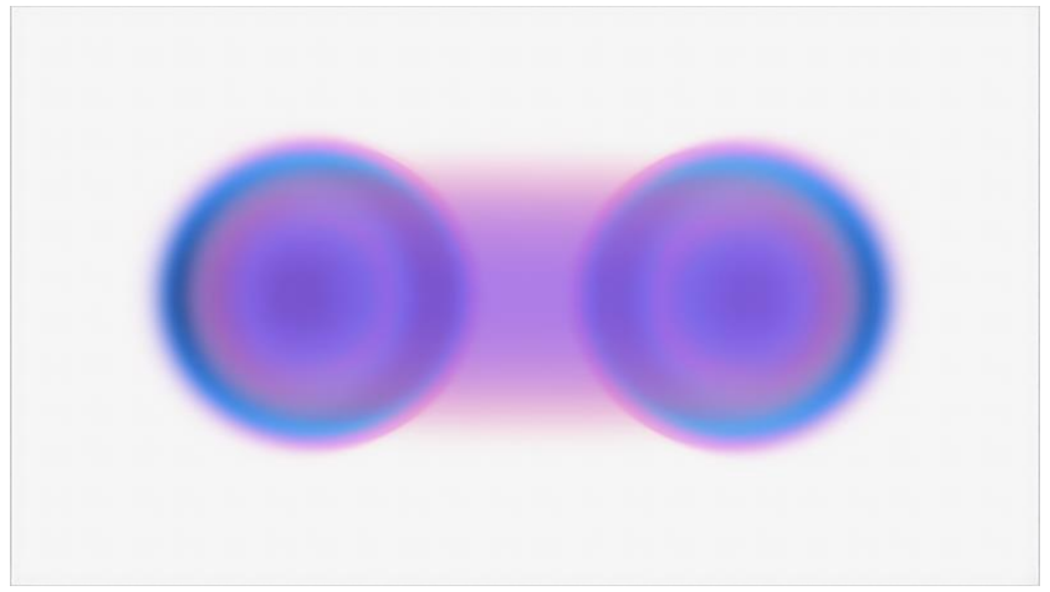
What is quantum computing?

Uniquely quantum

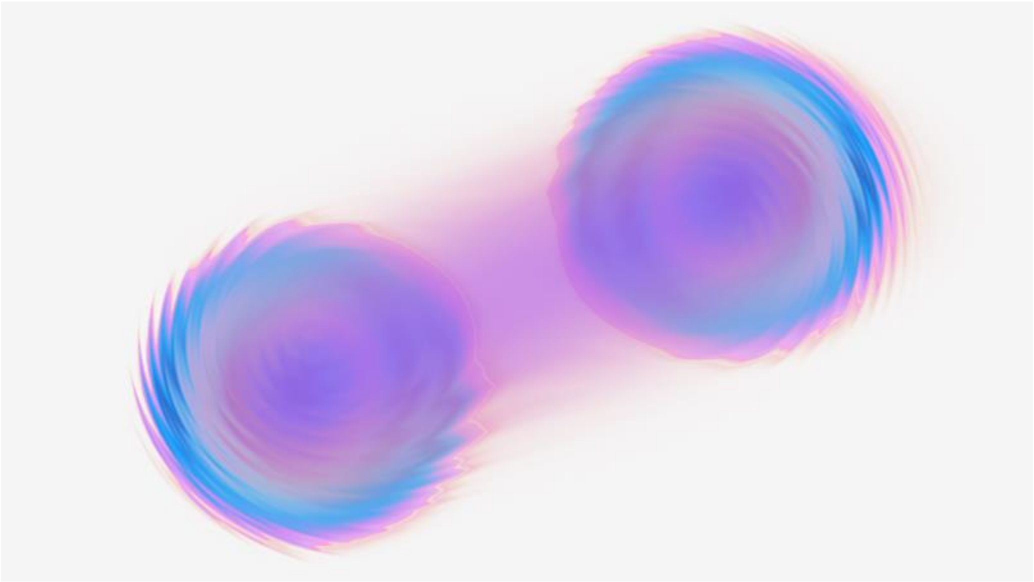
Some problems are classically intractable and will never be solvable with traditional computers



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

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

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

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.

0010011011100100100010010010011001001110010110
0111110010100100011100010001001010001001001010 1
0100101010111001001101110010010001001001001 1001
0011100101110011111001010010001110001000100101 0
0010010010101010010101011101110011100101011110

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

Bits and classical logic circuits

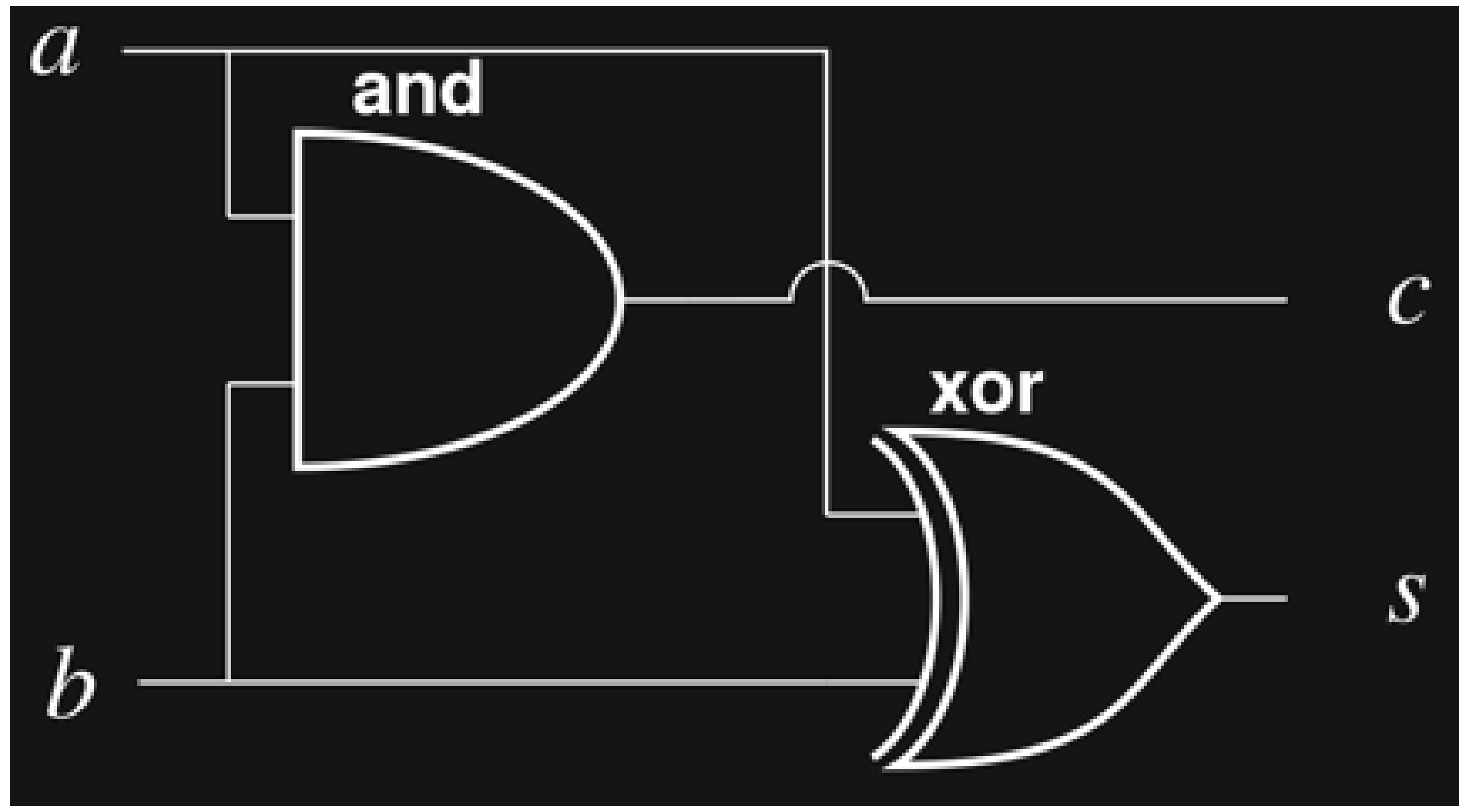
0

•

•

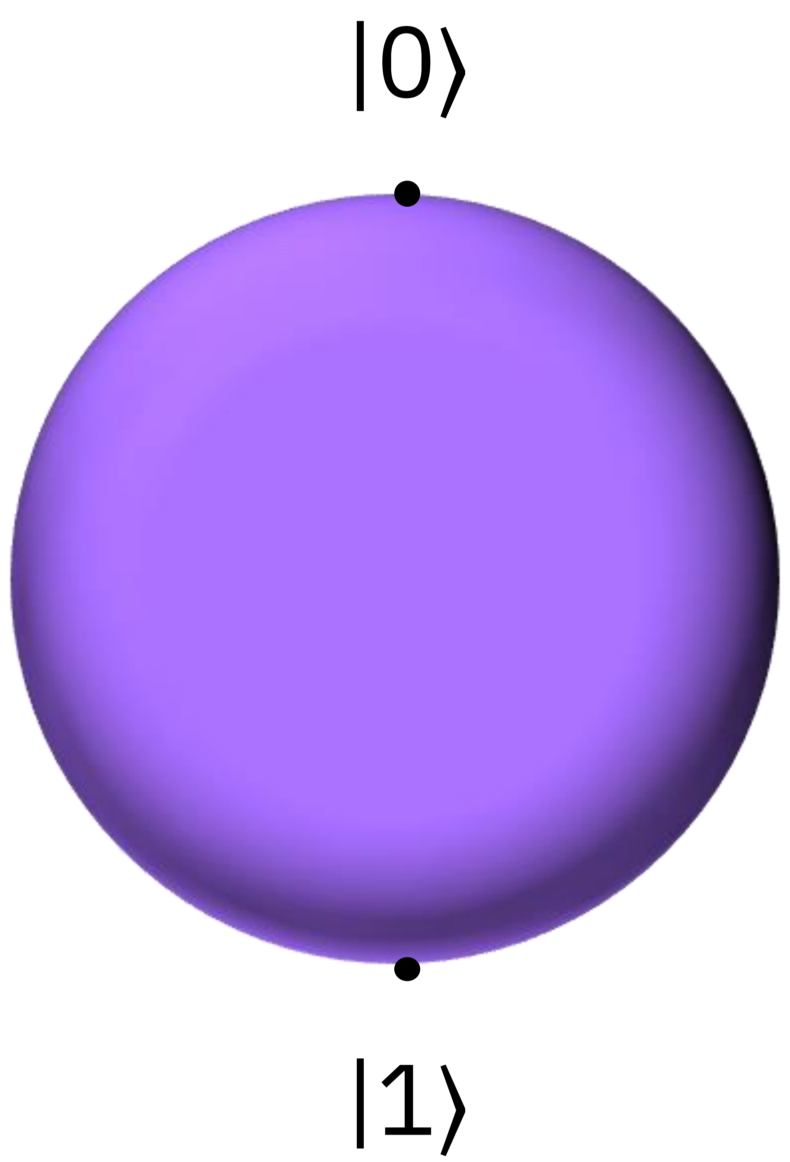
1

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

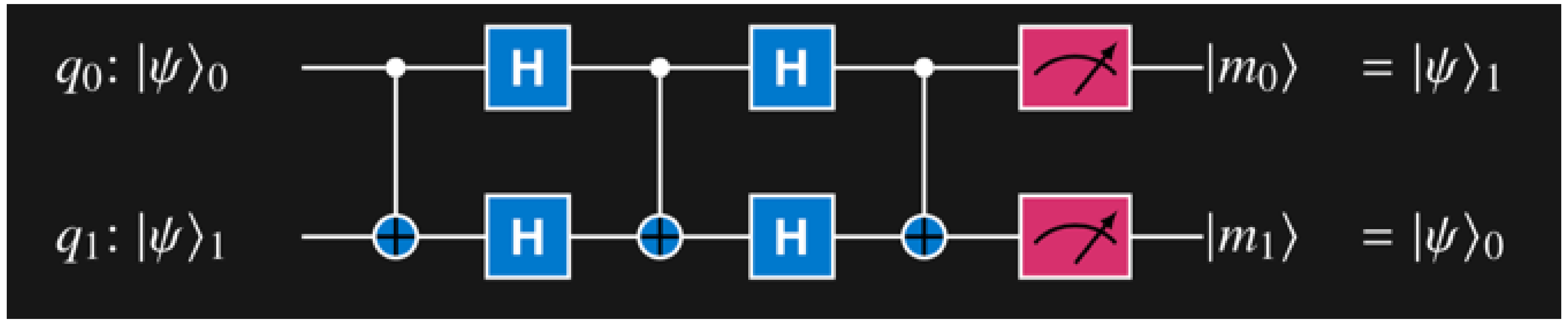


A classical logic circuit is a set of gate operations on bits and is the unit of computation

Quantum bits (qubits) and quantum circuits

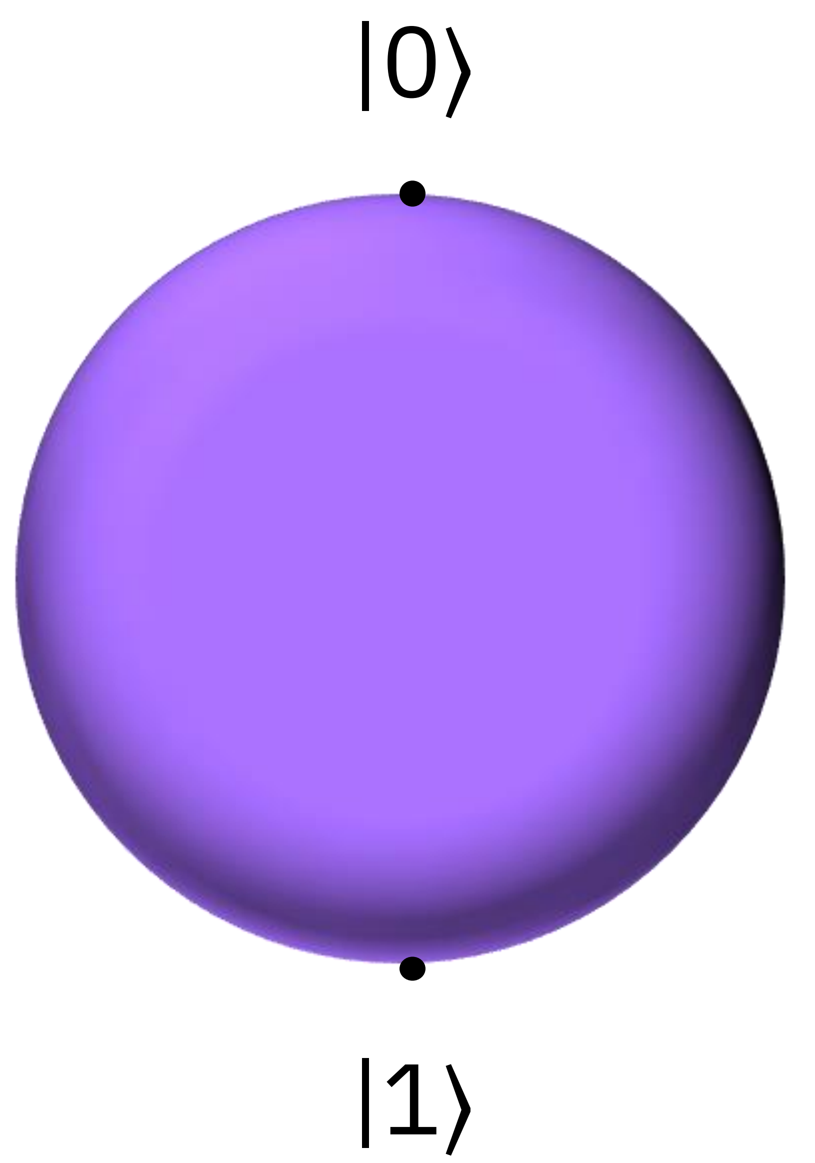


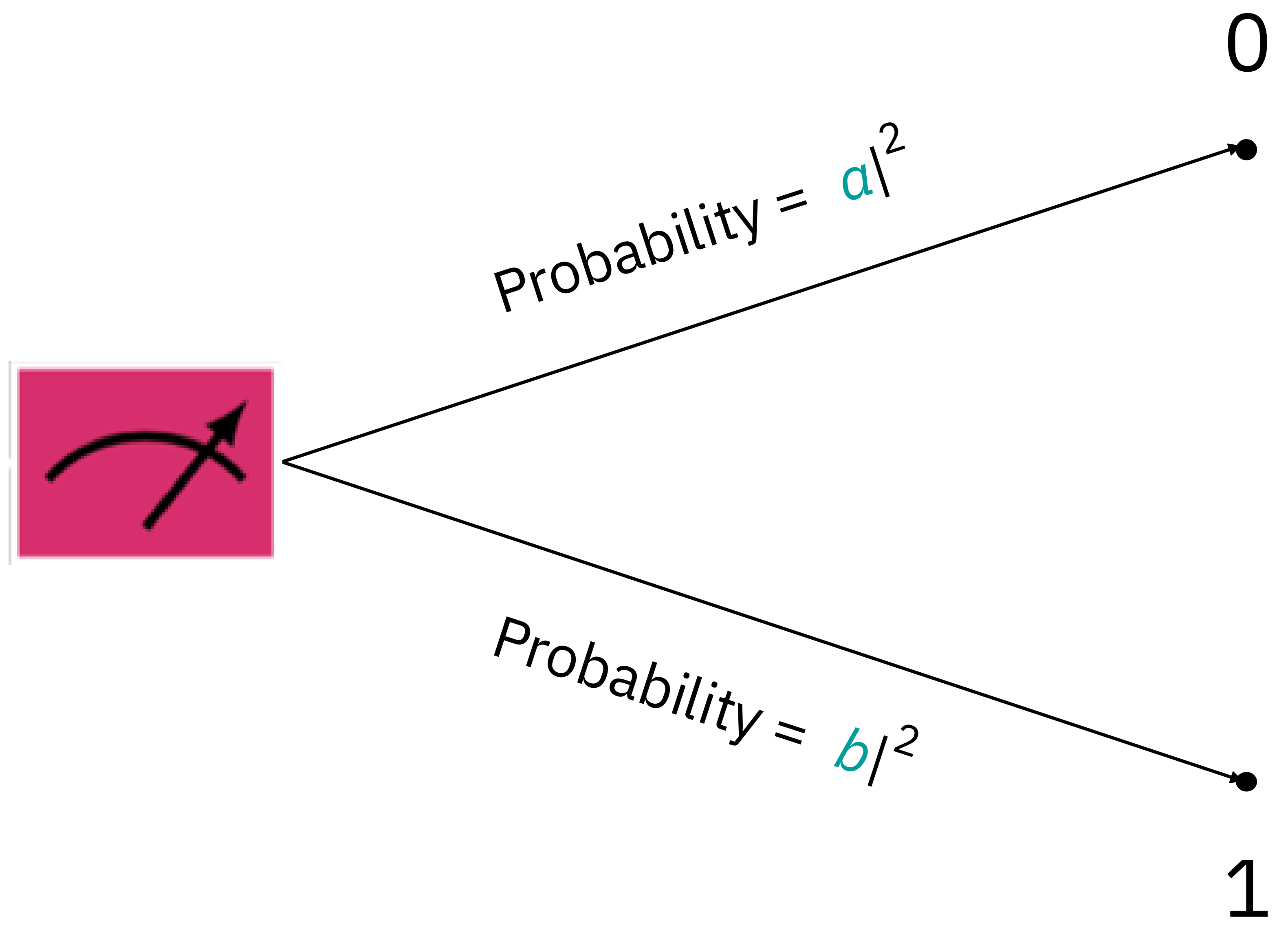
A quantum bit or qubit is a controllable quantum object that is the unit of information



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

Bits and qubits





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

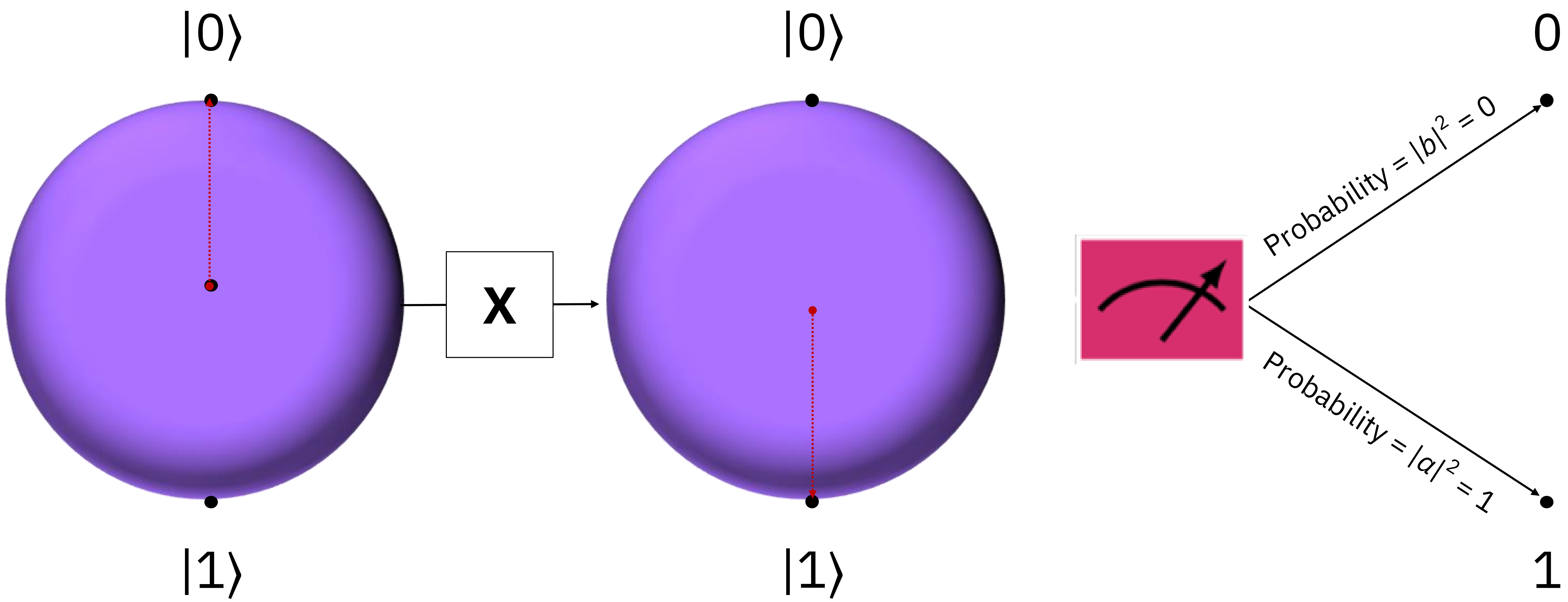
$$a\,|0\rangle + b\,|1\rangle$$

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 $|0\rangle$

IBM **Quantum**



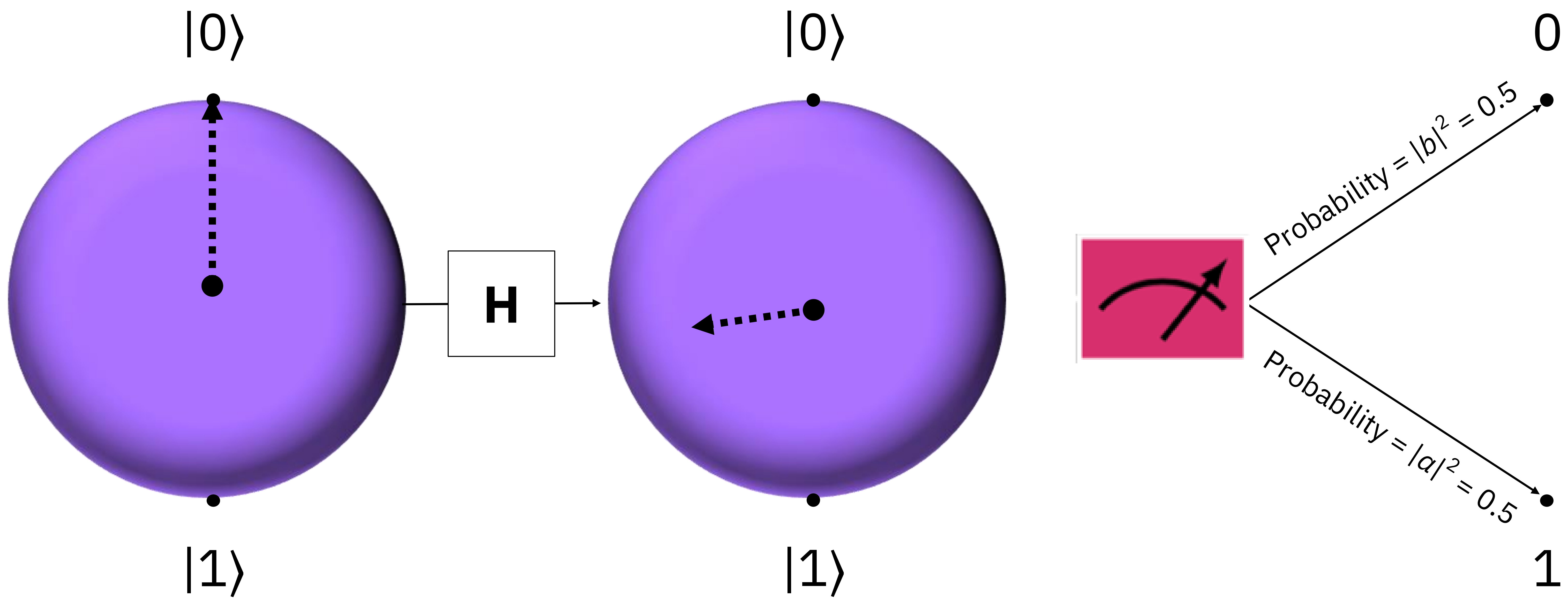
The **X** gate reverses $|0\rangle$ and $|1\rangle$:

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

$a = 1$ 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

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

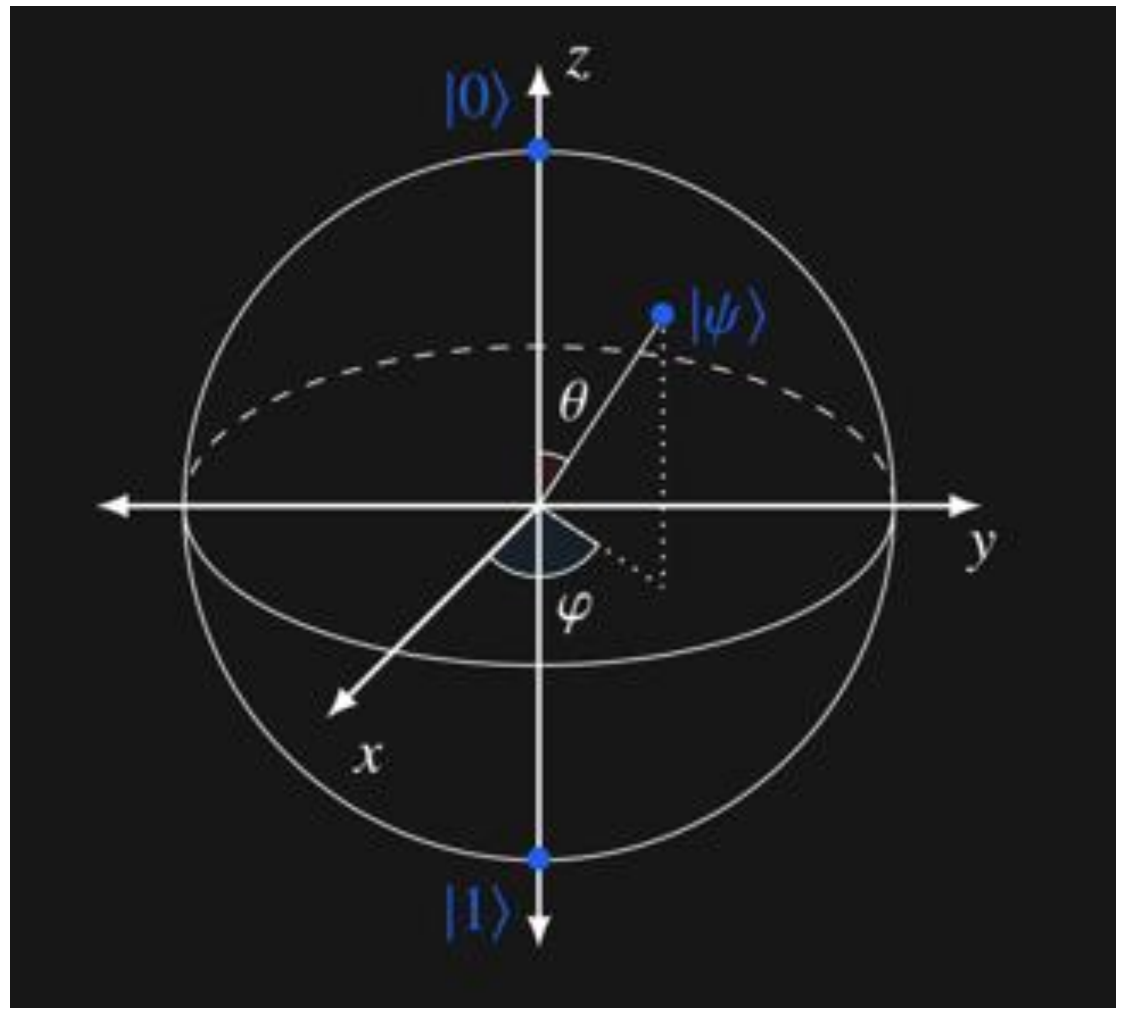
Two quantum states are equivalent if they differ only by a constant multiple u where $|u| = 1$.

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 $|1\rangle$

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

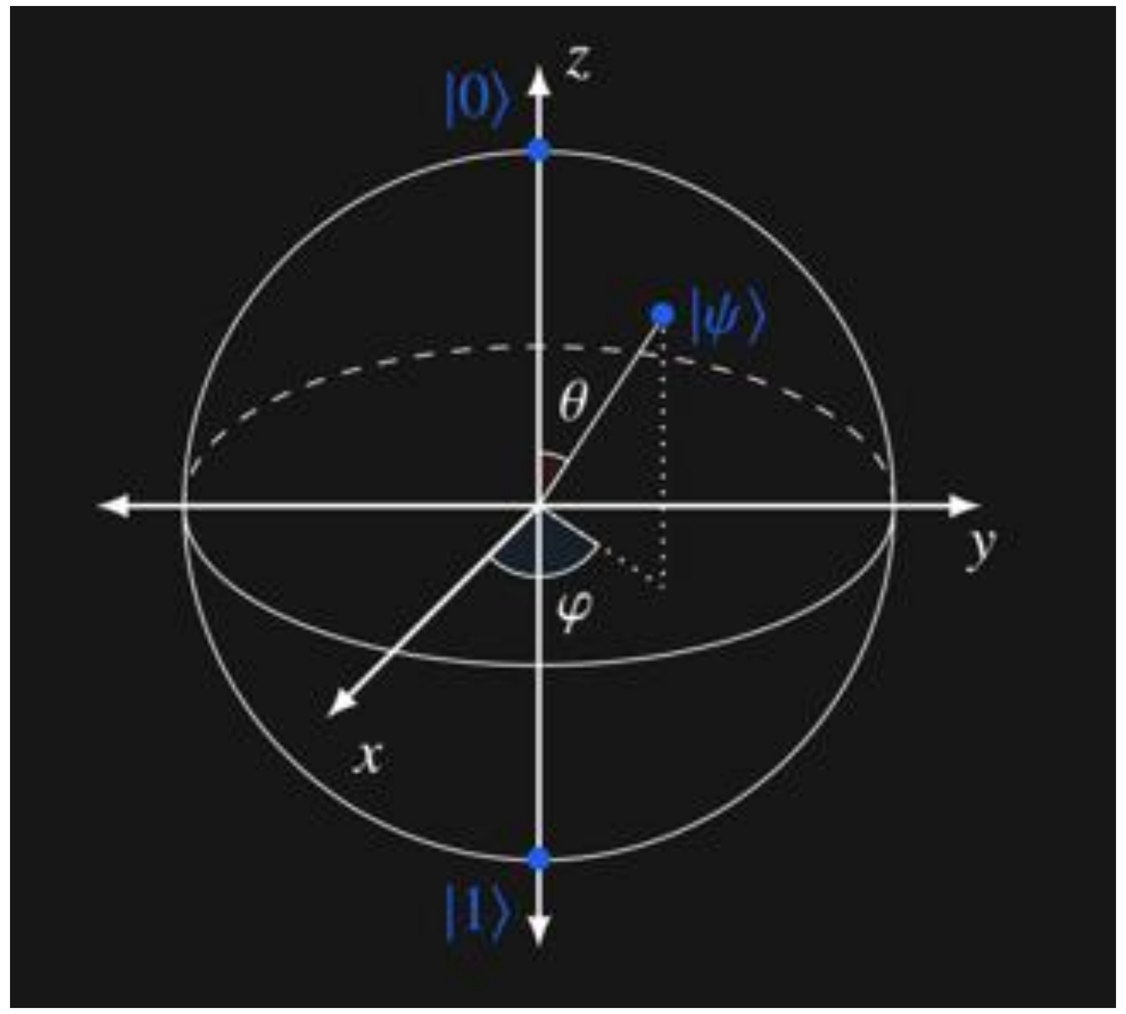
These conditions allow us to map the qubit onto the *Bloch Sphere*.

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,

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

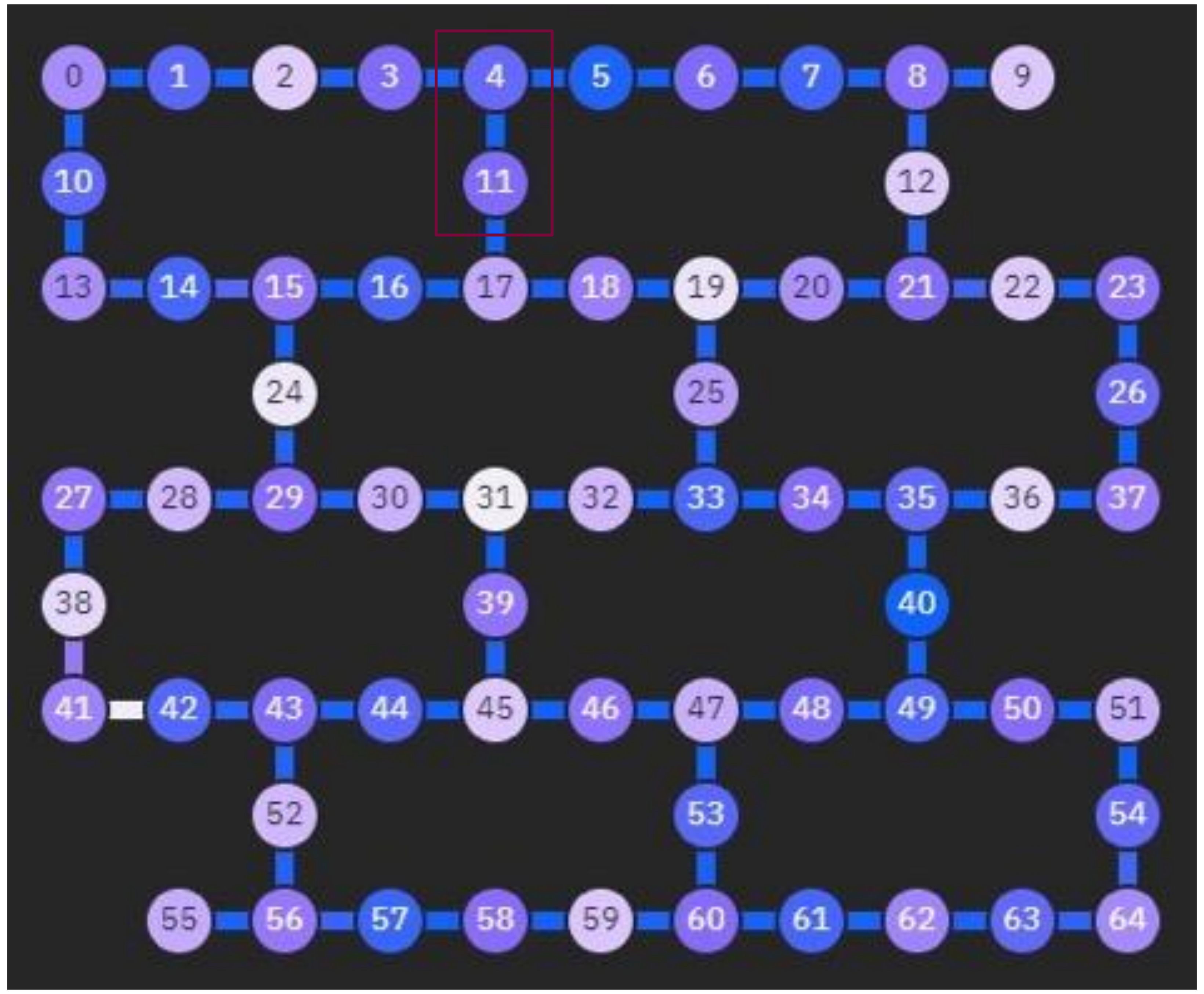
has an equal probability of becoming $|0\rangle$ or $|1\rangle$, and

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

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 $|1\rangle$

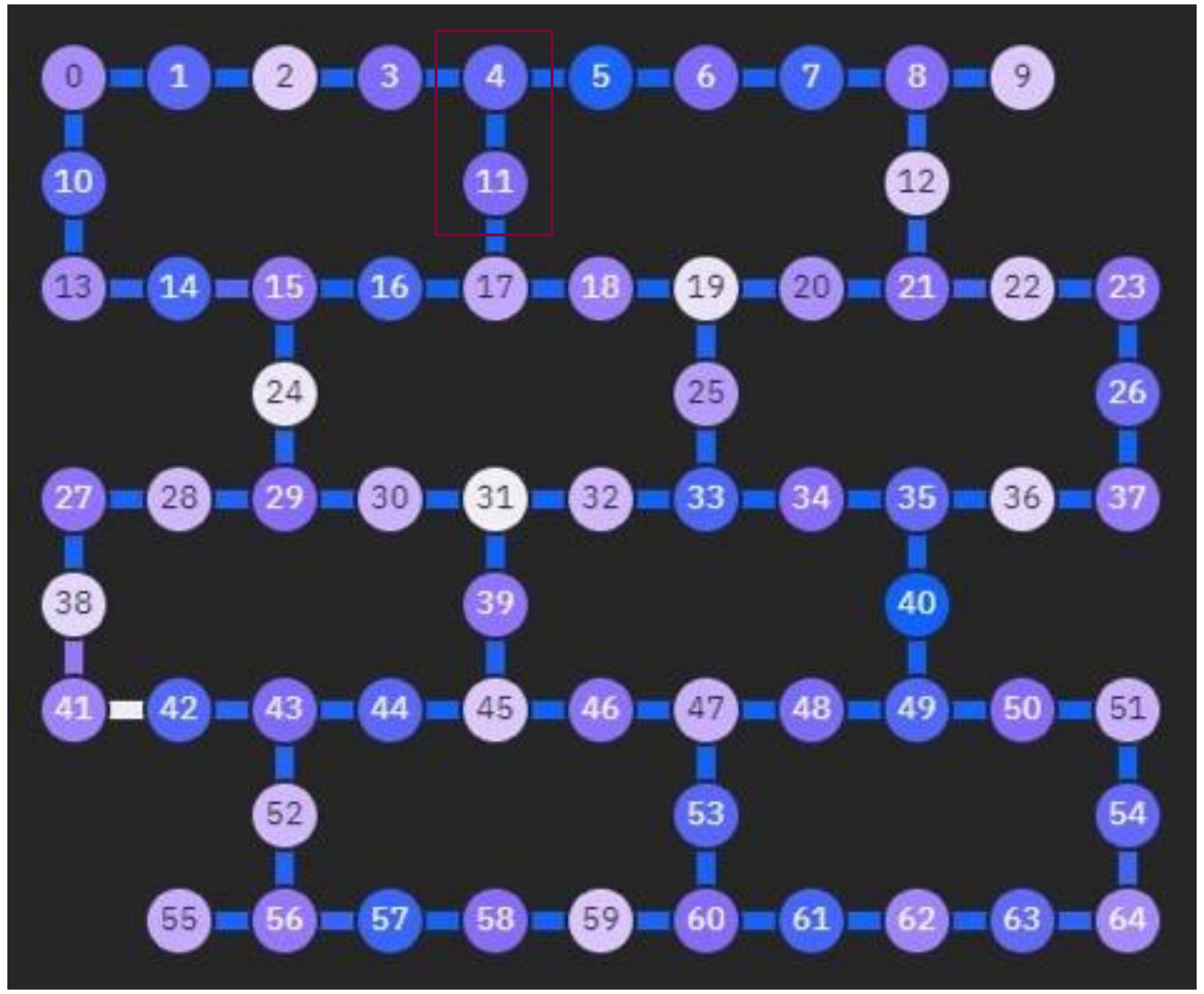
a, b, c, and d are complex numbers and

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

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,

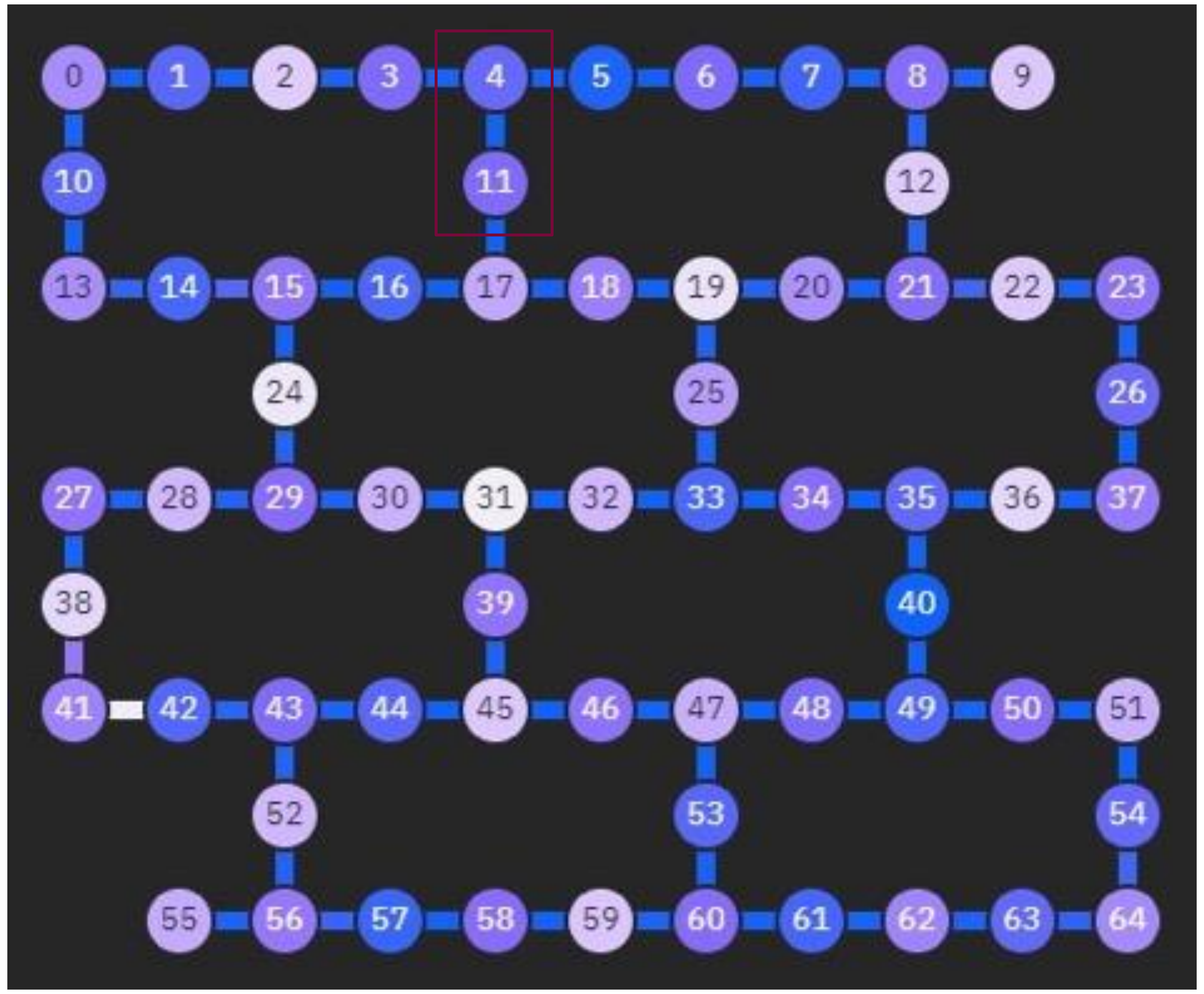
$$\frac{\sqrt{2}}{2}|00\rangle + \frac{\sqrt{2}}{2}|01\rangle$$ not entangled

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

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

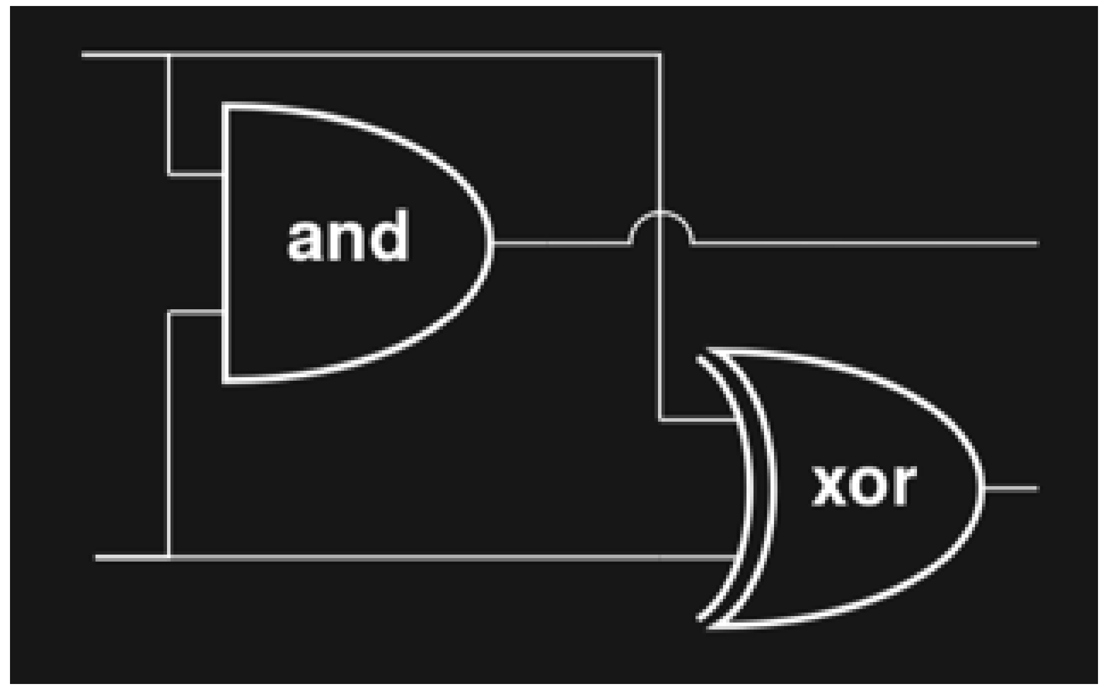
as the “product” of two single qubit states.

They are entangled!

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

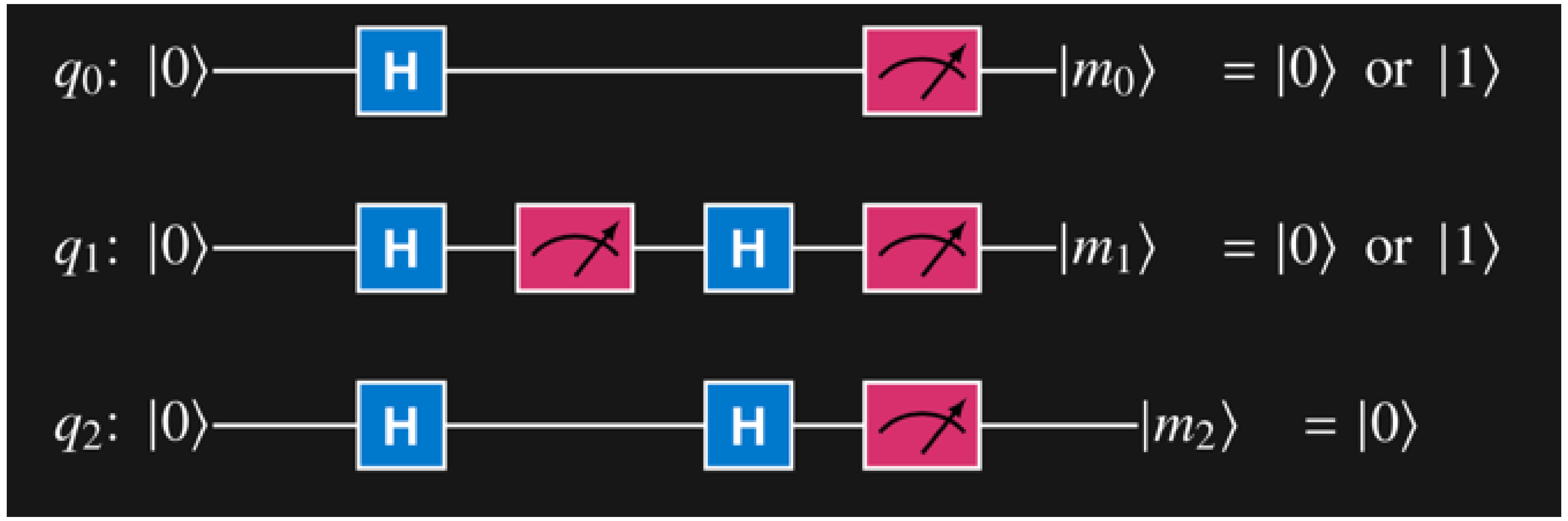
Quantum computing uses essential ideas from quantum mechanics

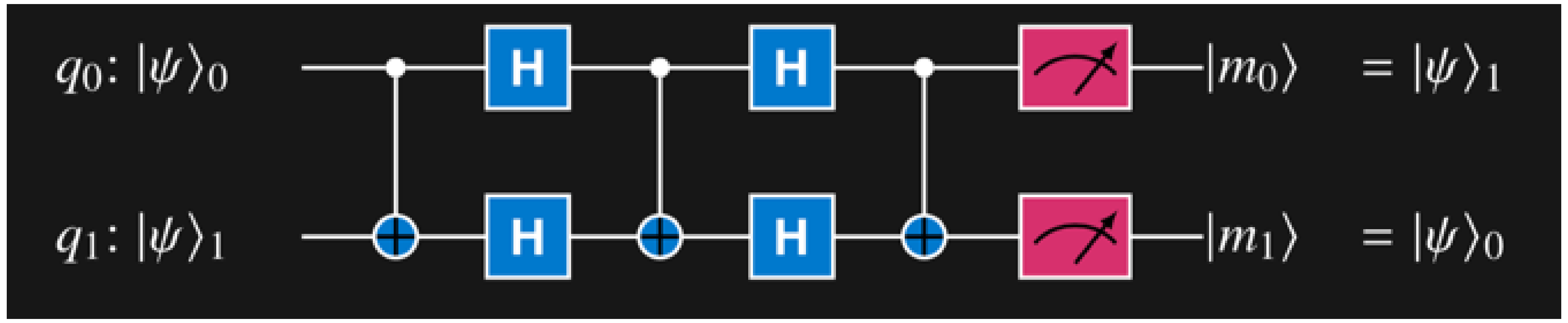
Gates / operations



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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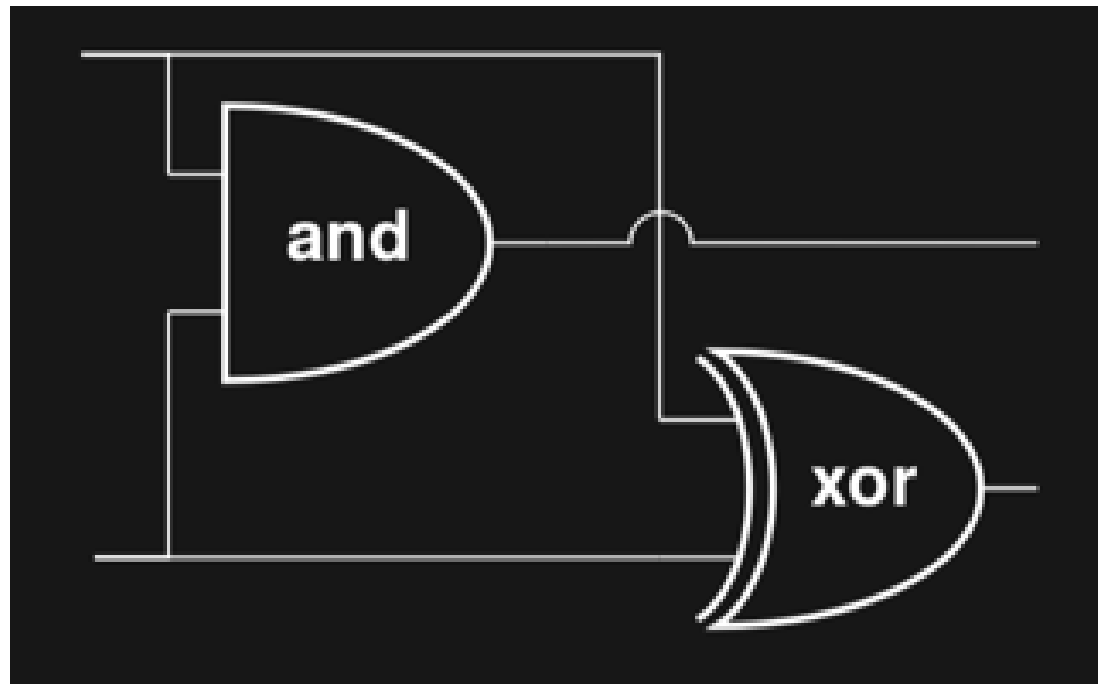

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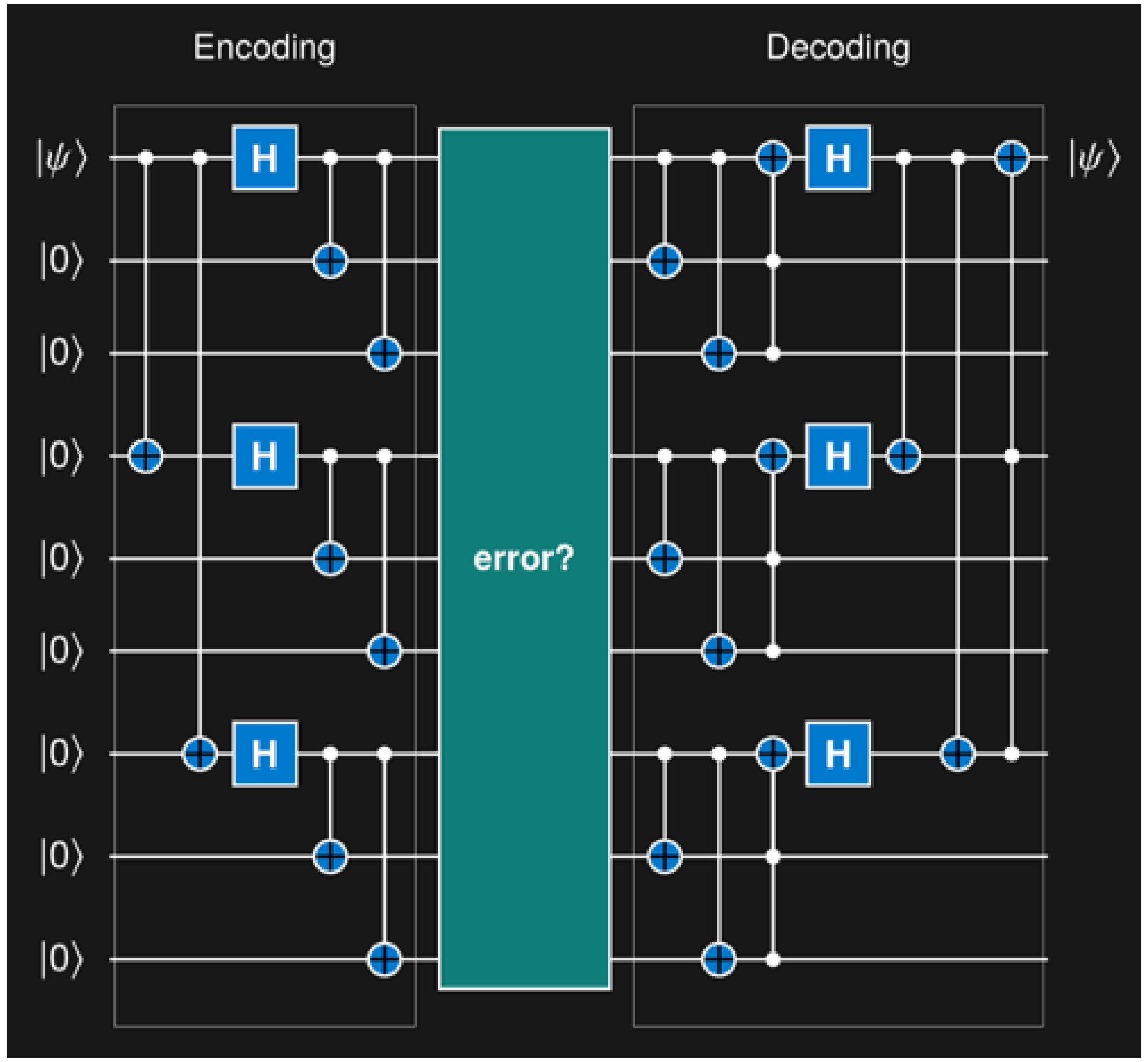
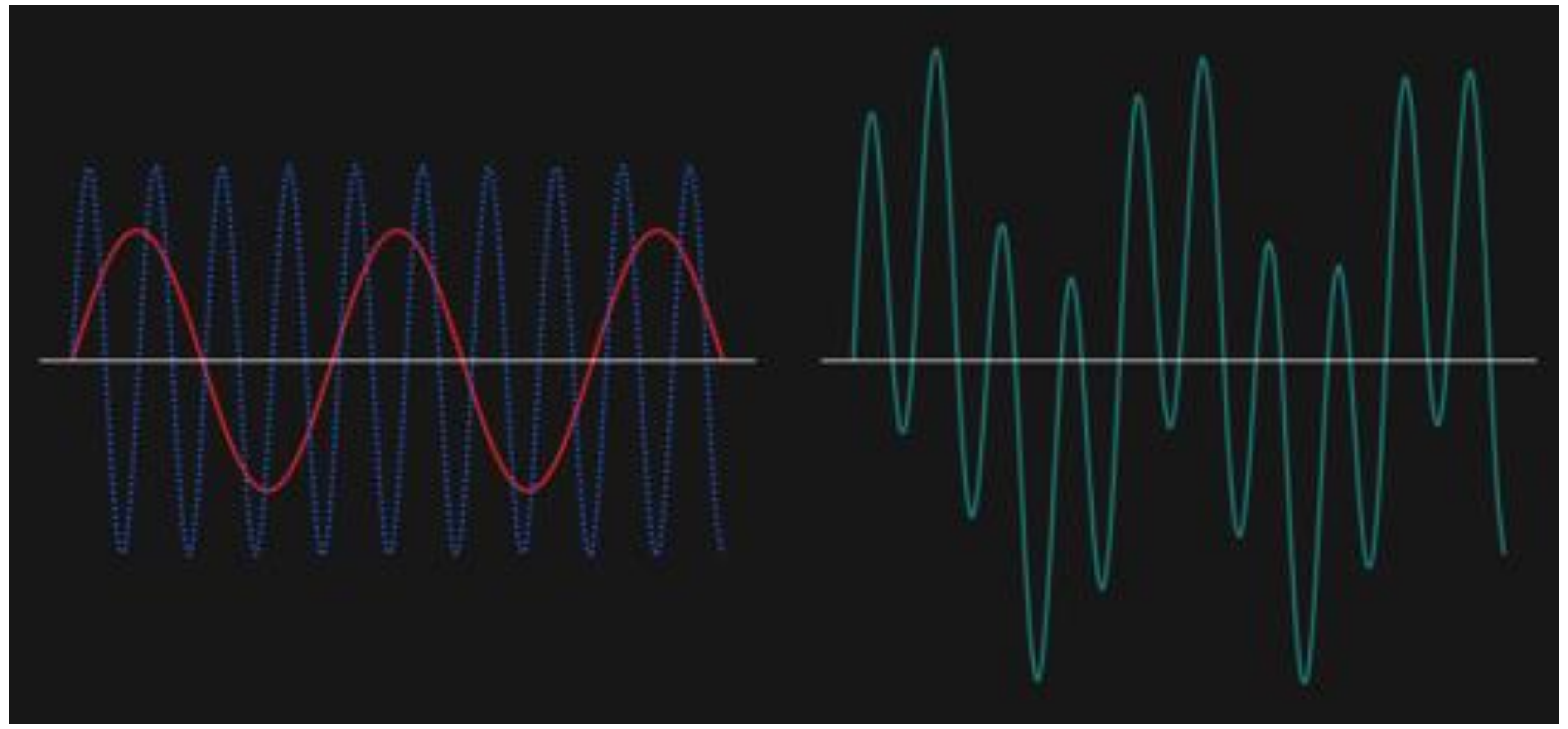
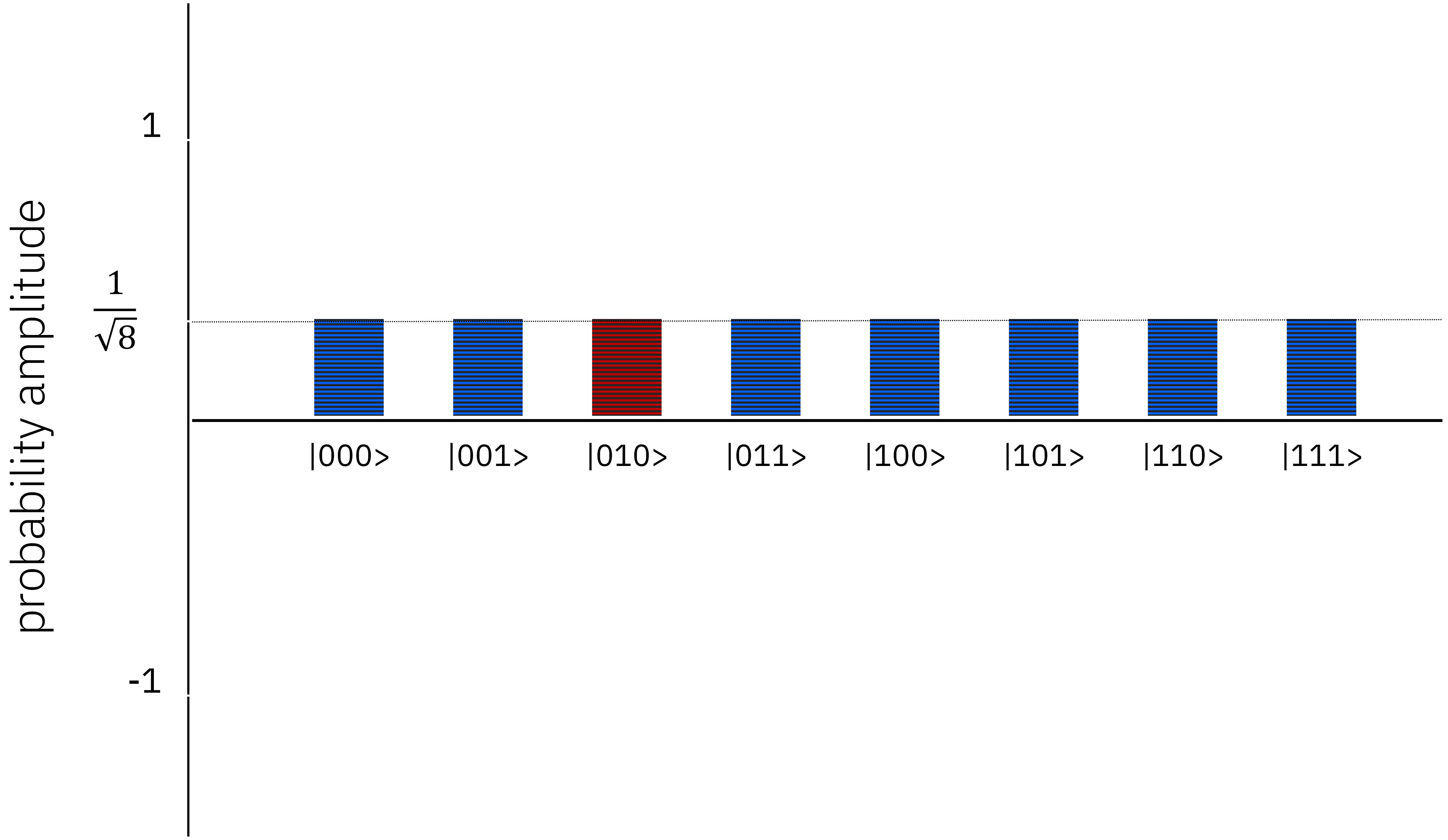


Quantum computing uses essential ideas from quantum mechanics

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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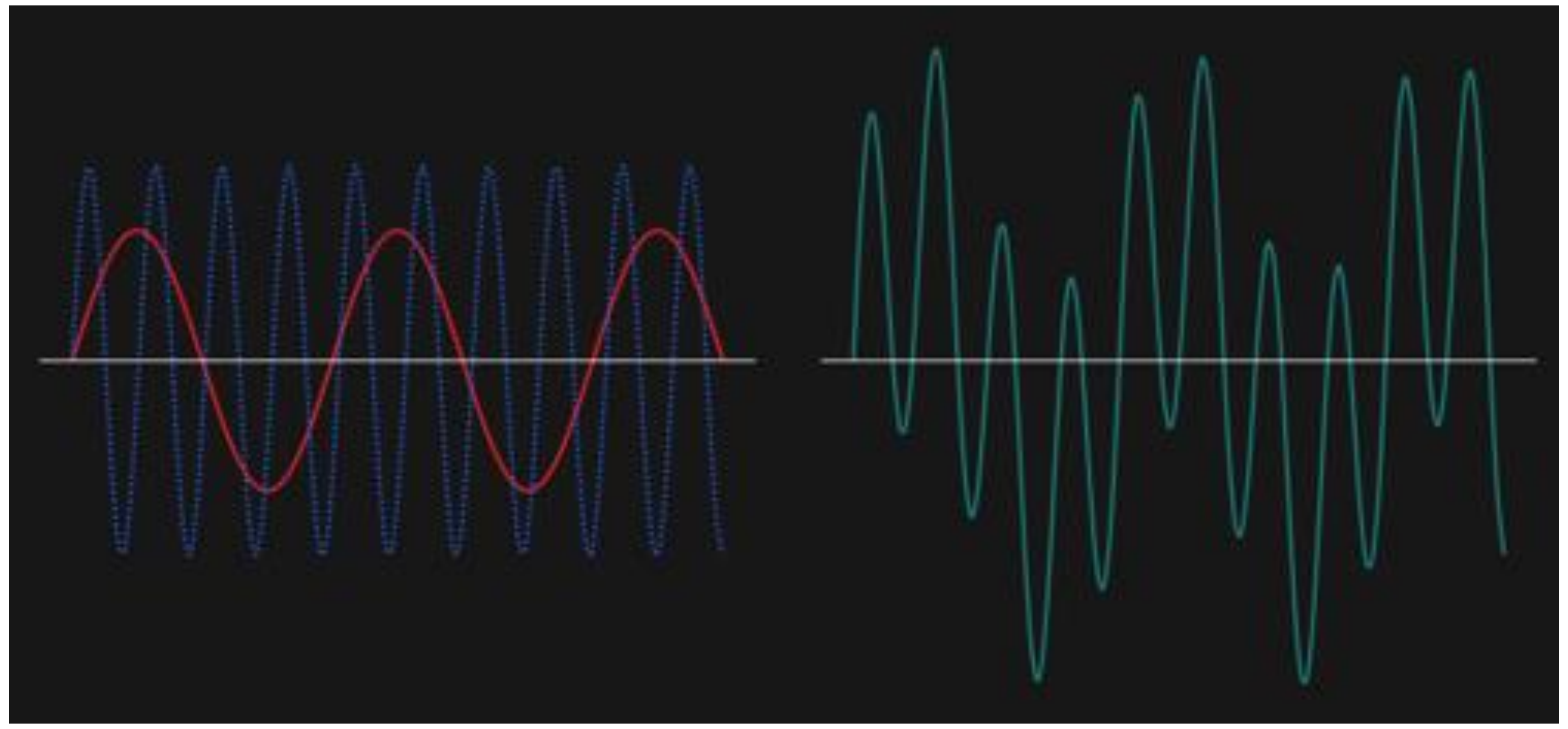

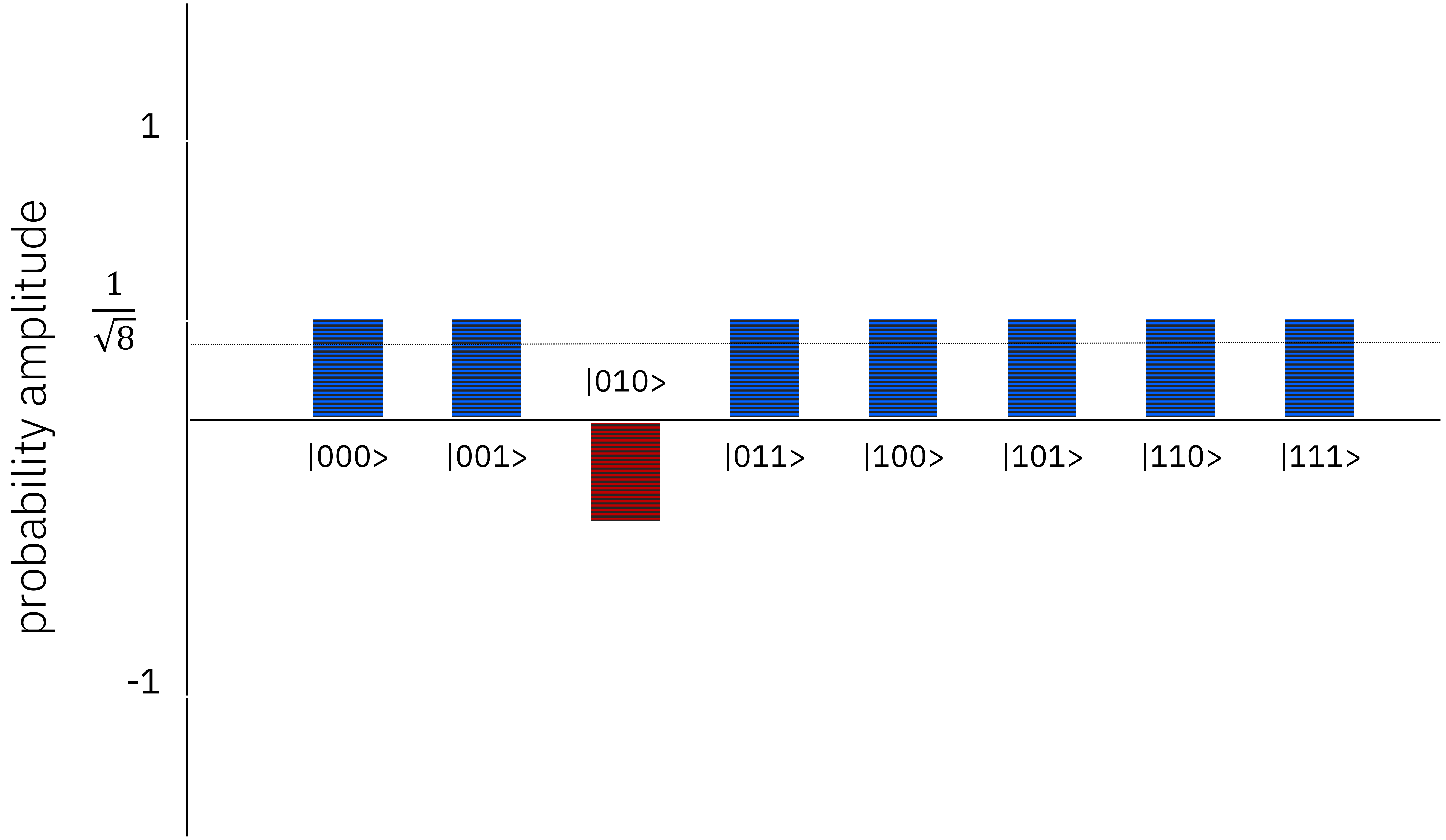

Quantum computing uses essential ideas from quantum mechanics

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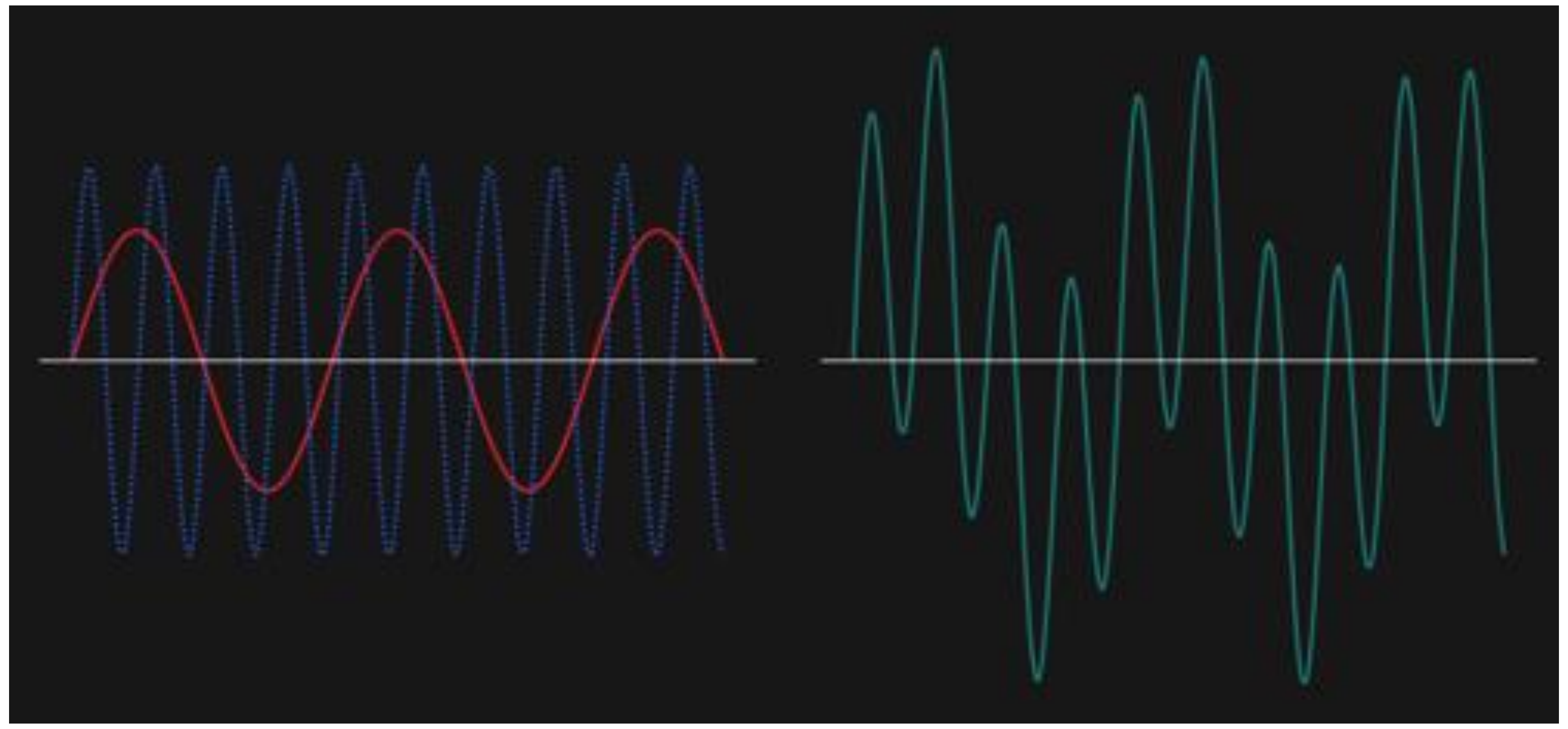
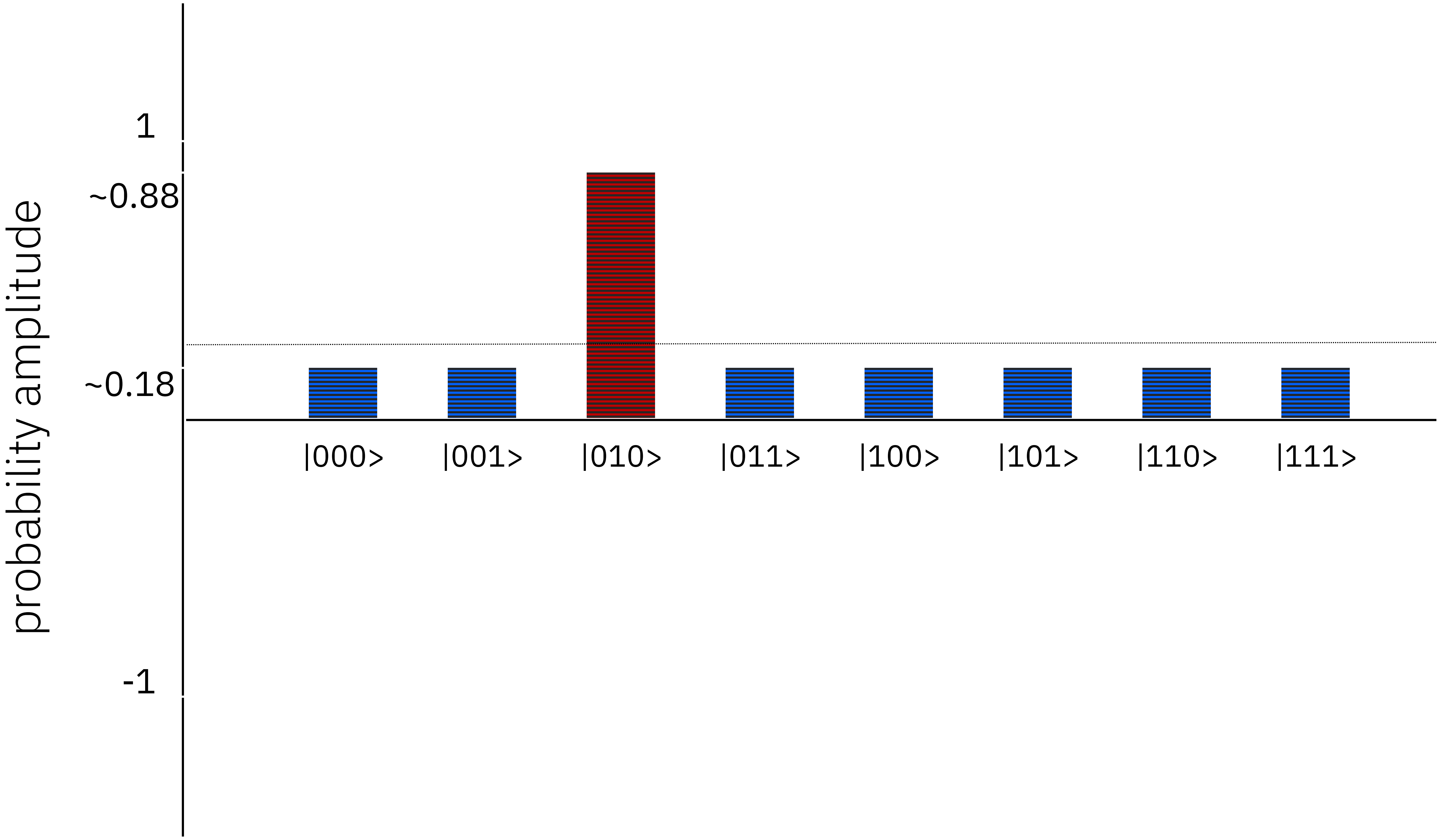
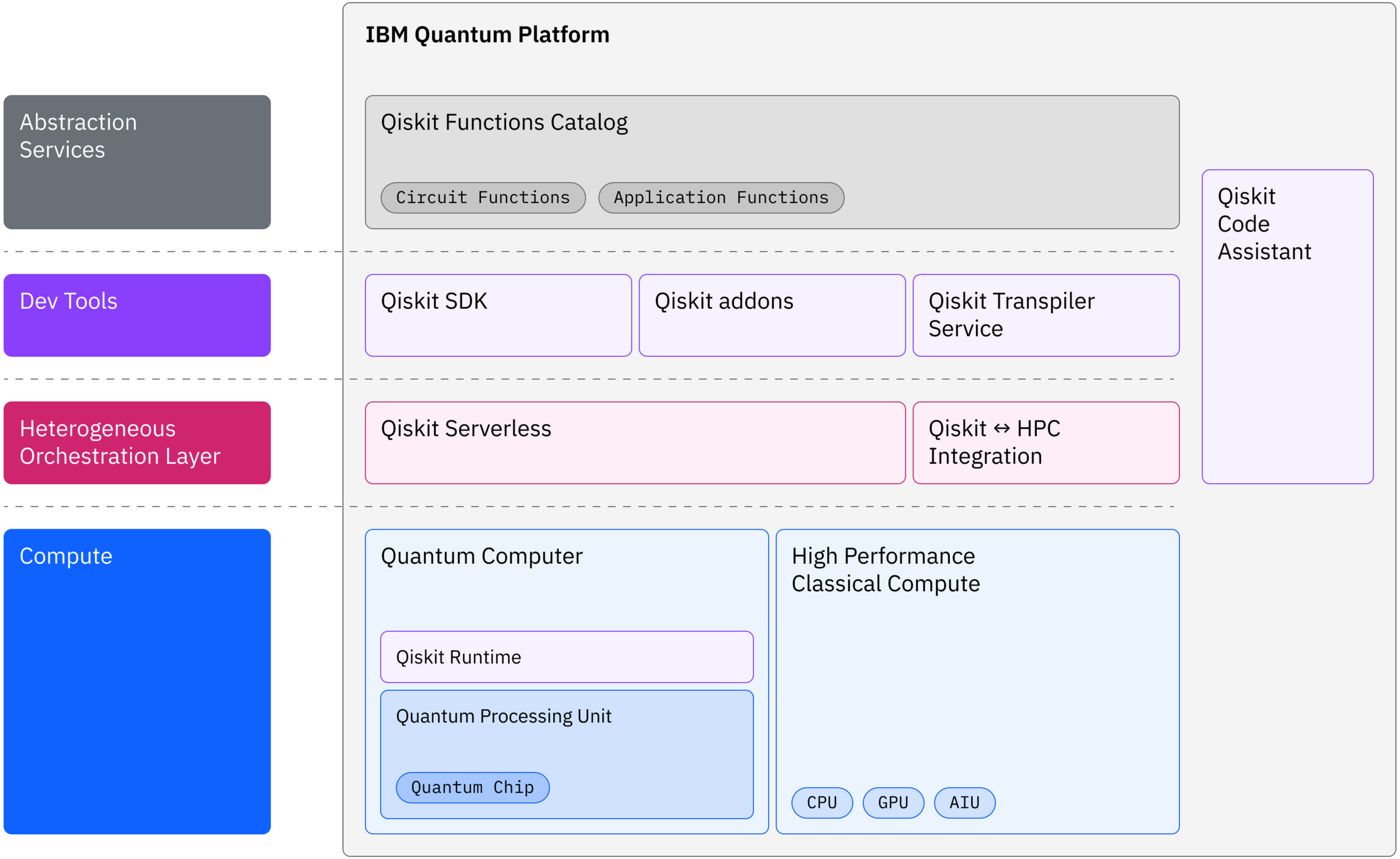
Interference

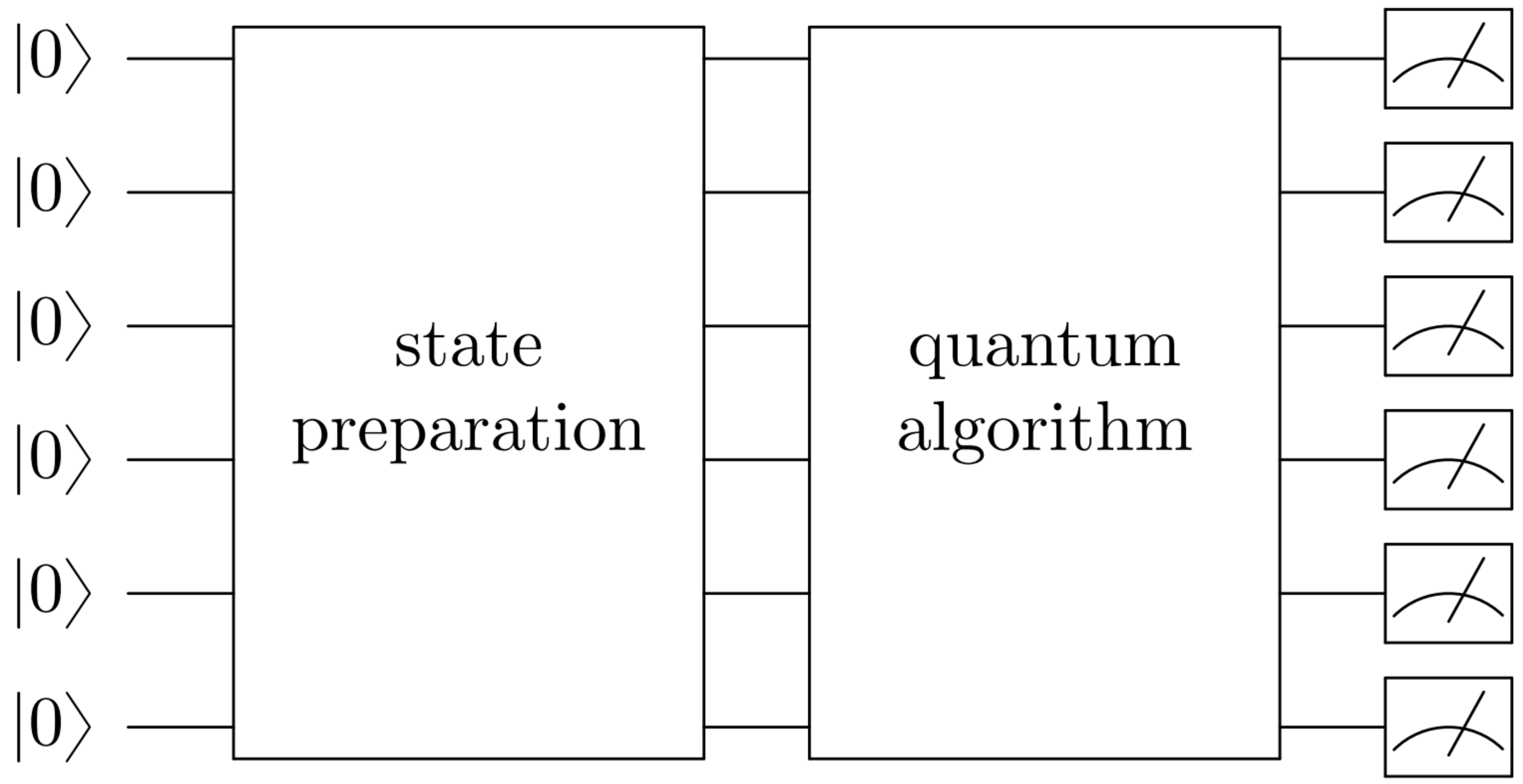




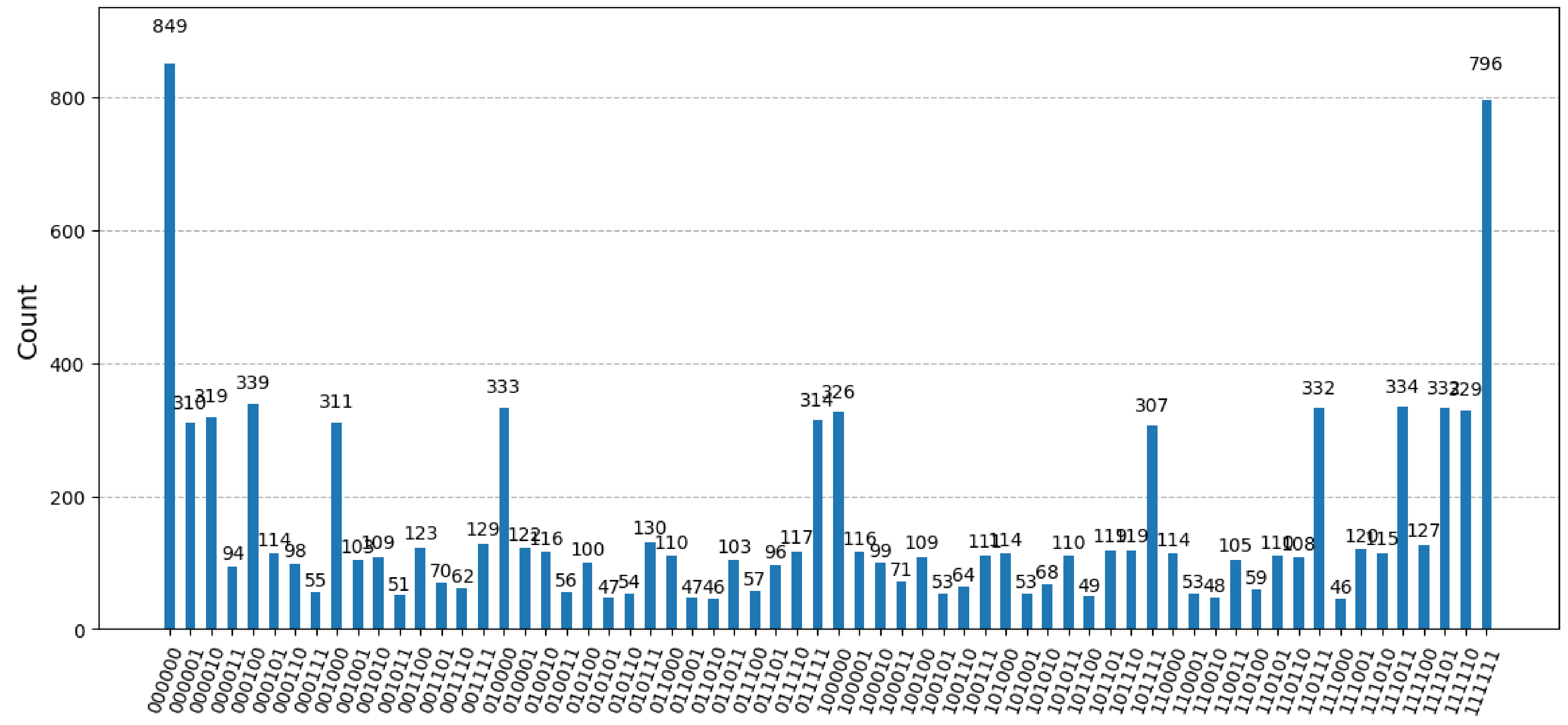
Qiskit SDK


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

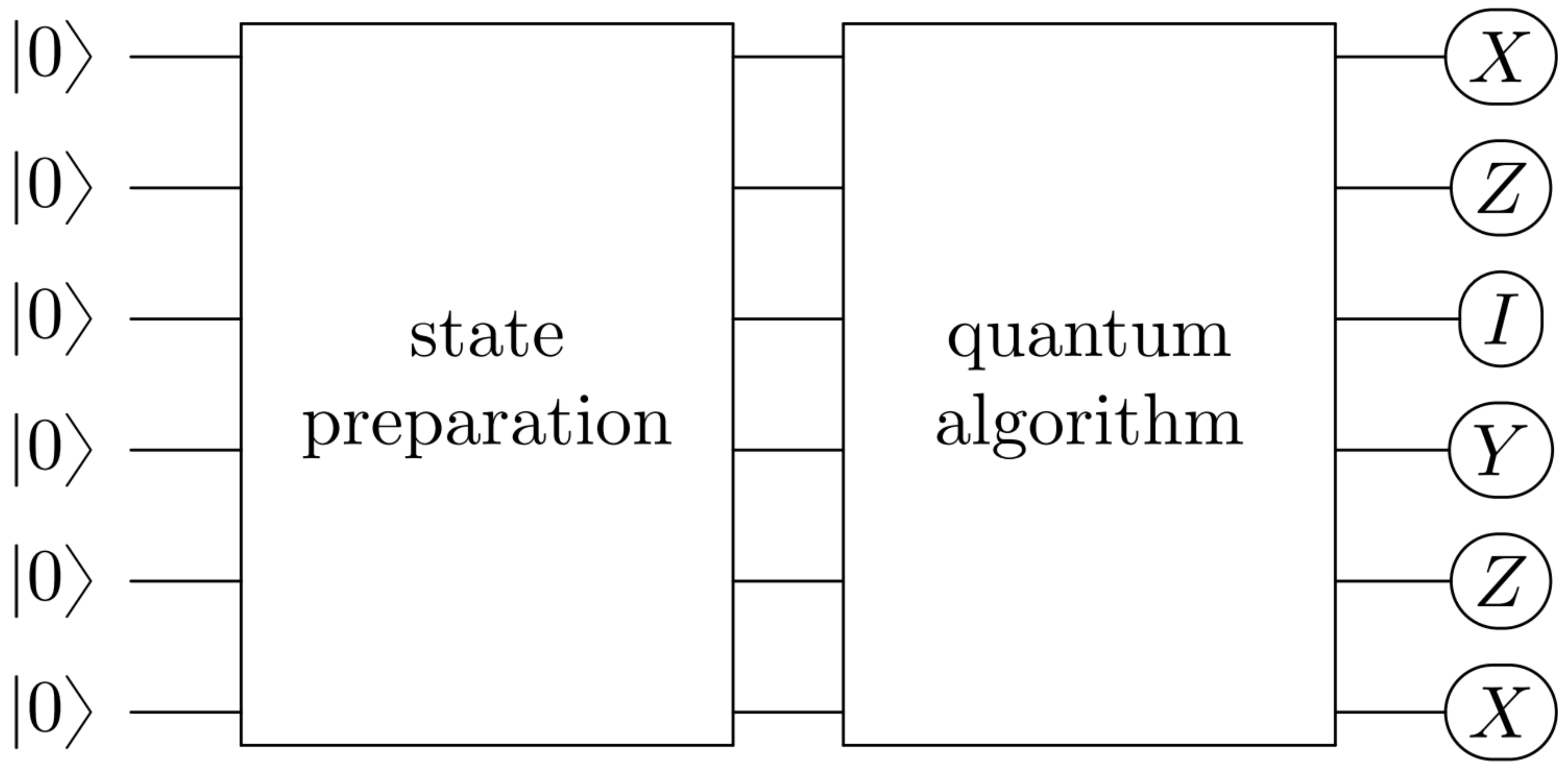
Samples



sample output = 101110



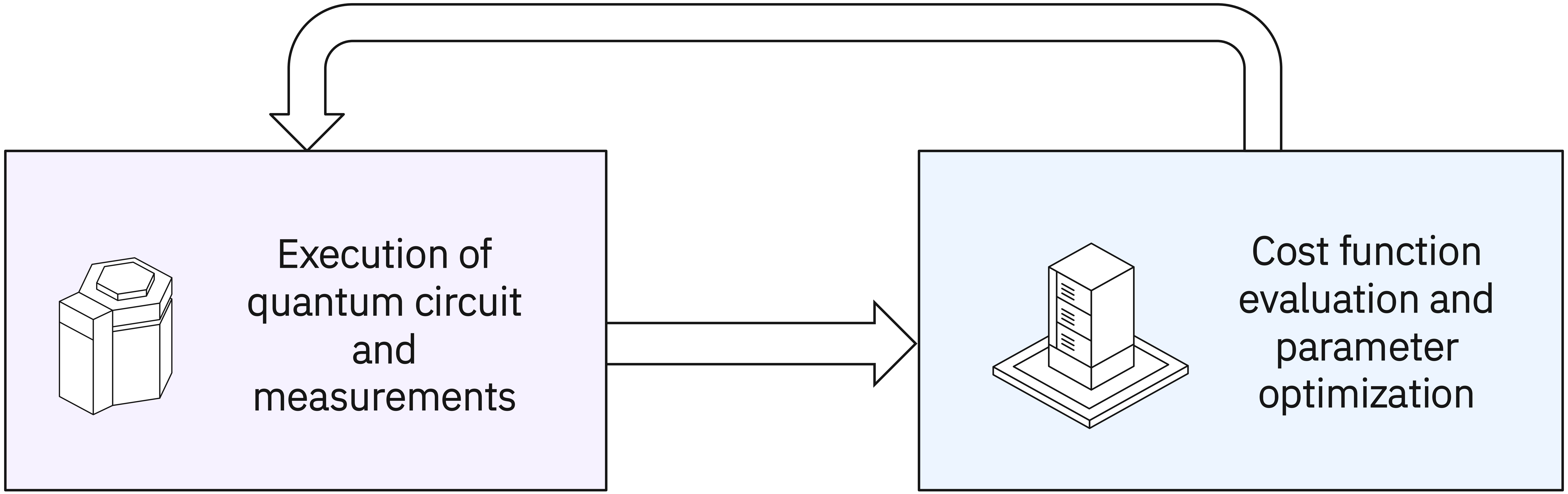
Observables



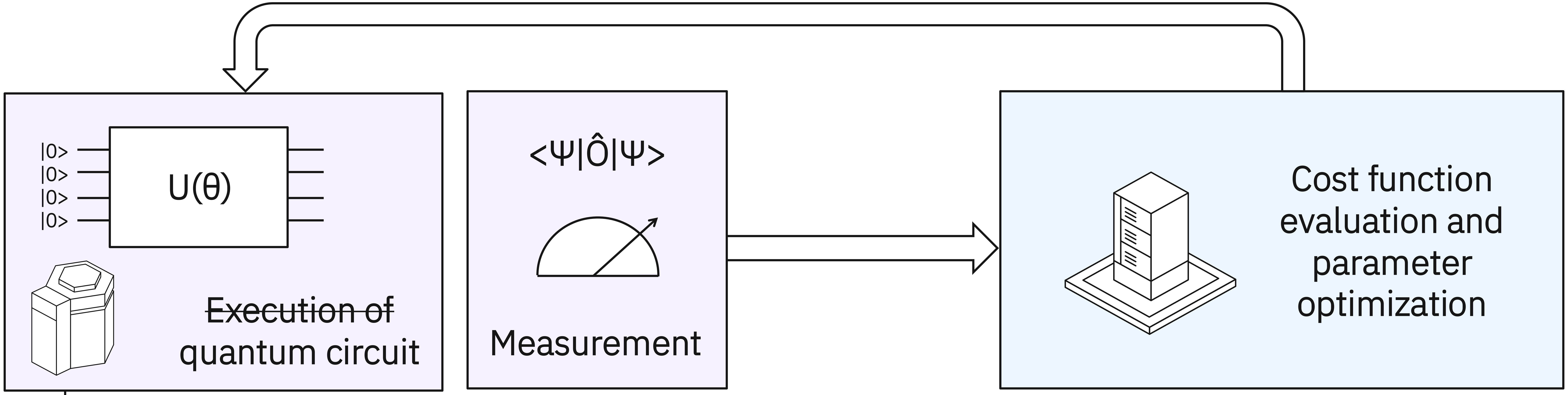
$$\langle \mathcal{O} \rangle = -0.34 \langle XZIYZX \rangle + 0.12 \langle XXYIZX \rangle + \ldots$$

corresponds to the value of a cost function, or a physical quantity such as energy or magnetization

Overview of Variational Quantum Algorithms

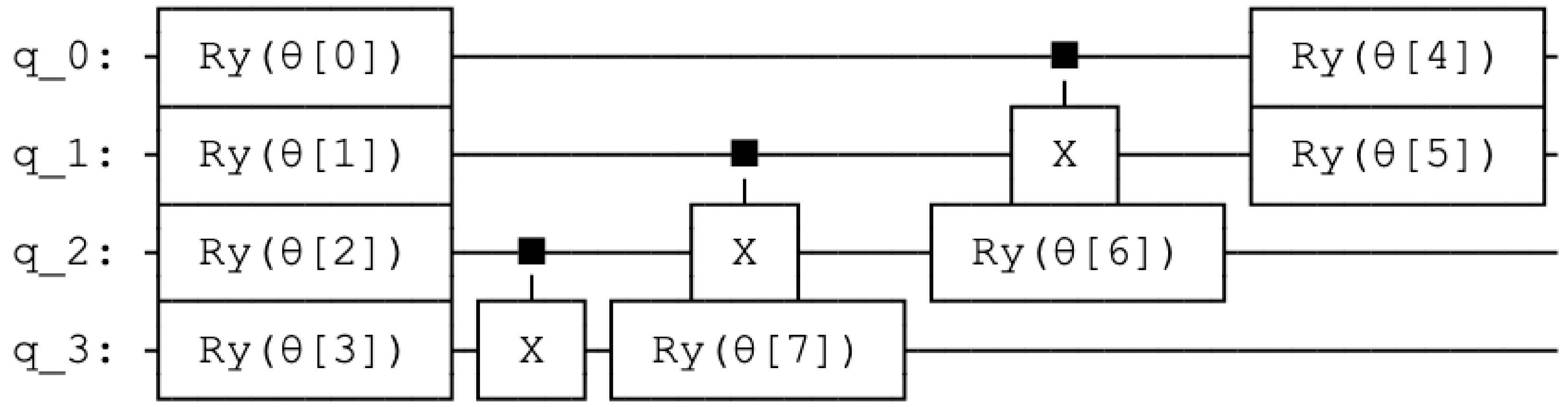


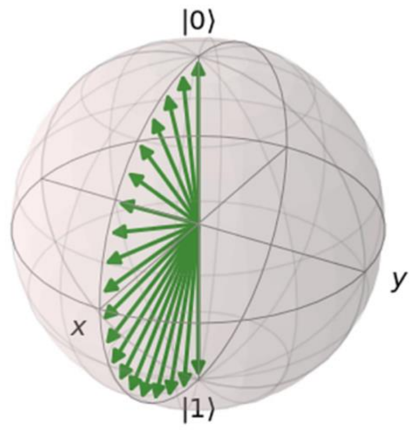
Overview of Variational Quantum Algorithms



- Choice of ansatz

`RealAmplitudes(4, reps=1)`





- Choice of initial parameters θ_0
(are there any constraints?)

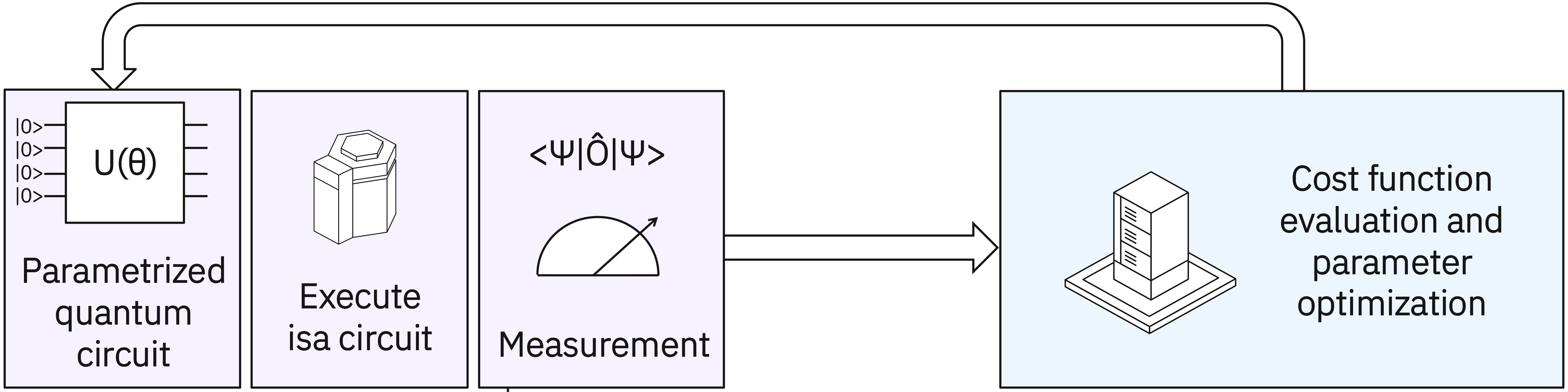
Qiskit circuit library

`n_local` (num_qubits, rotation_blocks, ...[, ...])	Construct an n-local variational circuit.
`efficient_su2` (num_qubits[, su2_gates, ...])	The hardware-efficient $SU(2)$ 2-local circuit.
`real_amplitudes` (num_qubits[, entanglement, ...])	Construct a real-amplitudes 2-local circuit.
`pauli_two_design` (num_qubits[, reps, seed, ...])	Construct a Pauli 2-design ansatz.
`excitation_preserving` (num_qubits[, mode, ...])	The heuristic excitation-preserving wave function ansatz.
`qaoa_ansatz` (cost_operator[, reps, ...])	A generalized QAOA quantum circuit with a support of custom initial states and mixers.
`hamiltonian_variational_ansatz` (hamiltonian)	Construct a Hamiltonian variational ansatz.
`evolved_operator_ansatz` (operators[, reps, ...])	Construct an ansatz out of operator evolutions.

arxiv.2402.15879

Overview of Variational Quantum Algorithms

Overview of Variational Quantum Algorithms



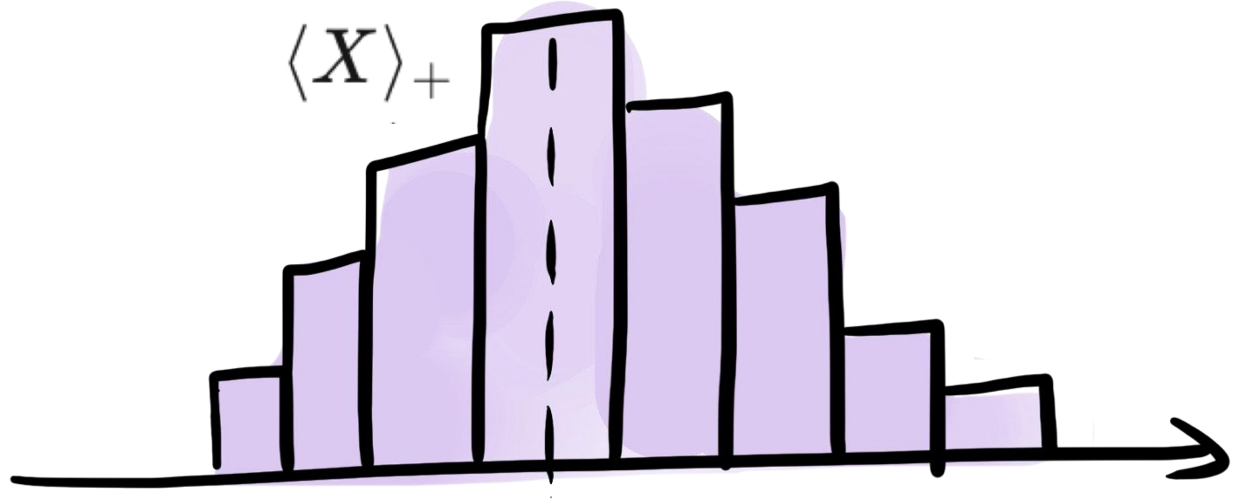
- Observable is given by the problem
- Expectation value is computed with finite num. of shots

Quantum state

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

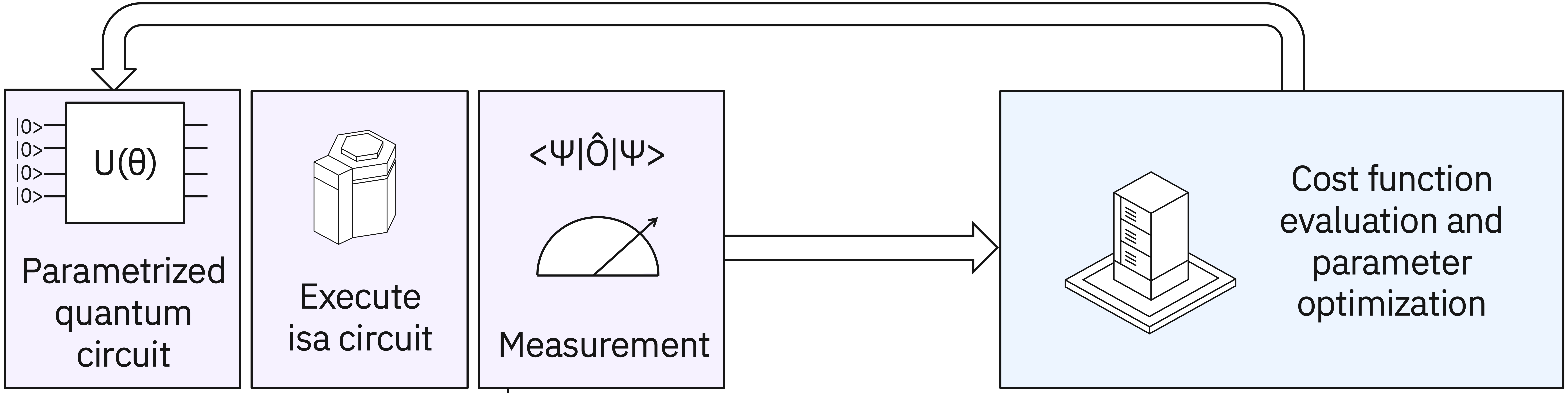
Observable

$$\hat{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$



measurement outcome on $|\psi\rangle$

Overview of Variational Quantum Algorithms

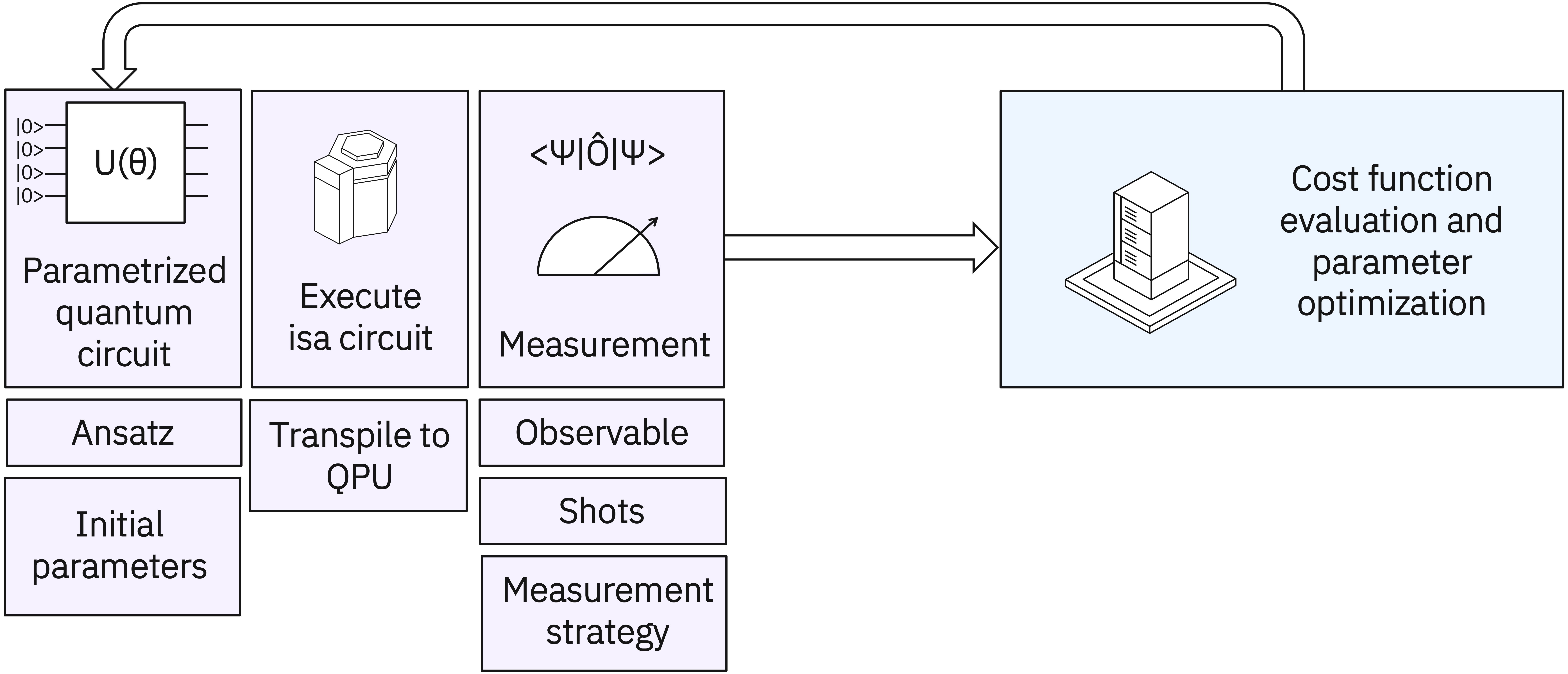


- Observable is given by the problem
- Expectation value is computed with finite num. of shots
- For complex observables we need grouping strategies

$\hat{O} = Z_0 \cdot X_1 + Y_1 \cdot X_2 + X_2 \cdot X_3 + X_0 + Z_3$ (5 terms)

Group 1: $Z_0 \cdot X_1 + X_2 \cdot X_3$
Group 2: $Y_1 \cdot X_2 + X_0 + Z_3$

Overview of Variational Quantum Algorithms



Inspired in “Introduction to VQAs”,
By Michał Stęchły, arxiv.2402.15879

Qiskit Pattern:
The anatomy of a quantum algorithm

01
Map problem instance to quantum circuits and operators

Map

02
Optimize for target hardware execution

Optimize

03
Execute via Qiskit Runtime

Execute

04
Result processing

Post-Process

Qiskit SDK sets the foundation

Qiskit SDK gives us a base layer of building blocks for building and running quantum algorithms

Qiskit Circuit Library

Input:
Domain inputs

Output:
Circuits, observable

Map

Transpiler

Input:
Circuits, observable

Output:
ISA circuit, observable

Optimize

Primitives

Input:
ISA circuit, observable

Output:
Expectation value/samples

Execute

Quantum Info

Input:
Expectation value/samples

Output:
Data objects/visualizations

Post-Process

Qiskit addons build on the Qiskit SDK

A collection of research capabilities developed as modular tools that can plug into a workflow to design new algorithms at the utility scale

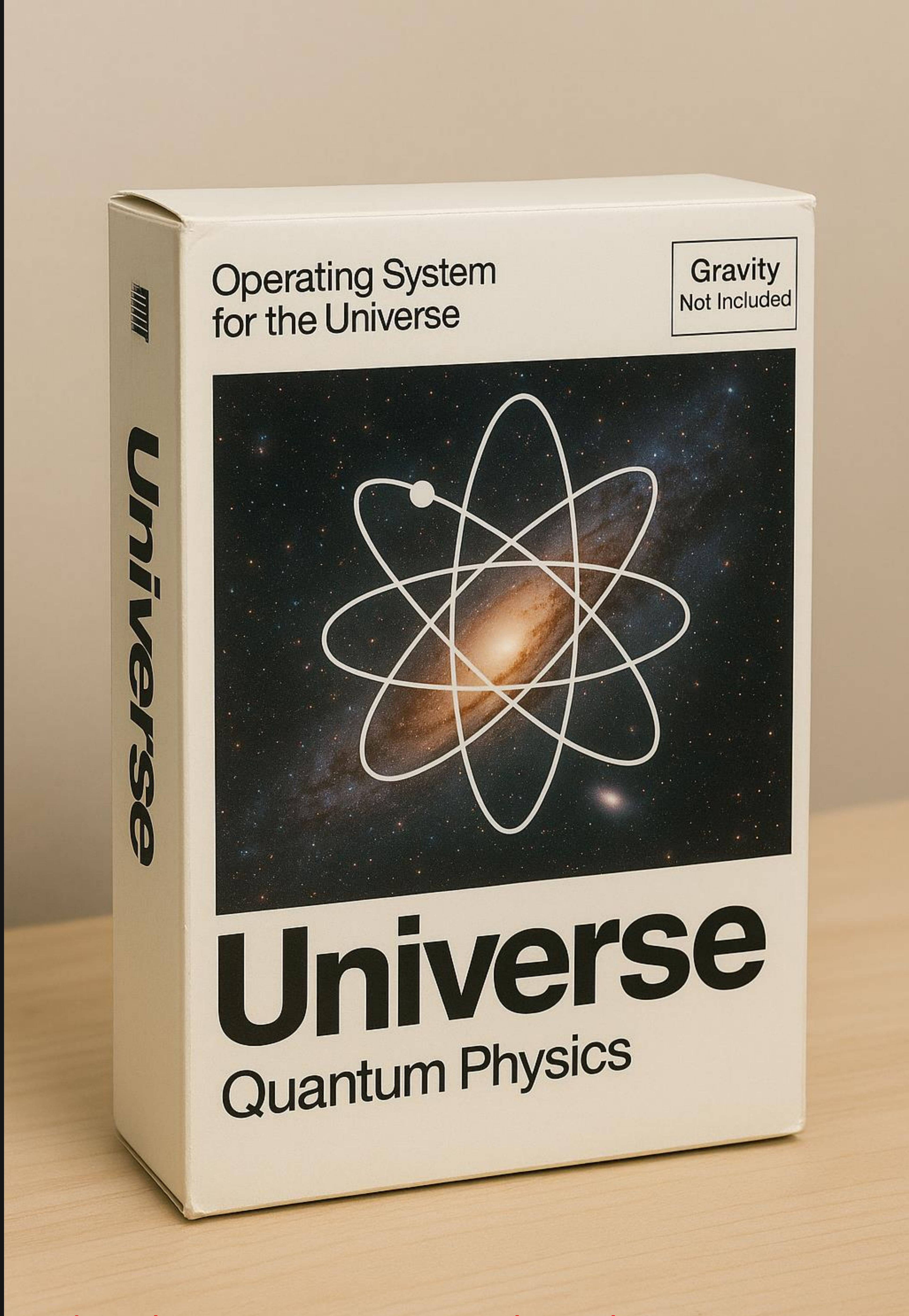
Starting with multi-product formulas (MPF), approximate quantum compilation (AQC-Tensor), operator backpropagation (OBP), and sample-based quantum diagonalization (SQD).

Map	Optimize	Execute	Post-Process
AQC-Tensor	OBP		SQD
MPF	Circuit cutting		M3
Qiskit Circuit Library	Transpiler	Primitives	Quantum Info
Input: Domain inputs	Input: Circuits, observable	Input: ISA circuit, observable	Input: Expectation value/samples
Output: Circuits, observable	Output: ISA circuit, observable	Output: Expectation value/samples	Output: Data objects/visualizations

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.

The new wave of computing

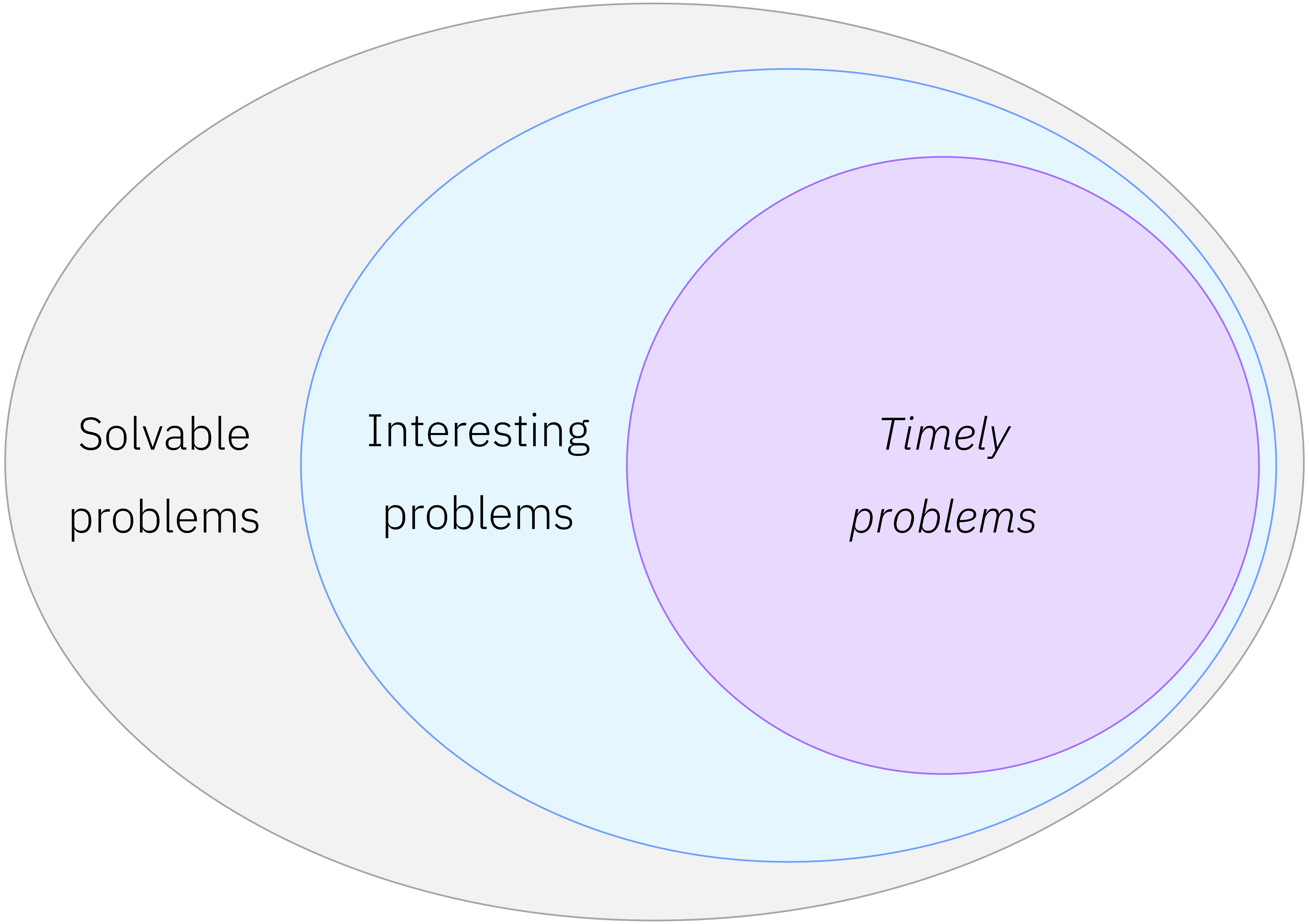
Classical computer
Well suited for many problems

Quantum computer
Unlock classically intractable problems

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

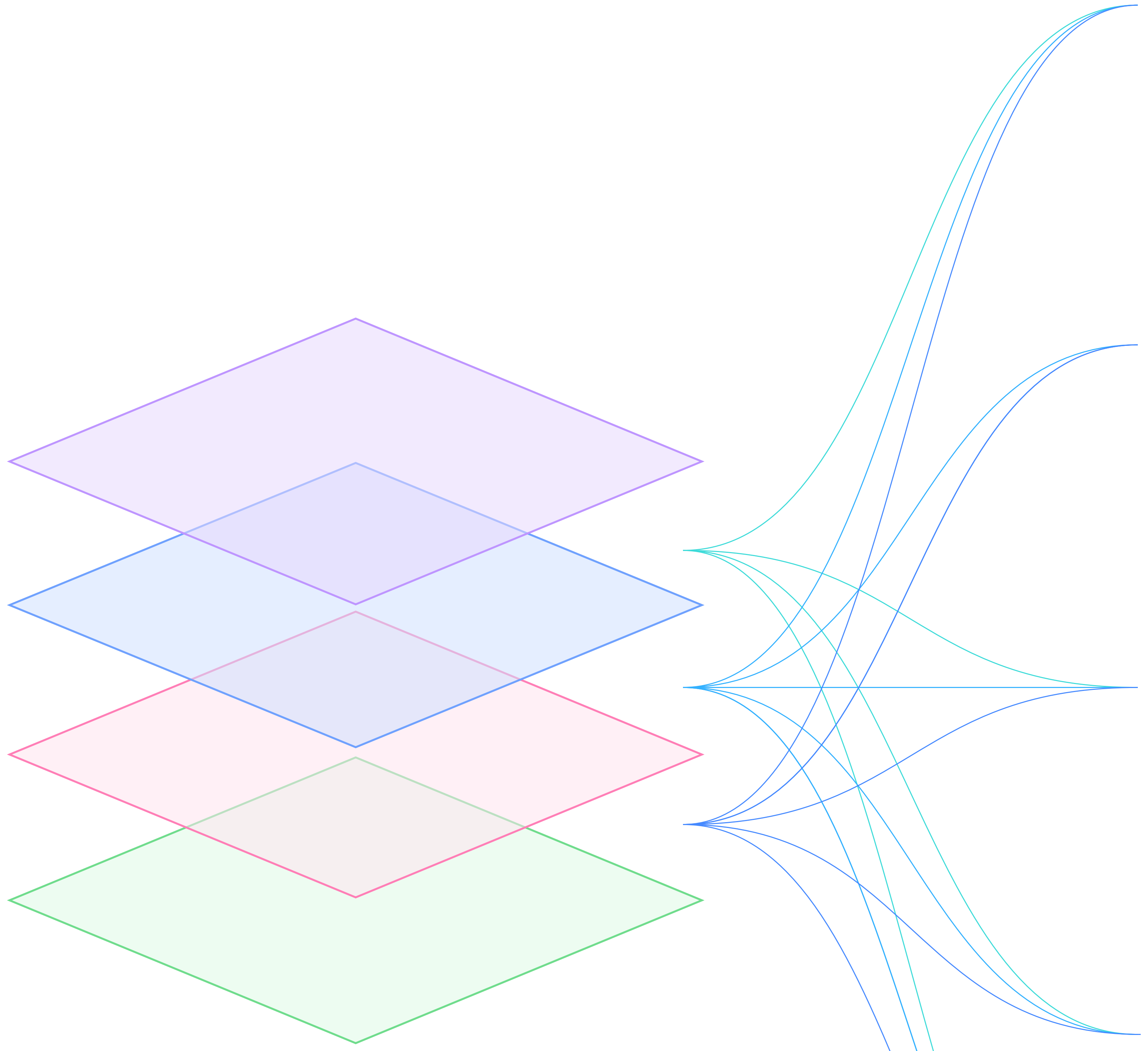
Nearer Term
Longer Term

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

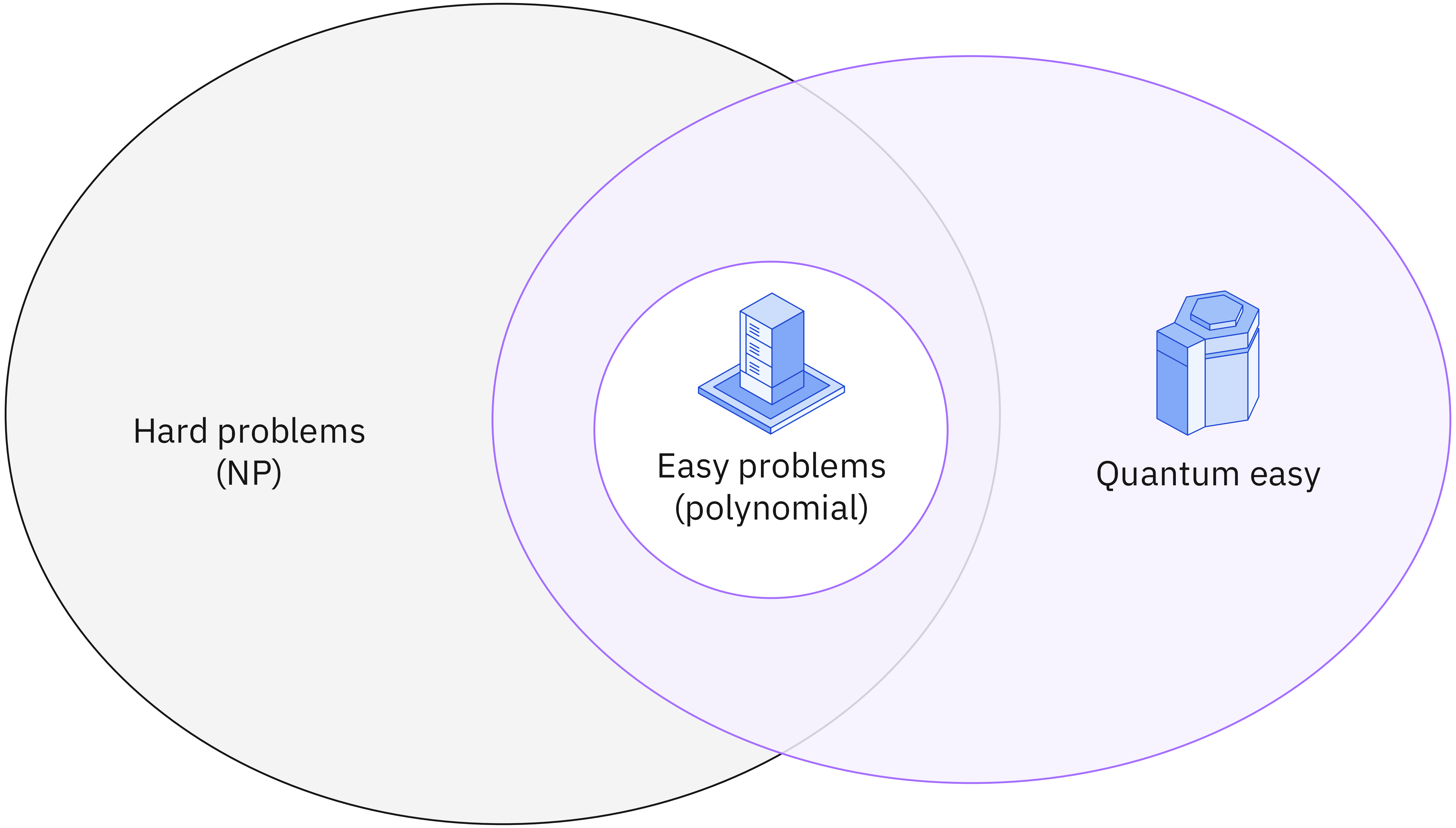
Energy
- Grid management
- Grid optimization with EV's
- Carbon Sequestration

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

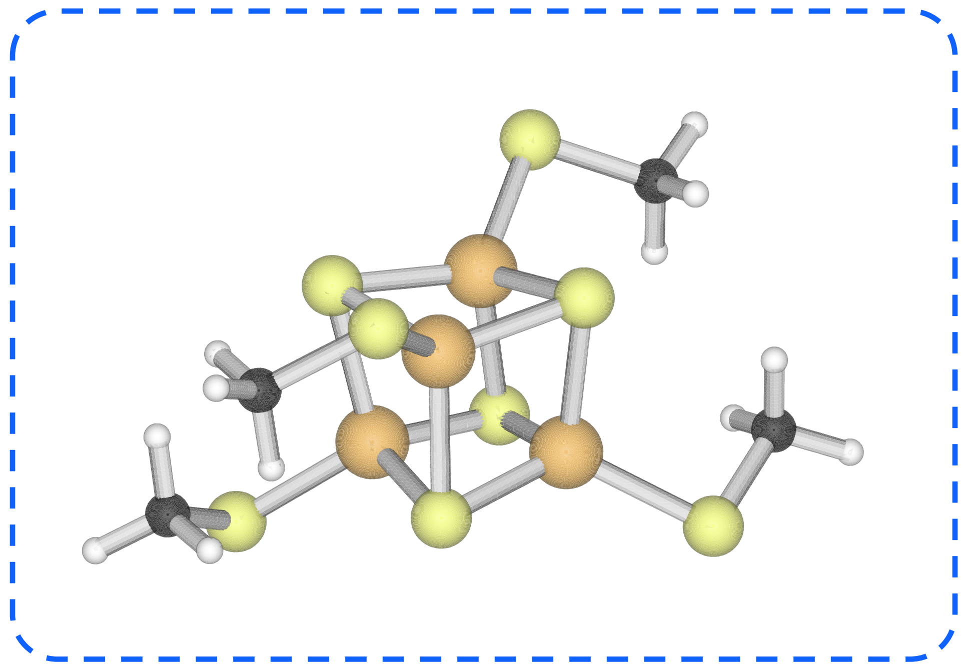
There is a rich seam of problems that cannot be solved by classical and AI supercomputing, and never will.

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

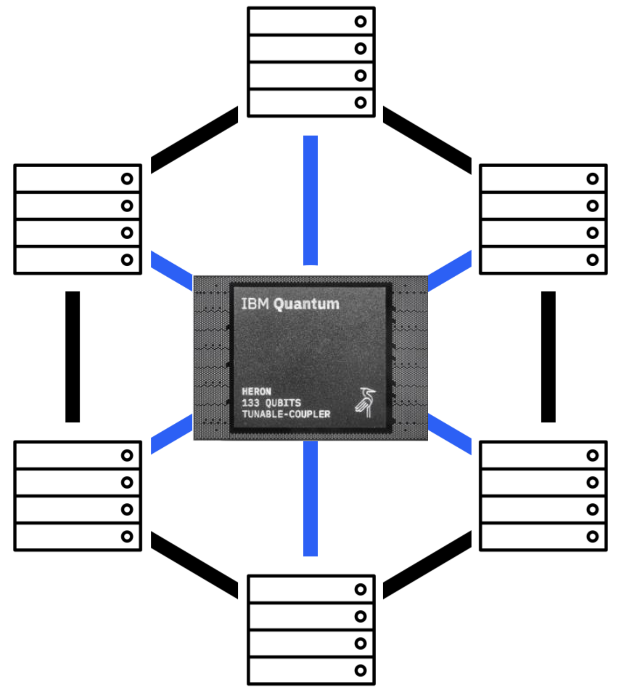


What are these problems?

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]

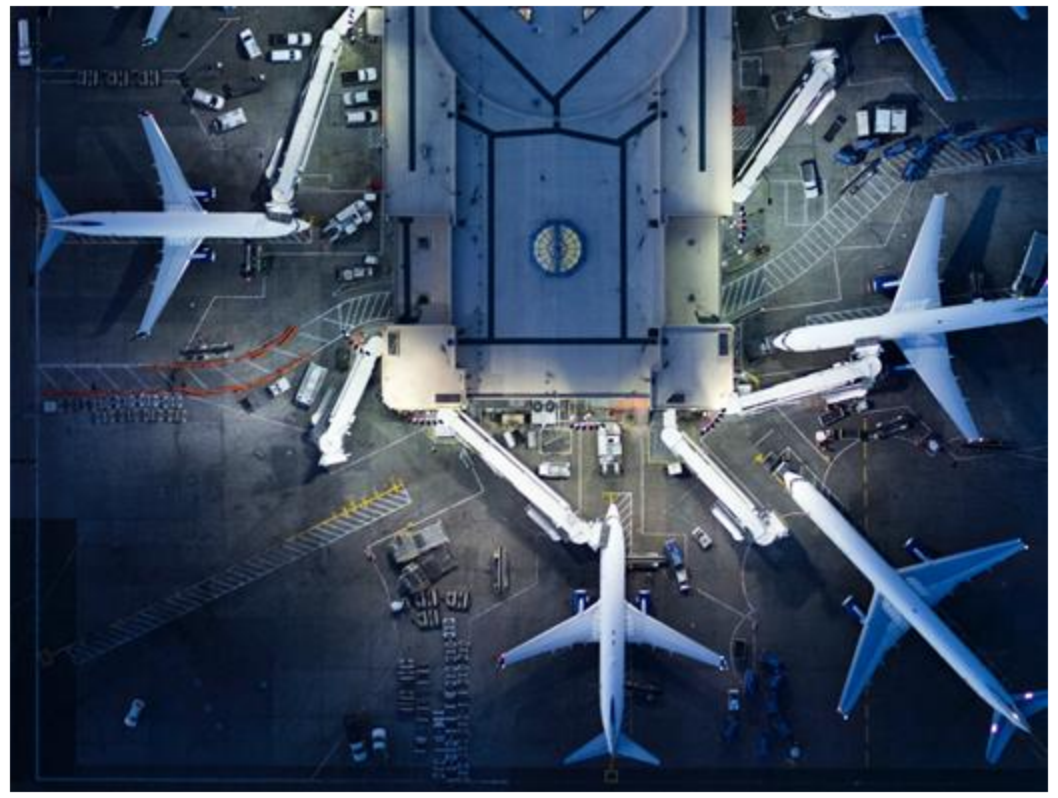
We are already using quantum (Heron, 77 qubits) and HPC (Supercomputer Fugaku) to achieve results comparable with the best classical approximate methods (DMRG) in accuracy and timing

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

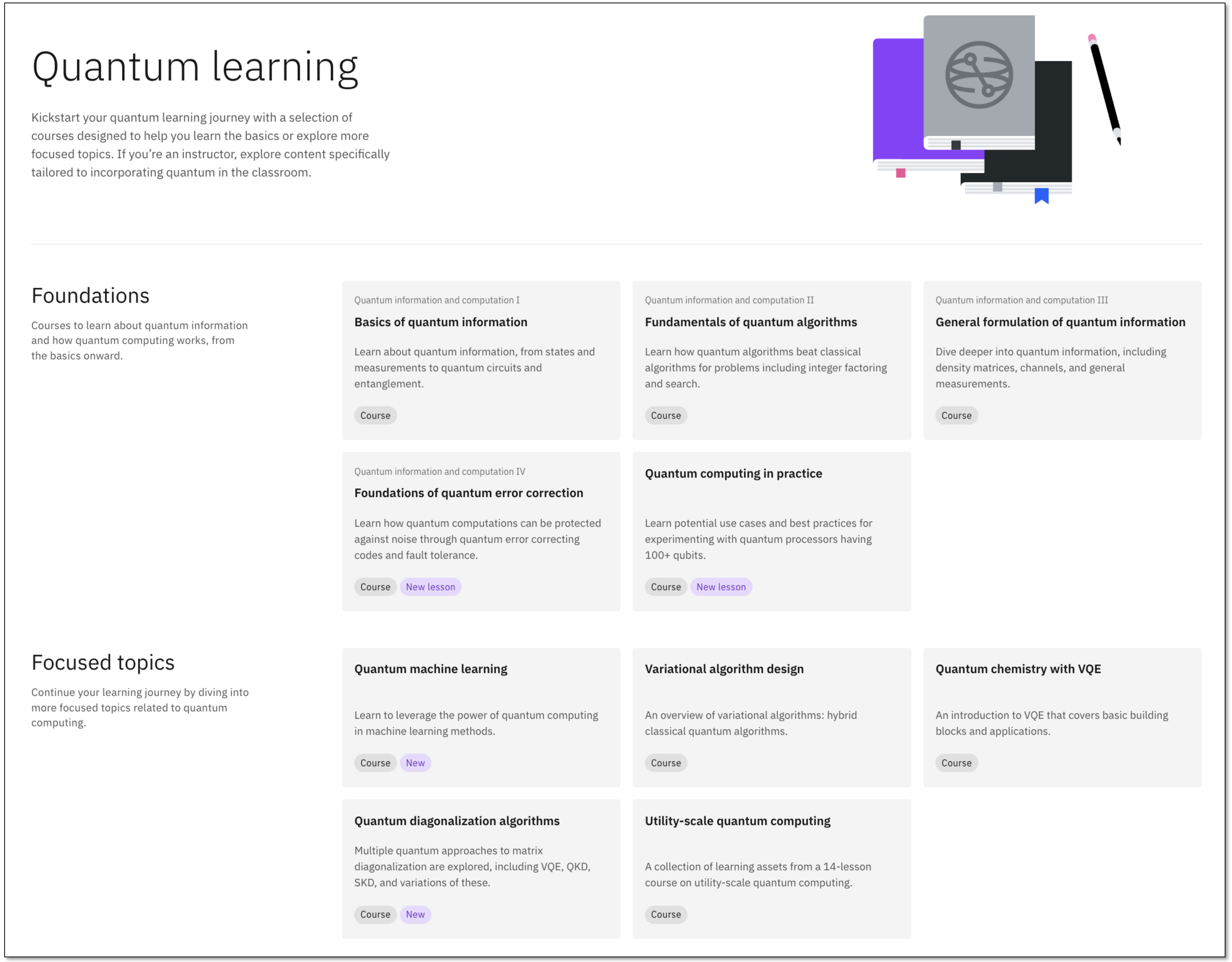
Designing optimal superconductors for MRI, electromobility, and renewable energies

Next steps!

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.



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.

What is the Qiskit advocate program?

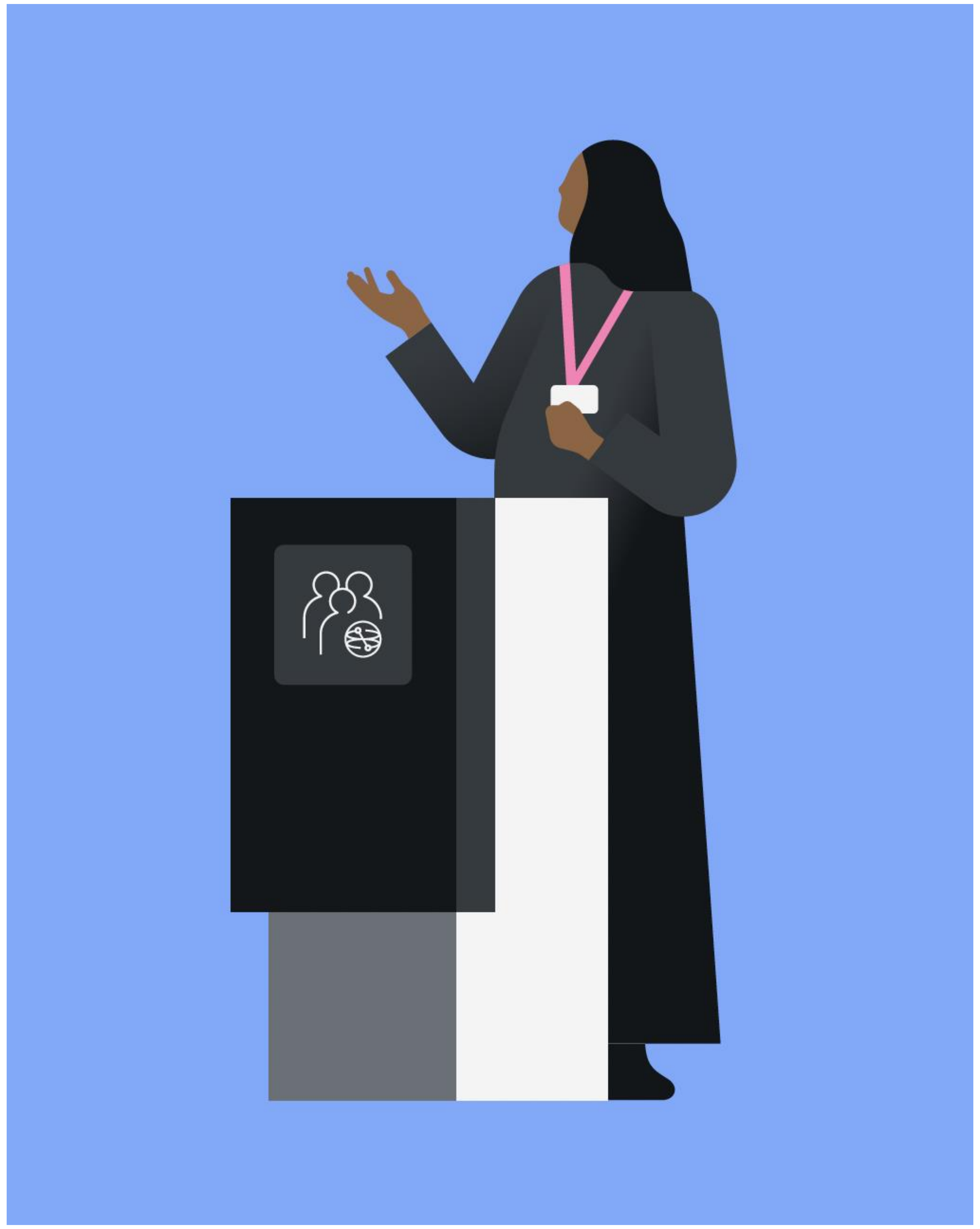
Join 544+ Qiskit Advocates across 50 countries in advancing quantum computing education and community.

The Qiskit advocate program is an external, global initiative that empowers and enables aspiring leaders in the Qiskit open-source community.

Qiskit advocates enhance their professional growth by:

- Building meaningful connections with quantum experts and peers
- Gaining exclusive access to Qiskit education and events
- Getting unique opportunities to contribute to quantum computing advancement
- Making open-source contributions and sharing knowledge through mentorship
- Participating in Qiskit events, networking, and quantum research and so much more.

Perfect for: Students, software developers, quantum researchers, educators, and anyone looking to upskill and advance their career in quantum computing.



Bring useful quantum computing to the world

IBM **Quantum**