Data and Quantum Machine Learning

(Tutorial for CODS-2025)

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Nisarg Vyas

IISER Pune

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I-HUB QUANTUM TECHNOLOGY FOUNDATION

sites.iiserpune.ac.in/~santh

Part 1: Introduction to quantum computing and QML

Part 2: Hand-on quantum encoding techniques and qRAM

Part 3: qPCA, and qSVM algorithms

Part 4: Hands-on demonstrations of qPCA and qSVM

Summary

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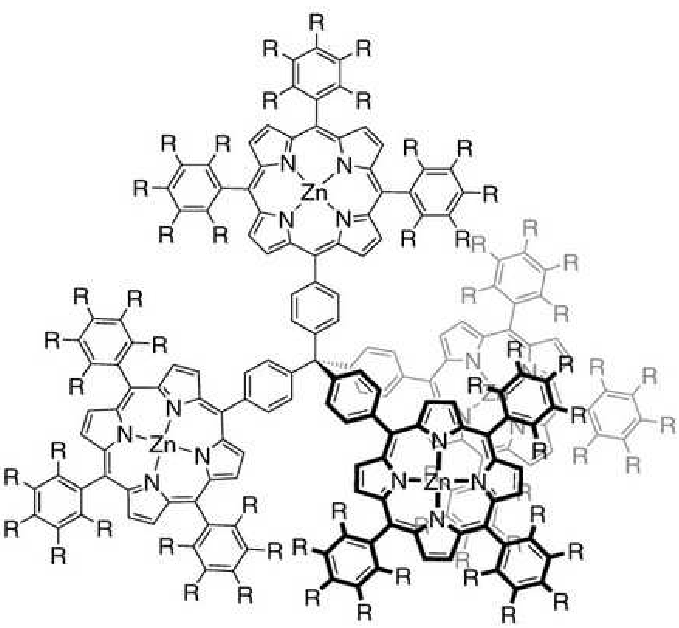
17.12.2021

Physics

Tardigrade is first multicellular organism to be quantum entangled

A tardigrade cooled to near absolute zero and placed in a state of quantum entanglement survived its ordeal

3Dstock/Shutterstock



$R = F$ or $C_{10}H_4F_{17}S$

Oligo-tetraphenylporphyrins (2000 atoms)

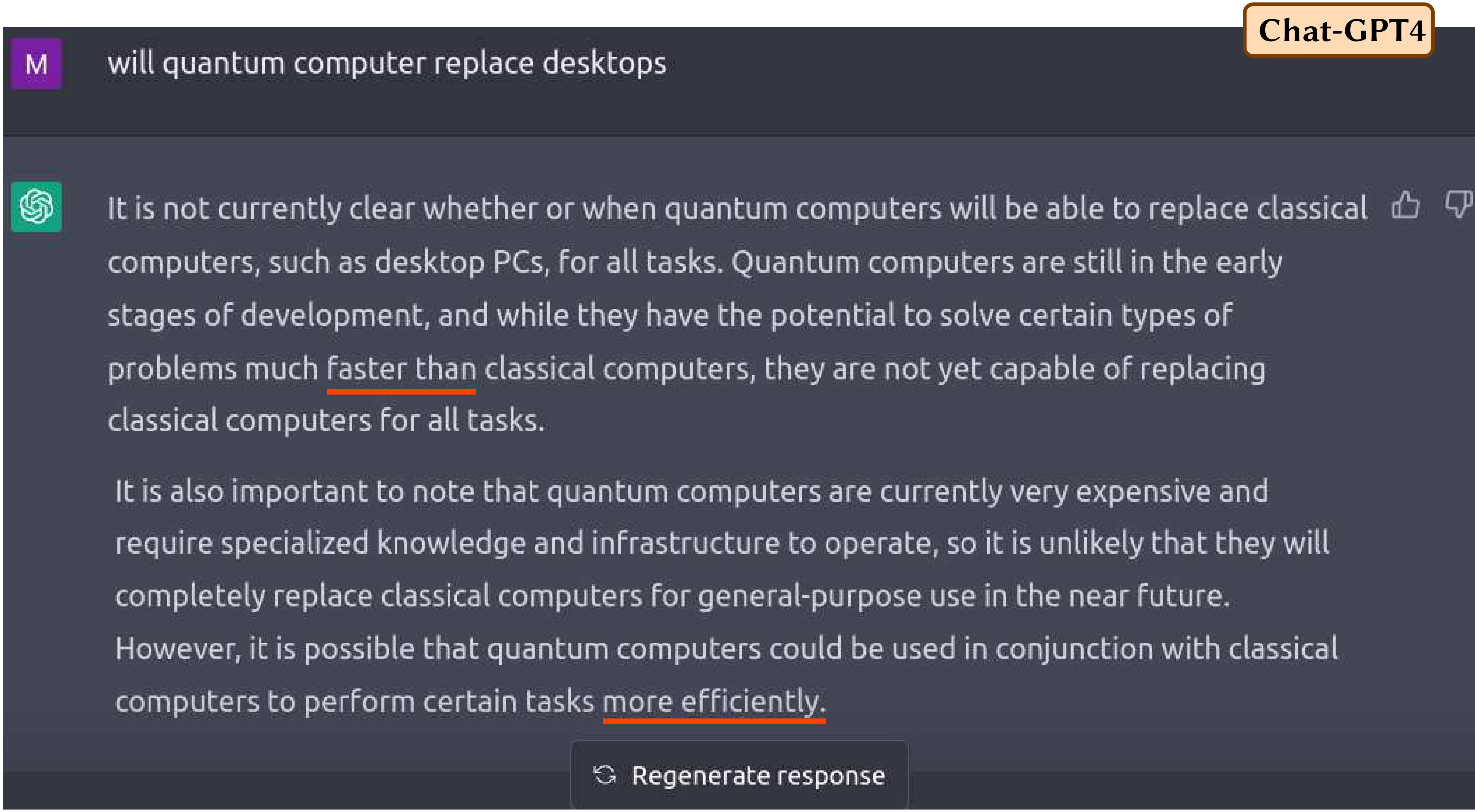
Superposition state of a large molecule (about 2000 atoms).
In two places at the same time.

Nature Physics **15**, 1242 (2019)

What quantum computing is NOT ?

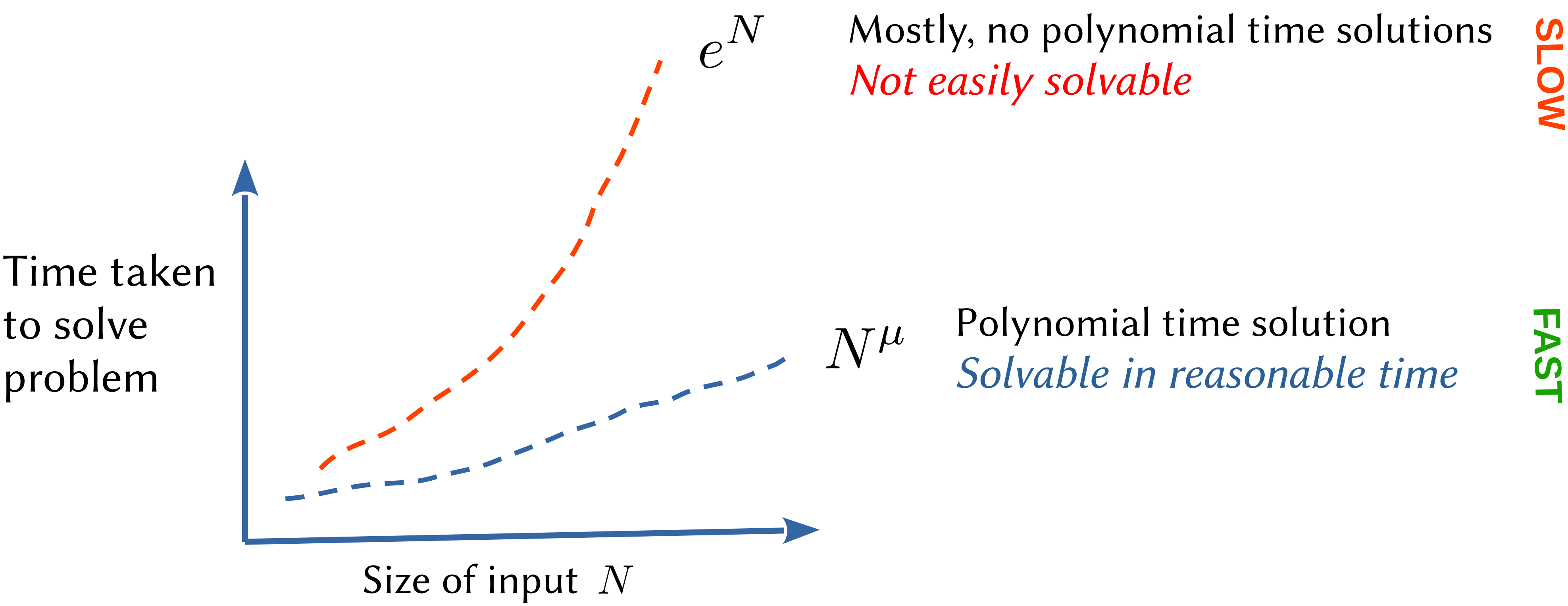
- It is not just a faster version of classical computers.
- It is not ONE new kind of technology, there are many quantum computing technologies.
- It might not replace our desktops and laptops for a several decades from now.
- It does not look like our familiar classical computers.

Credit : IBM

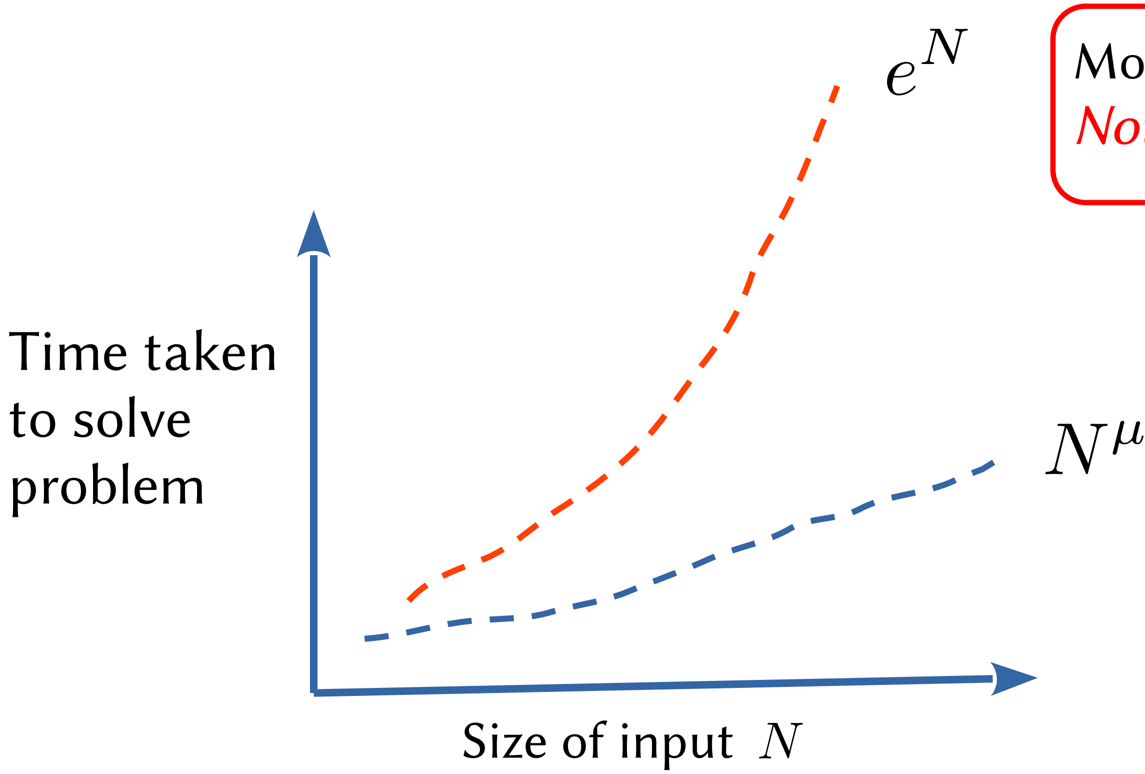


What do these terms mean ?

What is fast and efficient ?



e^N
Mostly, no polynomial time solutions
Not easily solvable
SLOW
Time taken to solve problem
N^μ
Polynomial time solution
Solvable in reasonable time
FAST
Size of input N



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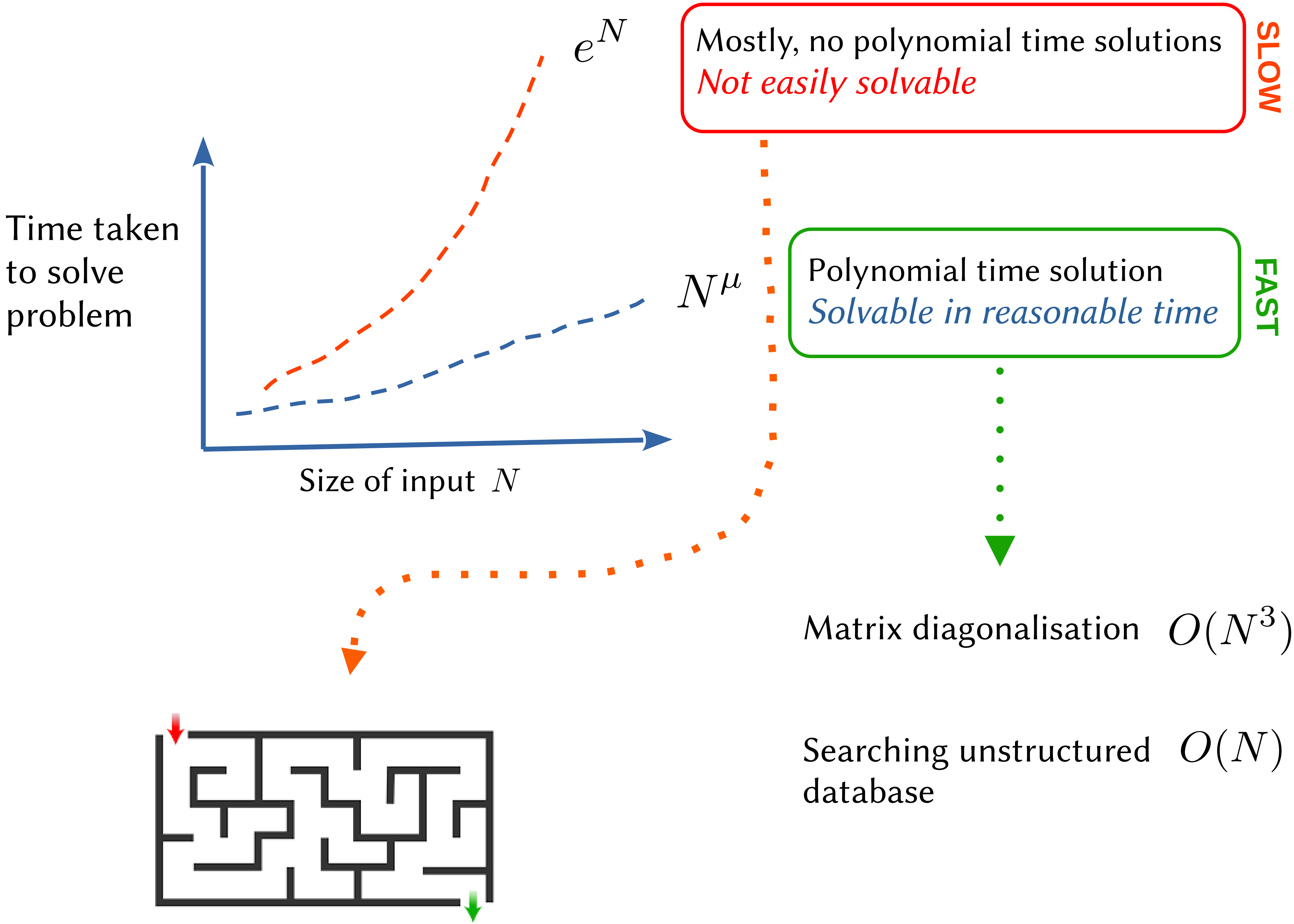
Polynomial time solution
Solvable in reasonable time

Matrix diagonalisation $O(N^3)$

Searching unstructured database $O(N)$



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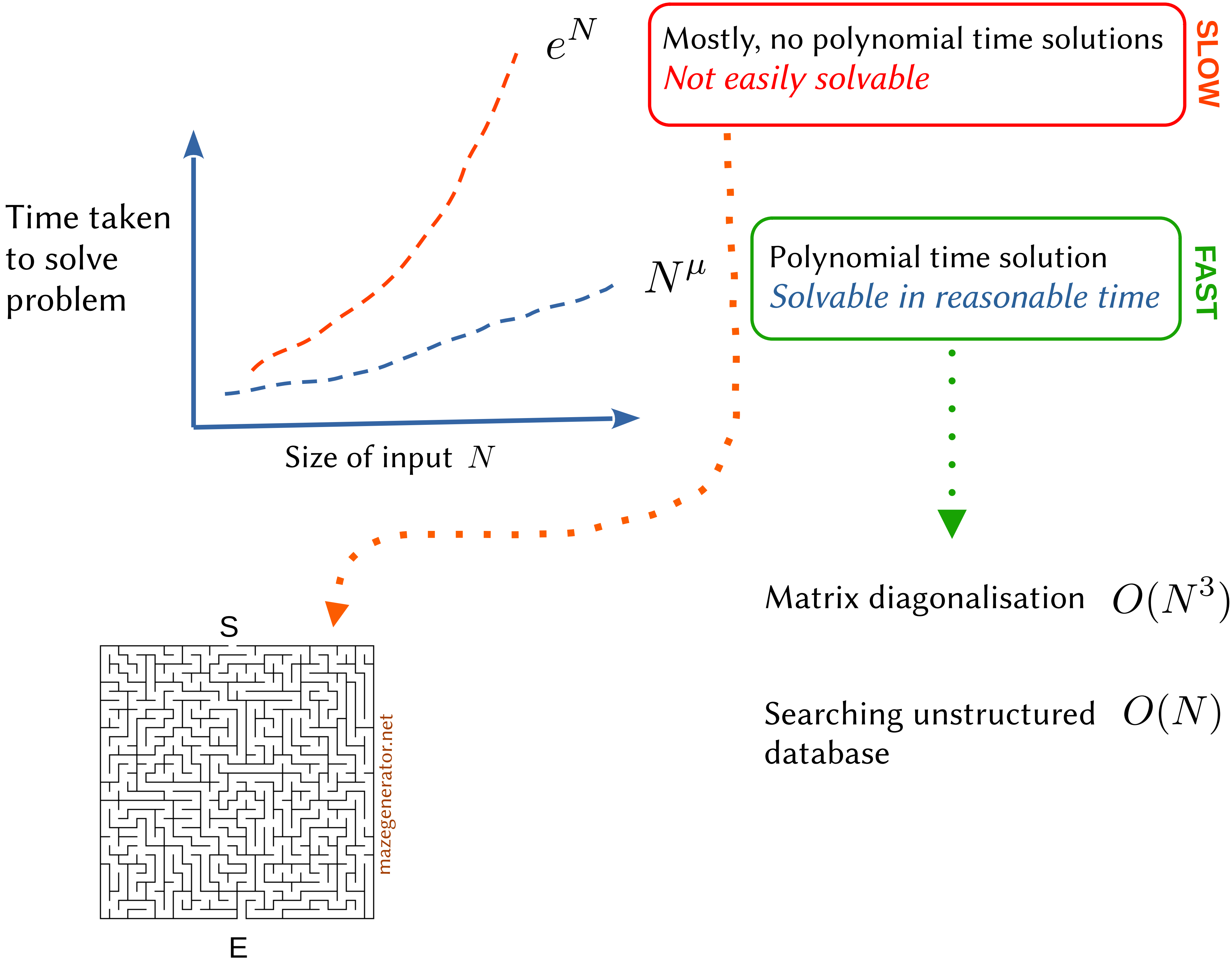

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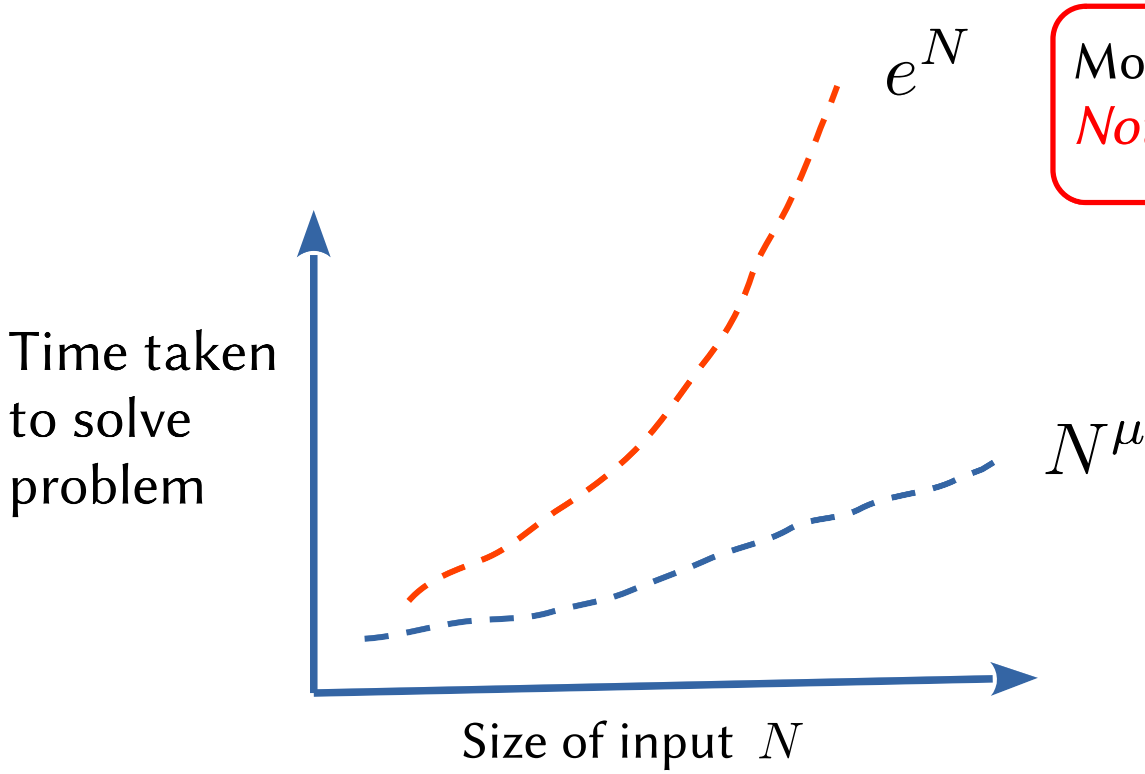


Mostly, no polynomial time solutions
Not easily solvable

SLOW

Polynomial time solution
Solvable in reasonable time

FAST

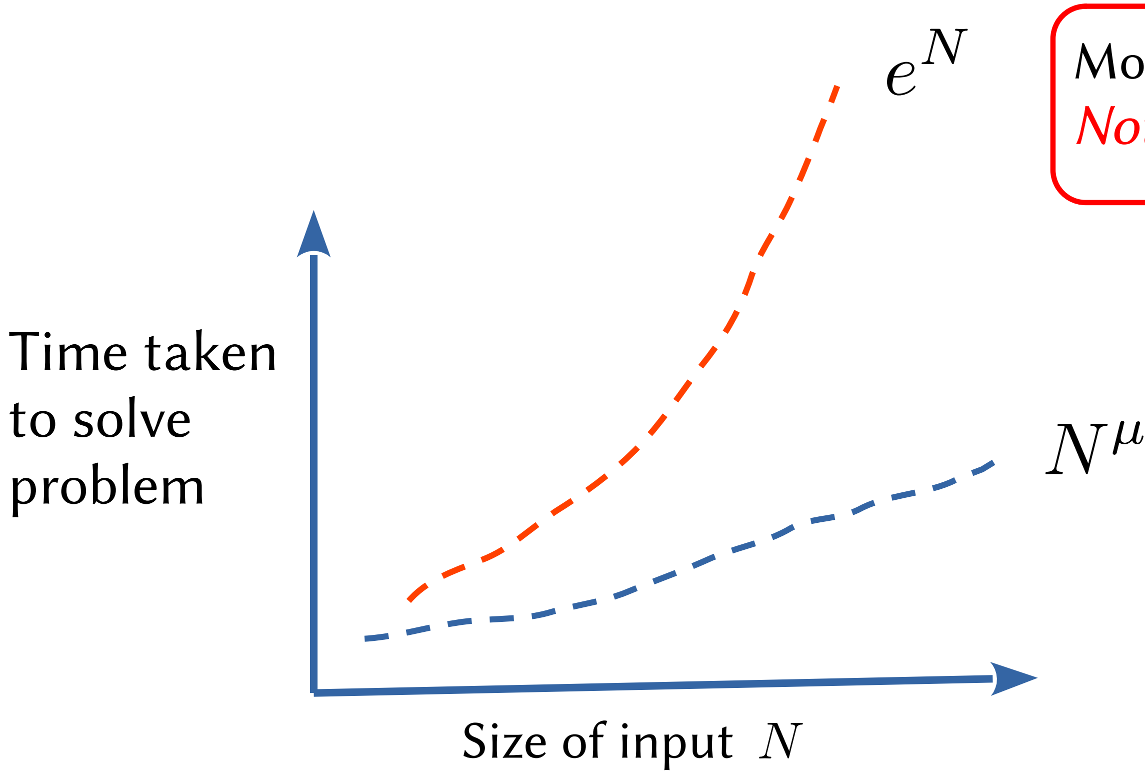
- Prime factorisation

$$15 = 5 \times 3$$

$$8245935632 = n_1 \times n_2$$

Matrix diagonalisation $O(N^3)$

Searching unstructured database $O(N)$



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Not easily solvable

SLOW

- Prime factorisation

$$M = n_1 \times n_2$$

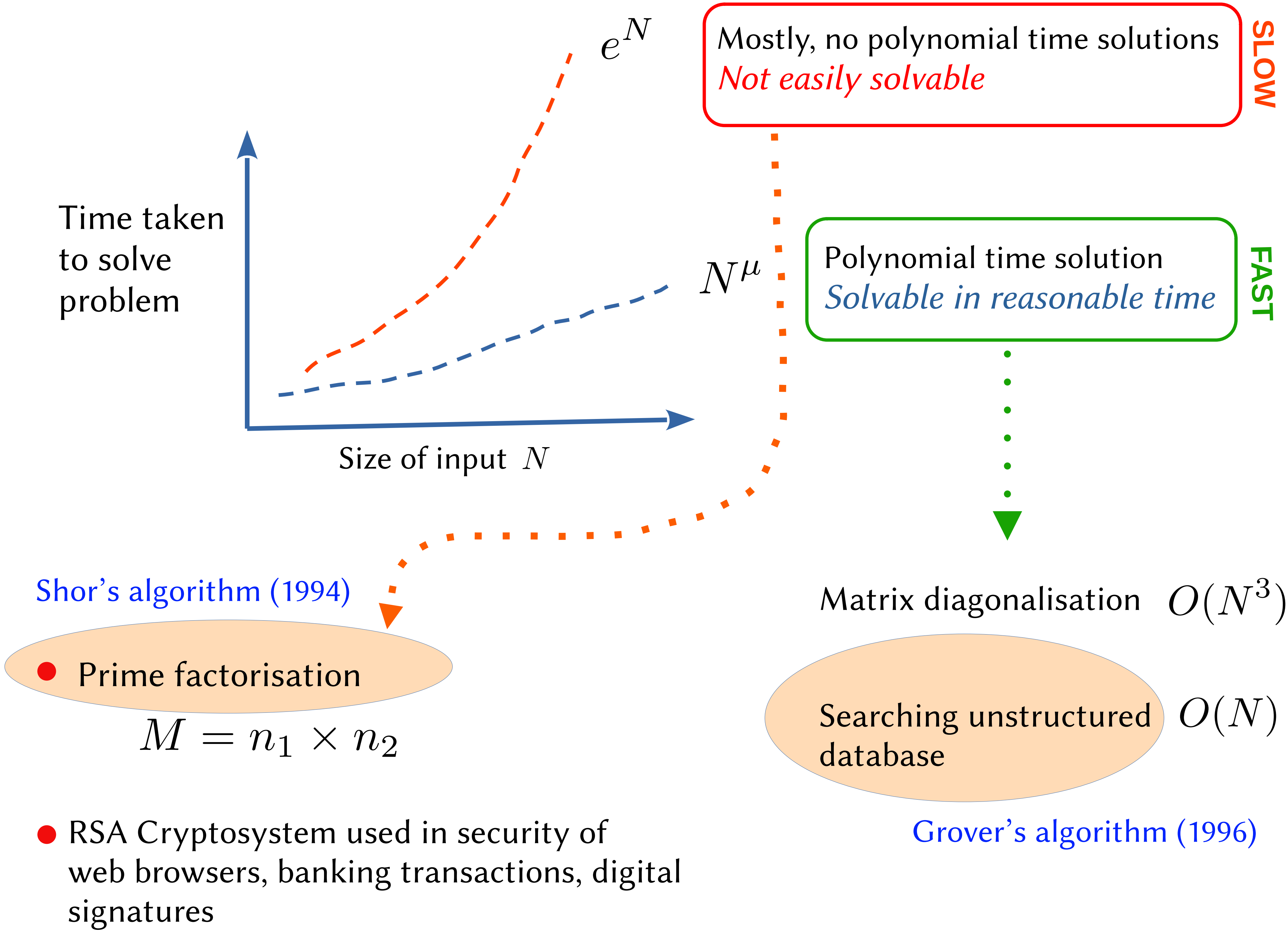
- RSA Cryptosystem used in security of web browsers, banking transactions, digital signatures

Polynomial time solution
Solvable in reasonable time

FAST

Matrix diagonalisation $O(N^3)$

Searching unstructured database $O(N)$



e^N
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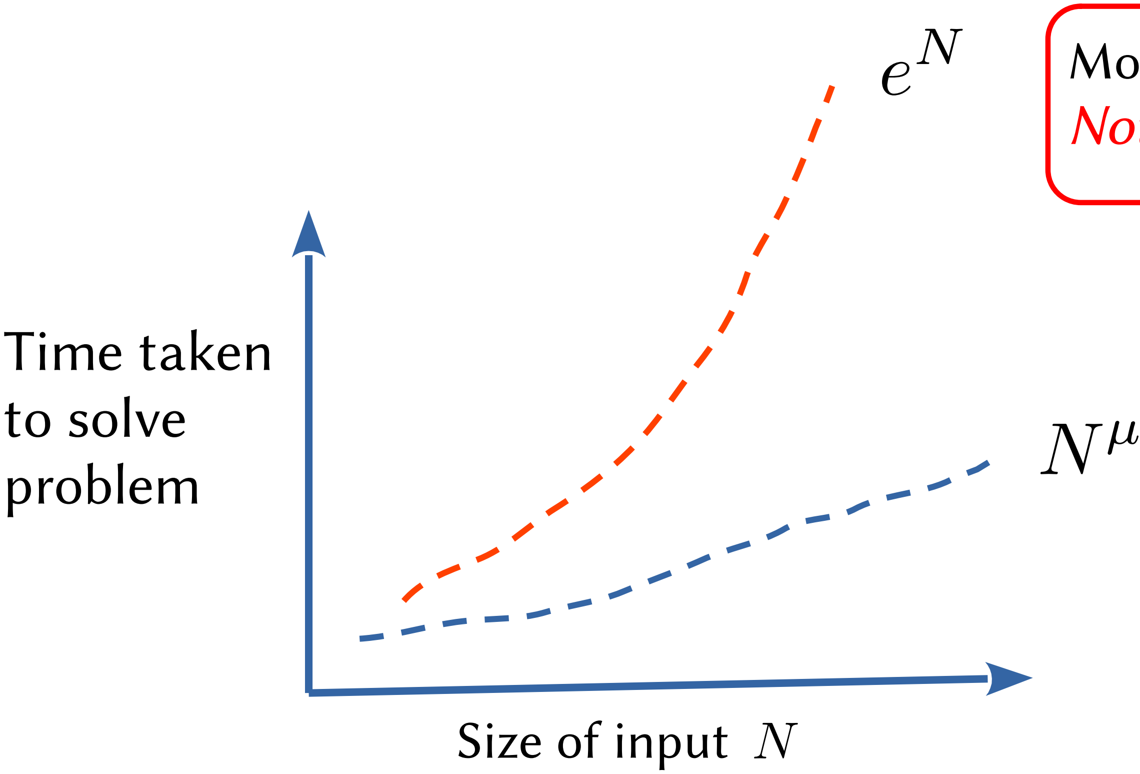
Time taken to solve problem
N^μ
Polynomial time solution
Solvable in reasonable time
FAST
Size of input N
Shor's algorithm (1994)
Prime factorisation
$M = n_1 \times n_2$
Matrix diagonalisation $O(N^3)$
Searching unstructured database
$O(N)$
Grover's algorithm (1996)
RSA Cryptosystem used in security of web browsers, banking transactions, digital signatures



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Polynomial time solution
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Matrix diagonalisation $O(N^3)$

- Prime factorisation

$$M = n_1 \times n_2$$

Searching unstructured database $O(N)$

- RSA Cryptosystem used in security of Web browsers, banking transactions, digital signatures

Quantum computing promises speedup for many such problems.

Can it help solve practical problems ?

Uncertainty principle

Some quantities such as position and momentum cannot be determined with infinite precision.

$$\Delta x \Delta p \geq \hbar$$

Quantum superposition

A linear combination of quantum States is also a valid quantum state

$$\psi(x) = \sum_{n=0}^{\infty} a_n \phi_n(x)$$

Quantum entanglement

Quantum systems display stronger than classical *non-local* correlations

$$\psi_{AB} \neq \phi_A \ \phi_B$$

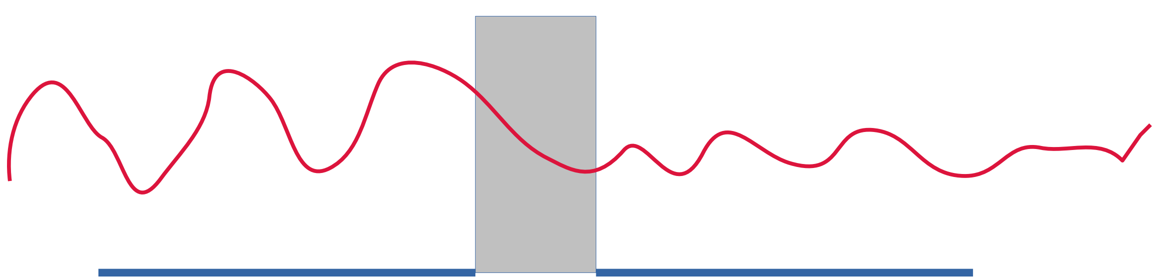
Decoherence

Quantum systems are delicate. They lose their quantumness when interacting with the environment.

This is one of main impediment In building large quantum computers.

Quantum Tunelling

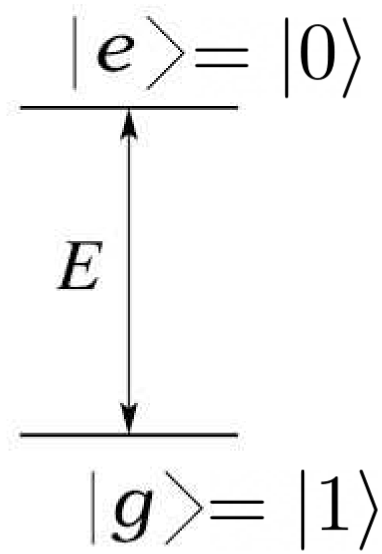
Purely quantum phenomenon with no classical analogue.



Classical bit is either 1 or 0.
In circuits, it represents different voltages.

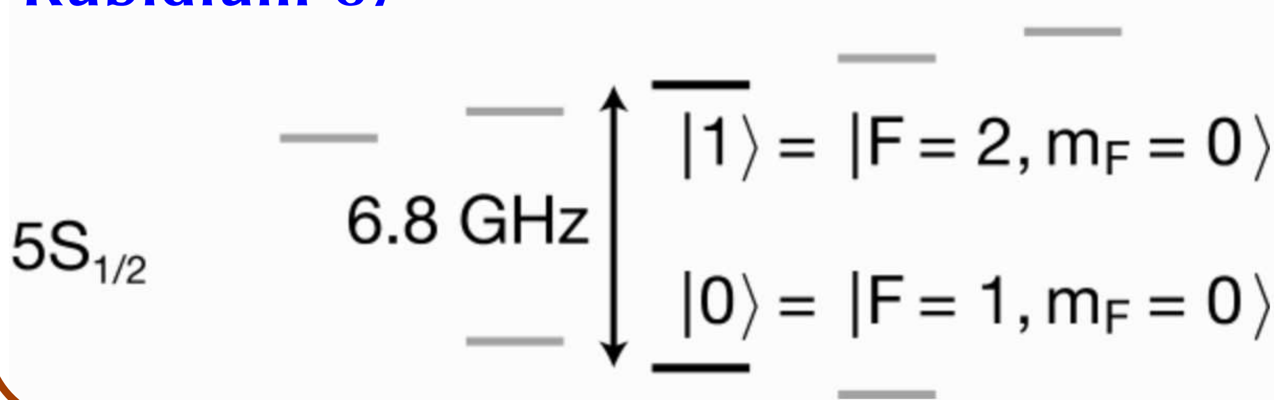
1 or 0

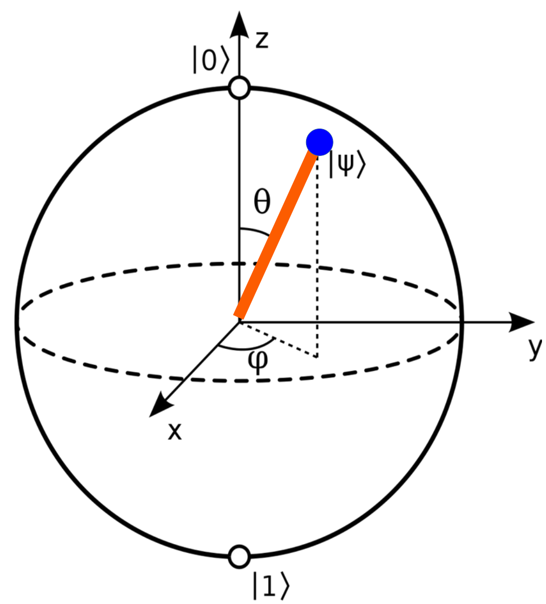
Quantum bit or qubit
represents two quantum states or energy levels



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

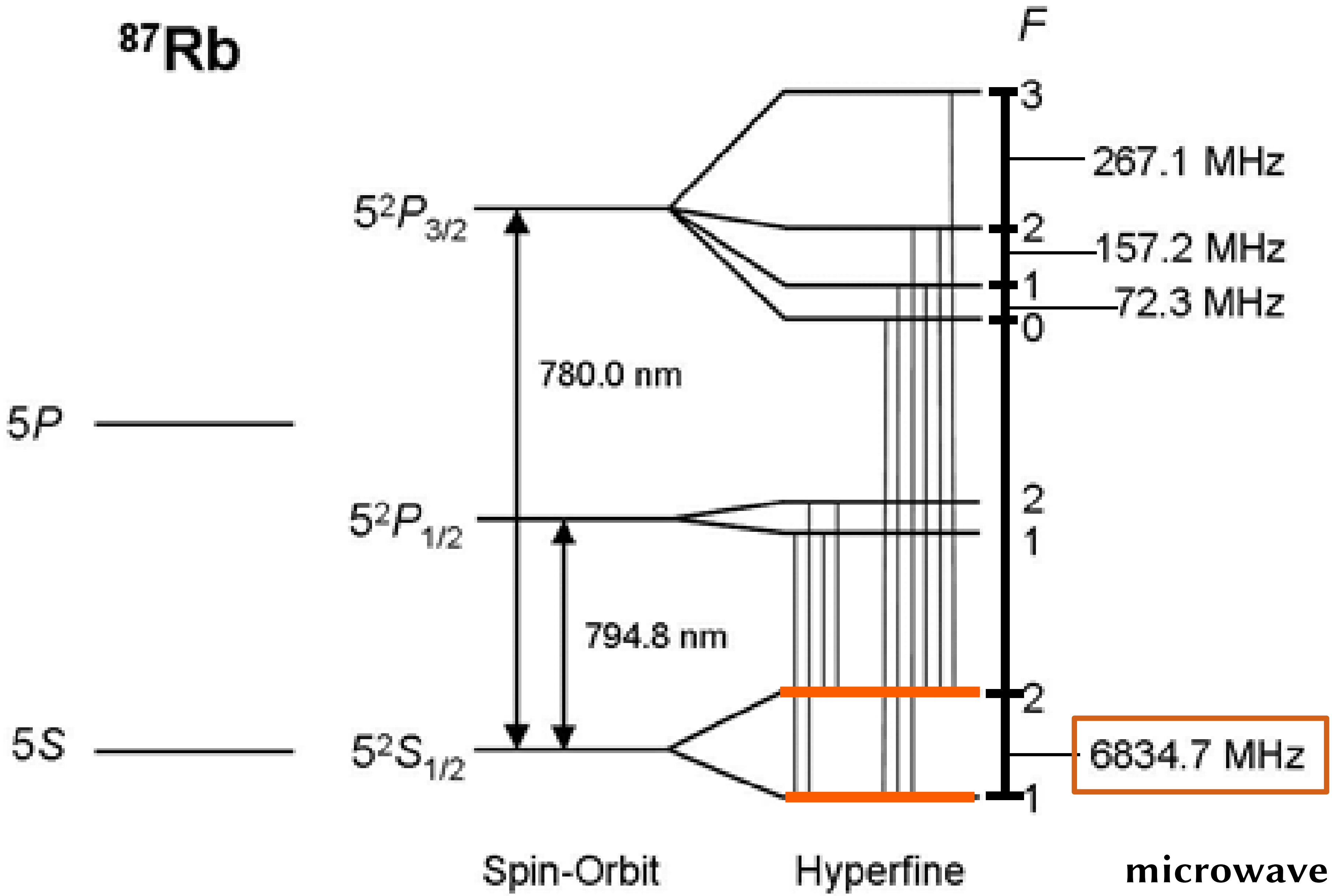
Rubidium-87



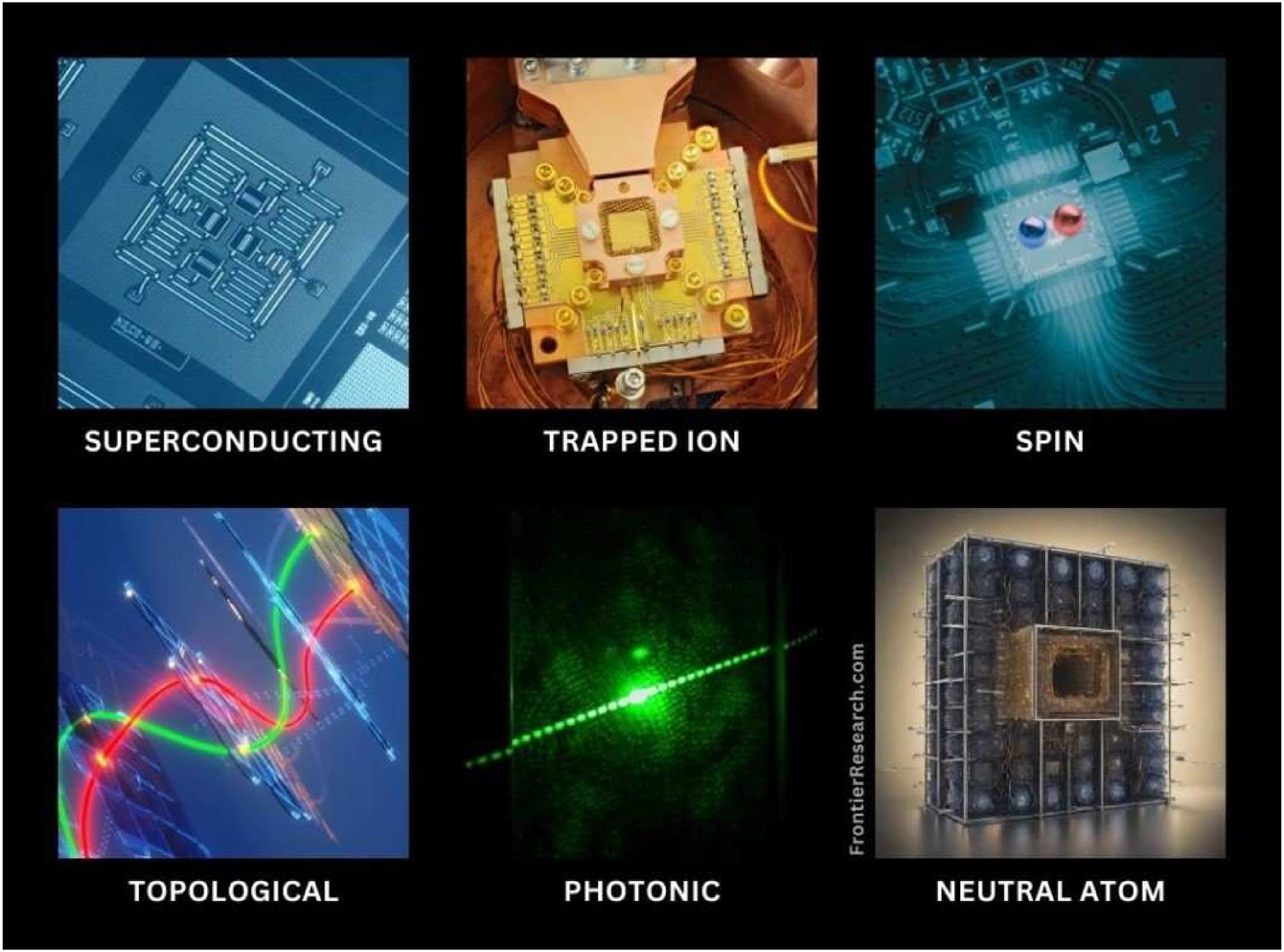


Source: wikipedia

Rubidium-87 levels



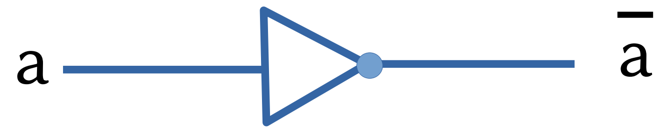
Source : advlabs.aapt.org



credits : exoswan.com

quantum gates

Classical gates manipulate bits.
Example : NOT gate

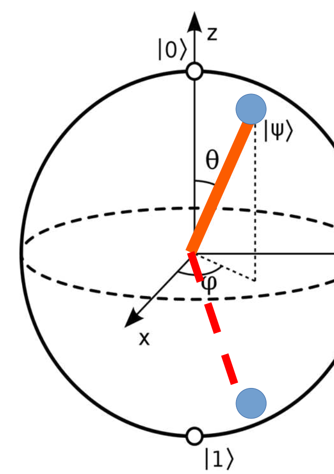


$$0 \to 1, \quad \text{or} \quad 1 \to 0$$

Quantum gates manipulate qubits.

$$a|0\rangle + b|1\rangle \; \text{—} \boxed{\hat{X}} \text{—} \; a' \; |0\rangle + b' \; |1\rangle$$

$$|0\rangle \; \text{—} \boxed{\hat{X}} \text{—} \; |1\rangle$$



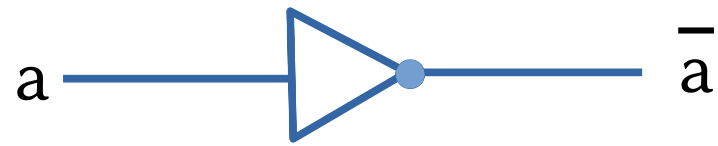
Mathematically,
quantum gates are
unitary operators
(unitary matrices)

$$\begin{bmatrix} a' \\ b' \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix}$$

All of quantum computing is matrix-vector manipulations

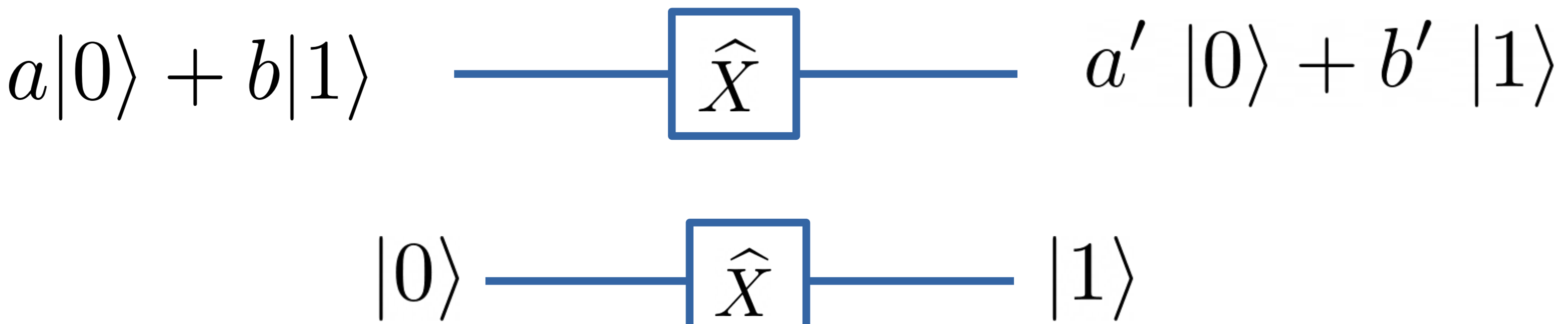
quantum gates

Classical gates manipulate bits.
Example : NOT gate

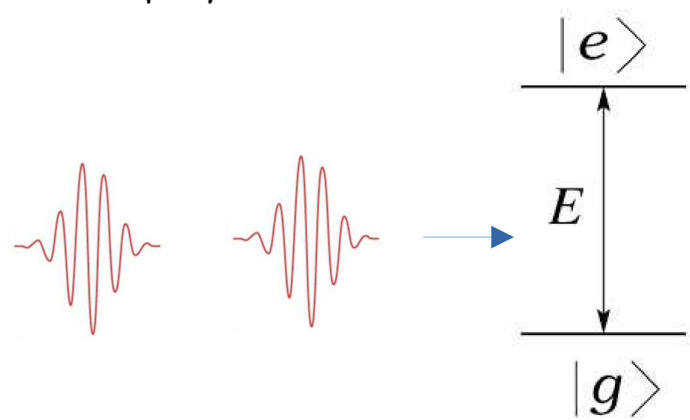


$$0 \to 1, \quad \text{or} \quad 1 \to 0$$

Quantum gates manipulate qubits.

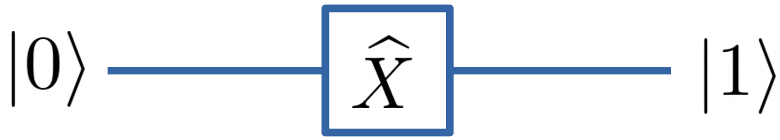


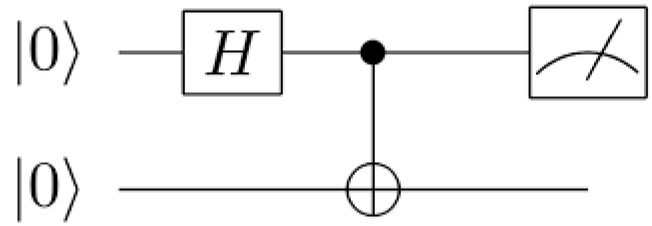
In quantum computers,
quantum gates are implemented
by sending microwave pulses.

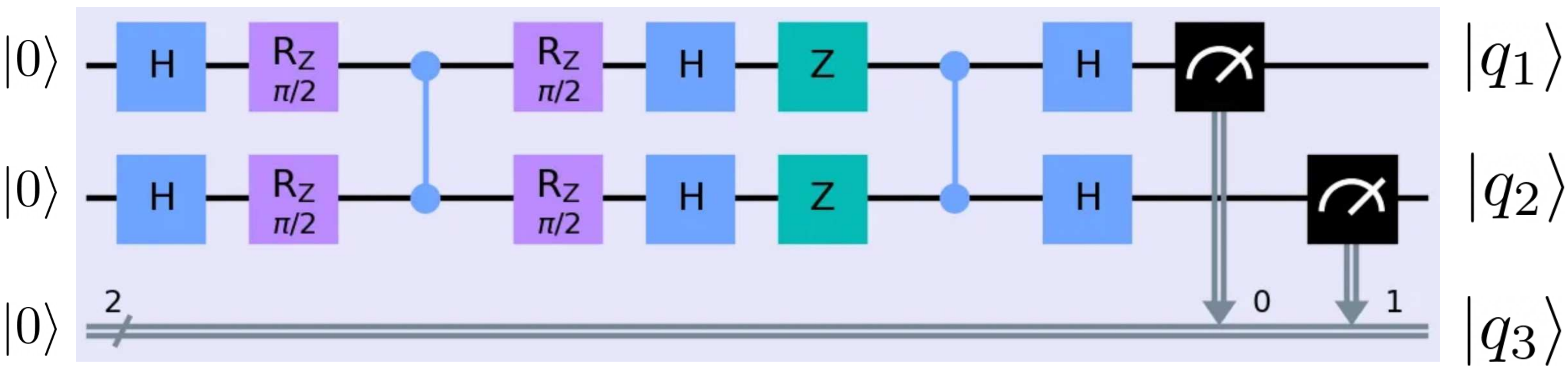


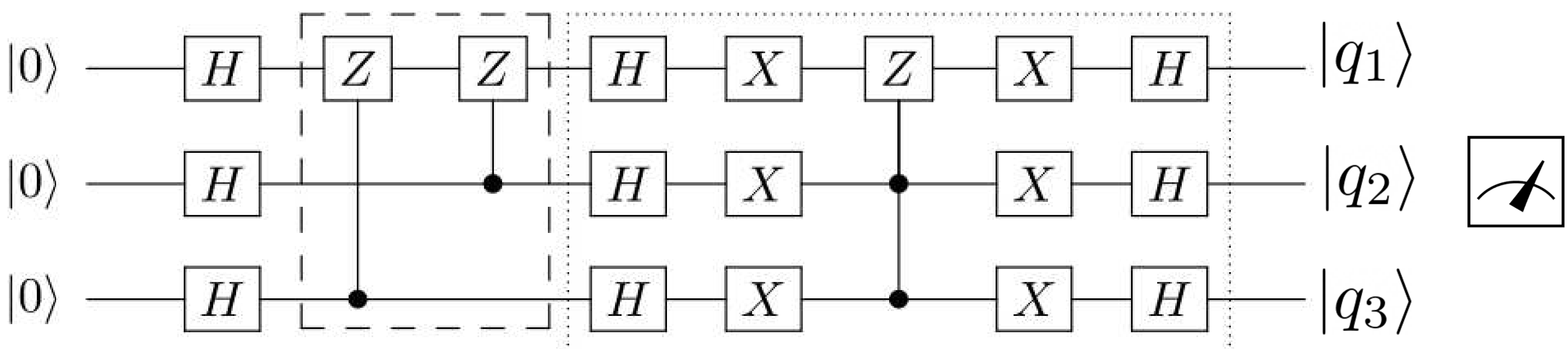
All of quantum computing is precision quantum control problem

quantum circuits



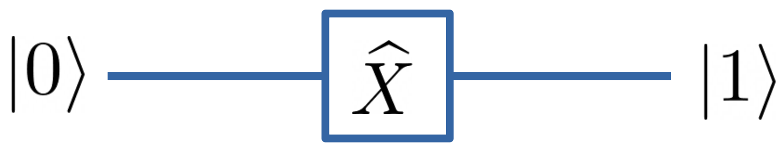


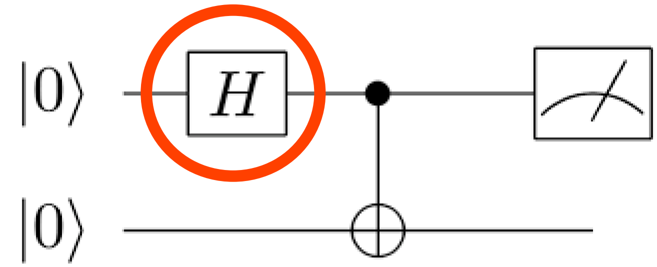


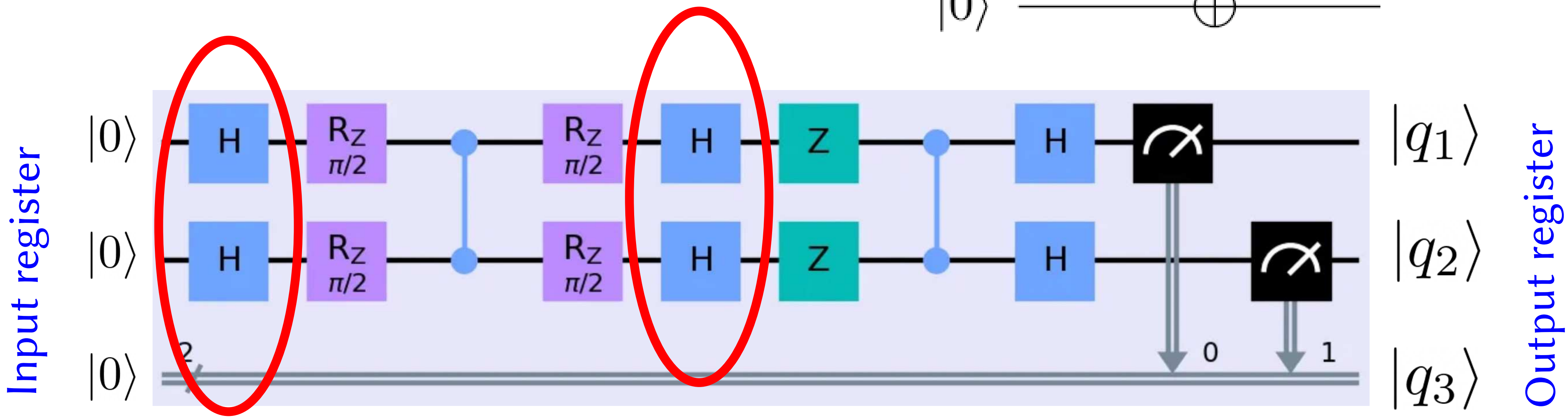


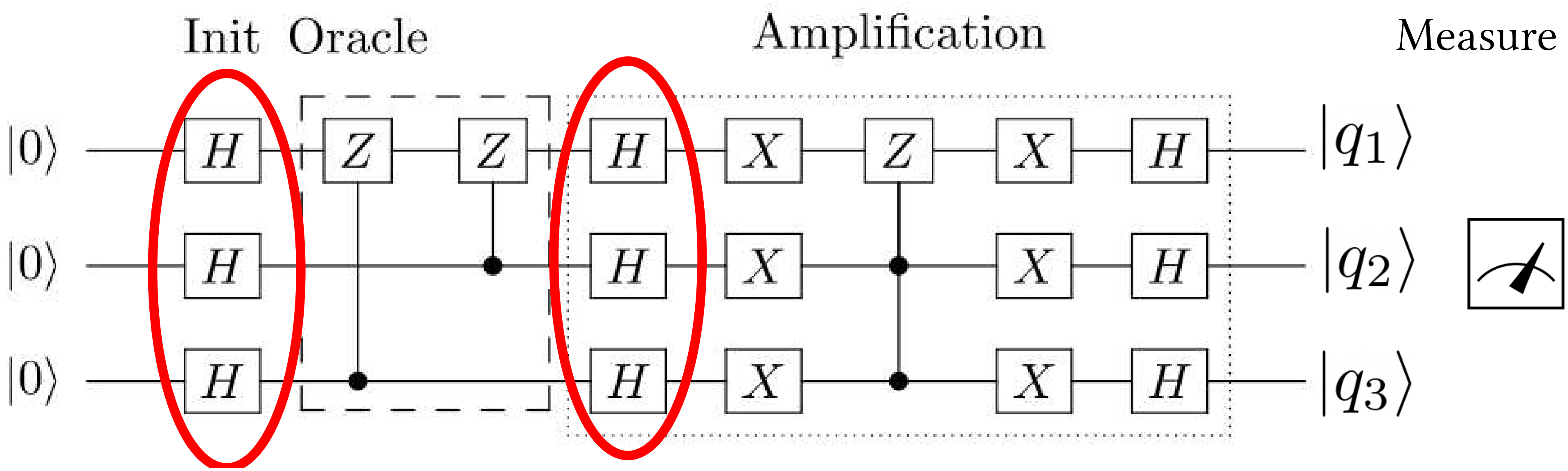
quantum circuits

Hadamard gates

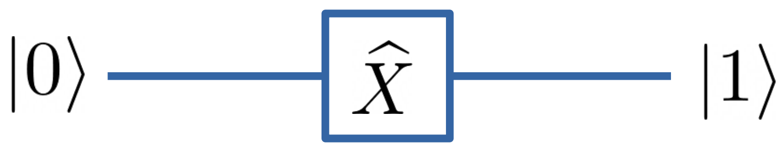




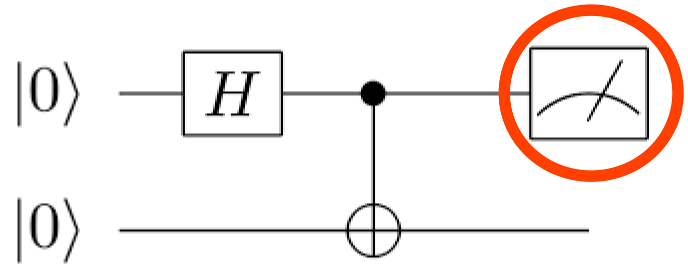


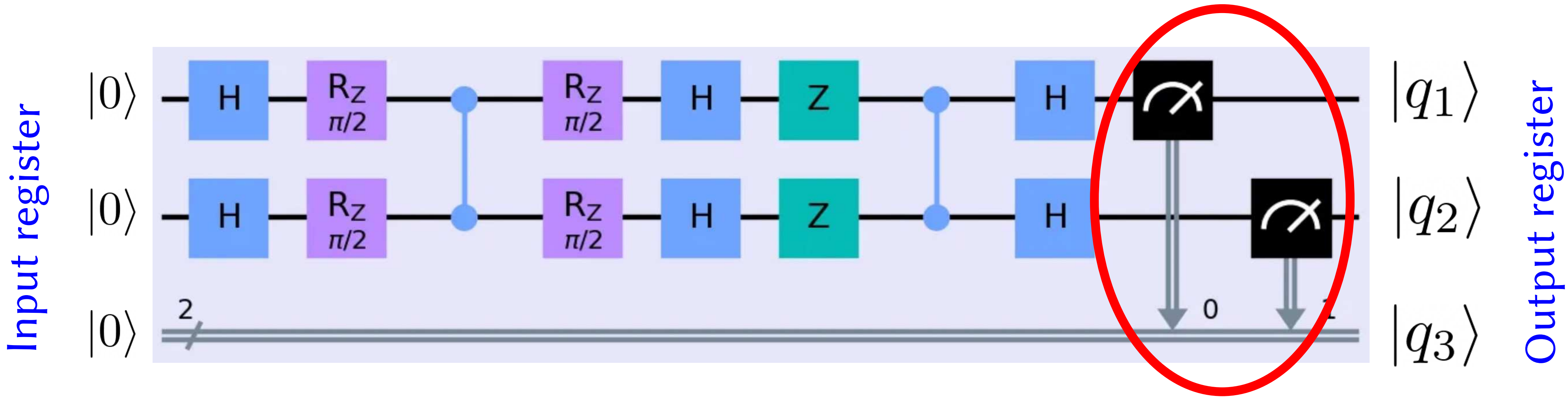


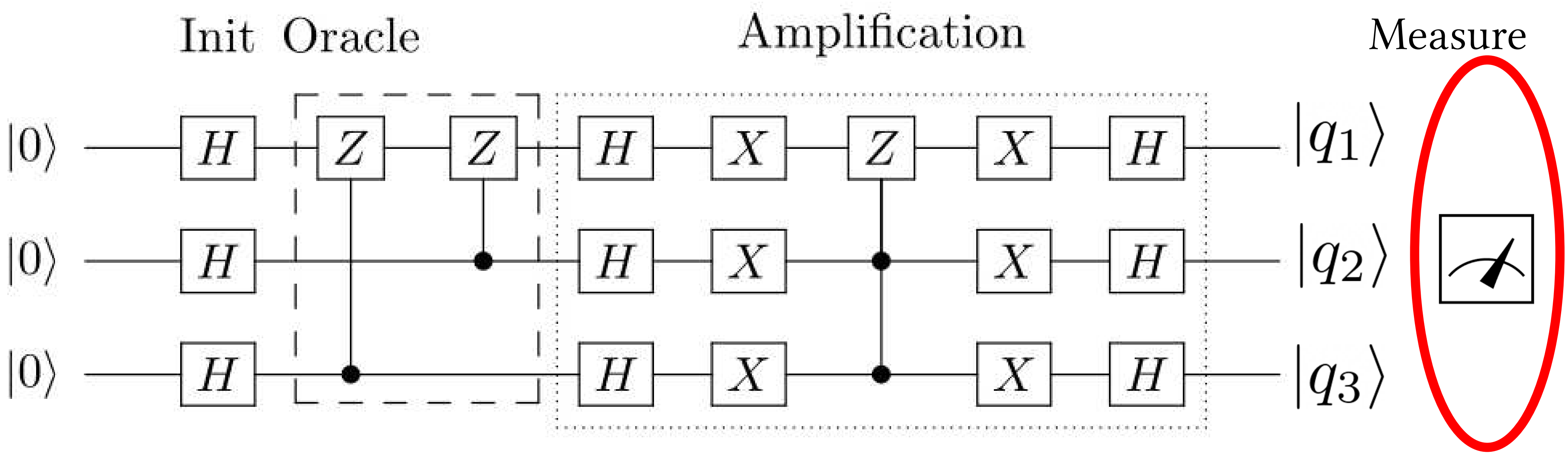
quantum circuits



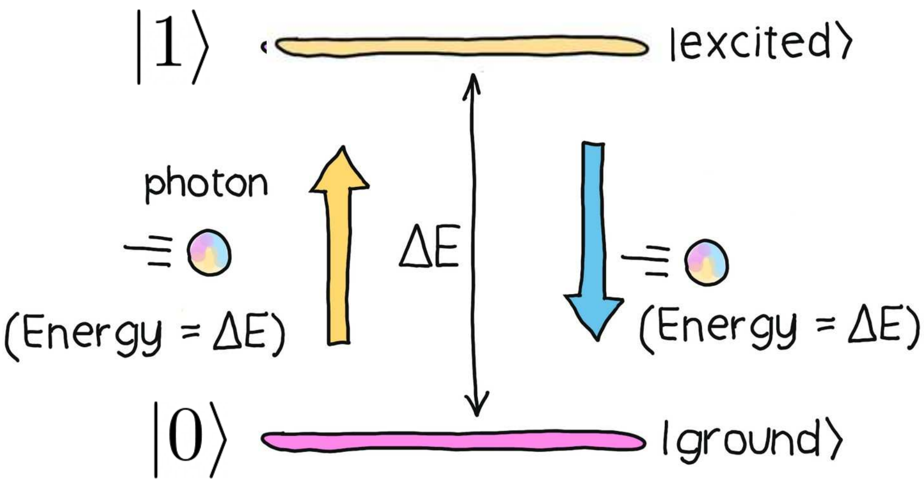
Measuring device

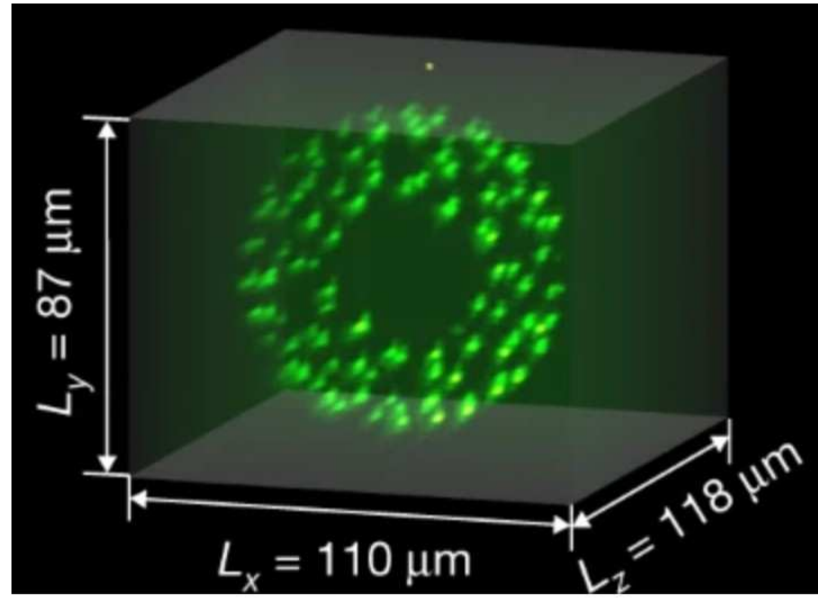






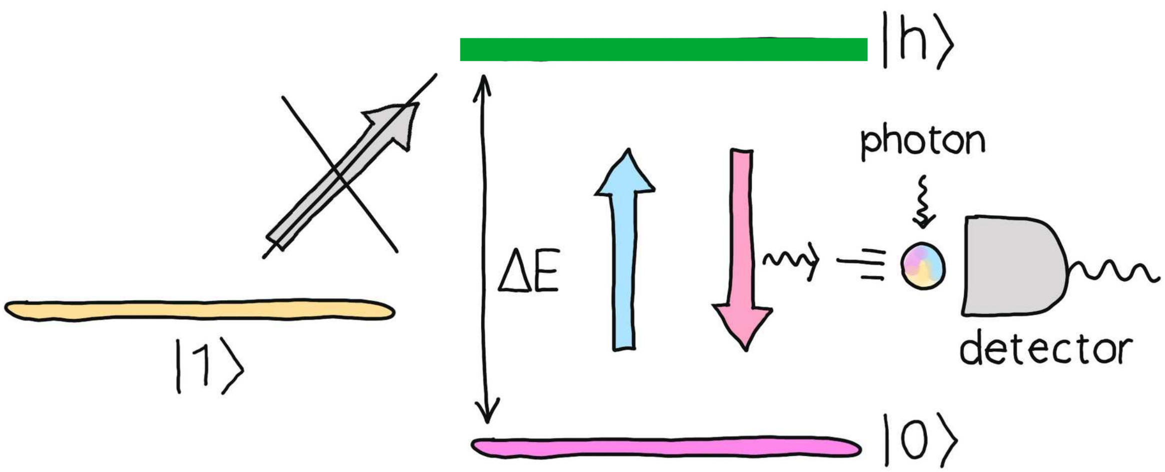
measurements





$25\mu K$

Nature **561**, 79 (2018)



Flourescence imaging

Credits : pennylane.ai

Registers

Single qubit $$a|0\rangle + b|1\rangle$$

Two qubits $$a_1|00\rangle + a_2|01\rangle + a_3|10\rangle + a_4|11\rangle$$

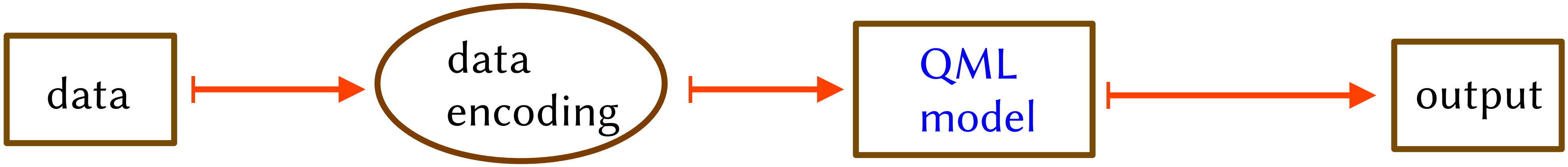
Three qubits $$a_1|000\rangle + a_1|100\rangle + a_2|010\rangle + \ldots\ldots a_8|111\rangle$$

N=300 qubits $$2^{300} \approx 2 \times 10^{90}$$ More than the number of atoms in the universe !

$$\psi = \sum_{i=1}^{N} (a_i|0\rangle + b_i|1\rangle)$$

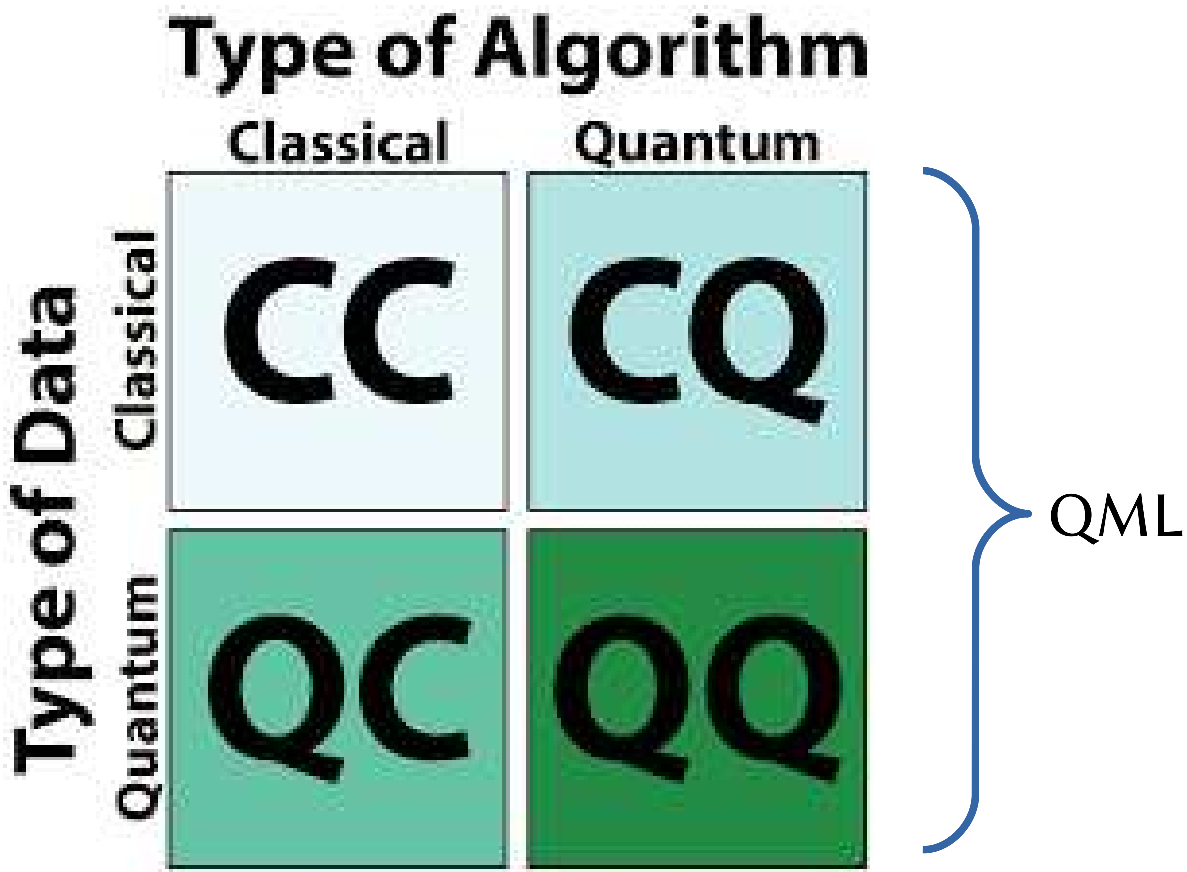
Creating and sustaining such large registers is technically challenging

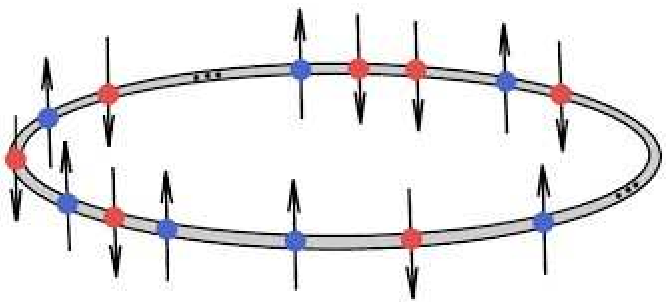
Quantum Machine Learning



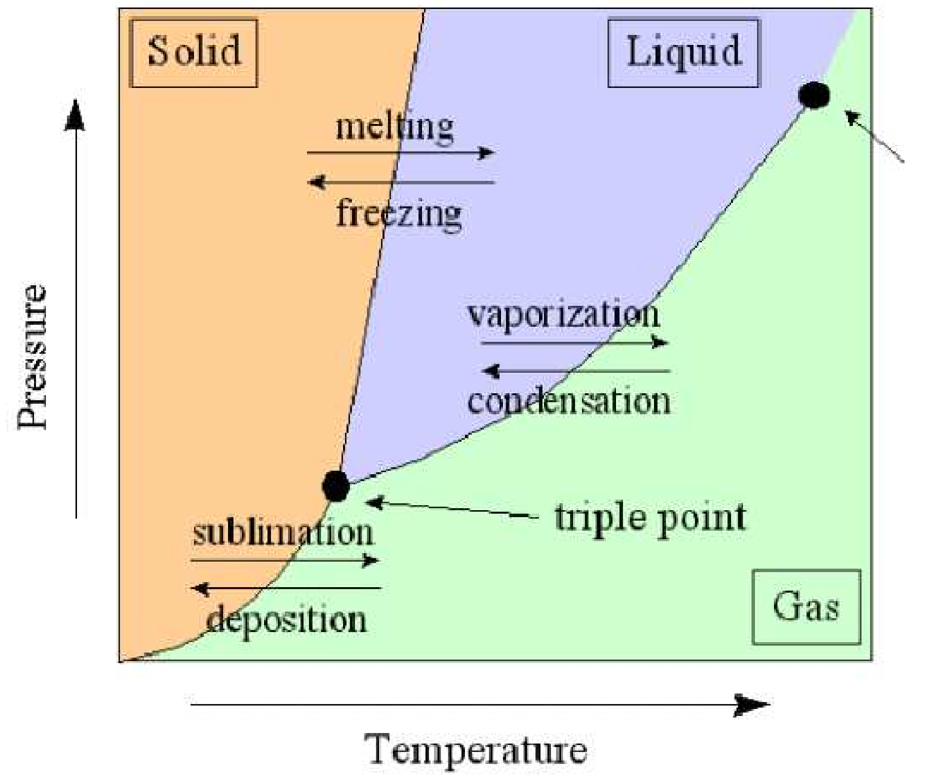
Usual ML
paradigm

Using classical ML to
solve quantum problems





- Ising type of models :
  Ferromagnetic to paramagnetic transition



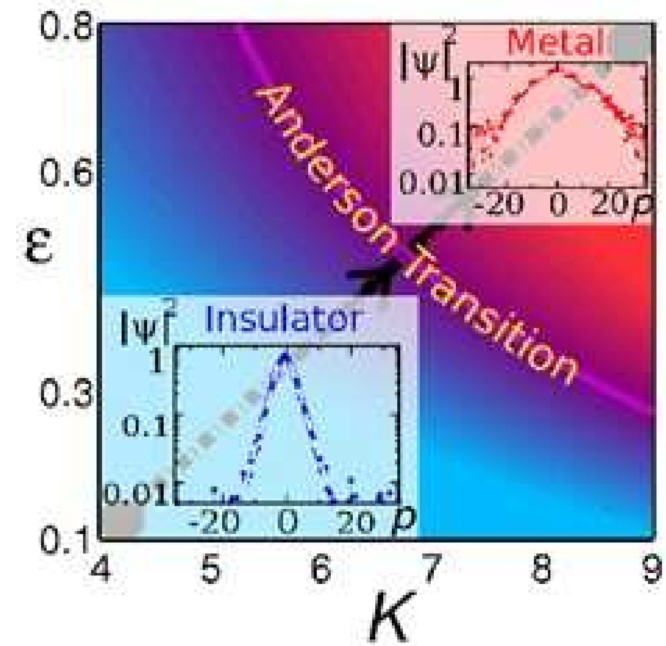
nature > nature physics > letters > article

Letter | Published: 13 February 2017

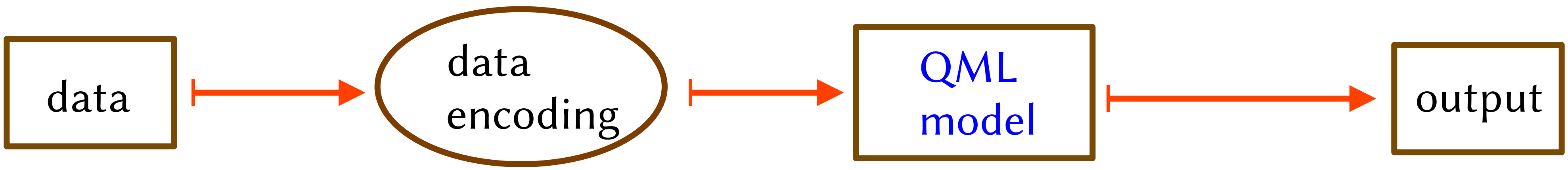
Machine learning phases of matter

Juan Carrasquilla & Roger G. Melko

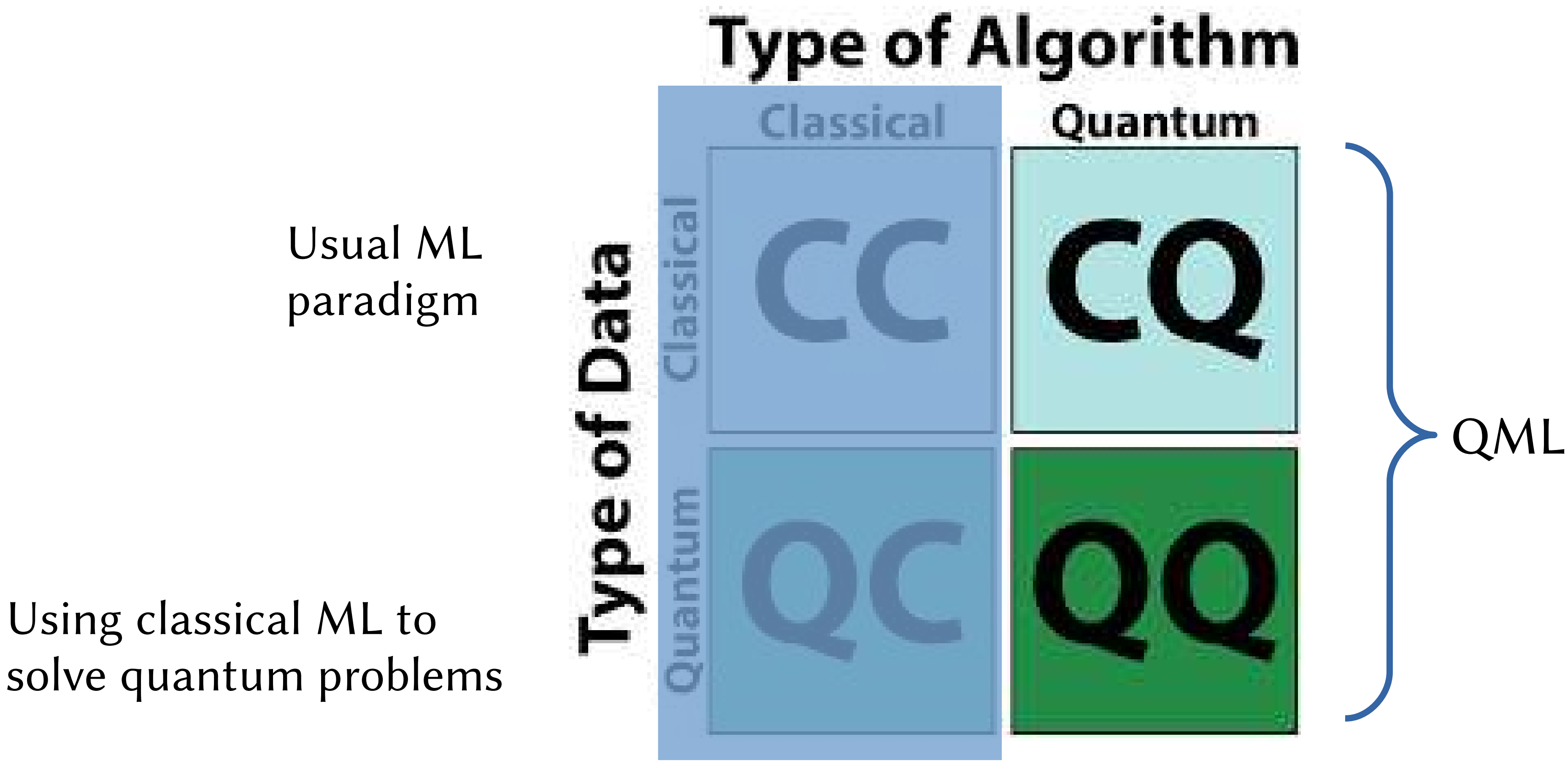
Nature Physics **13**, 431–434 (2017) | Cite this article



- Anderson type of models :
  Metal to insulator transitions



data
data encoding
QML model
output



Type of Algorithm
Classical
Quantum
Type of Data
Classical
Quantum
CC
CQ
QC
QQ
Usual ML paradigm
Using classical ML to solve quantum problems
QML

The promise and gaps in quantum machine learning

Some quantum algorithms can solve certain class of problems faster than classical algorithms

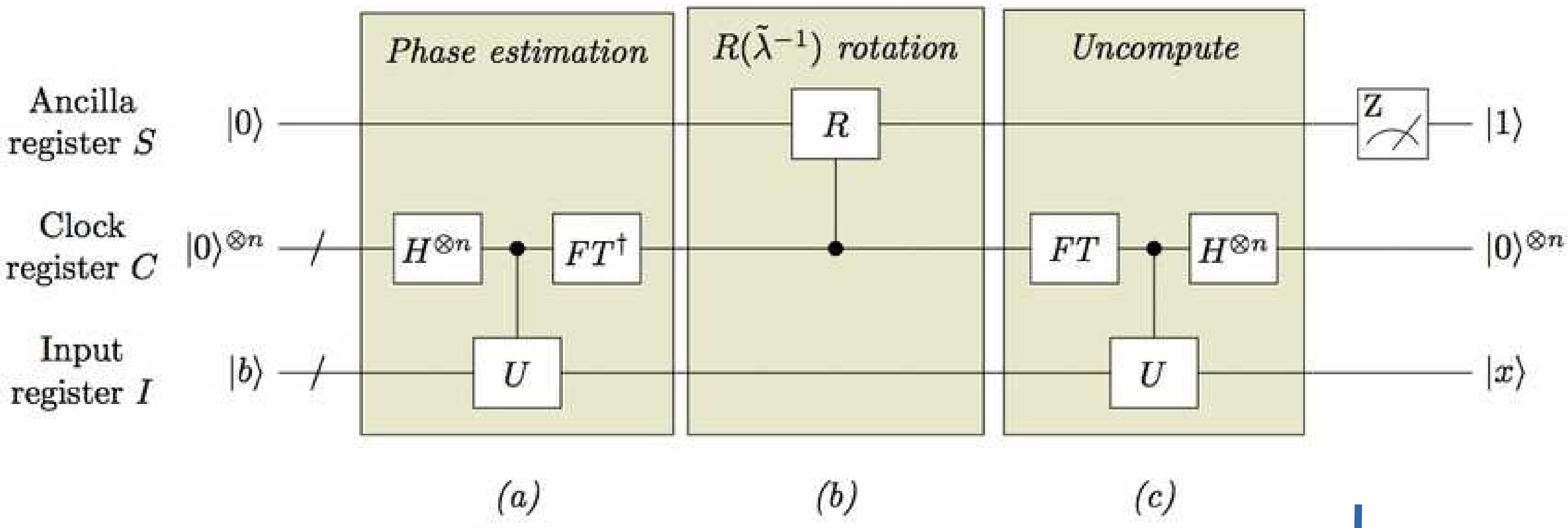
Example 1 : Linear system solver (HHL algorithm)

- *N* equations with *N* unknowns. Classical algorithm $\sim O(N\kappa)$

  HHL algorithm $\sim O(\log N\kappa^2)$

- Exponential speed-up over classical algorithm

Harrow, Hassidim and Lloyd, Phys. Rev. Lett. **103**, 150502 (2009)



Operator acting on quantum states

Matrix-vector multiplications

$$A\,\mathbf{x} = \mathbf{b}$$

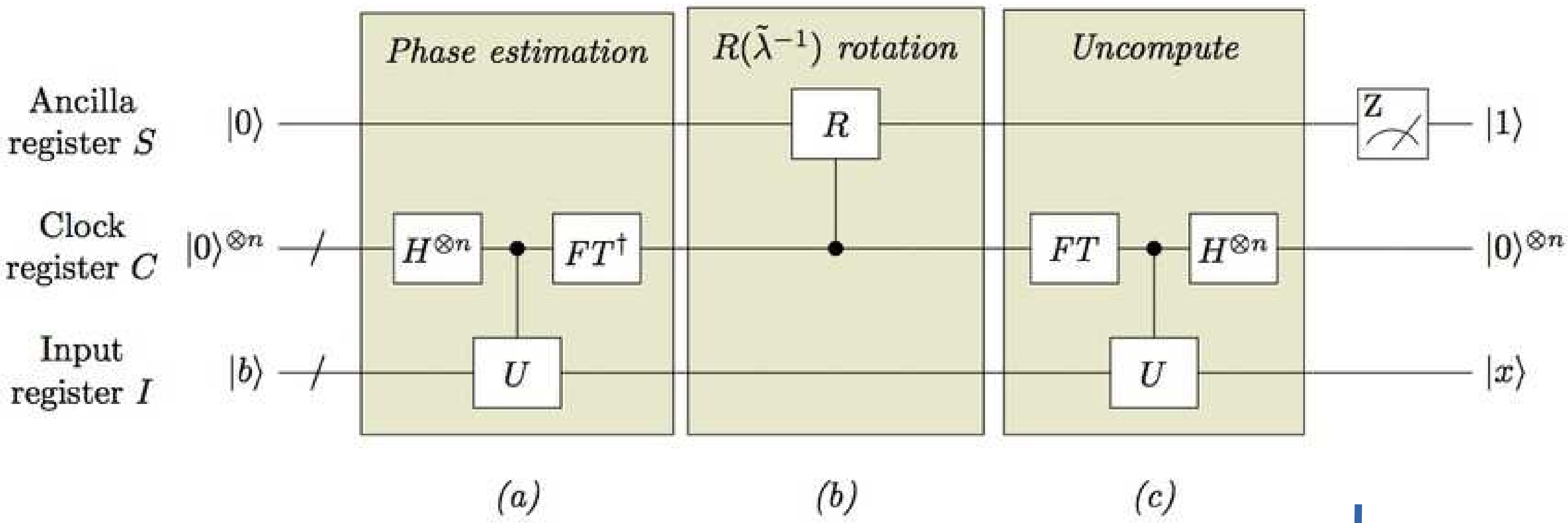
- We should be able to efficiently prepare initial state; Amplitude encoding of vector b
- Information about *A* goes into *U* (a unitary operator); Efficient implementation of *U*.

$$\mathrm{A} = \begin{pmatrix} 1 & -1/3 \\ -1/3 & 1 \end{pmatrix}$$

$$\mathrm{x} = \begin{pmatrix} 3/8 \\ 9/8 \end{pmatrix}$$

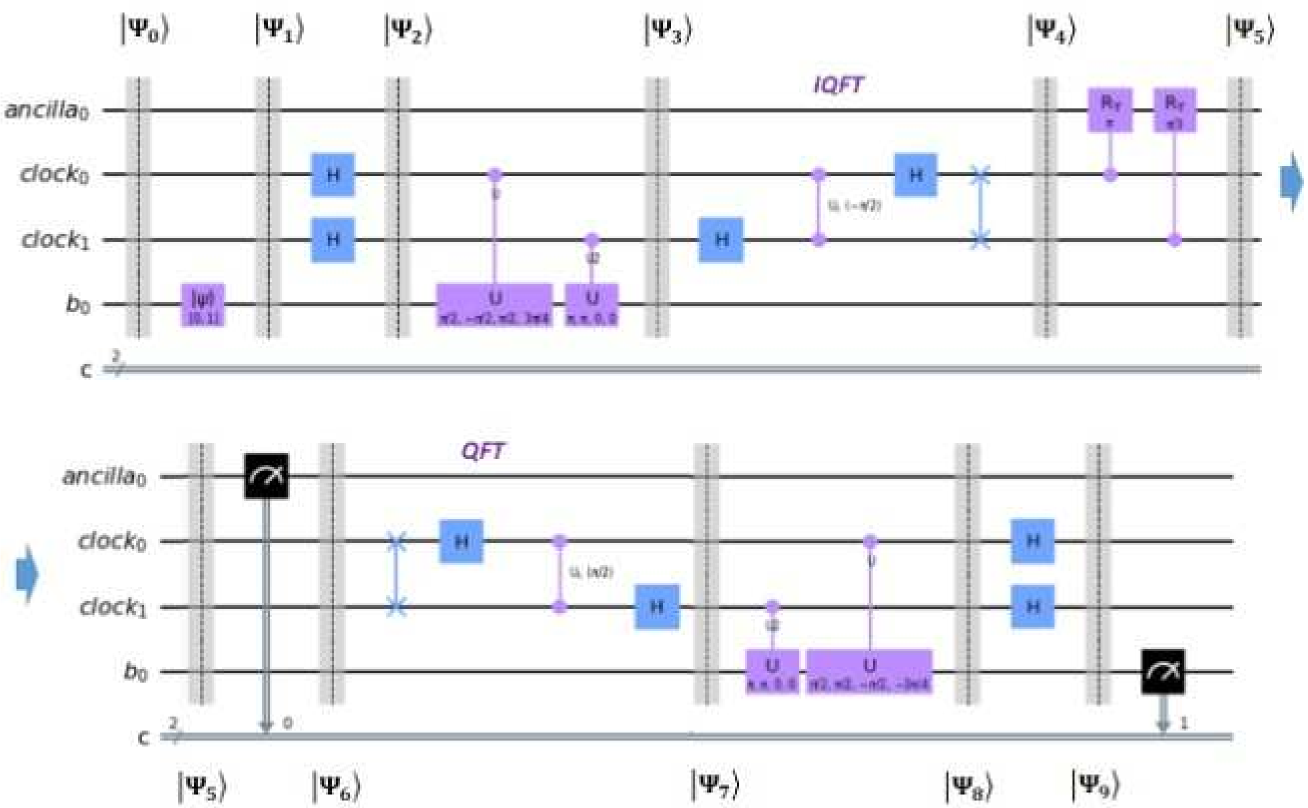
$$|x_0|^2 : |x_1|^2 = 1 : 9$$

A. Zaman *et. al.*
IEEE Access **11**, 77117 (2023)



Operator acting on quantum states

Matrix-vector multiplications



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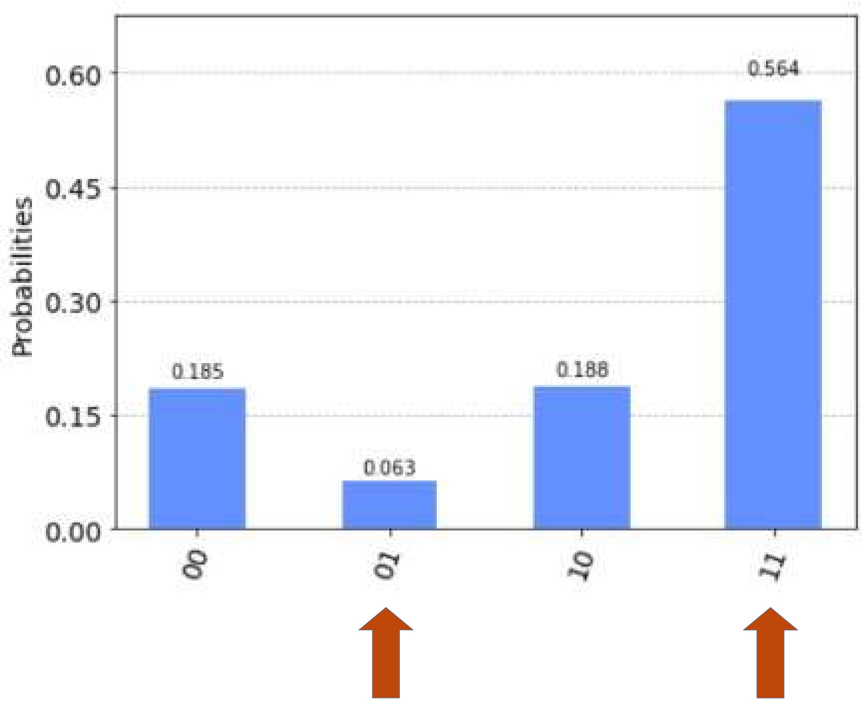
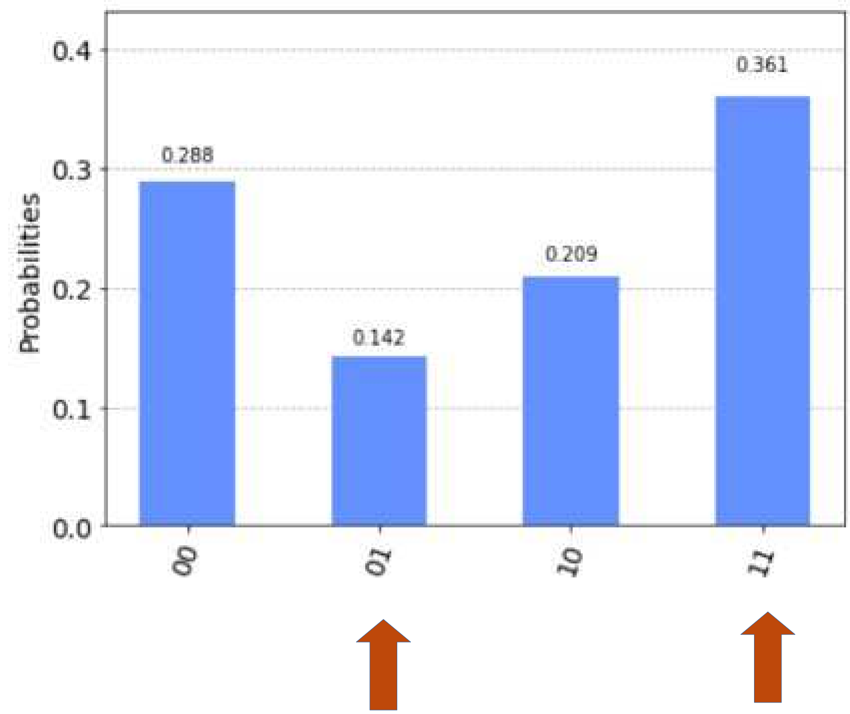




1 : 8.95

1 : 2.57

Using circuit simulation

Using IBM hardware

A. Zaman *et. al.*
IEEE Access **11**, 77117 (2023)

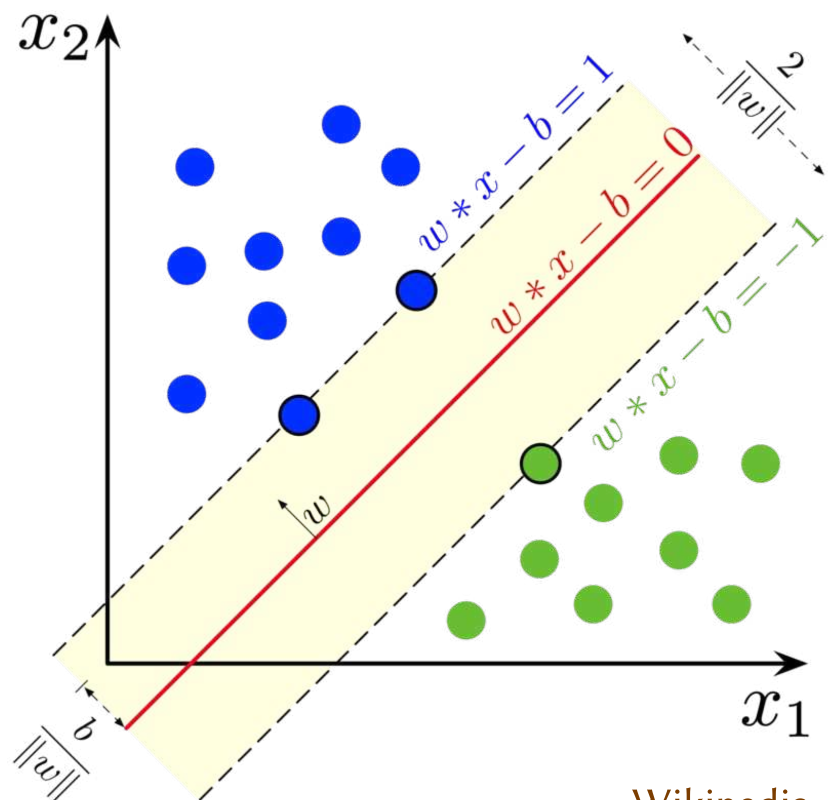
Experimental demonstration of HHL : *Phys Rev Lett* **110**, 230501 (2013)

The promise and gaps in quantum machine learning

Some quantum algorithms can solve certain class of problems faster than classical algorithms

Example 2 : Support vector machine

- A supervised ML algorithm
- Classifies vectors in a feature space In to one of two possible sets
- Requires training data set which determines the matrix *w*.



Wikipedia

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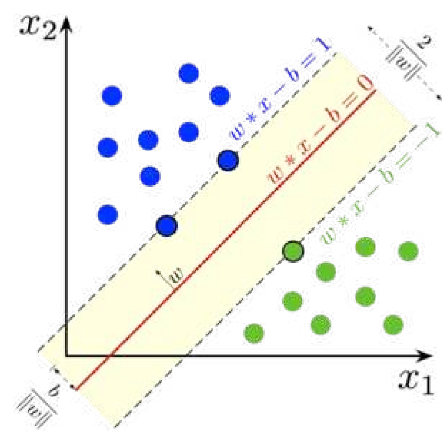
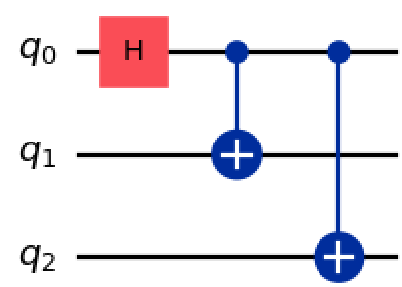


Example 2 : Quantum support vector machine

- Classical SVM → Quadratic programming problem
- Can be solved in time $O(\text{poly}(N, M))$

  Dim of feature space — Number of training vectors

- qSVM provides solution in $O(\log MN)$
  Uses HHL and efficient inner product evaluation



Phys. Rev. Lett. 113, 130503 (2014)

Method	Speedup
Bayesian Inference [107, 108]	$O(\sqrt{N})$
Online Perceptron [109]	$O(\sqrt{N})$
Least squares fitting [9]	$O(\log N^{(*)})$
Classical BM [20]	$O(\sqrt{N})$
Quantum BM [22, 62]	$O(\log N^{(*)})$
Quantum PCA [11]	$O(\log N^{(*)})$
Quantum SVM [13]	$O(\log N^{(*)})$
Quantum reinforcement learning [30]	$O(\sqrt{N})$

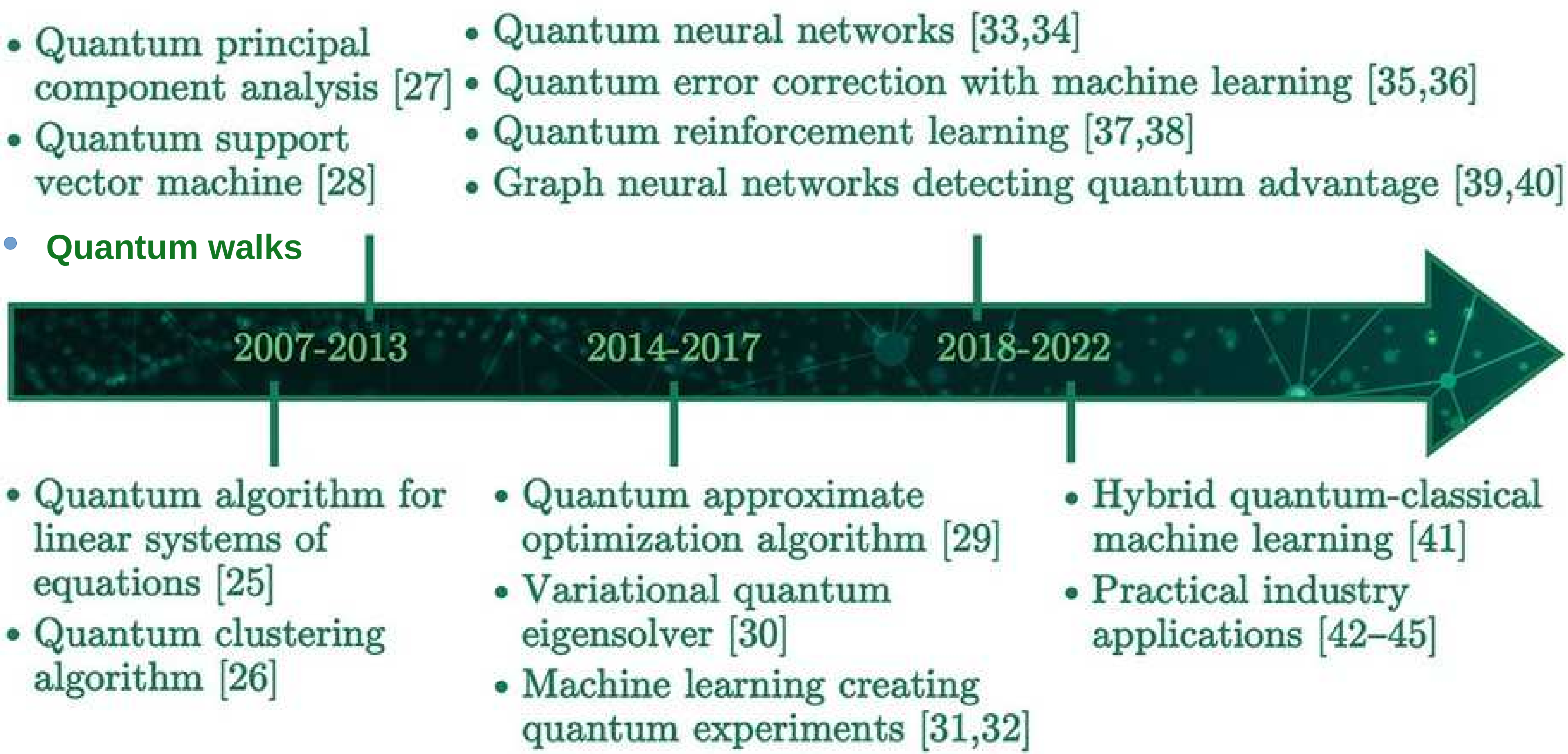
Biamonte et. al., Nature **549**, 195 (2017)

The promise and gaps in quantum machine learning

Applications

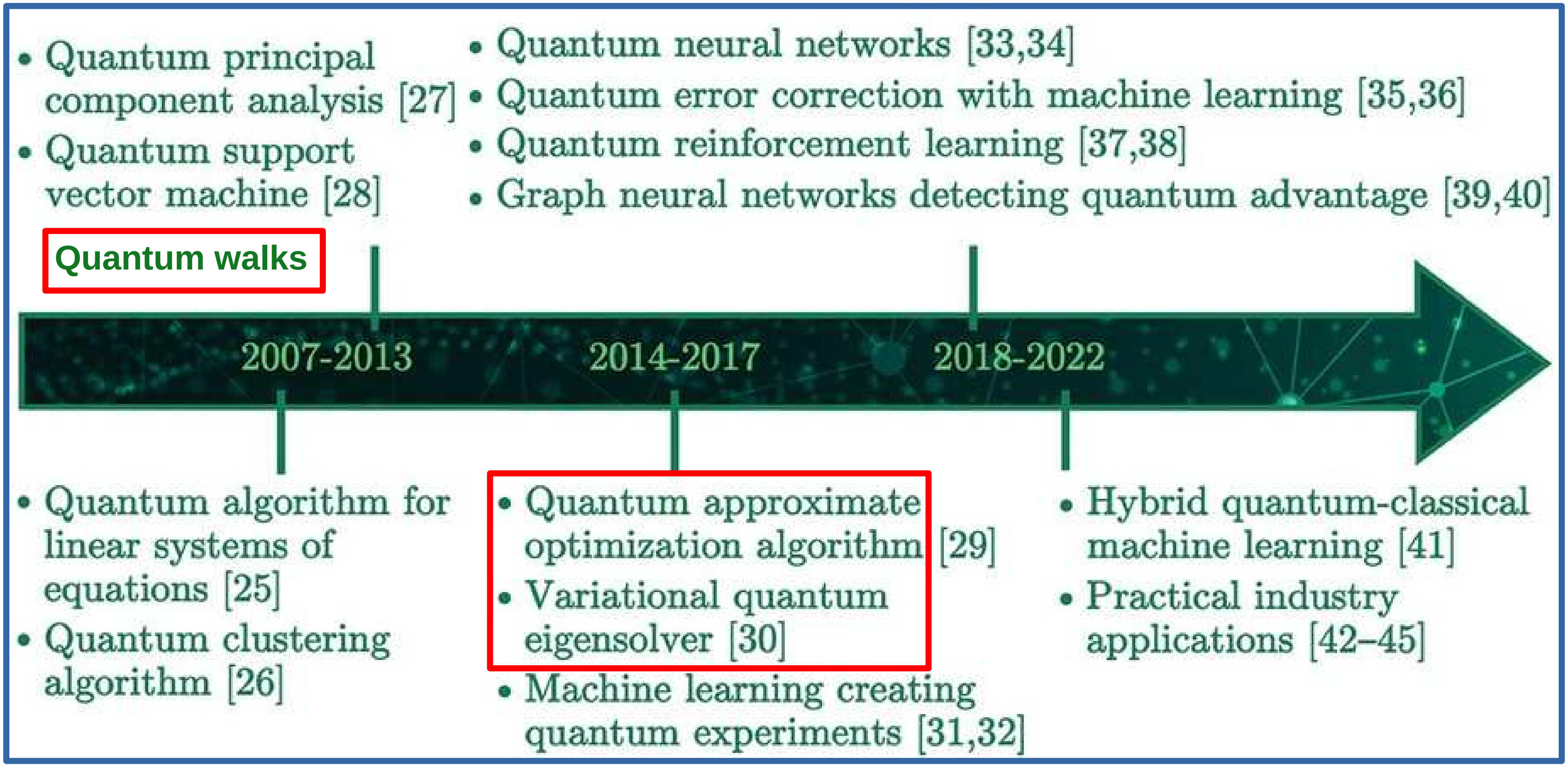
Biamonte et. al., Nature **549**, 195 (2017)

A brief history of QML



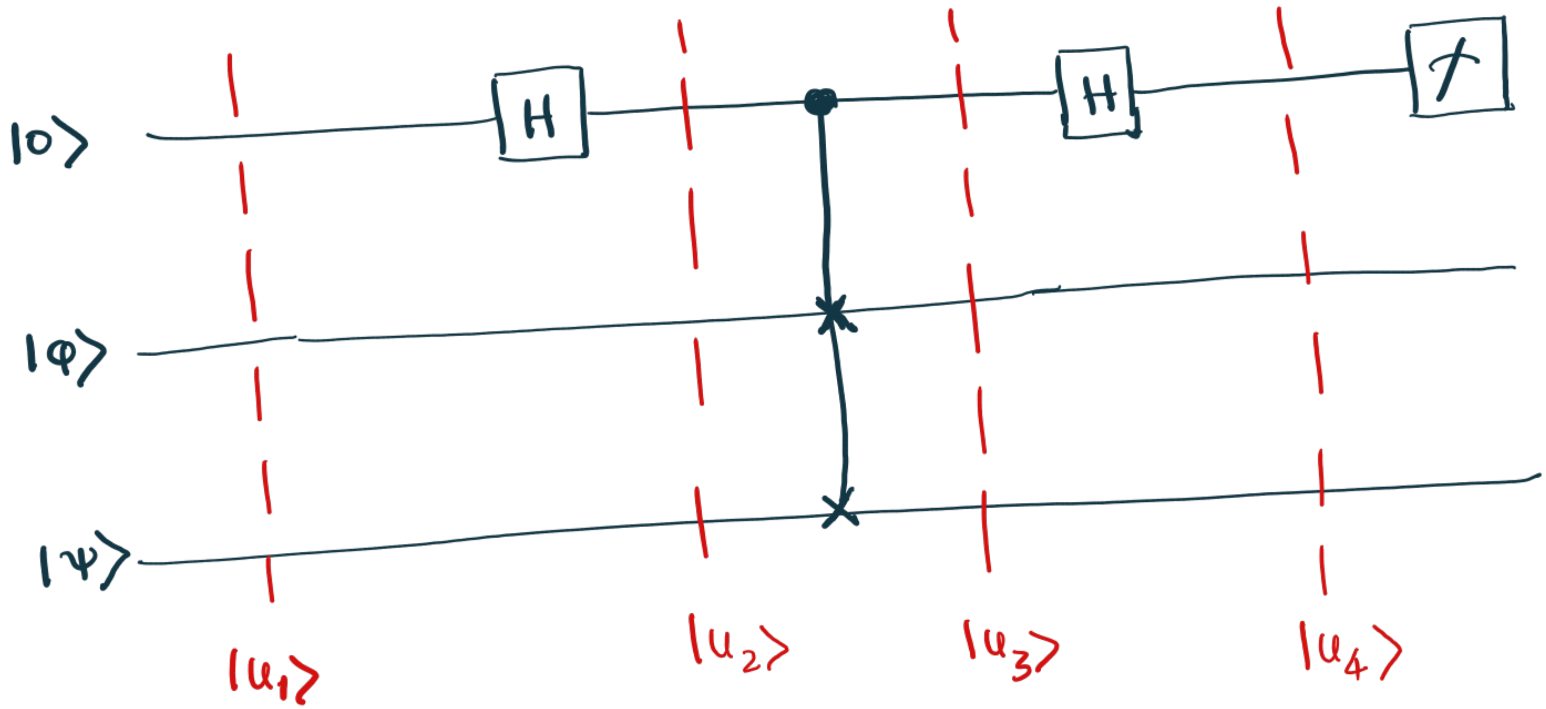
- **Quantum walks**

A brief history of QML



Fault-tolerant
quantum computer

SWAP test



Input register

$$|u_1\rangle = |0\ \varphi\ \psi\rangle$$

$$|u_2\rangle = \hat{H}\,|0\rangle \; I\,|\varphi\,\psi\rangle$$

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

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

$$|u_3\rangle = \frac{1}{\sqrt{2}}\left(|0\,\varphi\,\psi\rangle + |1\,\psi\,\varphi\rangle\right)$$

$$|u_4\rangle = H\,\frac{1}{\sqrt{2}}\left(|0\,\varphi\,\psi\rangle + |1\,\psi\,\varphi\rangle\right)$$

$$|u_4\rangle = \frac{1}{2}\left[|0\,\varphi\,\psi\rangle + |1\,\varphi\,\psi\rangle + |0\,\psi\,\varphi\rangle - |1\,\psi\,\varphi\rangle \right]$$

$$|u_4\rangle = \frac{1}{2}\,|0\rangle\left(|\varphi\,\psi\rangle + |\psi\,\varphi\rangle \right) + \frac{1}{2}\,|1\rangle\left(|\varphi\,\psi\rangle - |\psi\,\varphi\rangle \right)$$

measure the first qubit

Probability of getting 0 :

$$P(0) = \frac{1}{2} + \frac{1}{2}\,|\langle\varphi|\psi\rangle|^2$$

knowing $P(0)$, overlap can be estimated.

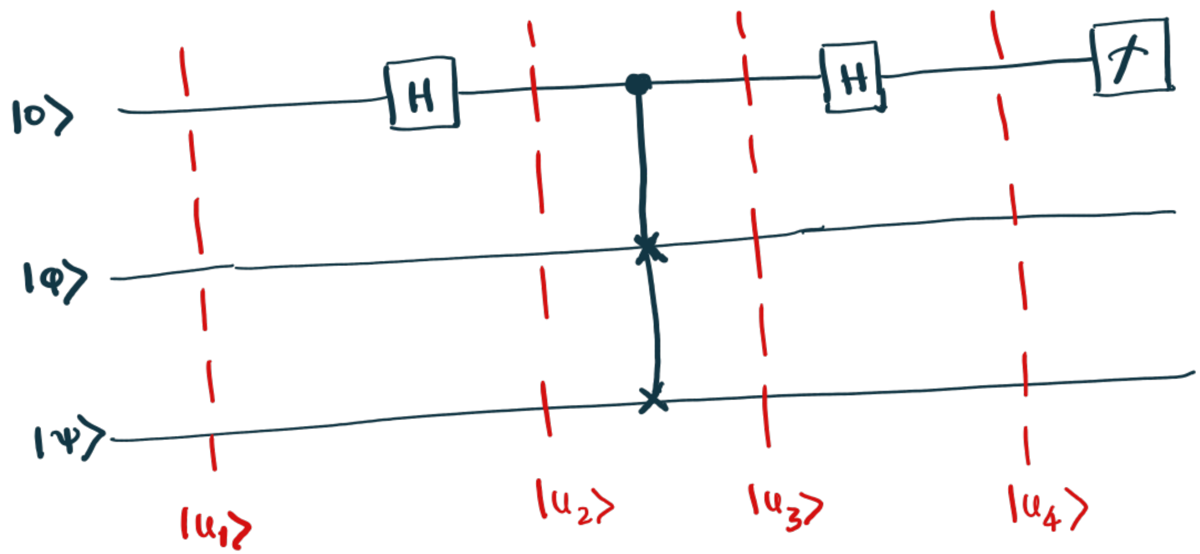
- Classical technique to estimate overlap for two vectors with 2^n components

$$2^n + (2^n - 1) \approx 2^{n+1} = O(2^n)$$

- Quantum swap test

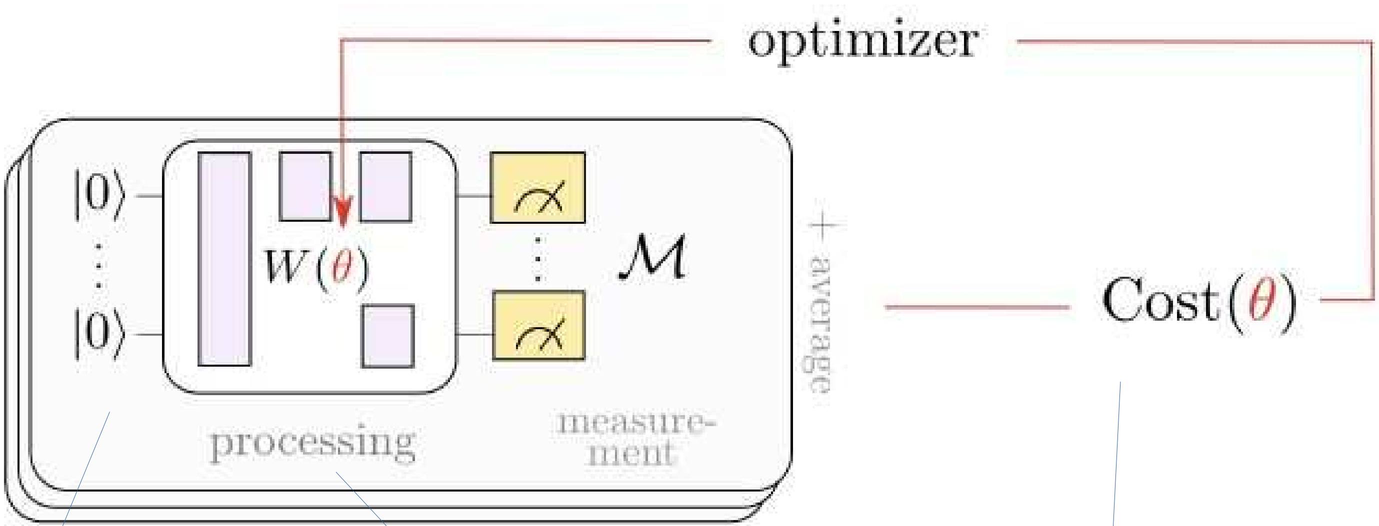
$$O(n)$$

Exponential advantage !



Variational quantum circuits :

Typically, in NISQ era quantum computers, noise destroys quantumness quickly (decoherence). Better to perform core computation on quantum devices and off-load the rest to classical computers.



Data encoded in Qubits and Represented as $|\phi\rangle$

ansatz $W(\theta)$

"Pauli Rotations"

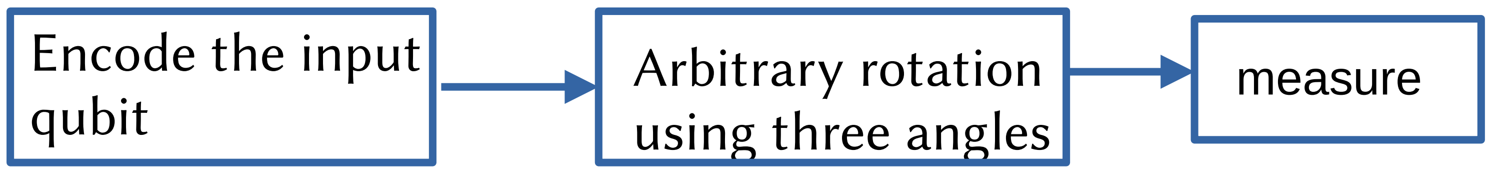
$$|\psi(\theta)\rangle = W(\theta)\ |\phi\rangle$$

θ → parameters

Optimise suitable loss function Using classical techniques

A simple variational quantum classifier :

- Given an input, classify it as belonging to one of the two sets.



- QML model

$$f_\theta(x) = \langle 0 | R_x(x)^\dagger \mathrm{Rot}(\theta_1, \theta_2, \theta_3)^\dagger \sigma_z \mathrm{Rot}(\theta_1, \theta_2, \theta_3) R_x(x) | 0 \rangle.$$

- Apply binary classifier :

$$y = \begin{cases} 1 \text{ if } f_\theta(x) > 0 \\ -1 \text{ else} \end{cases}$$

Variational quantum eigensolver

- Based on variational technique in standard quantum physics
- Useful in solving some quantum chemistry or optimisation problems

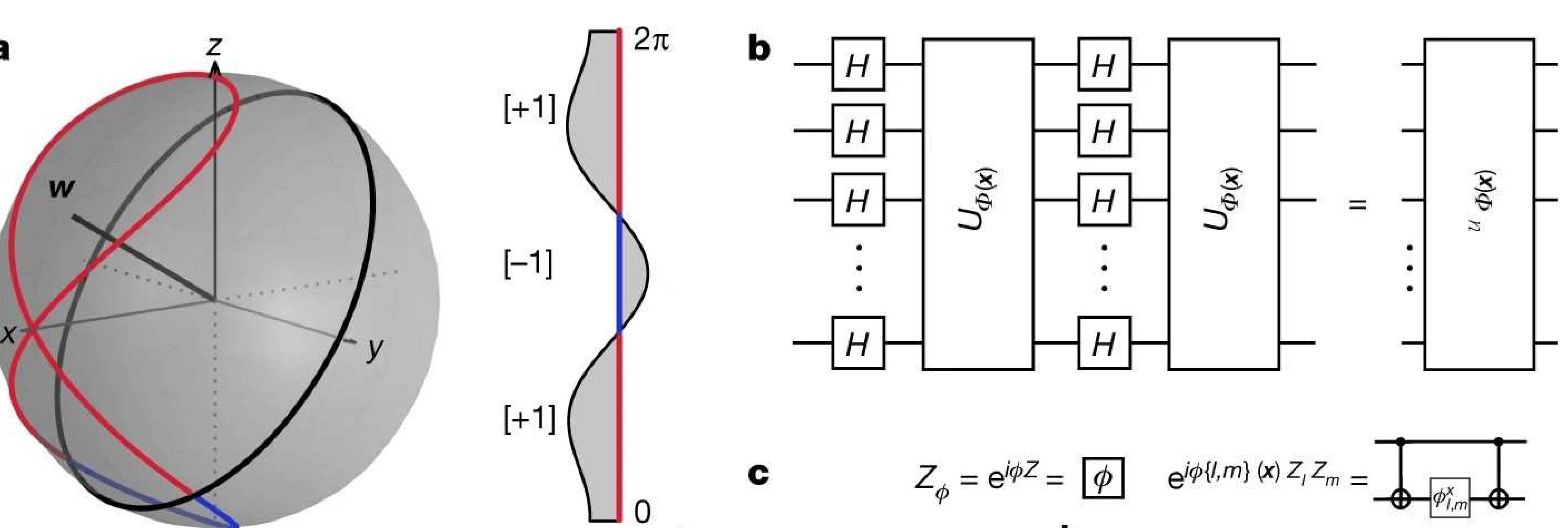
- Optimise the parameters such that $E(\theta_1, \ldots, \theta_n)$ is minimised

$$E(\theta_1, \cdots, \theta_n) = \langle \hat{H} \rangle = \sum_i \alpha_i \langle \psi(\theta_1, \cdots, \theta_N) | \hat{P}_i | \psi(\theta_1, \cdots, \theta_N) \rangle$$

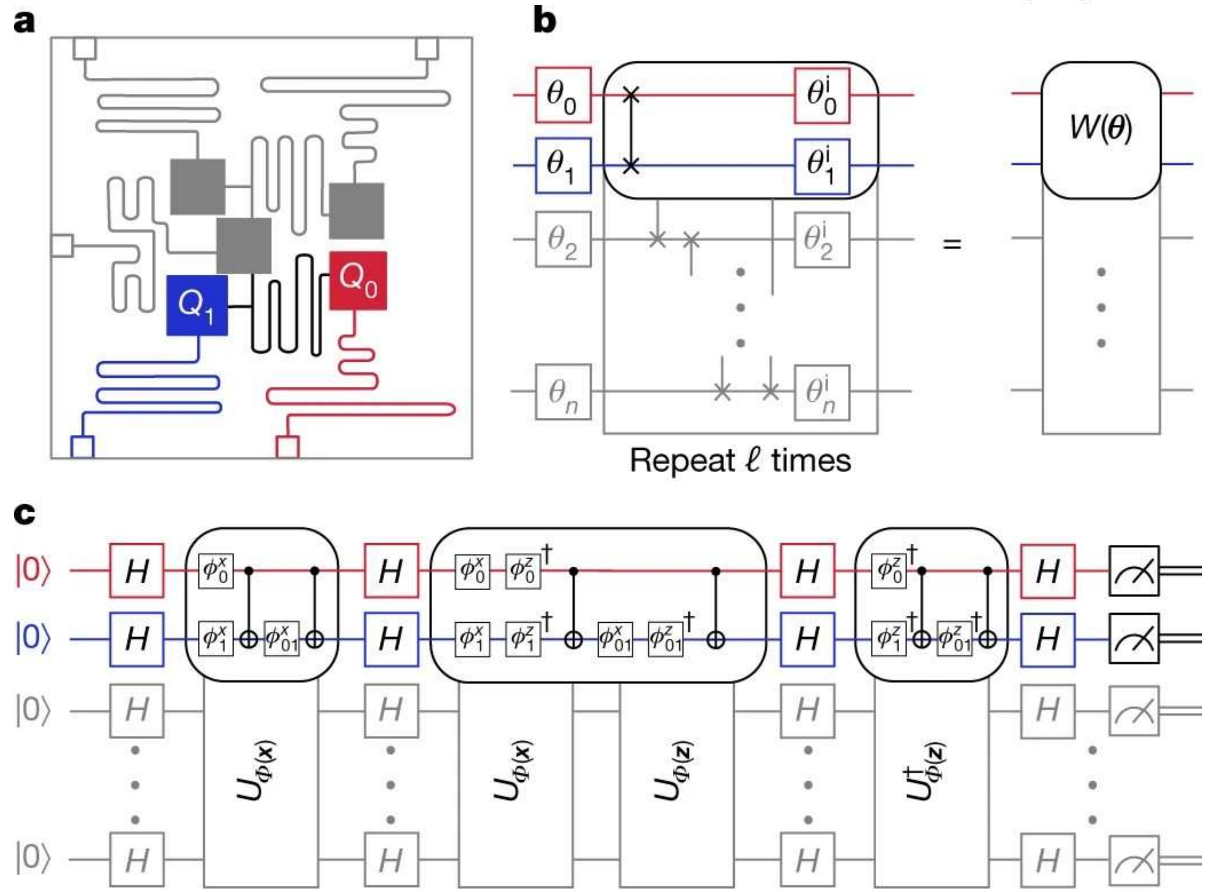
The Hamiltonian function must be written in terms of Pauli operators

Write the Hamiltonian function (think of it as your cost function)
in terms of Pauli operators

Optimise and Measure

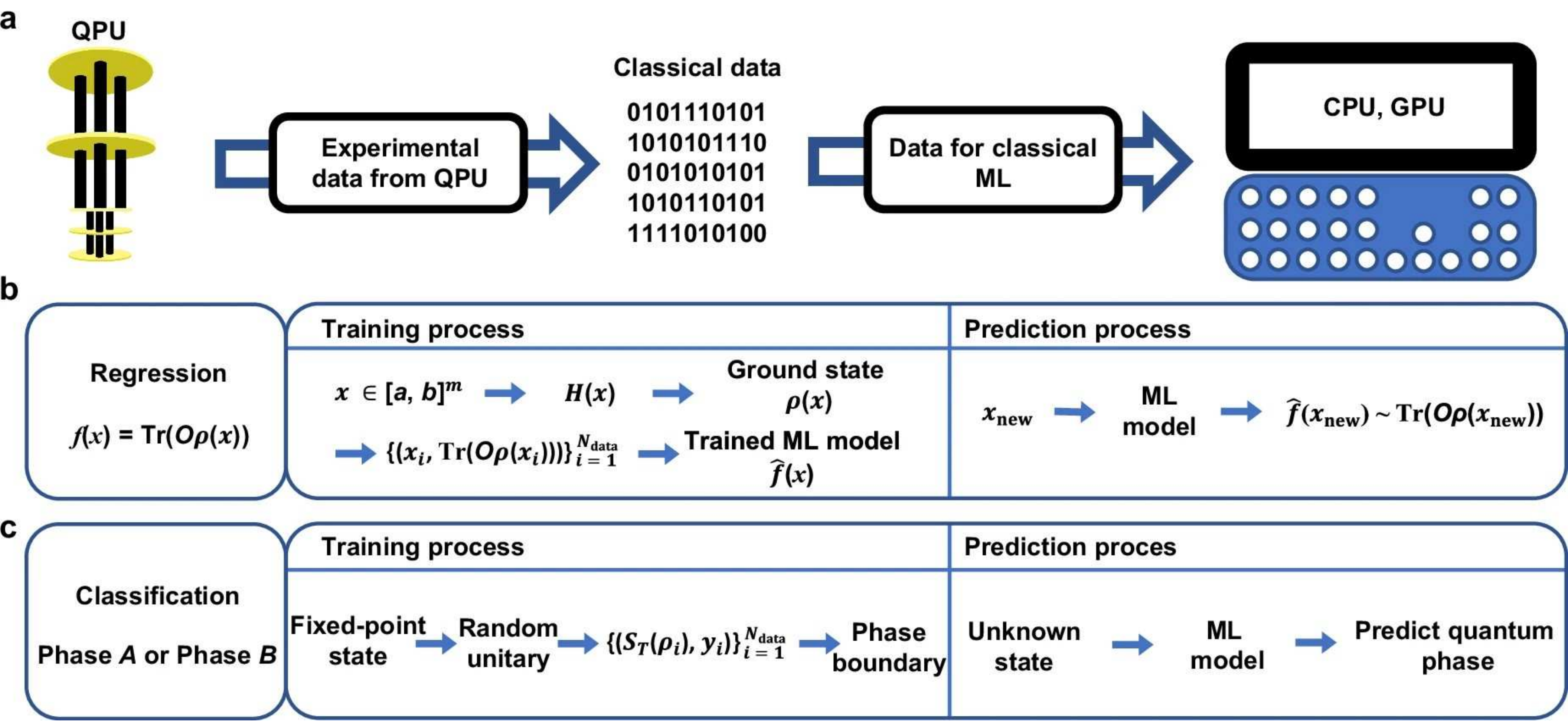


A more involved classification experiment with transmons



Classification problem implemented with 5 transmons

Nature 567, 210 (2019)

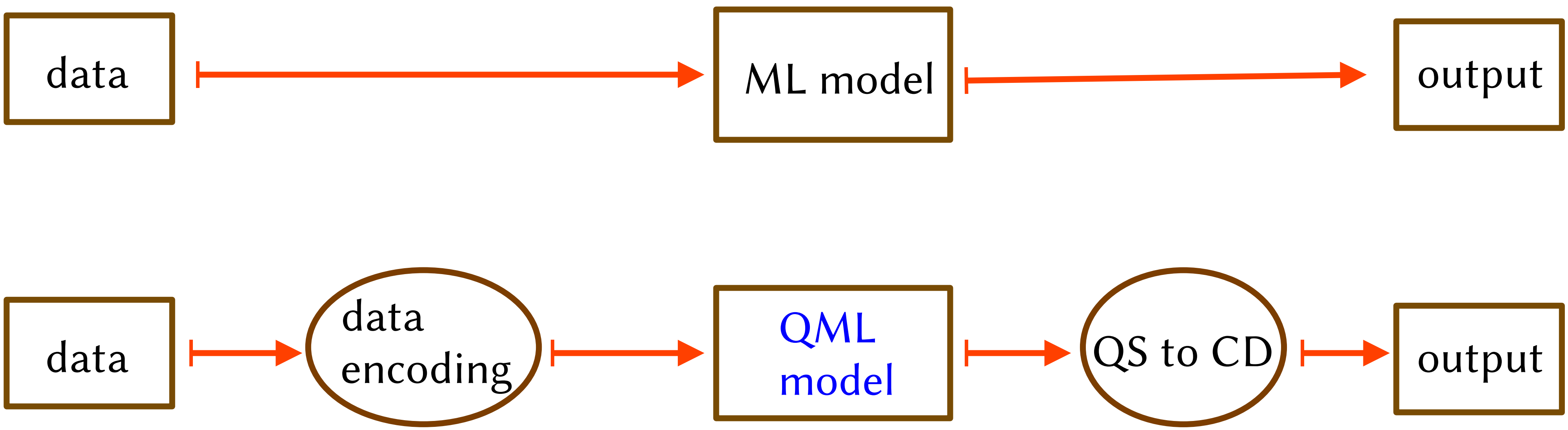


Quantum data from experiments processed using classical ML methods predicting phases of quantum matter.

Nature Communications 15, 7552 (2024).

The promise and gaps in quantum machine learning

- Large quantum computers not available yet
- Data encoding can be a major constraint
- Answers are probabilistic, repetition needed
- Other issues such as decoherence exist, but not QML specific

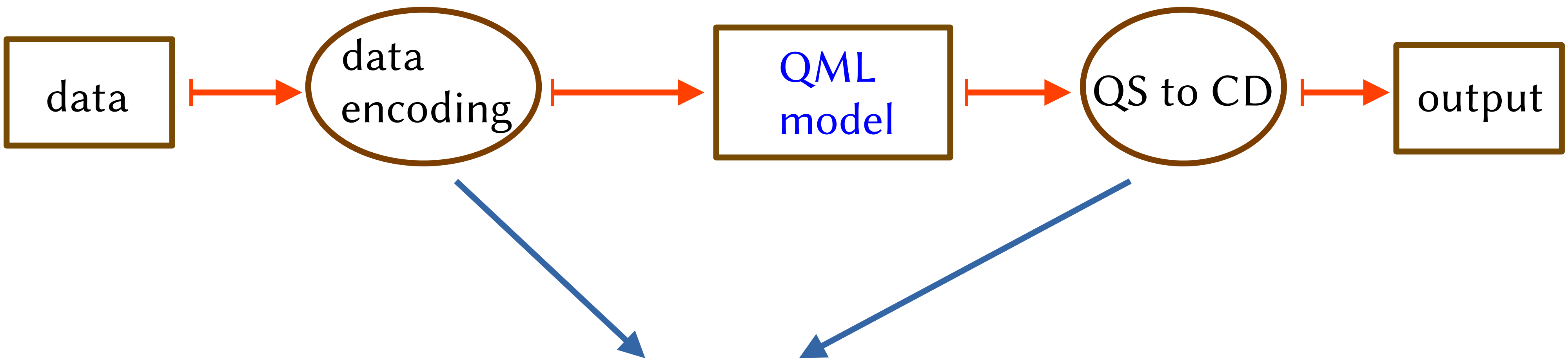


$$b_0 \ b_1 \ b_2 \ b_3 \longmapsto |b_0 \ b_1 \ b_2 \ b_3\rangle$$

Classical data $\longmapsto$ Quantum states

The promise and gaps in quantum machine learning

- Data encoding can be a major constraint



For complexity calculations,
these were not accounted for

$$b_0 \; b_1 \; b_2 \; b_3 \longmapsto |b_0 \; b_1 \; b_2 \; b_3\rangle$$

Classical data ⟼ Quantum states