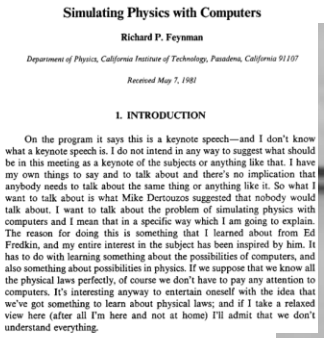
DCM4: Quantum Computing Challenge

Training

What is a Quantum Computer?

- A **quantum computer** is a device that uses quantum properties, namely *superposition* and *entanglement, to process information*



Simulating Physics with Computers

Richard P. Feynman

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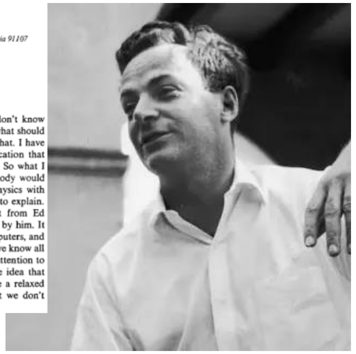
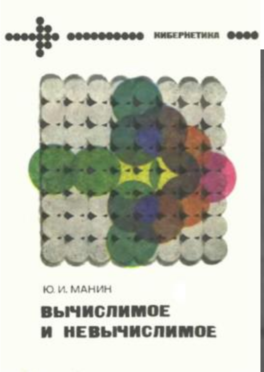
Received May 7, 1981

1. INTRODUCTION

On the program it says this is a keynote speech—and I don't know what a keynote speech is. I do not intend in any way to suggest what should be in this meeting as a keynote of the subjects or anything like that. I have my own things to say and to talk about and there's no implication that anybody needs to talk about the same thing or anything like it. So what I want to talk about is what Mike Dertouzos suggested that nobody would talk about. I want to talk about the problem of simulating physics with computers and I mean that in a specific way which I am going to explain. The reason for doing this is something that I learned about from Ed Fredkin, and my entire interest in the subject has been inspired by him. It has to do with learning something about the possibilities of computers, and also something about possibilities in physics. If we suppose that we know all the physical laws perfectly, of course we don't have to pay any attention to computers. It's interesting anyway to entertain oneself with the idea that we've got something to learn about physical laws; and if I take a relaxed view here (after all I'm here and not at home) I'll admit that we don't understand everything.



Richard Feynman



Yuri Manin

- The information is stored in the state of qubits

- The quantum computer acts on the qubits using quantum gates

What is a Quantum Computer?

- A **qubit** (quantum bit) is the quantum analogue to a classical bit; while a bit can be in two states (0 or 1), a qubit can be in a *superposition* of the *basis states* $|0\rangle$ and $|1\rangle$.

- We describe a qubit's **superposition** state by

$$|q\rangle = c_0|0\rangle + c_1|1\rangle$$

where the *amplitudes* c_0 and c_1 are complex numbers such that

$$|c_0|^2 + |c_1|^2 = 1$$

- Note: the normalisation condition $|c_0|^2 + |c_1|^2 = 1$ must hold for $|q\rangle$ to be a valid quantum state (i.e., satisfy the Schrödinger equation).

Complex Numbers: A brief aside...

We are familiar with ***real numbers*** like

$$0, 1, e, \pi, 1.23, 3/4, -10...$$

Complex numbers can be seen as an extension of real numbers, by introducing the *imaginary* unit i, and are essential to the field of quantum mechanics. The imaginary unit's defining property is that

$$i^2 = -1$$

A **complex number** has a ***real*** part and an ***imaginary*** part, which we define as

$$c = a + i \times b$$

Complex Numbers: A brief aside...

One quantity associated with a complex number c is its *magnitude* $|c|$, defined as

$$|c| = \sqrt{a^2 + b^2}$$

The magnitude is the "**length**" of the complex number (i.e., the length of the associated vector in complex vector space).

E.g., consider the following complex numbers and their respective magnitudes:

c	$\lvert c \rvert$
-3	3
$4i$	4
$4 - 3i$	5
$2 + 2i$	$2\sqrt{2}$

Quantum Computing: Qubits

- A **qubit** in a **superposition** of the states $|0\rangle$ and $|1\rangle$:

$$|q\rangle = c_0|0\rangle + c_1|1\rangle \qquad |c_0|^2 + |c_1|^2 = 1$$

- We cannot observe this superposition directly, and only have access to **measurement** outcomes that will return $|0\rangle$ or $|1\rangle$, each with some probability.

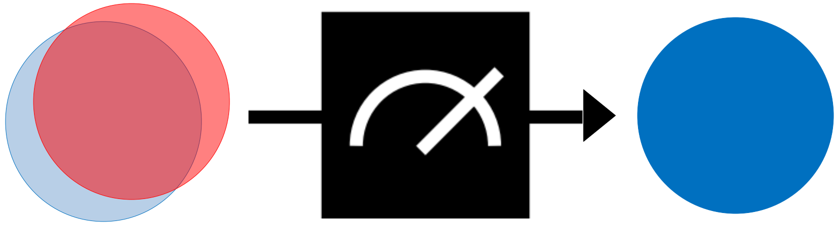
- However, the measurement outcome is ***correlated*** to the qubit's quantum state: probabilities of measuring $(|0\rangle, |1\rangle)$ are $(|c_0|^2, |c_1|^2)$ (i.e., the amplitude's absolute square $|c|^2 = c^*c = (a - bi)(a + bi)$ from the **Born rule**).

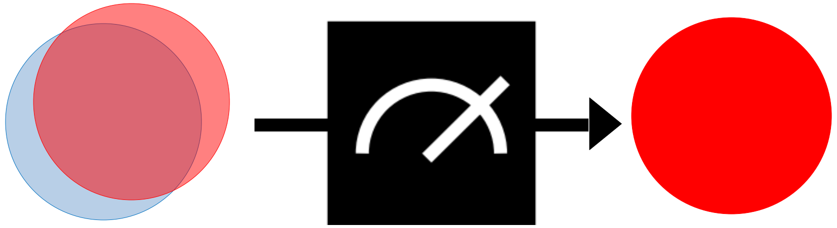
Quantum Computing: Qubits

- A **qubit** in a **superposition** of the states $|0\rangle$ and $|1\rangle$:

$$|q\rangle = c_0|0\rangle + c_1|1\rangle \qquad |c_0|^2 + |c_1|^2 = 1$$

- Following measurement, a qubit's superposition state ***collapses*** to the measured state





Quantum Computing: Qubits

- A **qubit** in a **superposition** of the states $|0\rangle$ and $|1\rangle$:

$$|q\rangle = c_0|0\rangle + c_1|1\rangle \qquad |c_0|^2 + |c_1|^2 = 1$$

- As previously described, we cannot observe $|q\rangle$ directly – we can only perform a measurement to obtain 0 and 1, each with some probability.

- E.g., consider the state

$$|q\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{i}{\sqrt{2}}|1\rangle$$

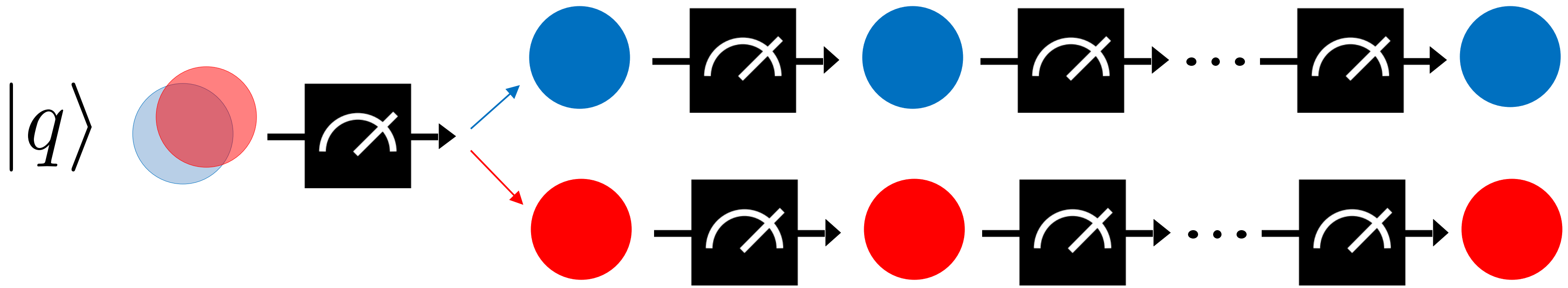
- Measuring $|q\rangle$ will return 0 with probability $|c_0|^2 = \left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{2}$ and 1 with probability $|c_1|^2 = \left|\frac{i}{\sqrt{2}}\right|^2 = \frac{1}{2}$.

Quantum Computing: Qubits

- A **qubit** in a **superposition** of the states $|0\rangle$ and $|1\rangle$:

$$|q\rangle = c_0|0\rangle + c_1|1\rangle \qquad |c_0|^2 + |c_1|^2 = 1$$

- Immediately after the initial measurement, that state collapses and all subsequent measurements will obtain the same result. If 0 is measured we will have $|q\rangle = |0\rangle$ but if 1 is measured we will have $|q\rangle = |1\rangle$.



Quantum Computing: Measurement

- Recall that we can't directly observe a quantum state, and that we can only measure (i.e., read out) a single bit, representing one of the basis states $(|0\rangle, |1\rangle)$.

- The **Born rule** states that the probability of obtaining a particular bit outcome equals the *absolute square* of its amplitude in the superposition state being measured.

- E.g., measuring $|+\rangle$ yields $|0\rangle$ or $|1\rangle$ with probability $\frac{1}{2}$ each.

Max Born

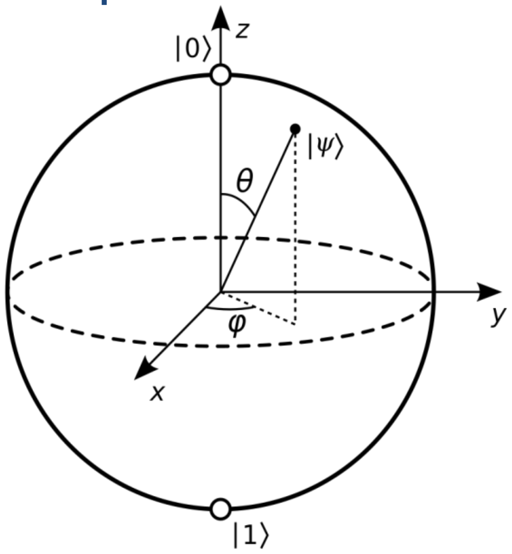
$$|+\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle) \rightarrow \begin{array}{l} \Pr(|0\rangle) = \left|\left(\frac{1}{\sqrt{2}}\right)\right|^2 = \frac{1}{2} \\ \Pr(|1\rangle) = \left|\left(\frac{1}{\sqrt{2}}\right)\right|^2 = \frac{1}{2} \end{array}$$

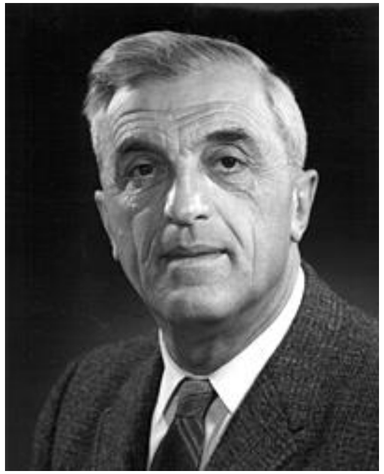
Quantum Computing: Bloch Sphere

- A **qubit** in a **superposition** of the states $|0\rangle$ and $|1\rangle$:

$$|q\rangle = c_0|0\rangle + c_1|1\rangle \qquad |c_0|^2 + |c_1|^2 = 1$$

- The **Bloch** sphere is a geometric representation of a quantum superposition state.

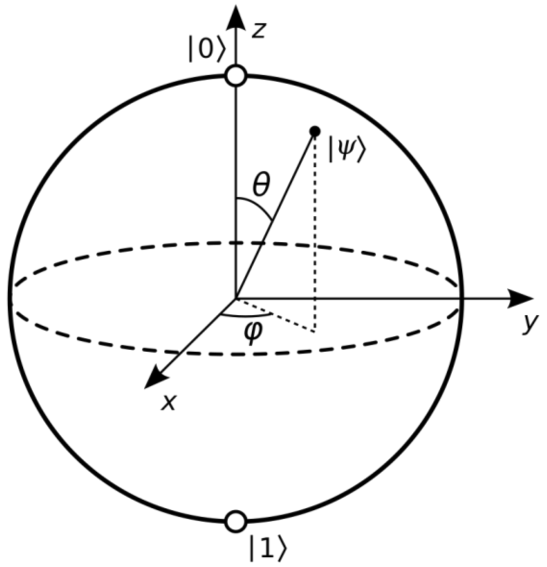




Felix Bloch

Quantum Computing: Bloch Sphere

Deriving the **Bloch sphere:** $|c_0|^2 + |c_1|^2 = 1$ can be re-expressed using *polar coordinates*



$$c_1 = \sin(\theta/2)e^{i\phi} \quad c_0 = \cos(\theta/2)$$

where

$$0 \leq \theta \leq \pi \quad 0 \leq \phi \leq 2\pi$$

and so we rewrite $|q\rangle \rightarrow |\psi\rangle$ as

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

The state $|\psi\rangle$ then corresponds to a point on the surface of a sphere where the north pole is $|0\rangle$ and the south pole is $|1\rangle$ with (θ, ϕ) as coordinates (colatitude and longitude).

Extending to Multiple Qubits

- Quantum computers store information on **multiple qubits** (just as classical computers use multiple bits).

- The 2-qubit system $|q_0\rangle|q_1\rangle = |q_0 q_1\rangle$ can be in a superposition of $2^2 = 4$ *basis states*: $|00\rangle$, $|01\rangle$ $|10\rangle$, $|11\rangle$

$$|q_0 q_1\rangle = c_{00}|00\rangle + c_{01}|01\rangle + c_{10}|10\rangle + c_{11}|11\rangle$$

$$|c_{00}|^2 + |c_{01}|^2 + |c_{10}|^2 + |c_{11}|^2 = 1$$

Extending to Multiple Qubits

- In general, a system of *n* qubits can be in a superposition of 2^n states:

1 qubit $\qquad |q\rangle = c_0|0\rangle + c_1|1\rangle \qquad |c_0|^2 + |c_1|^2 = 1$

2 qubits $\qquad |q_0 q_1\rangle = c_{00}|00\rangle + c_{01}|01\rangle + c_{10}|10\rangle + c_{11}|11\rangle \qquad |c_{00}|^2 + |c_{01}|^2 + |c_{10}|^2 + |c + 11|^2 = 1$

⋮

n qubits $\qquad |\psi\rangle = |q_0 q_1 \cdots q_n\rangle = \sum_{j=0}^{2^n-1} c_{\mathrm{bin}(j)} |\mathrm{bin}(j)\rangle \qquad \sum_{j=0}^{2^{n-1}} |c_{\mathrm{bin}(j)}|^2 = 1$

Extending to Multiple Qubits

- E.g., a two-qubit state:

$$|q_0 q_1\rangle = \frac{1}{3}|00\rangle + \frac{\sqrt{3}i}{3}|01\rangle + \frac{1+i}{3}|10\rangle - \frac{\sqrt{3}}{3}|11\rangle$$

A three-qubit state:

$$|q_0 q_1 q_2\rangle = -\frac{2}{5}|001\rangle + \frac{3}{5}|010\rangle - \frac{\sqrt{2}i}{5}|011\rangle + \frac{\sqrt{5}}{5}|101\rangle + \frac{\sqrt{3}}{5}|110\rangle + \frac{1-i}{5}|111\rangle$$

where $c_{000} = c_{100} = 0$.

Extending to Multiple Qubits

- Multi-qubit systems can also exhibit **entanglement**. An entangled system exists in a superposition state such that individual qubits cannot be described independently (even if separated in space).

- E.g., consider the separable 2-qubit state $|q_0 q_1\rangle = \frac{1}{2}|00\rangle - \frac{1}{2}|01\rangle + \frac{1}{2}|10\rangle - \frac{1}{2}|11\rangle$

which can be factored:

$$|q_0 q_1\rangle = \left(\frac{1}{2}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right)\left(\frac{1}{2}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle\right) = |q_0\rangle|q_1\rangle$$

- Now consider the entangled 2-qubit state. $|q_0 q_1\rangle = \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$

This state cannot be factored, and neither qubit's state can be individually described (i.e., $|q_i\rangle$ can't be written as a superposition $c_0|0\rangle + c_1|1\rangle$).

Measuring a Multi-Qubit System

- Similarly, recalling the *absolute square*

$$|c|^2 = c^*c = (a - bi)(a + bi)$$

measuring the state

$$|q_0q_1\rangle = \frac{1}{2}|01\rangle - \frac{i}{2}|10\rangle + \frac{1+i}{2}|11\rangle$$

- Yields the following probability table:

$\|\mathbf{ab}\rangle$	$\|c_{ab}\|^2$	$\Pr[\|\mathbf{q_0 q_1}\rangle = \|\mathbf{ab}\rangle]$
$\|00\rangle$	0	0
$\|01\rangle$	$\left\|\left(\frac{1}{2}\right)\right\|^2$	$\frac{1}{4}$
$\|10\rangle$	$\left\|\left(\frac{-i}{2}\right)\right\|^2$	$\frac{1}{4}$
$\|11\rangle$	$\left\|\left(\frac{1+i}{2}\right)\right\|^2$	$\frac{1}{2}$

Measuring a Multi-Qubit System

- Also recall that measuring a qubit collapses its quantum state to a classical bitstring, destroying the superposition in the process.

- E.g., suppose measuring the previous 2-qubit system

$$|q_0q_1\rangle = \frac{1}{2}|01\rangle - \frac{i}{2}|10\rangle + \frac{1+i}{2}|11\rangle$$

yields $|10\rangle$. The 2-qubit system will remain in this state

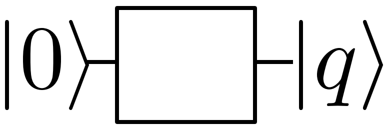
$$|q_0q_1\rangle = |10\rangle$$

such that all subsequent measurement return $|10\rangle$ with a probability of 1.

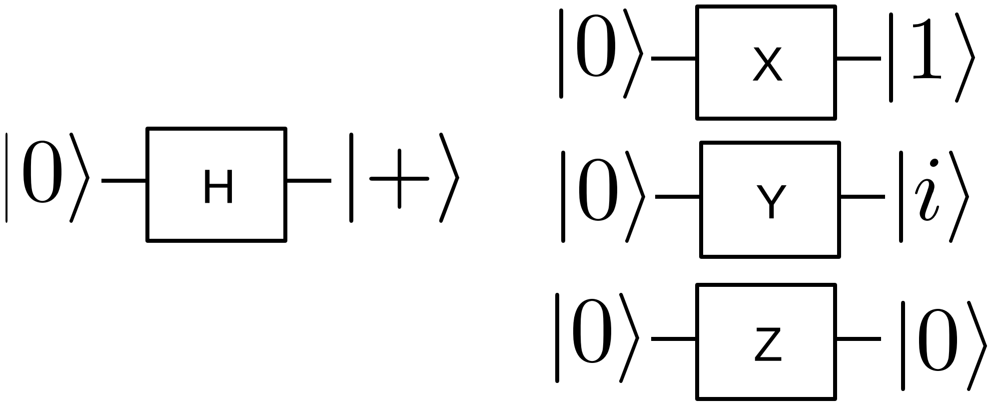
Quantum Logic Gates

- Qubits are typically initialised in the *ground state* $|0\rangle$; we generate superposition states and entanglement using **quantum logic gates.**

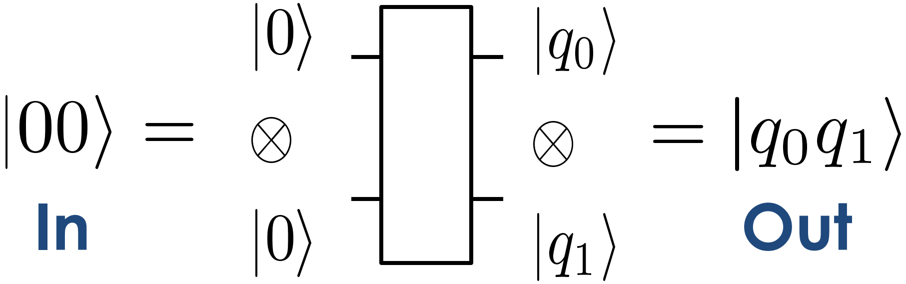
Single-qubit Gates



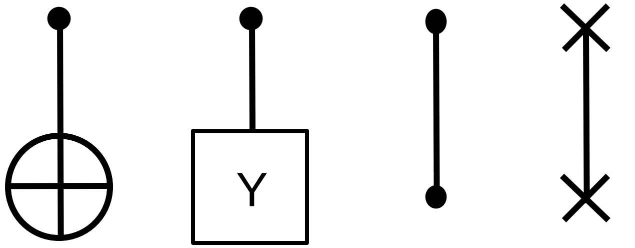
In **Out**



Two-qubit Gates



In **Out**



Quantum Logic Gates

- It is common and convenient to adopt a *matrix representation* for quantum operations. We consider the basis states $(|0\rangle, |1\rangle)$ as *vectors*

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

- Quantum computation can then be expressed in terms of matrix-vector operations. E.g., consider the matrix representation of the commonly used X gate and its effect on a qubit in the *ground state* $|0\rangle$:

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

- I.e., the X gate is the quantum analogue to a **classical NOT** that performs a (**qu**)**bit-flip** (takes the bit 0 → 1 and 1 → 0).

Quantum Logic Gates

- Another common gate is the Hadamard gate, represented as

$$\mathrm{H} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} = \left(\frac{1}{\sqrt{2}}\right) \cdot \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

- The effect of the Hadamard on a qubit in the ground state $|0\rangle$ is

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

the output of which is commonly labeled as $|+\rangle = \dfrac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$

- Similarly, its effect on a qubit in the *excited state* $|1\rangle$ is

$$\mathbf{H}|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = |-\rangle$$

Quantum Logic Gates

- We can also perform gates acting on more than one qubit, e.g., the **controlled-X gate** (CX) receiving as input a *control qubit* and a *target qubit*.

$$CX|00\rangle = |00\rangle \quad CX|10\rangle = |11\rangle$$
$$CX|01\rangle = |01\rangle \quad CX|11\rangle = |10\rangle$$

- CX performs an X on the target when the control is in state $|1\rangle$
- With matrix representation

$$\mathbf{CX} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Quantum Logic Gates

Matrix representations of common quantum gates:

$$\mathbf{X} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \mathbf{H} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$$

$$\mathbf{Y} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \mathbf{S} = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$$

$$\mathbf{Z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \qquad \mathbf{T} = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$$

$$\mathbf{CX} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$$\mathbf{SWAP} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Quantum Logic Gates

- Quantum gates are *linear* operations, and so they preserve superpositions: the output of applying a quantum gate to a qubit in superposition will also be a superposition. E.g., for $|q\rangle = a|0\rangle + b|1\rangle$ we have

$$\mathbf{H}|q\rangle = \mathbf{H}(a|0\rangle + b|1\rangle) = a\mathbf{H}|0\rangle + b\mathbf{H}|1\rangle = \frac{a+b}{\sqrt{2}}|0\rangle + \frac{a-b}{\sqrt{2}}|1\rangle$$

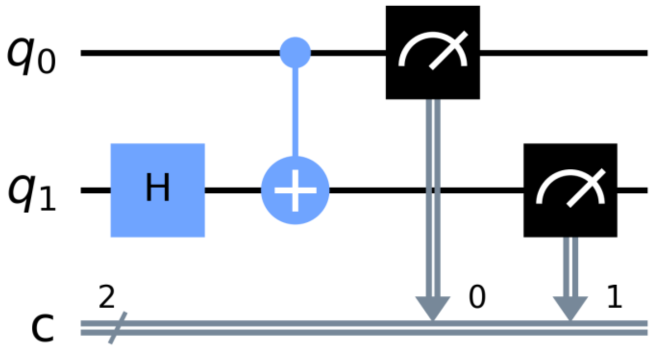
I.e., the output is also in a superposition of $|0\rangle$ and $|1\rangle$

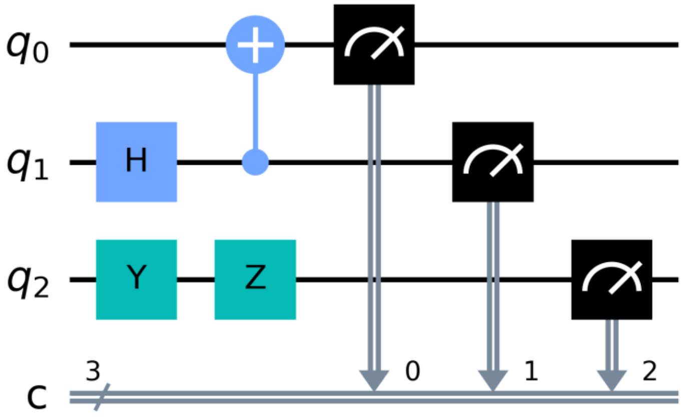
- We can also apply multiple gate sequentially:

$$\mathbf{CX}(\mathbf{H}\otimes\mathbf{I})|00\rangle = \mathbf{CX}\left(\frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|10\rangle\right) = \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$$

Quantum Circuits

- **Quantum circuits**, are sequences of quantum logic gates acting on qubits. They are the quantum analogue to classical (Boolean) logic circuits



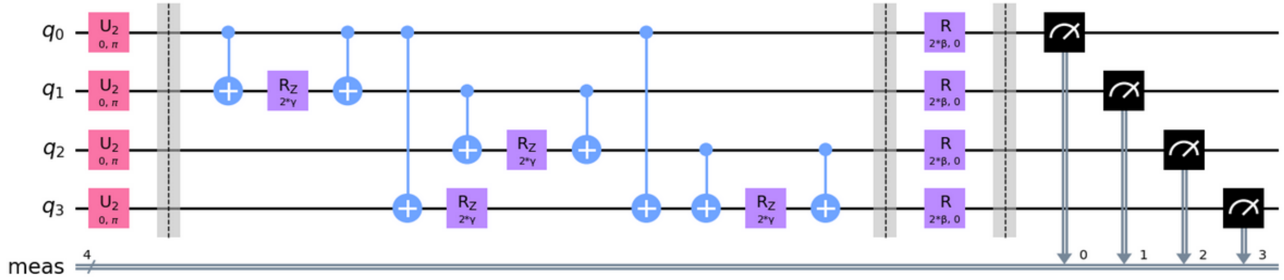


- We represent qubits with wires and gates with blocks placed over the wires corresponding to the qubits they operate on.

- Measurements are represented with meter symbols, and a double wire represents classical bit.

Quantum Algorithms

- Quantum computers allow building quantum circuits that create and manipulate quantum phenomena.



- **Quantum algorithms** use quantum circuits to solve a problem more efficiently than classical systems allow.
- E.g., variational quantum algorithms (e.g., QAOA, VQE); Quantum machine learning (QML) algorithms, Shor's algorithm (prime factorisation), Grover's algorithm (database search).

Quantum Algorithms: QAOA

- **Quantum Approximate Optimisation Algorithm** (QAOA) for solving (binary) **combinatorial optimisation**: making an optimal (binary) decision among a very large number of options

$$\arg\min_x f(x) \quad x \in \{0,1\}^N$$

$$h_j(x) = 0 \text{ for } j = 1, \dots, n$$

$$g_i(x) \leq 0 \text{ for } i = 1, \dots, m$$

N binary decisions

2^N options

n + m constraints

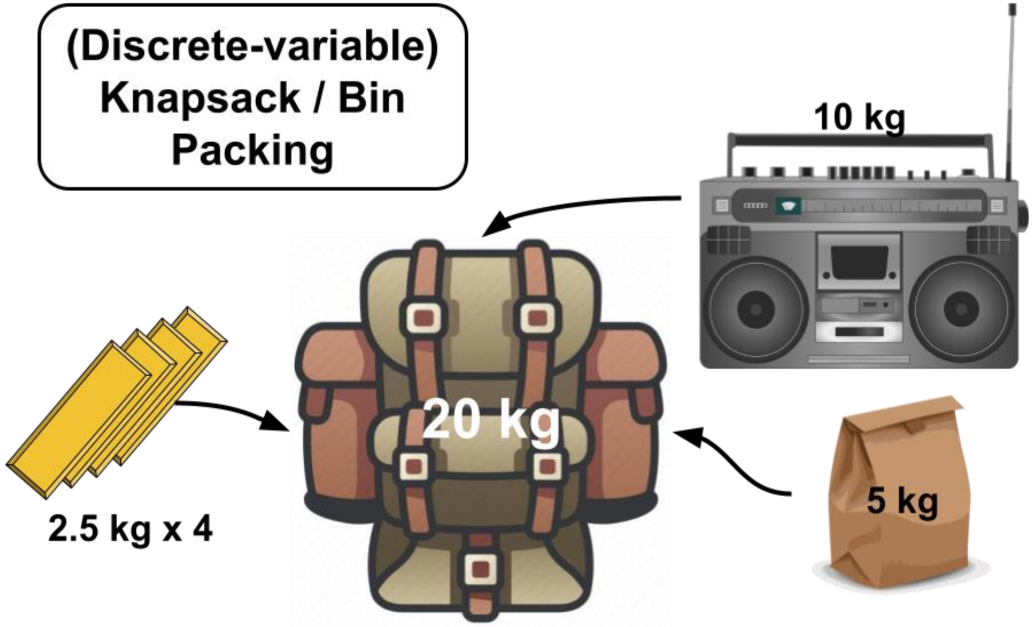
Objective function: f(x)

"Loss function", "Cost function"

- Examples of combinatorial optimisation problems:
  - Travelling Salesman Problem
  - Knapsack Problem (Bin Packing)
  - Job-Shop Scheduling

Quantum Algorithms: QAOA

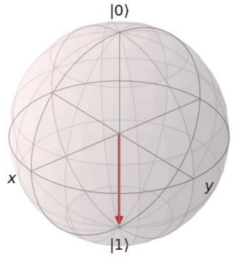
- **Knapsack Problem**
  - 6 items / binary decisions → 6 qubits



QAOA uses a **variational quantum circuit** to search the solution space: each gate is parameterised

q — R_Y γ — $\longrightarrow$

$\gamma \in [0, 2\pi]$

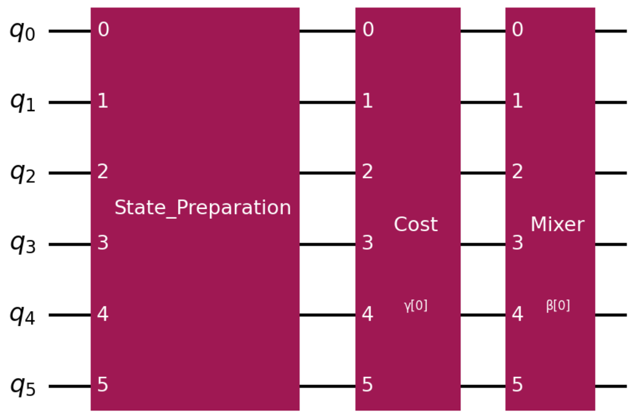


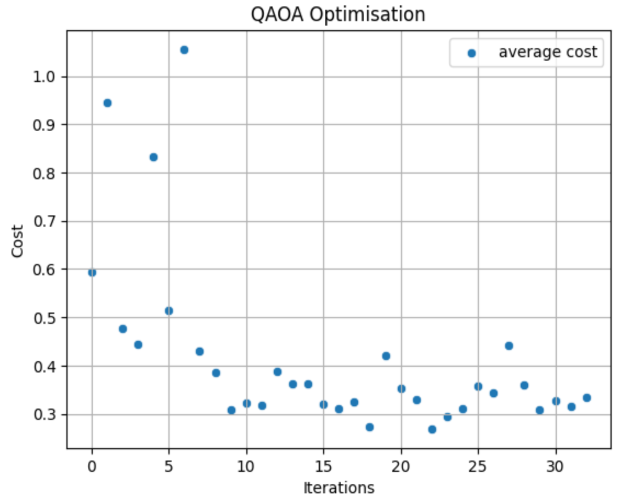
$\gamma = \pi/4$

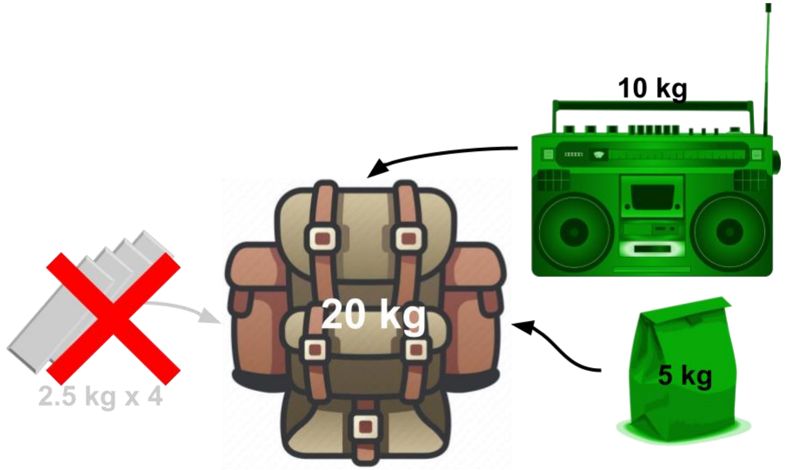
Optimisation loop
- Initialise quantum circuit with random gate parameters
- Compute circuit to get output bitstring
- Compute cost function for output bitstring
- Based on cost, choose next set of gate parameters

Quantum Algorithms: QAOA

- **QAOA** ansatz: quantum circuit used to compute output bitstring
- Iterate on gate parameters until **cost function is minimized**; final output bitstring corresponds to **optimal decision**





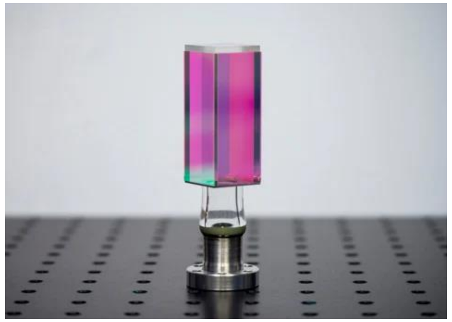


E.g., final output bitstring = 000011 → No/No/No/No/Yes/Yes

Quantum Computing Hardware

Quantum computing implementations include various technologies/hardware:

- Cold (neutral) atoms
- Trapped ions
- Superconducting transmons
- Semiconductor spin-qubits (quantum dots)



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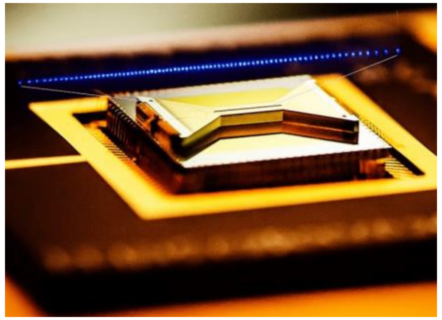

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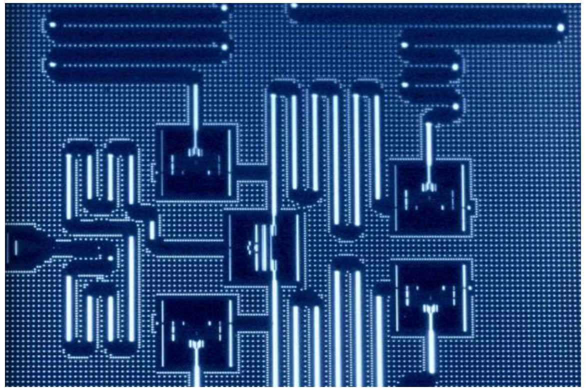
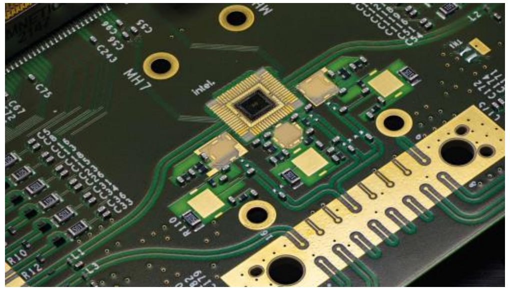


IBM Quantum



intel

Infleqtion Quantum Computing Stack

Qiskit, Cirq and other quantum software development kits

- Integration with Classical Workflow — Superstaq
- Industry-specific Quantum Solutions
  Chemistry, FinTech, Ai...
- Algorithms
  Grover, QFT, VQE, QAOA...
- Quantum Software Libraries
- Circuit Optimization — Superstaq
- Low-level Quantum Circuits — Superstaq

Quantum Hardware Control

Cold Atom Quantum Hardware