Machine Learning crash course

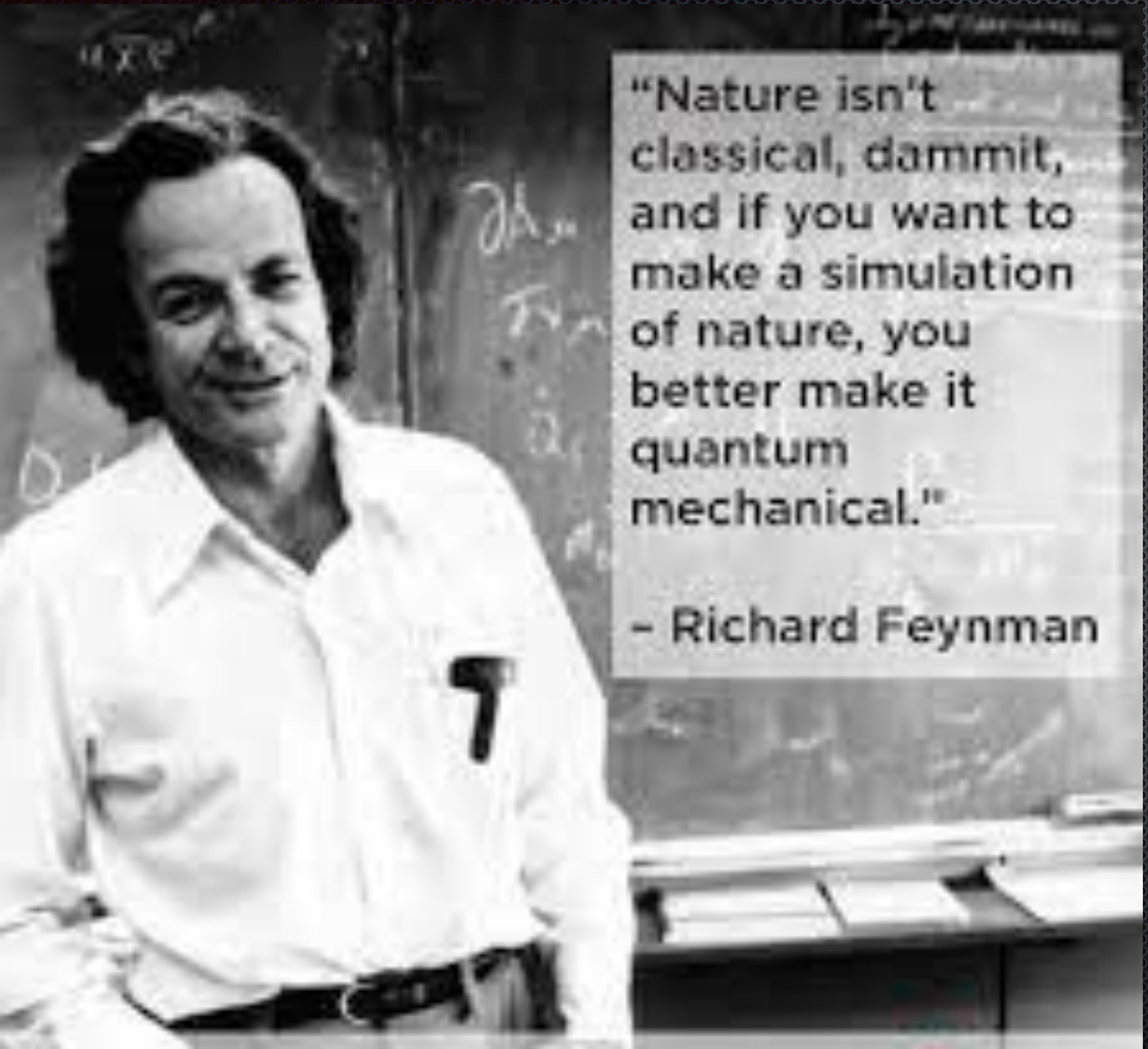
(Part-6)

Ahmed Hammad

Introduction to quantum machine learning, quantum gates, quantum feature map, data encoding and VQC

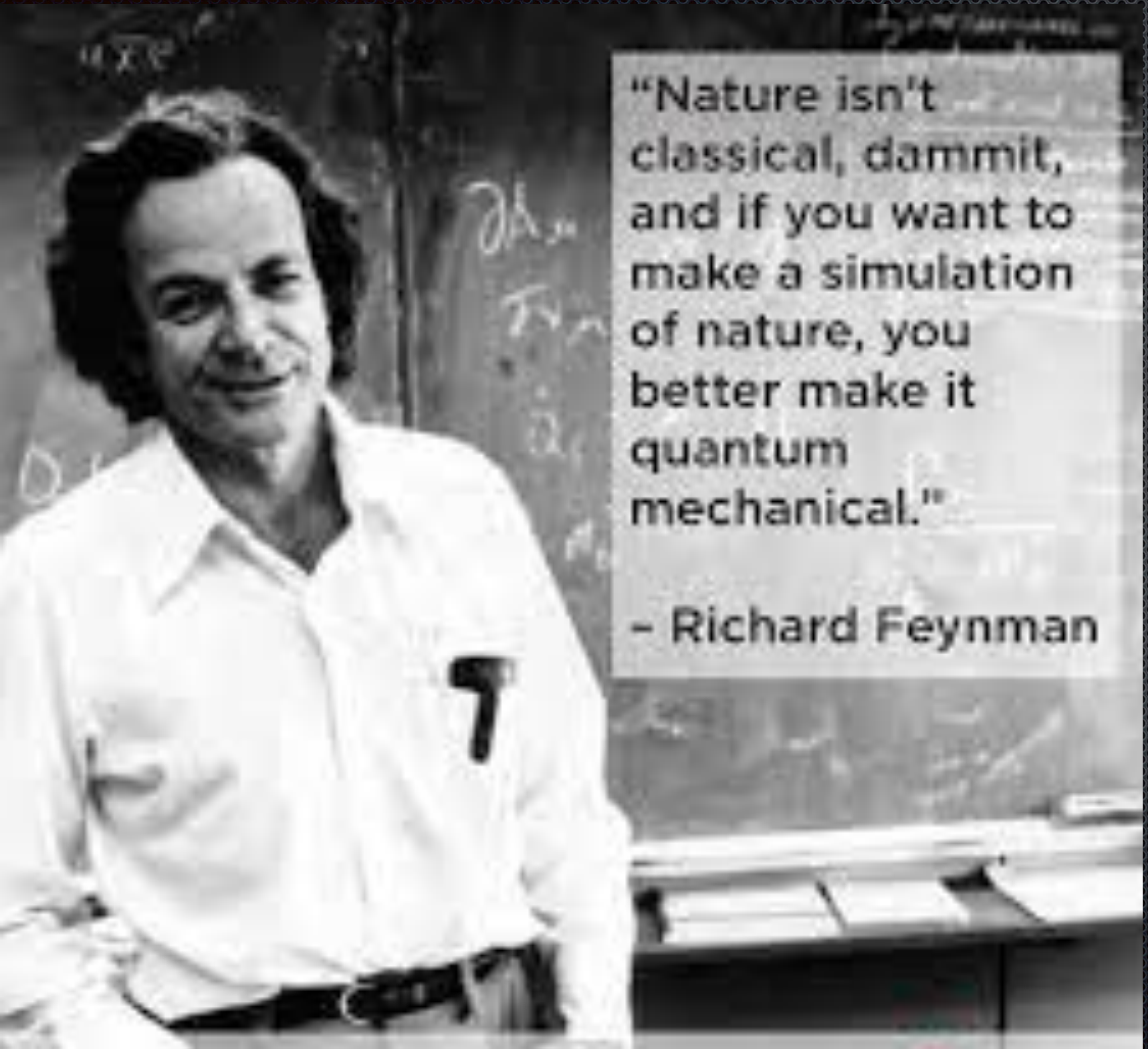
Introduction

In 1982 Richard Feynman had a dream to replace the classical simulation With the quantum one, but he didn't know how !!

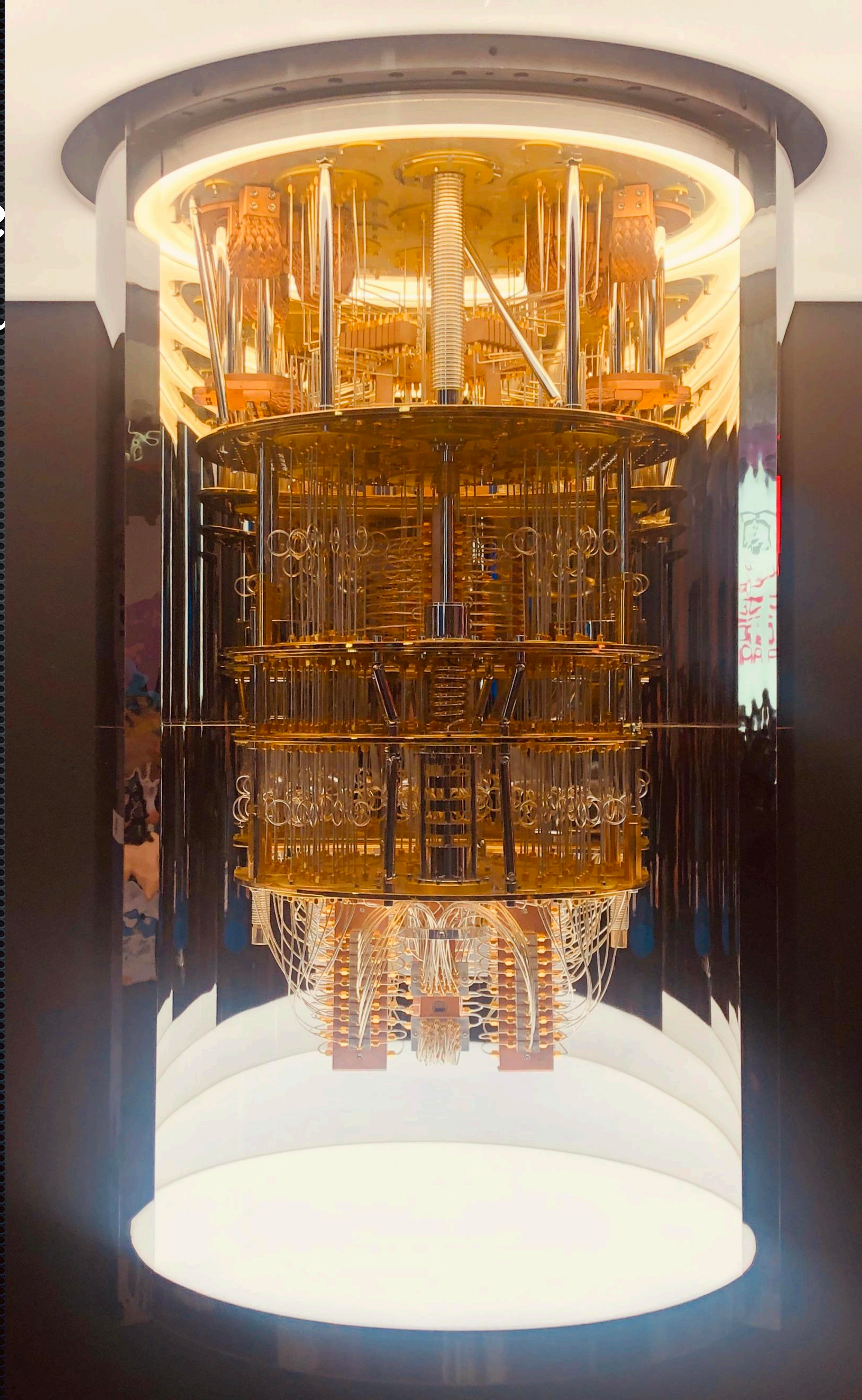


Introduction

In 1982 Richard Feynman had a dream to replace the
With the quantum one, but he didn't kno



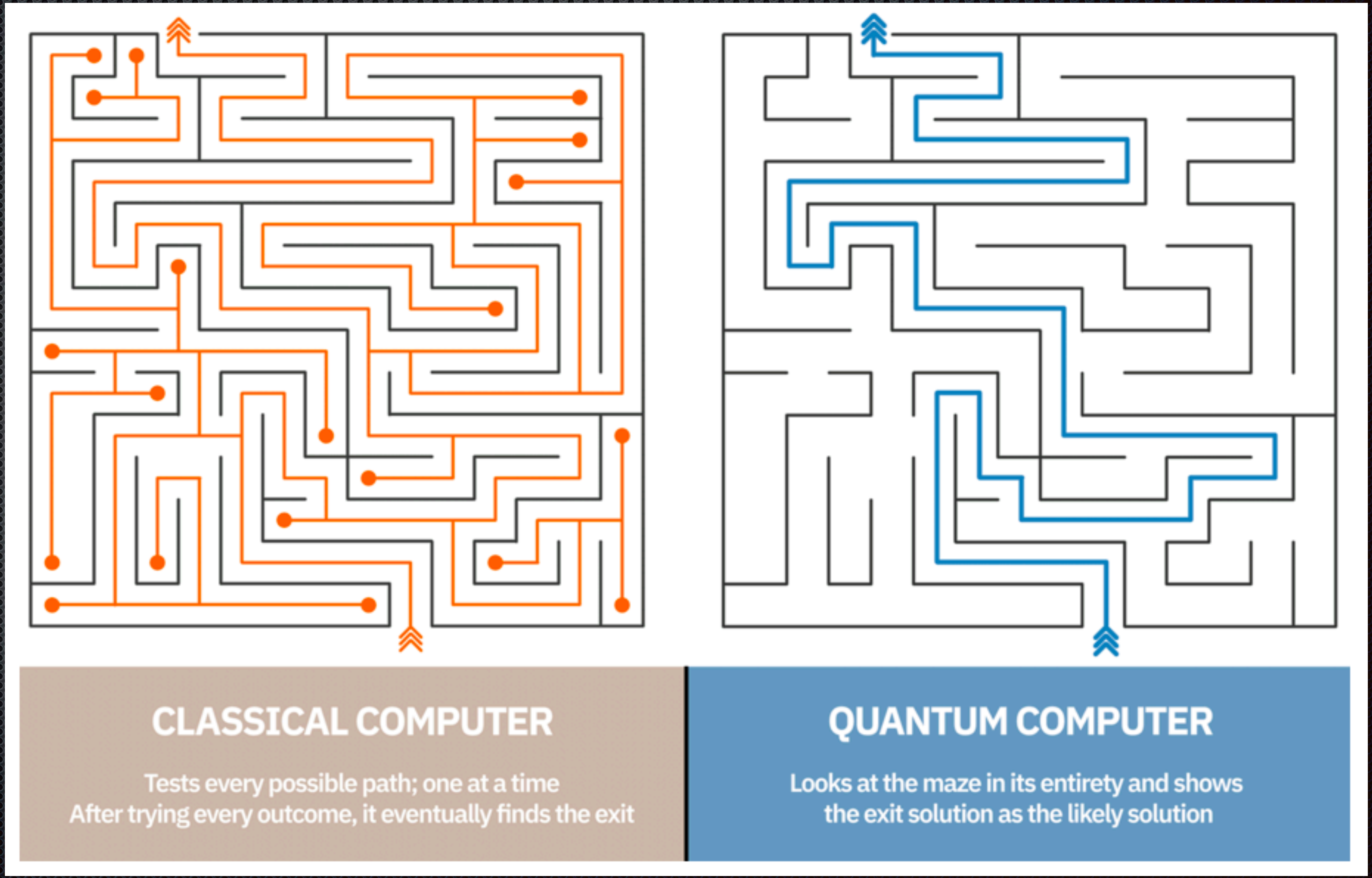
Now we know



Introduction

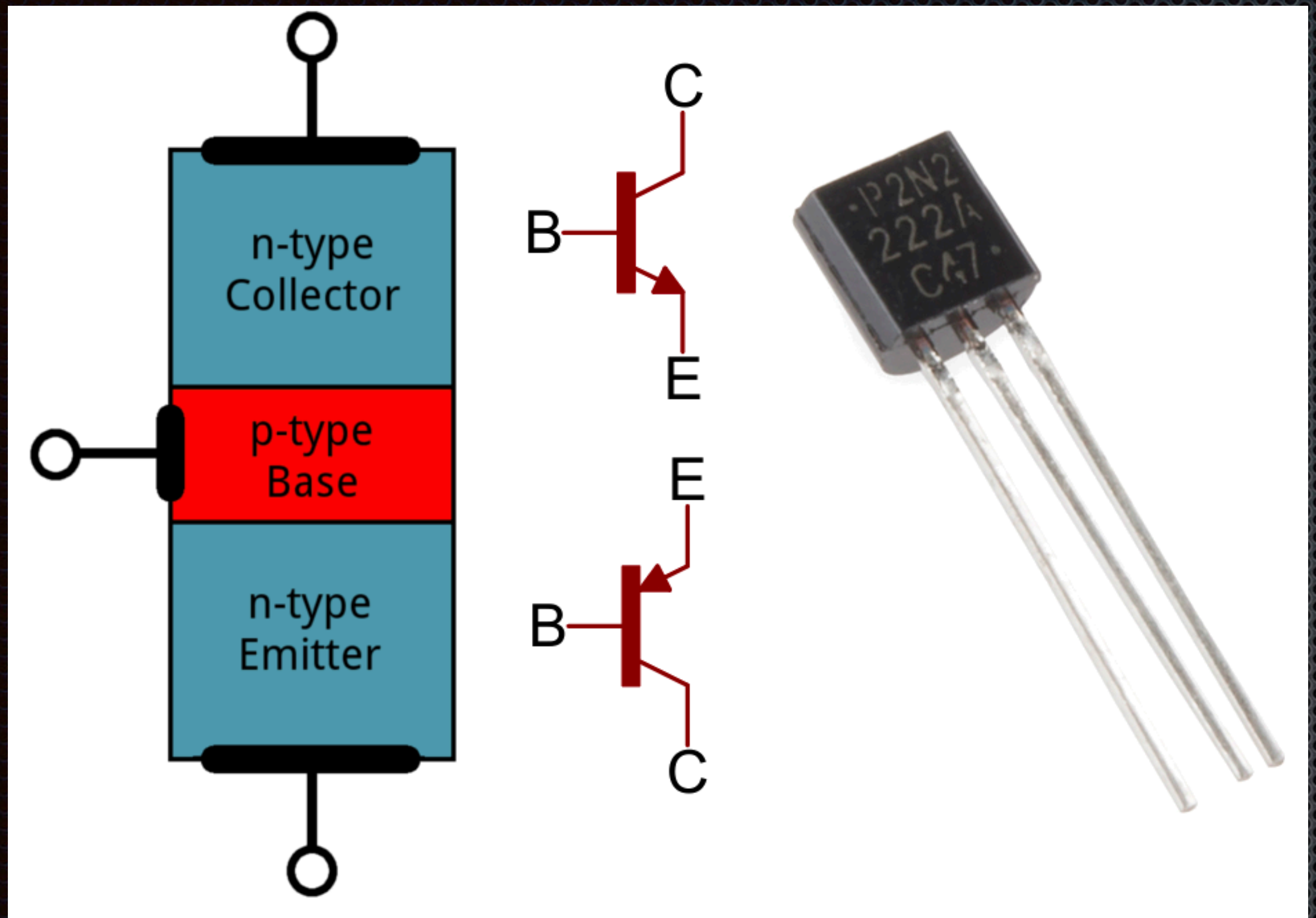
Using classical and quantum computers to search for unstructured data to find the exit of a maze

Quantum computer can access the whole maze structure at once exploiting the superposition of the qubits states; but how ?

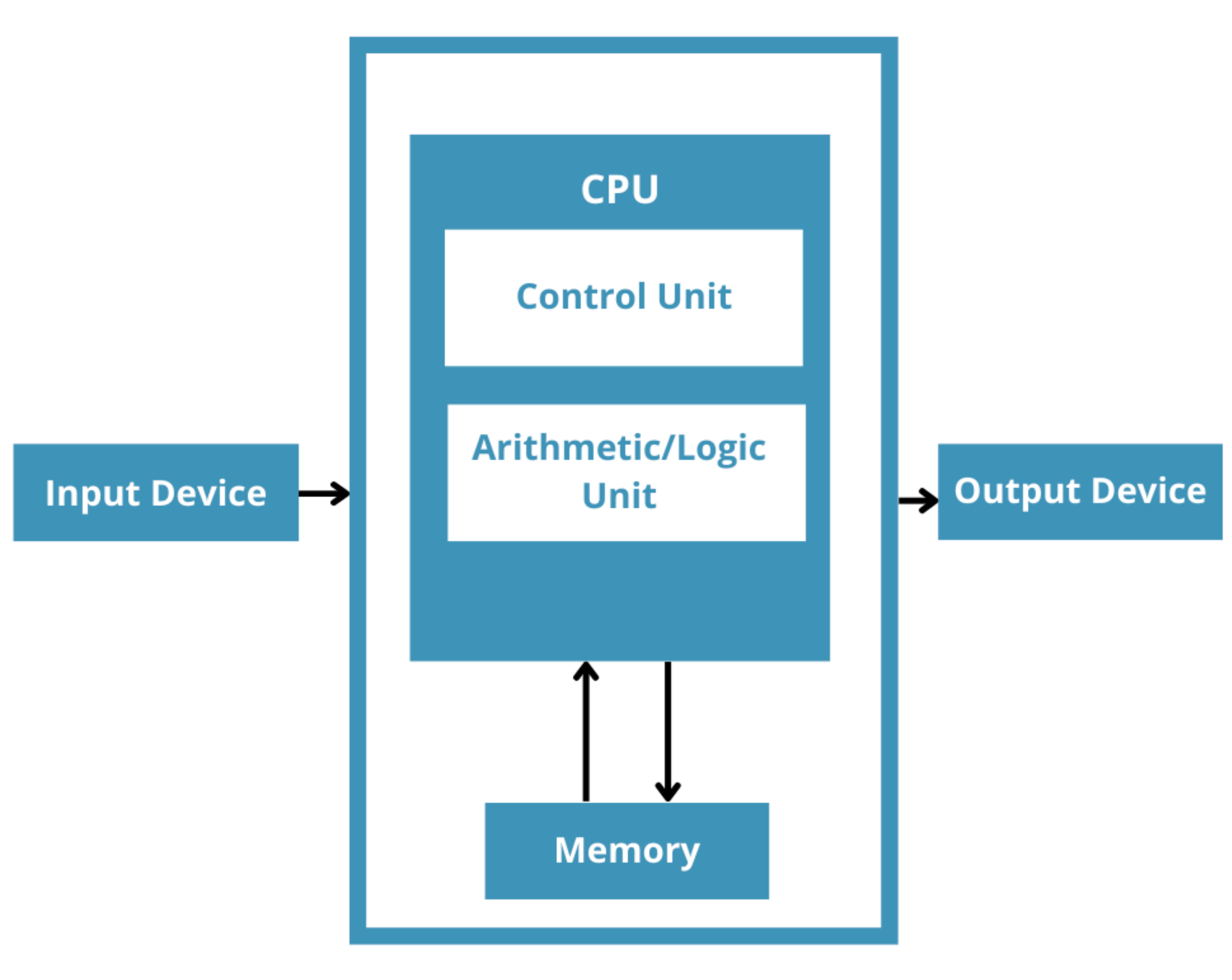


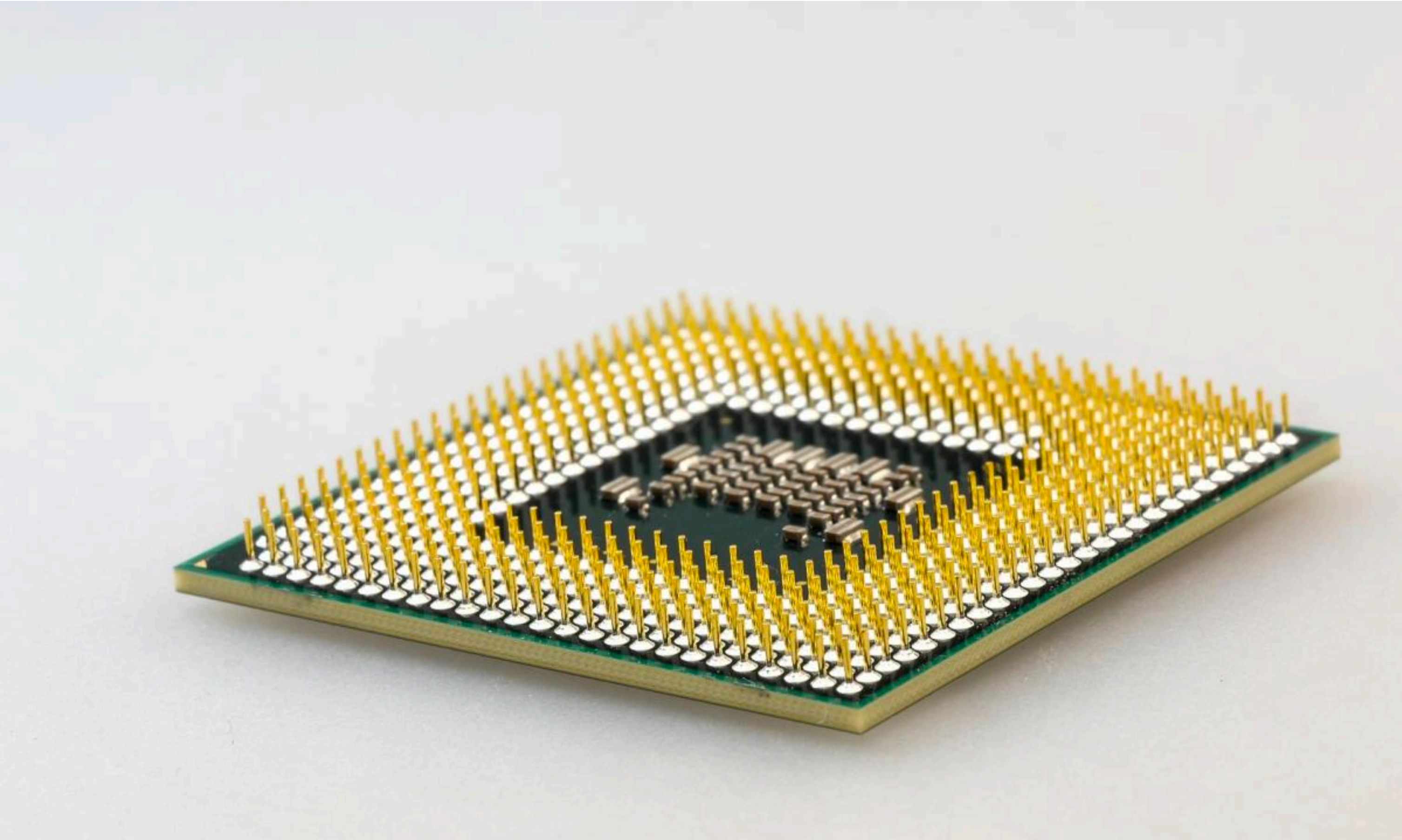
Introduction

Classical computers use a bunch of binary gates to construct the CPU



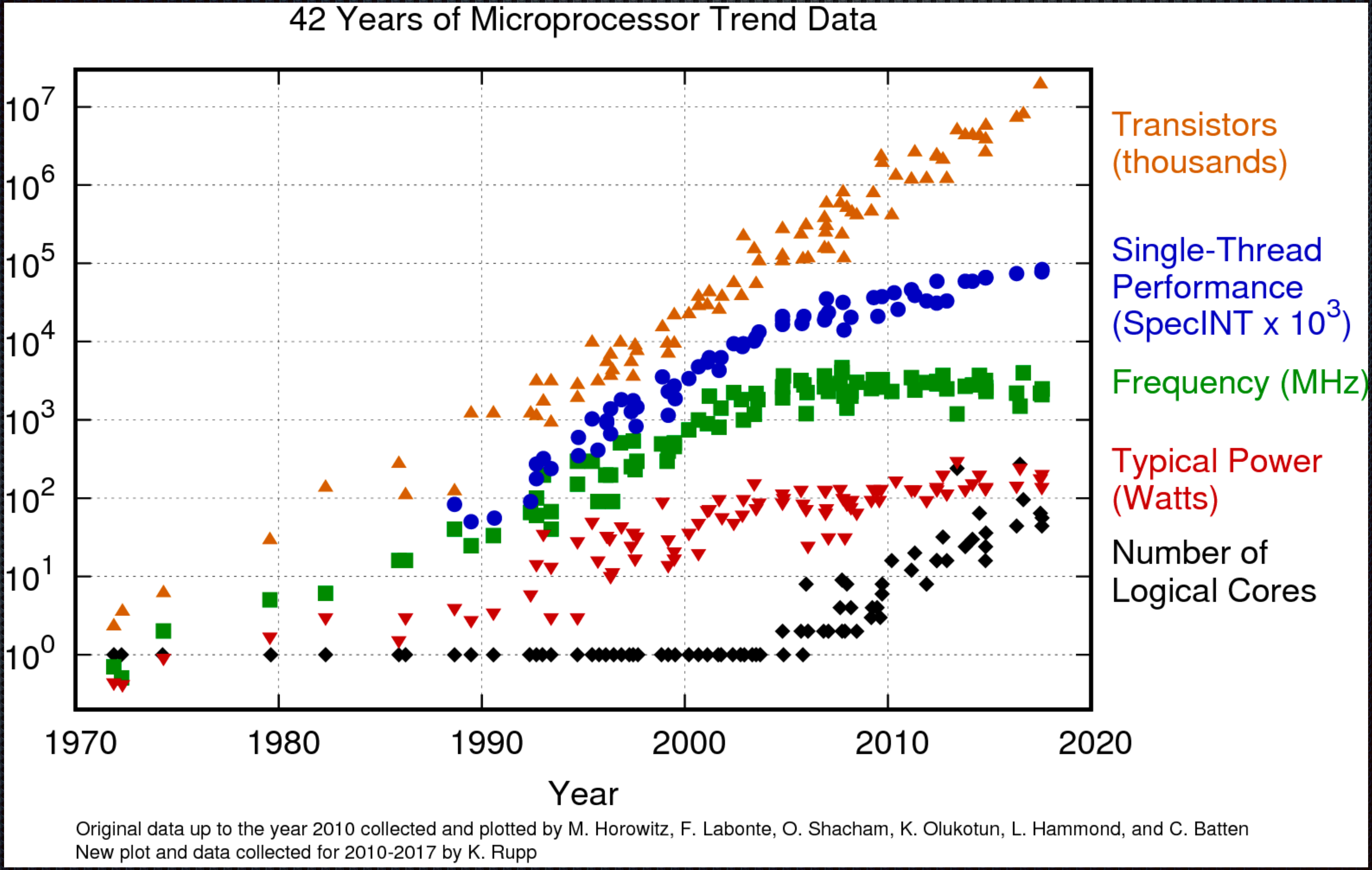
More and more gates
to construct a CPU





Introduction

Why do we need quantum computation



Introduction

Examples of quantum computers

Quantum annealers

Solving optimization problem to finding the ground state of the time evolution wave function

Photonic QC

Quantum computations done on the Polarization states of the photon

Quantum dots

Processing quantum information On the spin states of an electron in a Semiconductor dot.

Superconducting QC

Tiny electrical circuits to produce and manipulate qubits

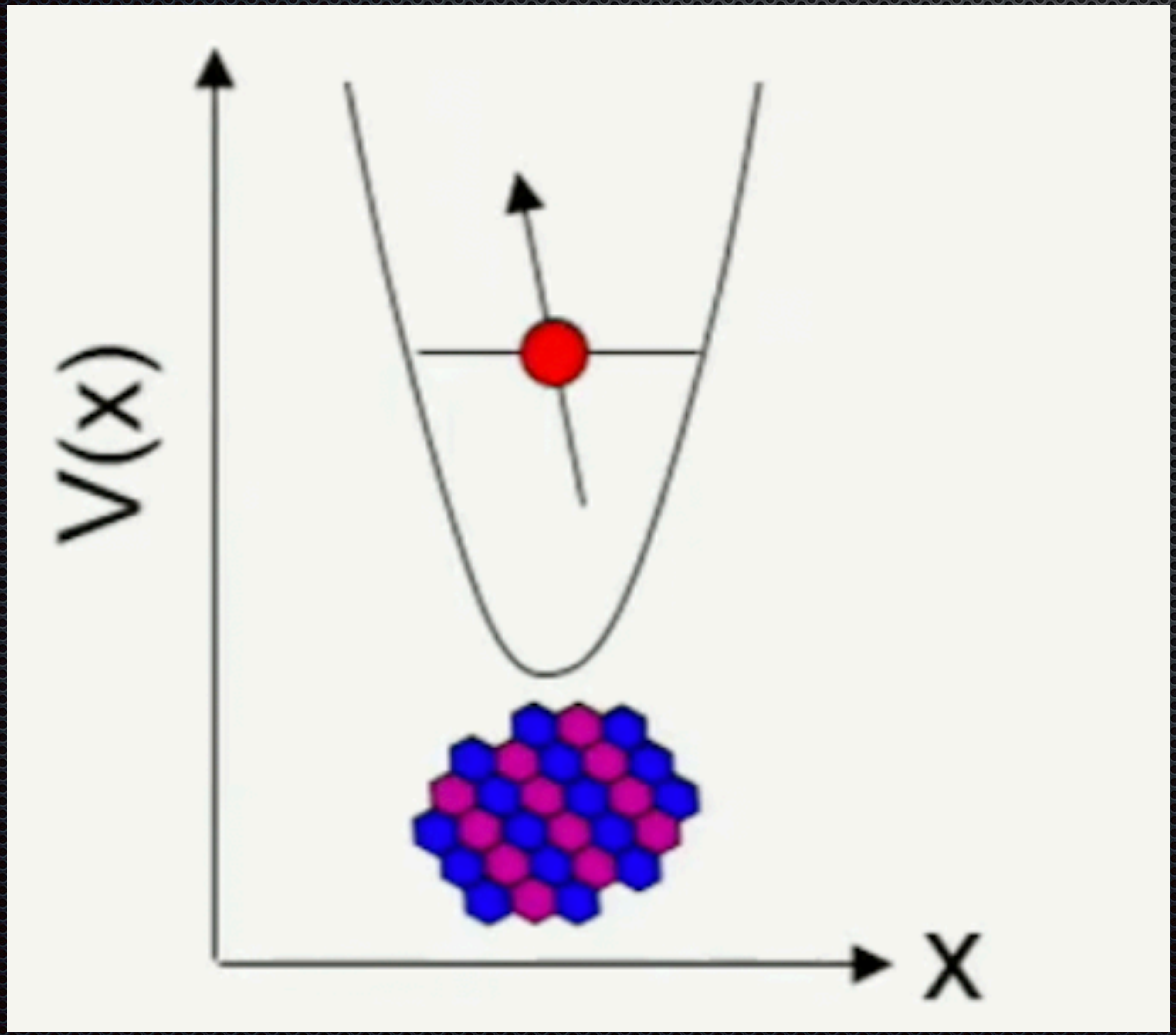
Trapped ions

Trapped ions are used to process Quantum information using electric and magnetic fields

Quantum dot

How to perform computations on quantum dots?

Quantum dot: A semiconducting confinement hole where single electrons can be trapped. While trapped electron can be excited to higher energy scale with EM pulses.



To perform quantum computations (gate operations) we need to confine the electron on a dot.

How to cook a quantum dot?

Quantum dot

Lets ask ChatGPT how to cook a quantum dot

A Hi GPT

Hello! How can I assist you today?

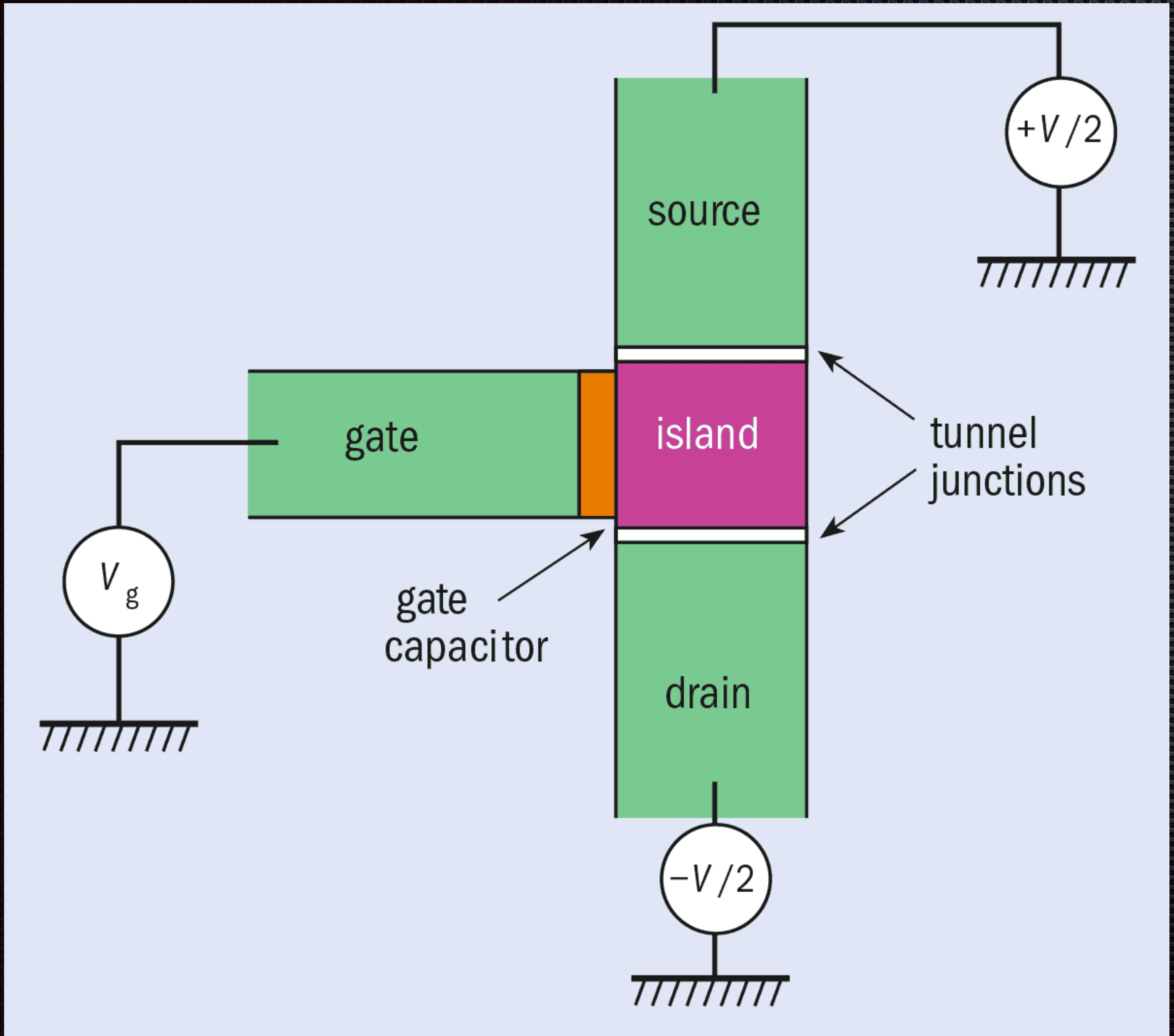
A How to cook a quantum dot at home? answer precisely

I'm sorry, but it is not safe or feasible to cook quantum dots at home. Quantum dots are nanoscale semiconductor particles that require specialized equipment and materials to synthesize. The process involves complex chemical reactions and precise control over reaction conditions.

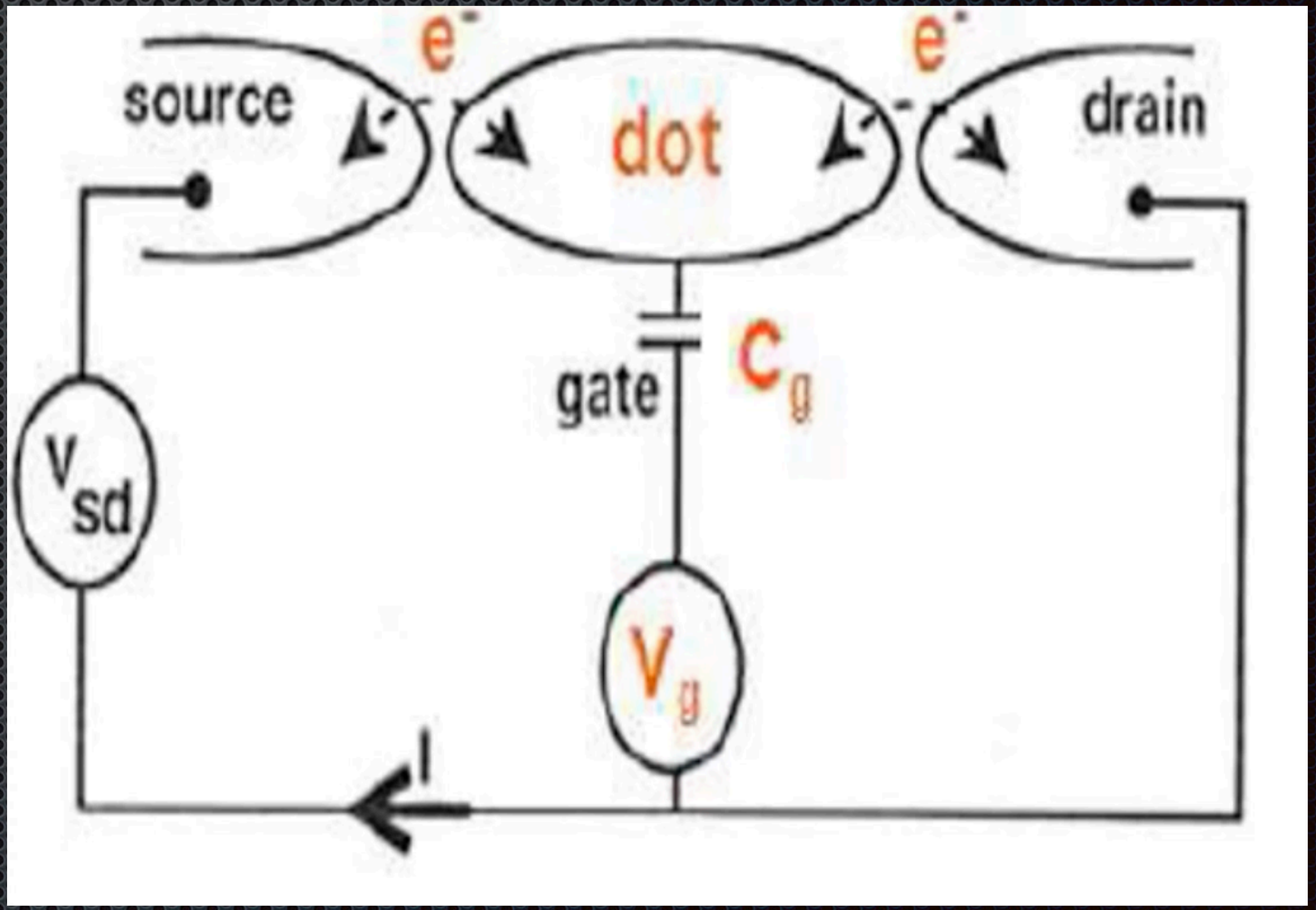
Furthermore, working with quantum dots typically requires a controlled environment, such as a laboratory setting, due to the potential health risks associated with handling certain chemicals and nanoparticles. It's important to prioritize safety and leave the synthesis of quantum dots to professionals in the field of nanotechnology.

Quantum dot

Single electron box



Electrons can tunnel to the island by controlling the gate voltage

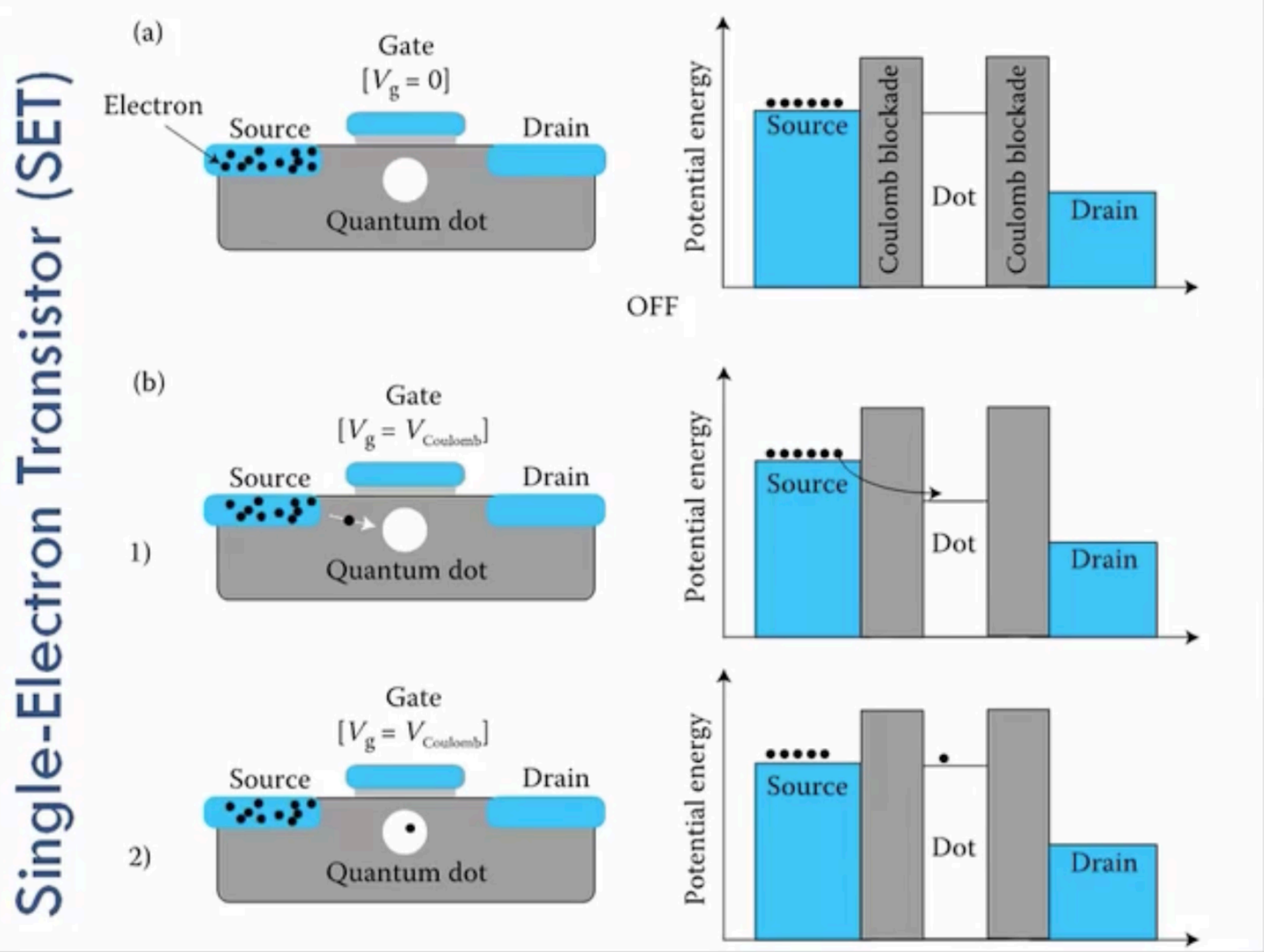


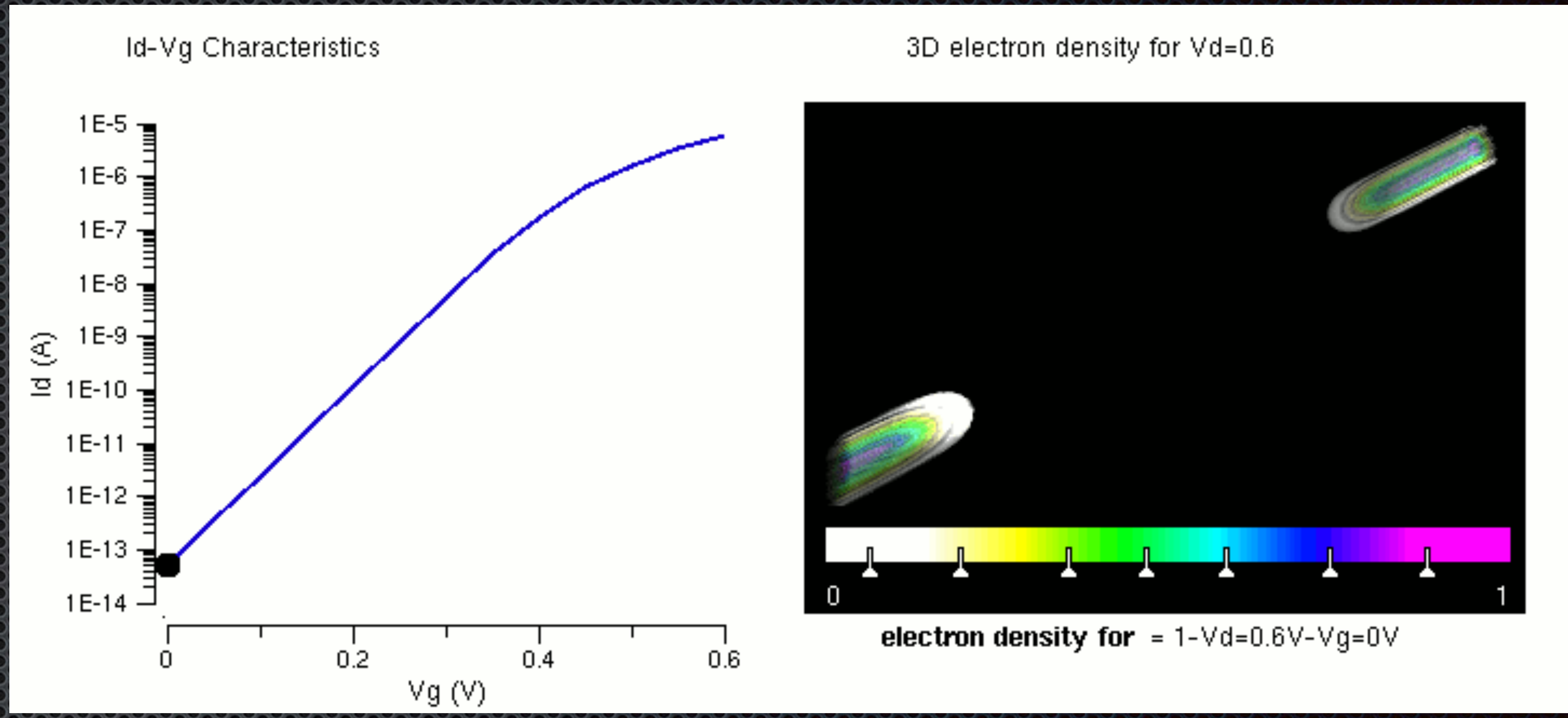
Due to Pauli exclusion principle, only a single electron can occupy the dot at a time. Once the dot is empty another electron can jump into the dot

Quantum dot

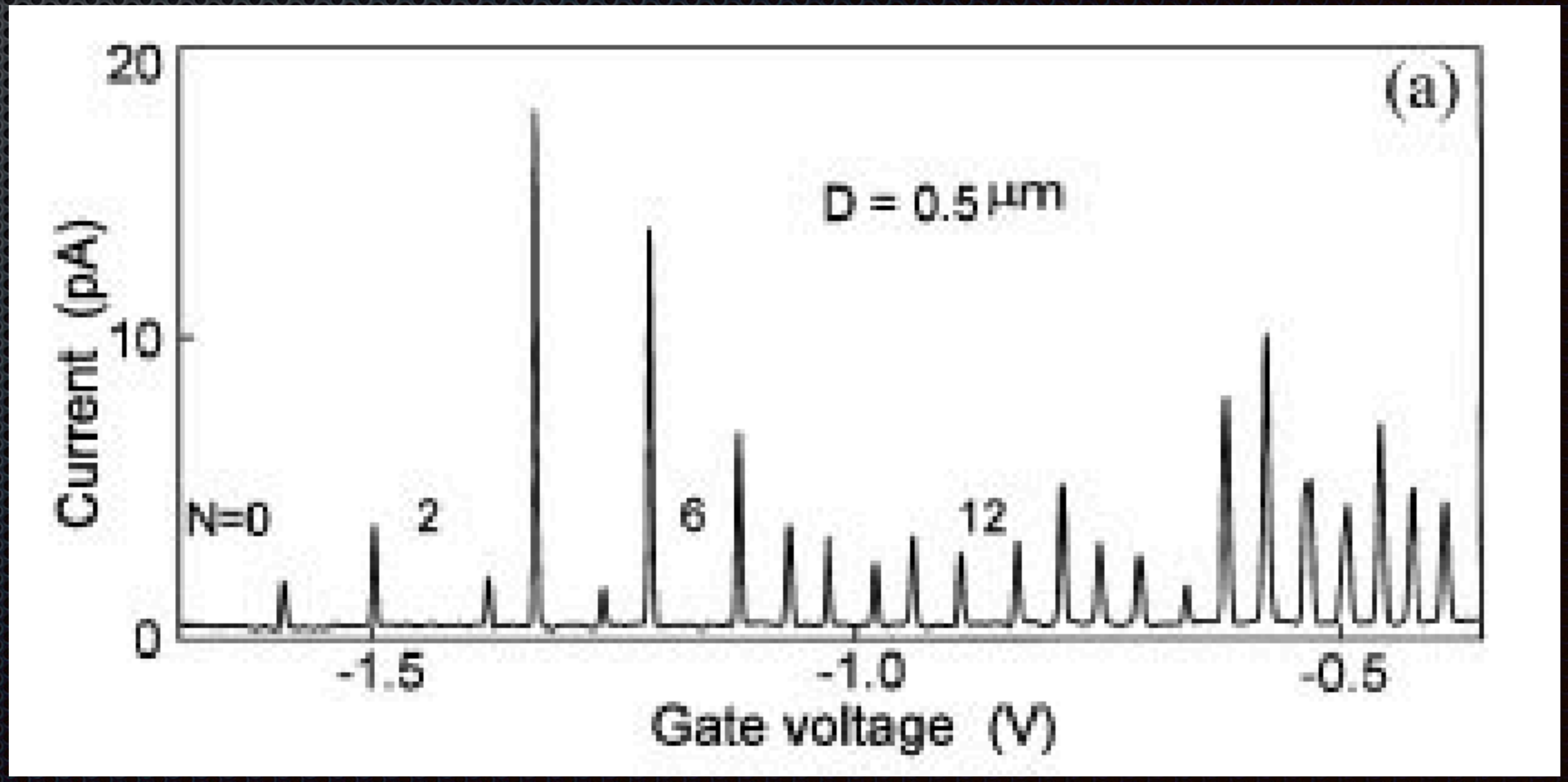
By controlling the gate voltage we can control the electron in the dot

Single electron box





https://en.wikipedia.org/wiki/Threshold_voltage#/media/File:Threshold_formation_nowatermark.gif

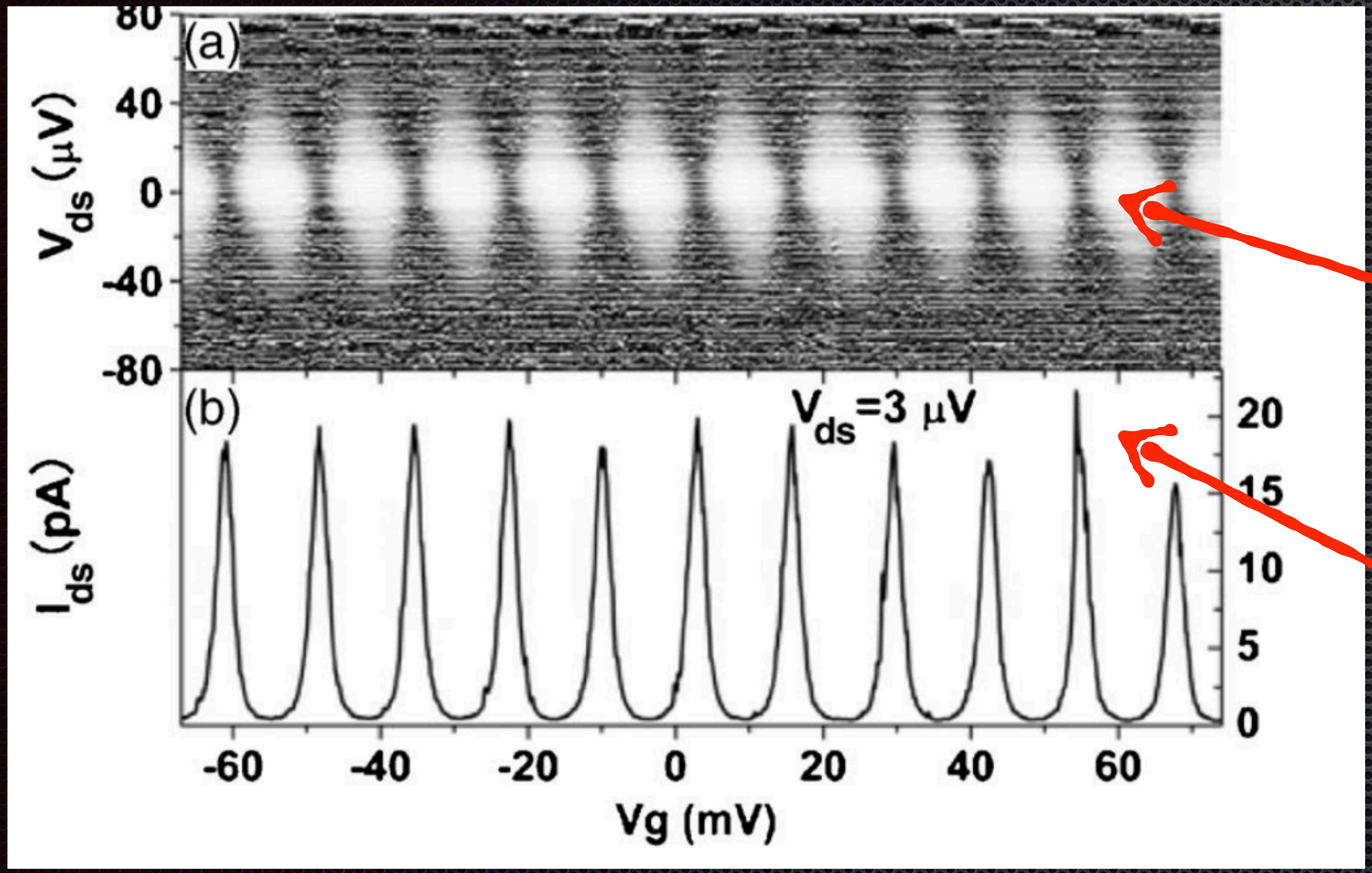


PhysRevLett.77.3613

Quantum dot

Coulomb blockade oscillations

From classical electrodynamics electrons cannot jump from the source to the drain unless it has enough energy.
In quantum mechanics there is a probability for quantum tunneling which is controlled by Coulomb blockade



213110-2 Huang et al. Appl. Phys. Lett. 92, 213110 2008

We can control the current flow by controlling the gate voltage (V_g) and the drain-source voltage V_sd

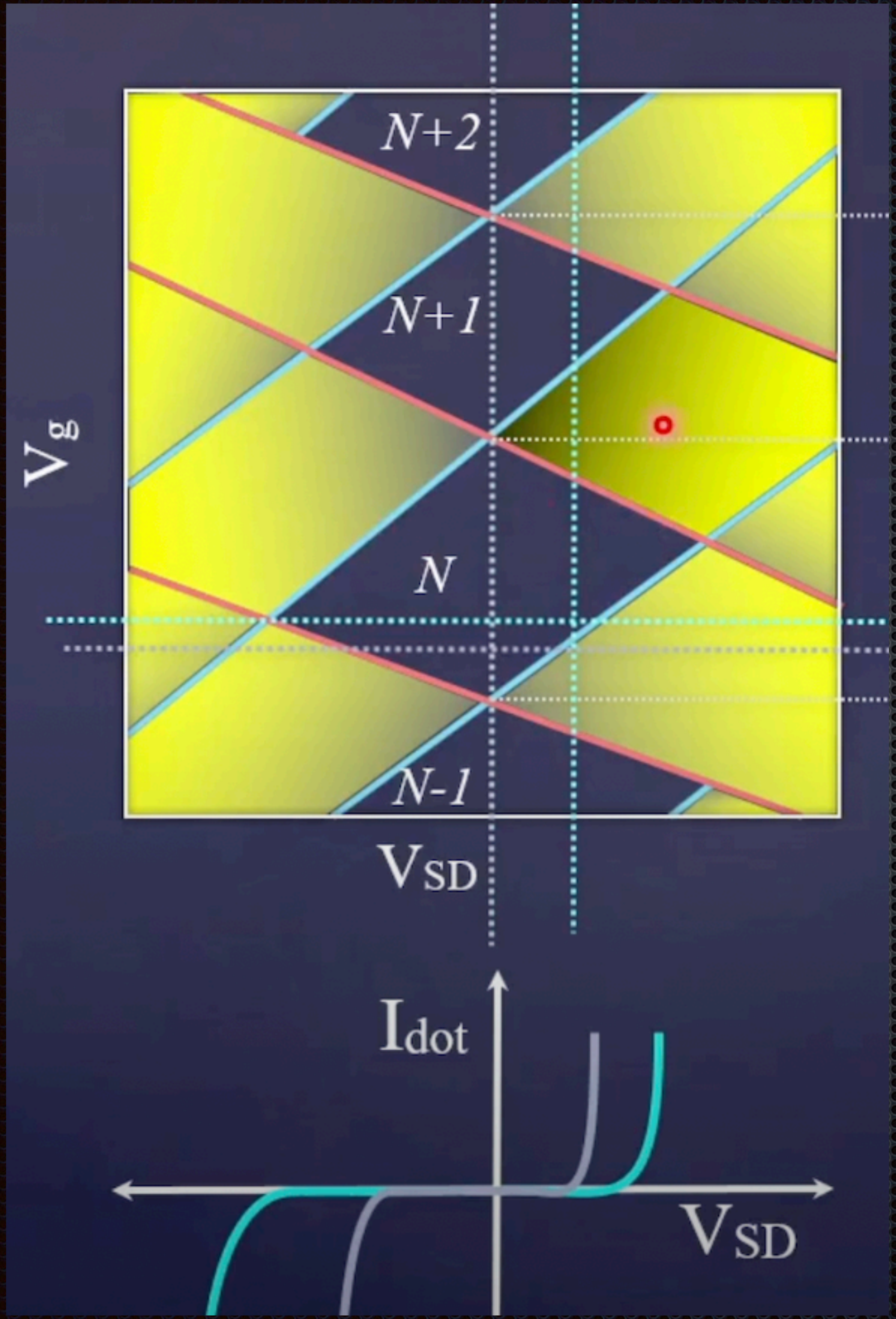
Diamond shape with no current flows inside
(Electron cage)

Current flows as pulses

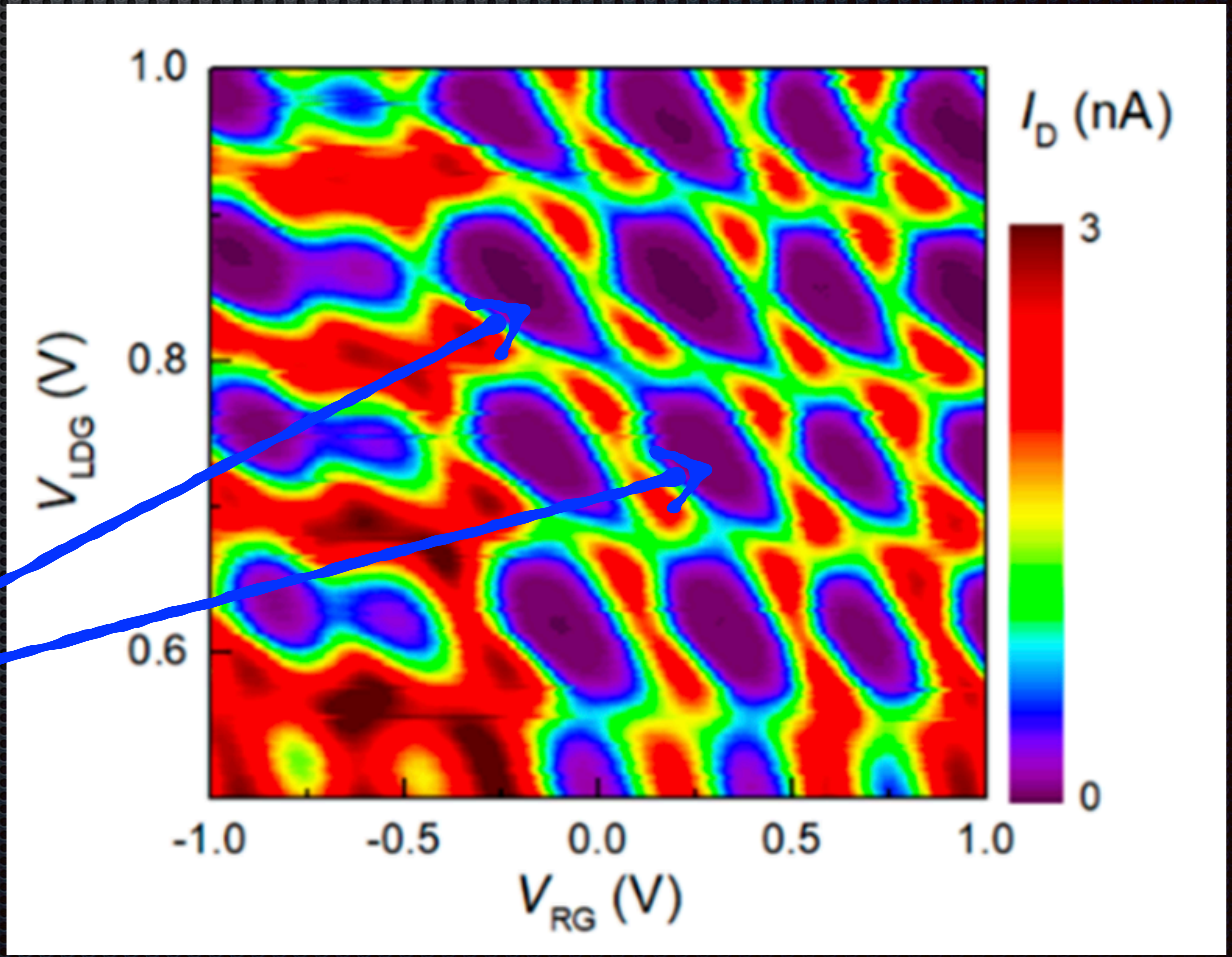
Quantum dot

Coulomb diamonds

Coulomb diamonds can act as traps for the electrons



Quantum dots

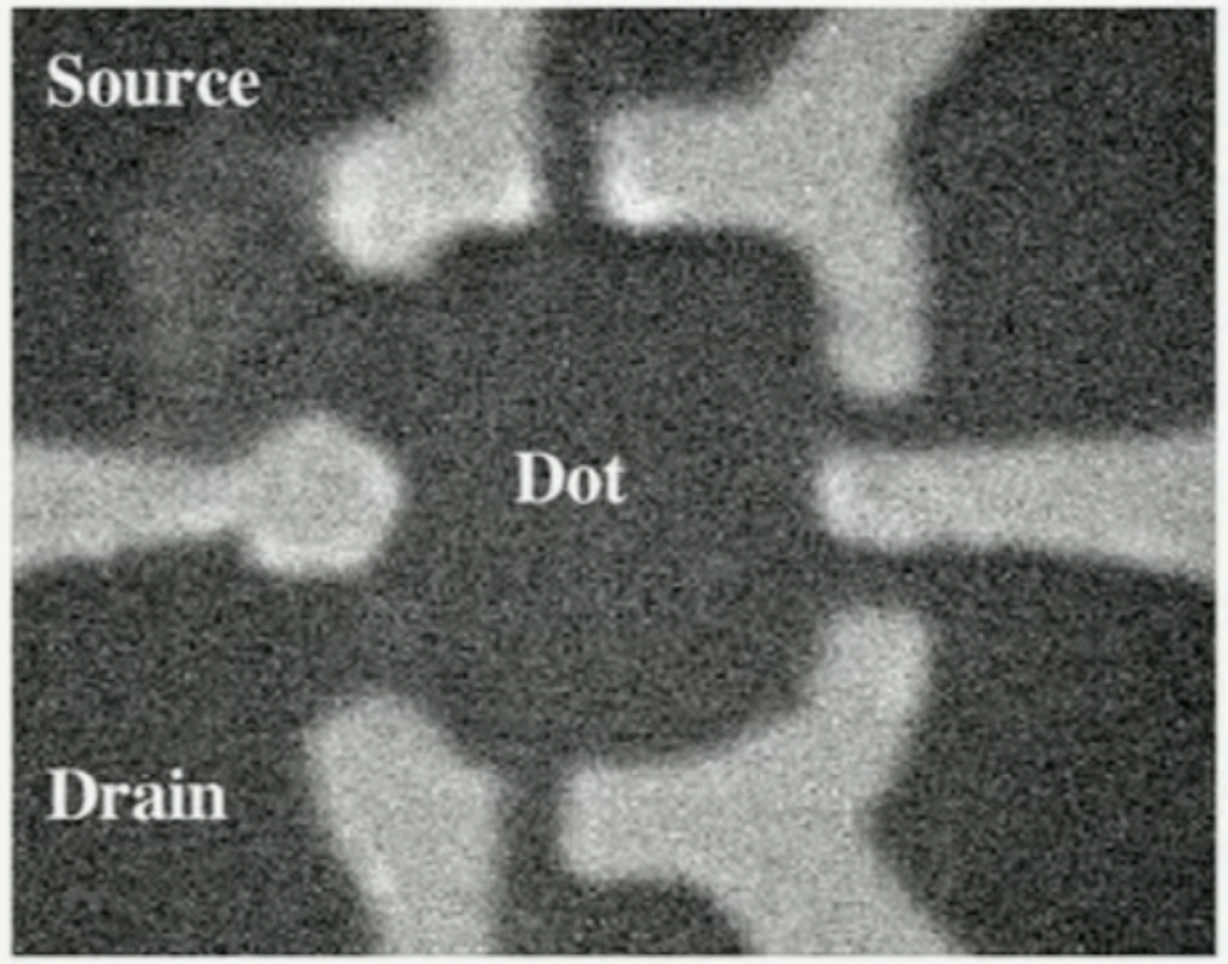


https://pubs.acs.org/doi/pdf/10.1021/acs.nanolett.9b05332

Quantum dot

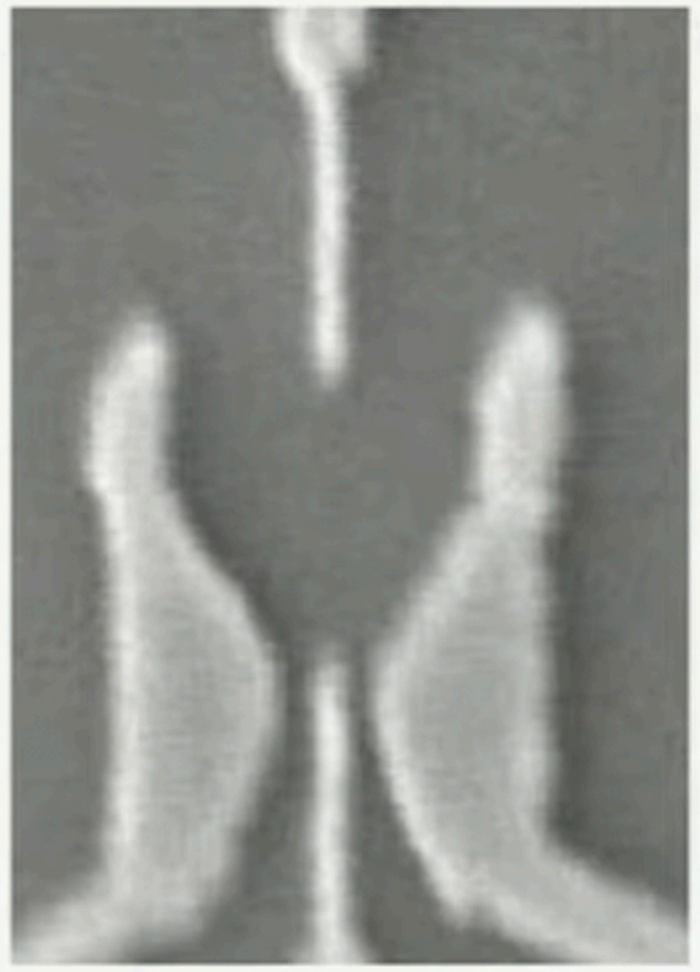
Quantum dots example

N_e~100 — 400 nm



Marcus group (1996)

N_e~1

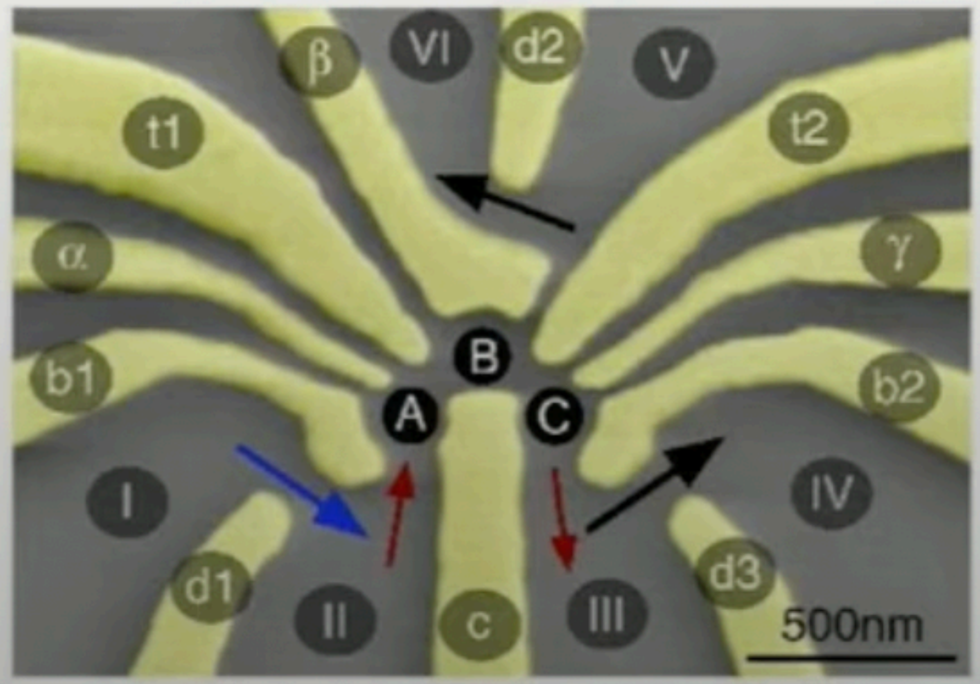


Ciorga *et al.*, PRB **61**, 16315 (2000)

Double dots

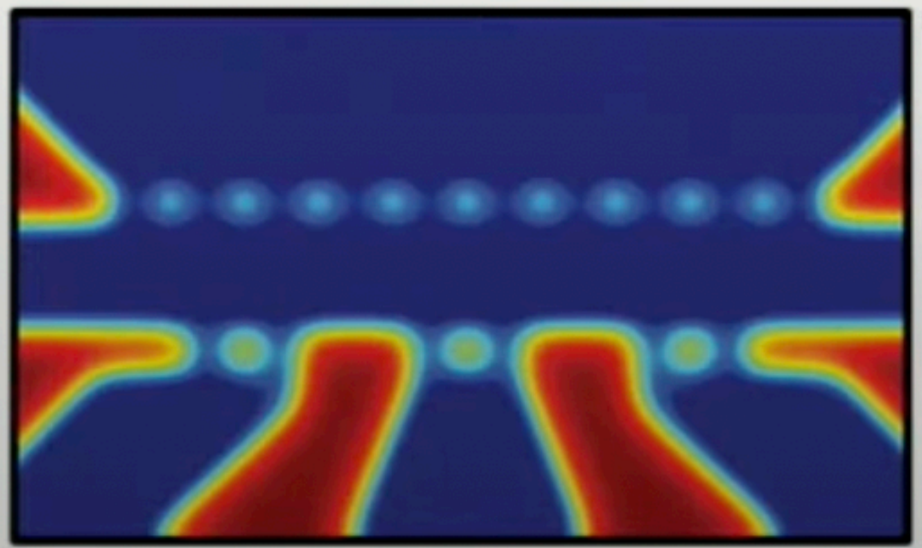
Elzerman (2003)
Petta (2004)

Triple dots



Gaudreau, Schroer (2007)

12 dots



Zajac *et al.* (2016)

Qubit dynamincs

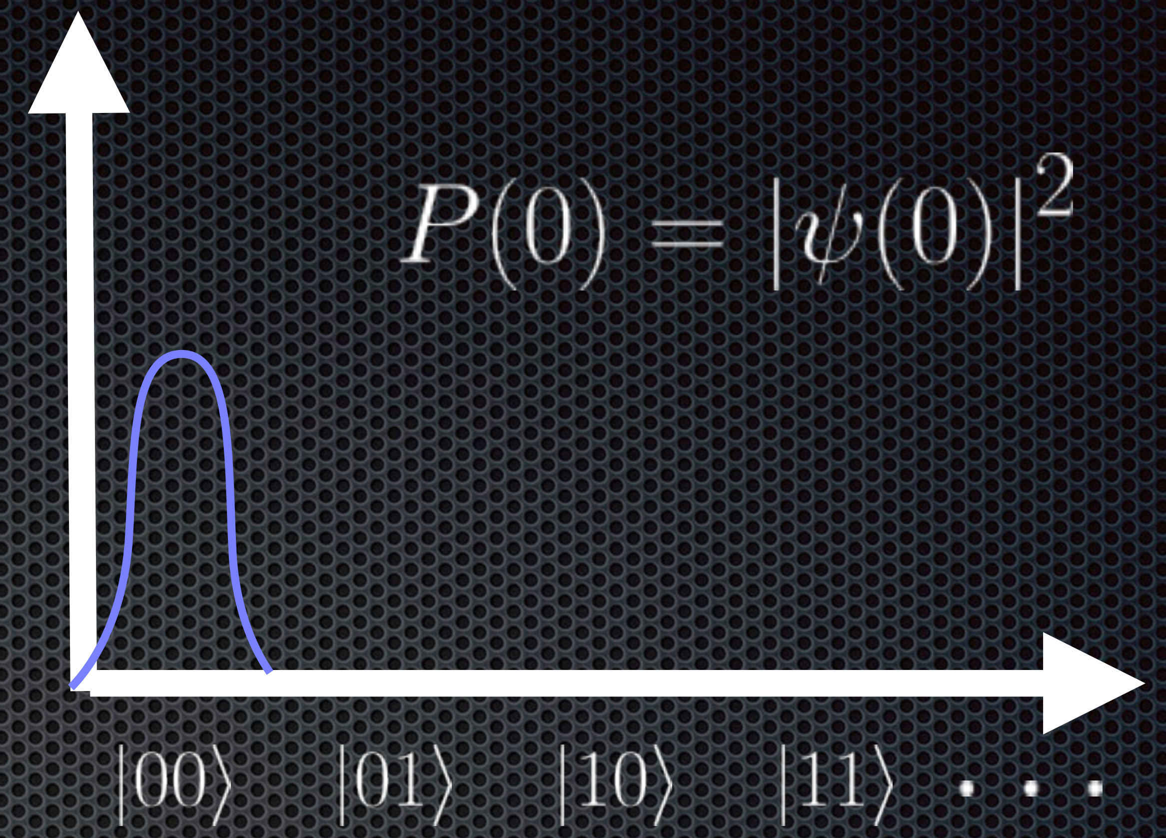
Well, now we know how to cook a quantum dot.

How to do computations on a qubit in a quantum dot?

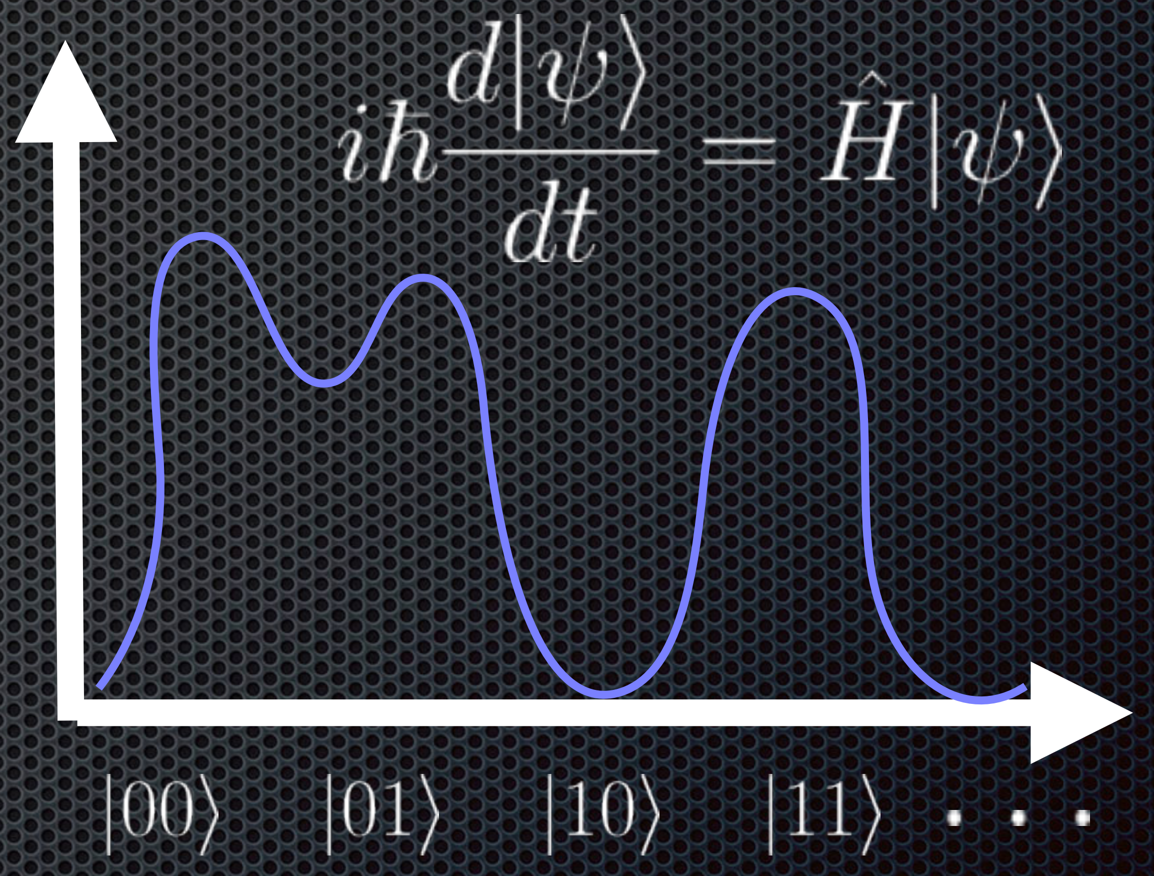
Qubit dynamincs

Quantum computation

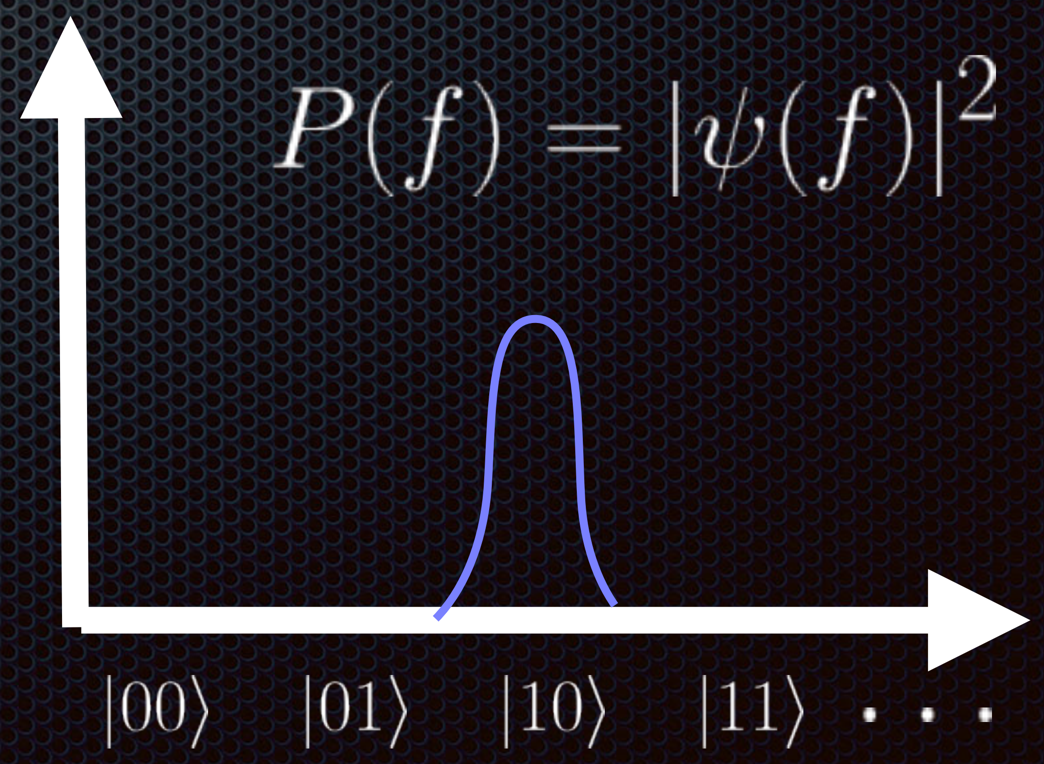
1- Initialize the qubits



2- Processing the qubits

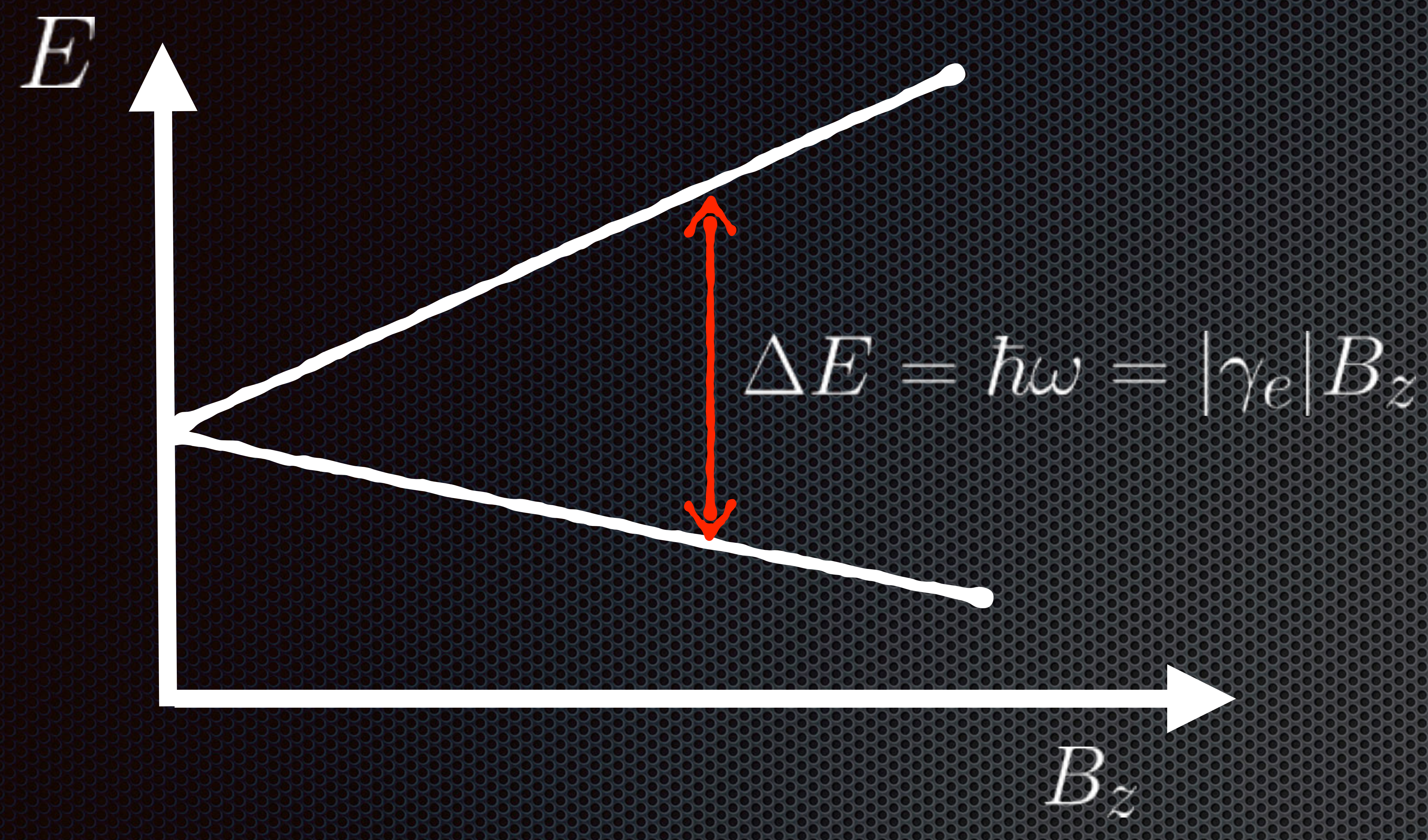


3- Measure the expectation value



Qubit dynamincs

Zeeman effect: Applying a static magnetic field the electron splits its spin states



$$\omega = \frac{|\gamma_e| B_z}{\hbar}$$

$$\gamma_e = \frac{g_e \, \mu_B}{\hbar} \vec{S}$$

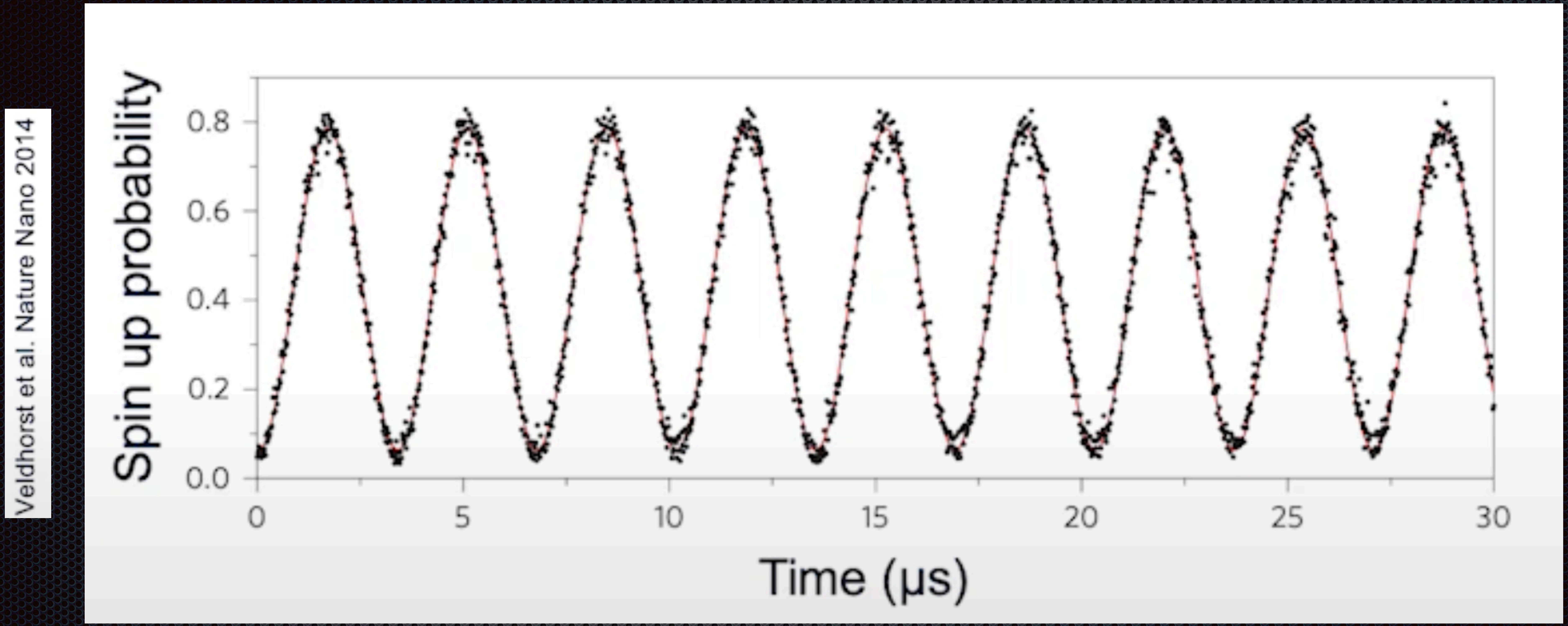
In the presence of magnetic field the electron spin will be randomly in any of the two states.
In the case of static magnetic field the spin states of the electron splits with energy difference.
We can initialize the electron in the zero state by lowering the energy of the quantum dot.

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Qubit dynamincs

To controls the qubit rotations we need to have extra AC magnetic field where the electron Oscillates between the two states according to "Rabi oscillations"



To understand the qubit dynamics we need to realize Rabi oscillations

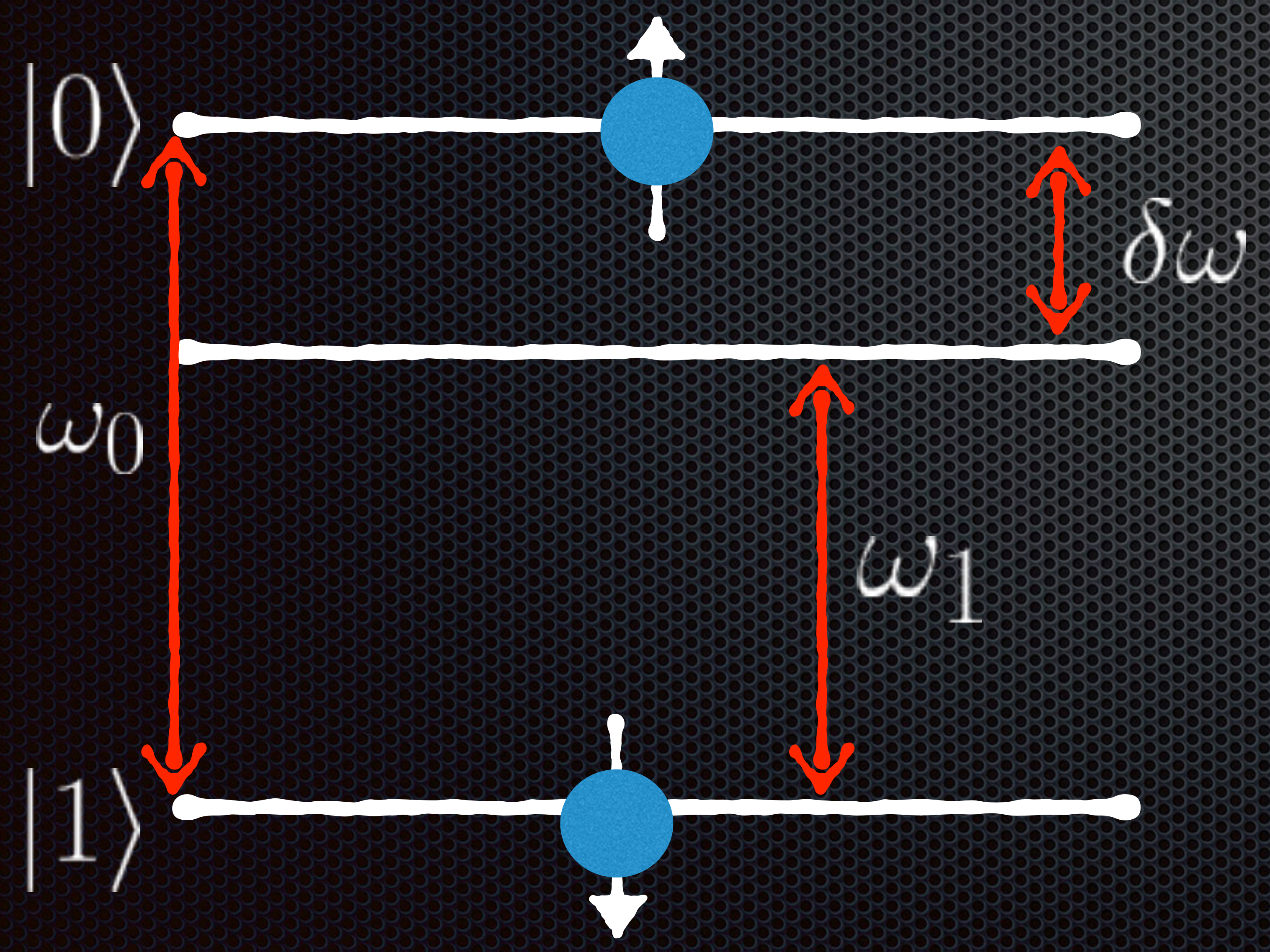
Qubit dynamincs

To controls the qubit rotations we need to have extra AC magnetic field orthogonal to the DC magnetic field

$$B_z = B_0 \qquad B_x = B_1 \cos(\omega\, t + \phi)$$

$$\hat{H}_{\text{Lab}} = \hat{H}_0 + \hat{H}_1 = \frac{\omega_0}{2}\sigma_z + \frac{\omega_1}{2}(\cos\omega\, t + \phi)\sigma_x$$

$$\omega_0 = |\gamma_e| B_z$$
$$\omega_1 = |\gamma_e| B_1$$



The goal is to find the Hamiltonian in a time independent Schrödinger picture. We use the rotating frames.

Qubit dynamincs

After tedious calculations, the Hamiltonian in the rotating frame

$$\hat{H}_{\text{rot}} = \frac{1}{2}\left(\delta\omega\sigma_z + \frac{\omega_1}{2}(\cos\phi\sigma_x - \sin\phi\sigma_y)\right) = \frac{1}{2}\begin{pmatrix} \delta\omega & \frac{\omega_1}{2}(\cos\phi - i\sin\phi) \\ \frac{\omega_1}{2}(\cos\phi + i\sin\phi) & -\delta\omega \end{pmatrix}$$

Generic form of the Hamiltonian in a rotating frames

$$\hat{H}_{\text{rot}} = \frac{1}{2}\Omega_t \vec{n}.\vec{\sigma}$$

$$\Omega_t = \sqrt{\left(\frac{\omega_1}{2}\right)^2 + (\delta\omega)^2}$$

Off-diagonal terms that
Couples the two spin states

Qubit dynamincs

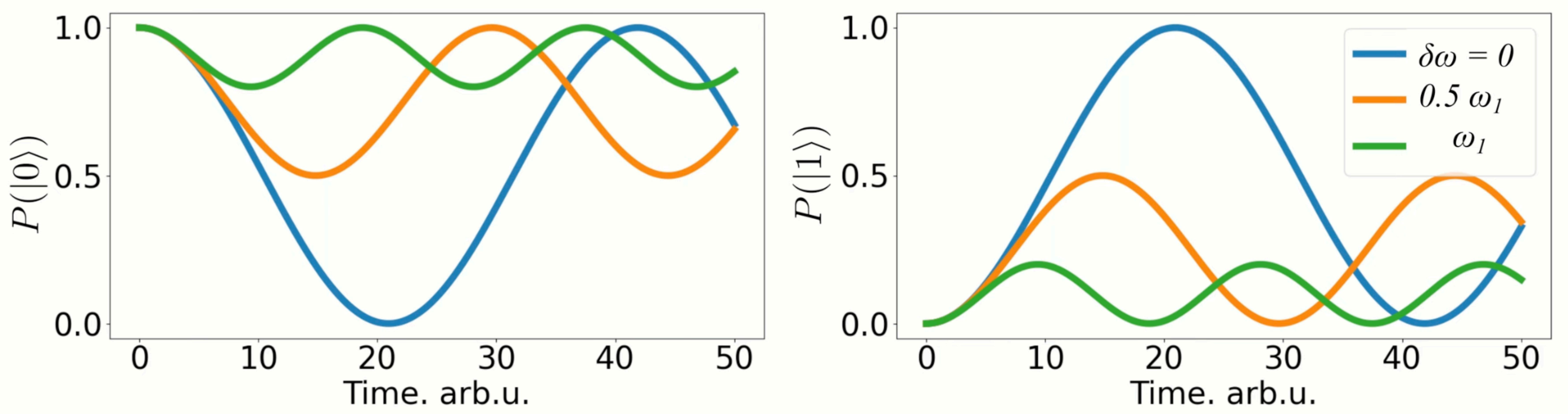
Well, but how to find the state of the system at a given time ?

$$|\psi_{\text{rot}}(t)\rangle = \left(\cos\frac{\Omega_t}{2} - i\sin\frac{\Omega_t\delta\omega}{2}\right)|0\rangle - i\sin\frac{\Omega_t\omega_1}{4}e^{-i\phi}|1\rangle$$

With the probability of measuring the electron in state 1

$$P(|0\rangle) = \left|\langle 1|\psi_{\text{rot}(t)}\rangle\right|^2 = \left(\frac{\omega_1}{2\Omega}\right)\left(\frac{1-\cos\Omega_t}{2}\right)$$

With Rabi frequency $\Omega = \sqrt{\left(\frac{\omega_1}{2}\right)^2 + \delta\omega^2}$



In the non-resonance case the oscillation never reach the state 1 or zero

Qubit dynamincs

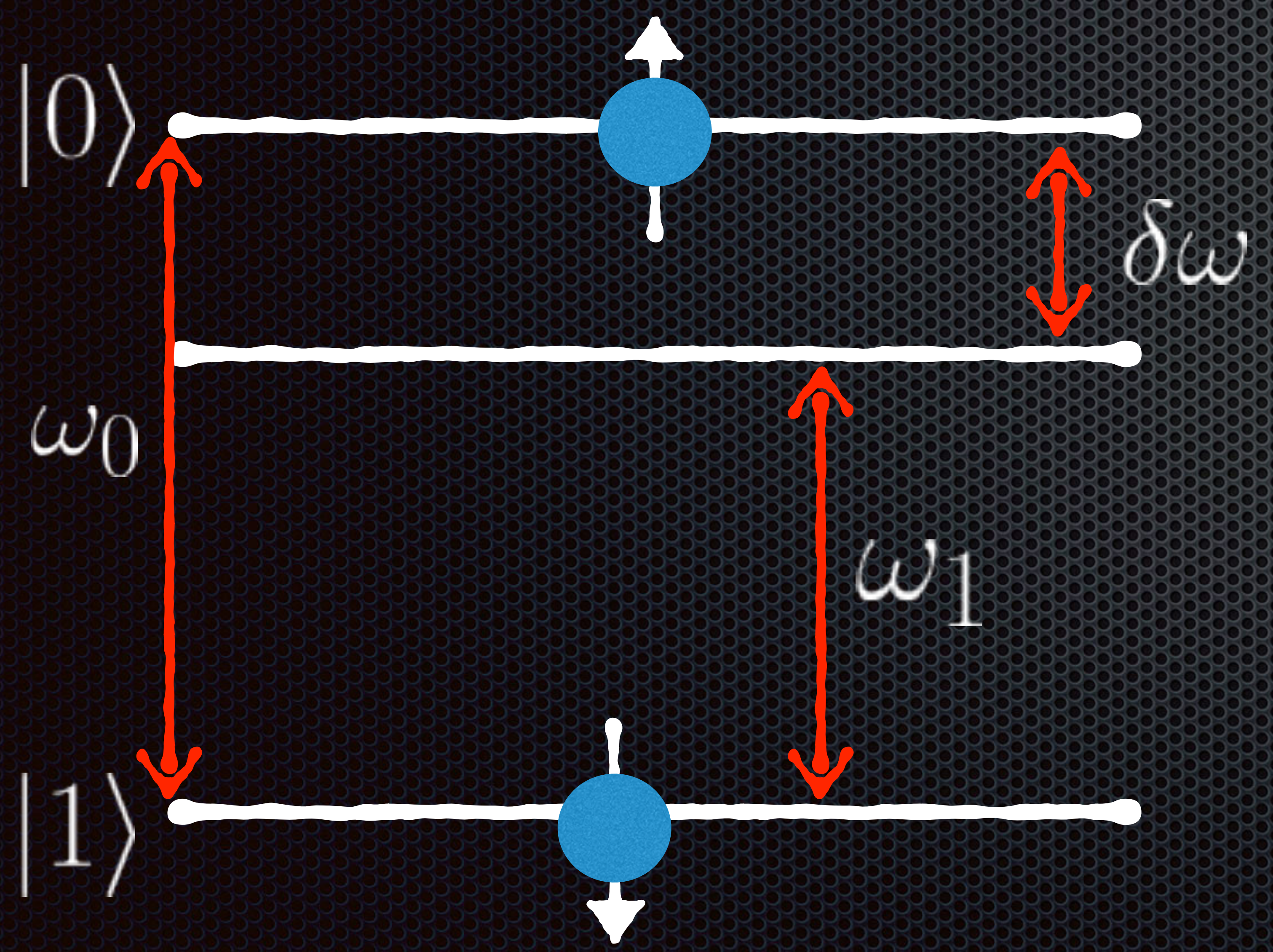
In the resonance case:

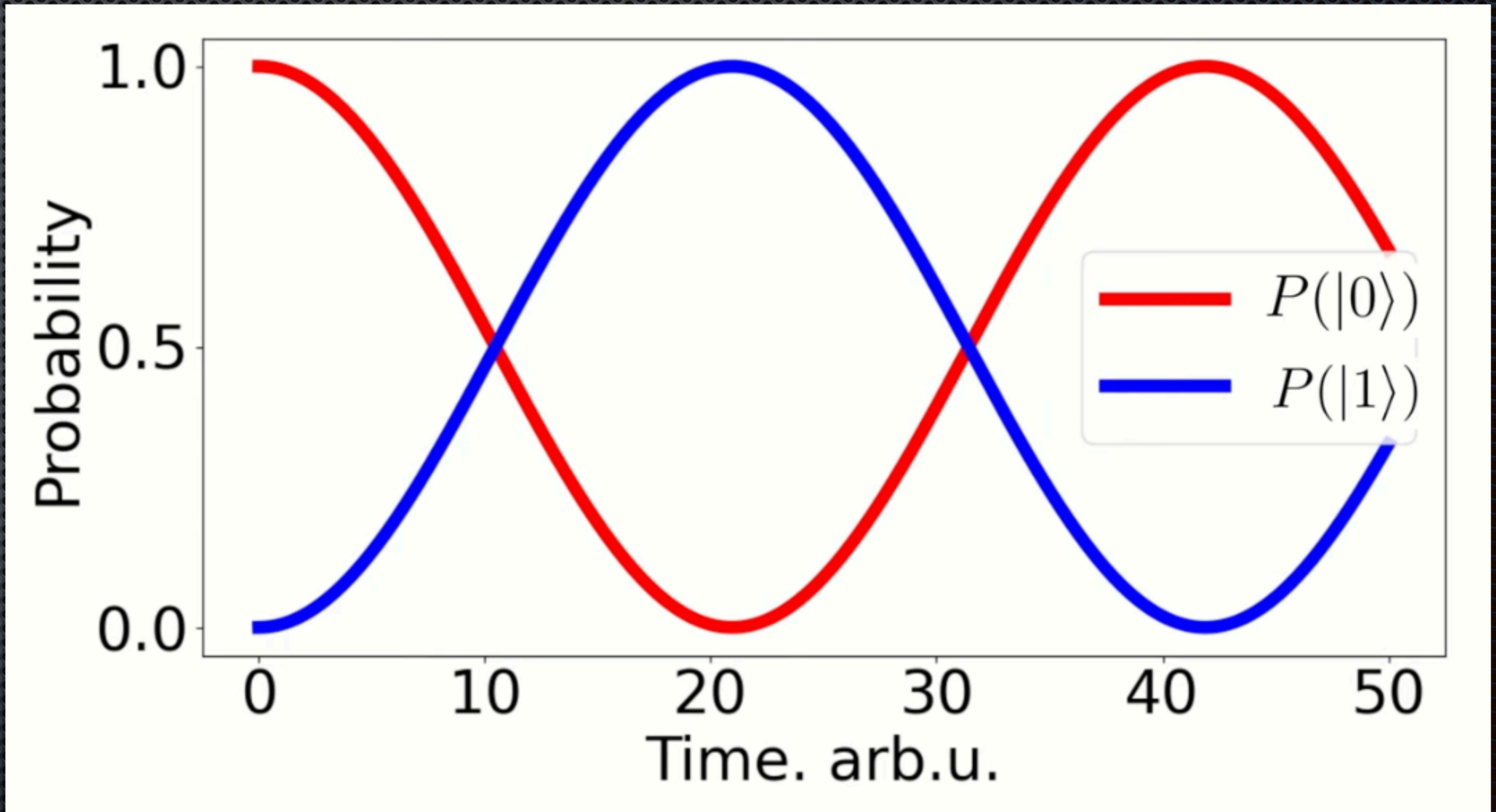
$$\delta\omega = 0$$

$$\Omega = \frac{\omega_1}{2}$$

$$P(|1\rangle) = \frac{1 - \cos\Omega_t}{2}$$

$$P(|0\rangle) = \frac{1 + \cos\Omega_t}{2}$$



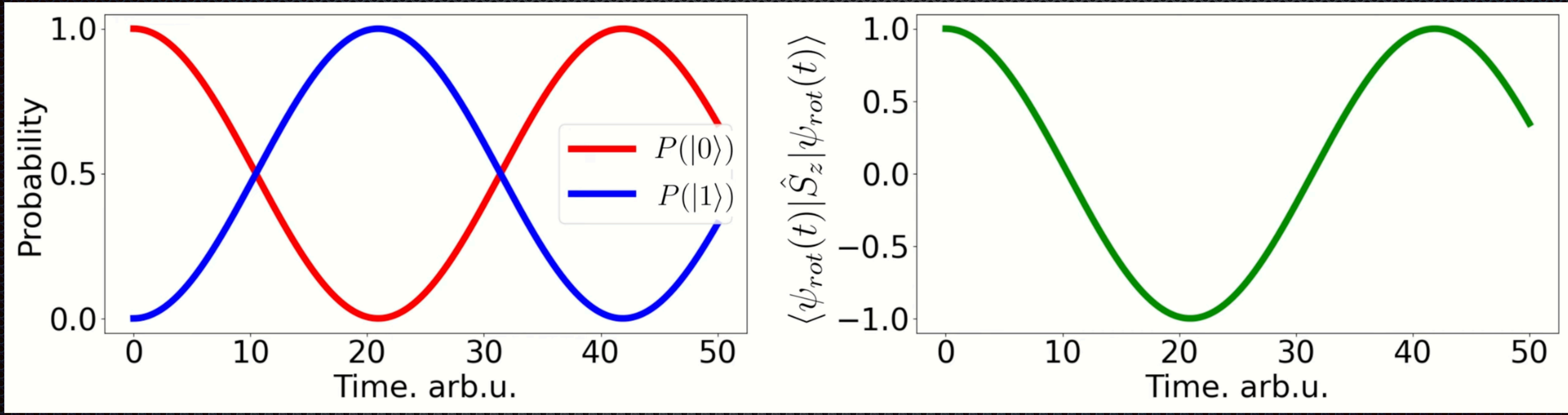


Maximal Rabi Oscillations

Qubit dynamincs

The expectation value of rotating qubit

$$\langle\psi(t)|\hat{S}_z|\psi(t)\rangle = P(|0\rangle) - P(|1\rangle) = \frac{1+\cos\Omega_t}{2} - \frac{1-\cos\Omega_t}{2} = \cos\Omega_t$$

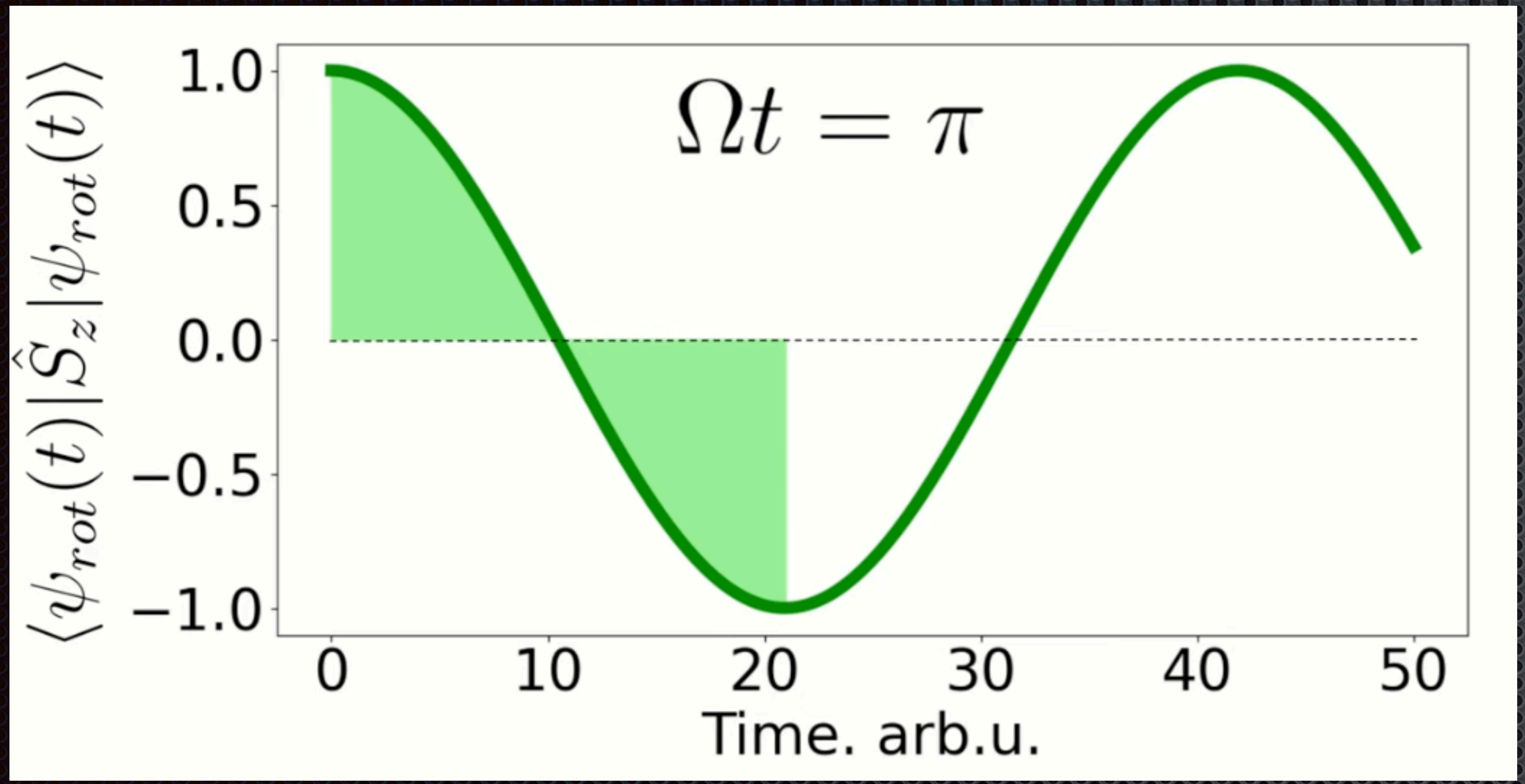


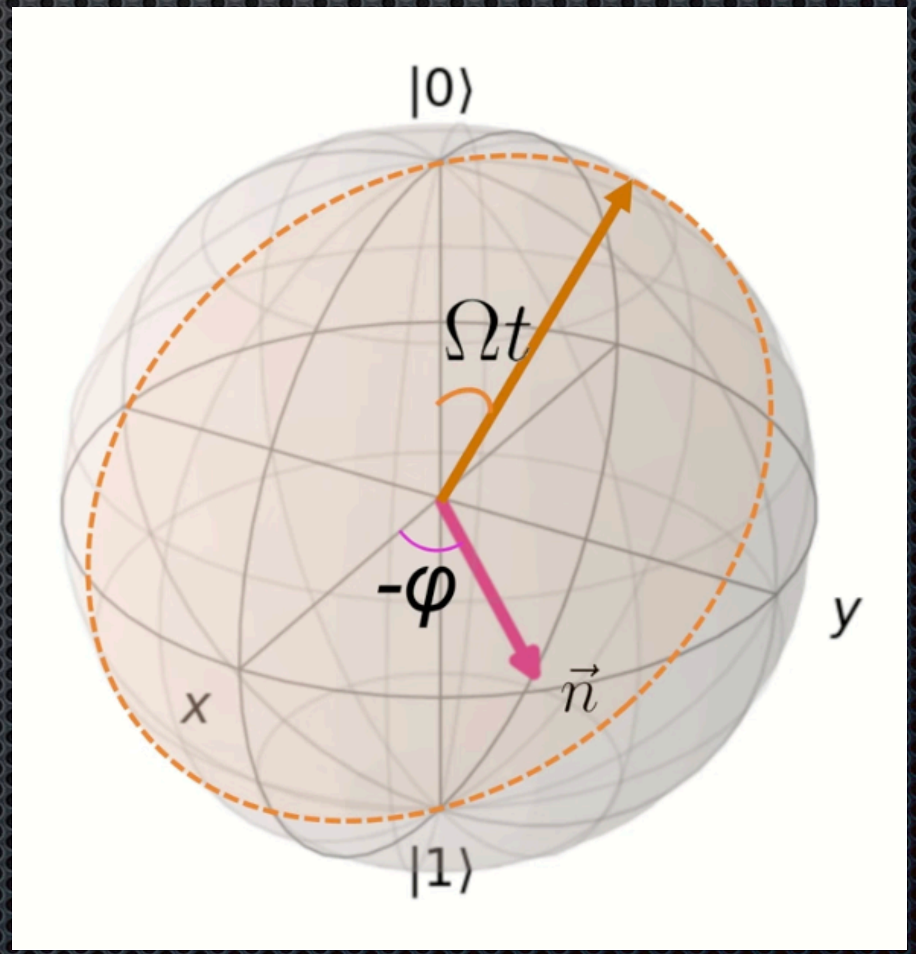
Qubit dynamincs

Both static and dynamic magnetic fields define the rotation of the qubit

$$\hat{H} = \frac{\omega_1}{4}\left(\cos\phi\sigma_x - \sin\phi\sigma_y\right)$$

$$\delta\omega = 0 \qquad \vec{n} = (\cos\phi; -\sin\phi, 0) \qquad \Omega = \frac{\omega_1}{2}$$



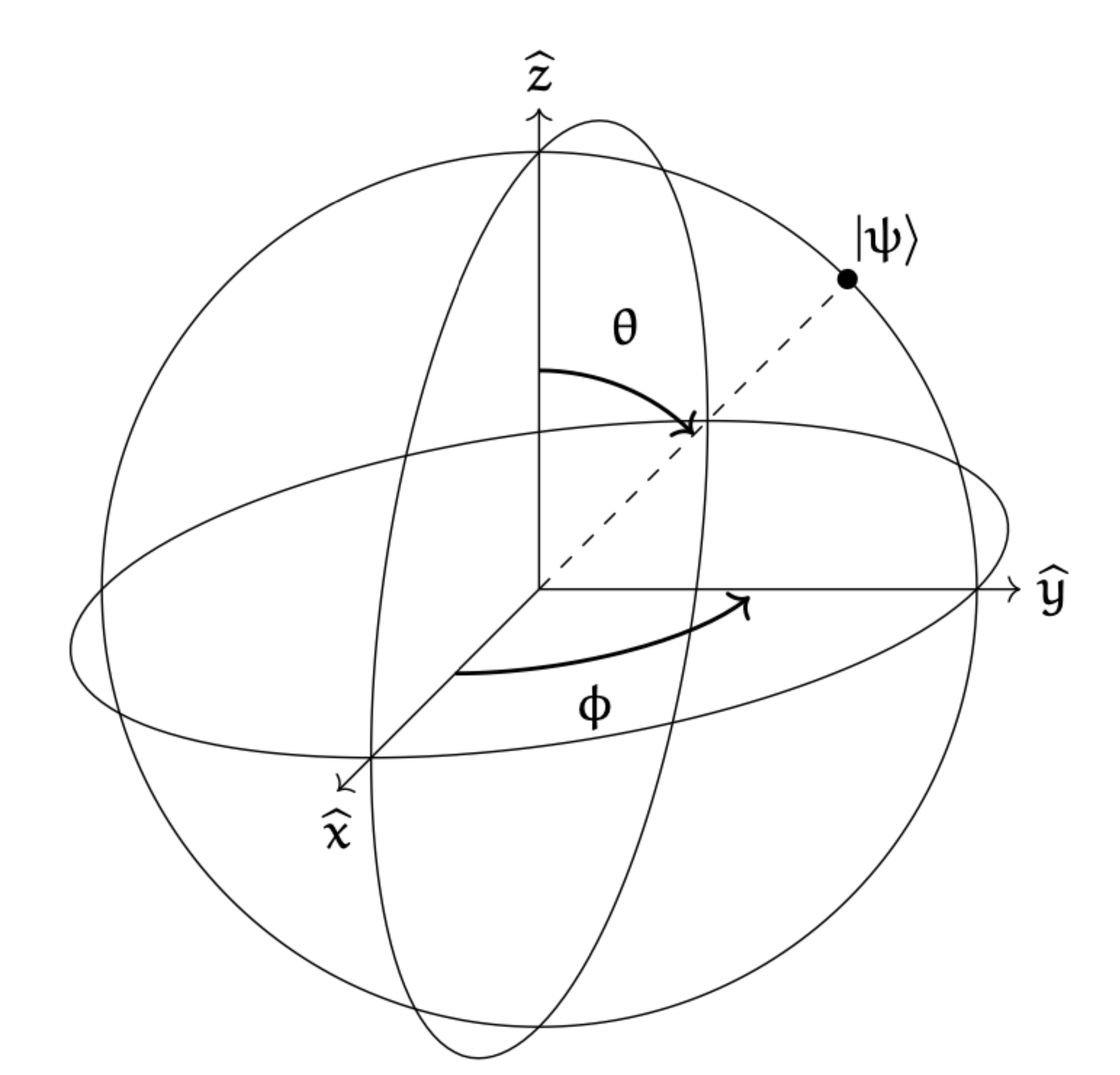


Pi pulses lead to the quantum gates

φ	$\hat{H}_{rot}$	gate
0	$\frac{\omega_1}{4}\hat{\sigma}_x$	$\hat{X}$
- $\pi/2$	$\frac{\omega_1}{4}\hat{\sigma}_y$	$\hat{Y}$

Single qubit gates

Bloch sphere representation of single qubit states

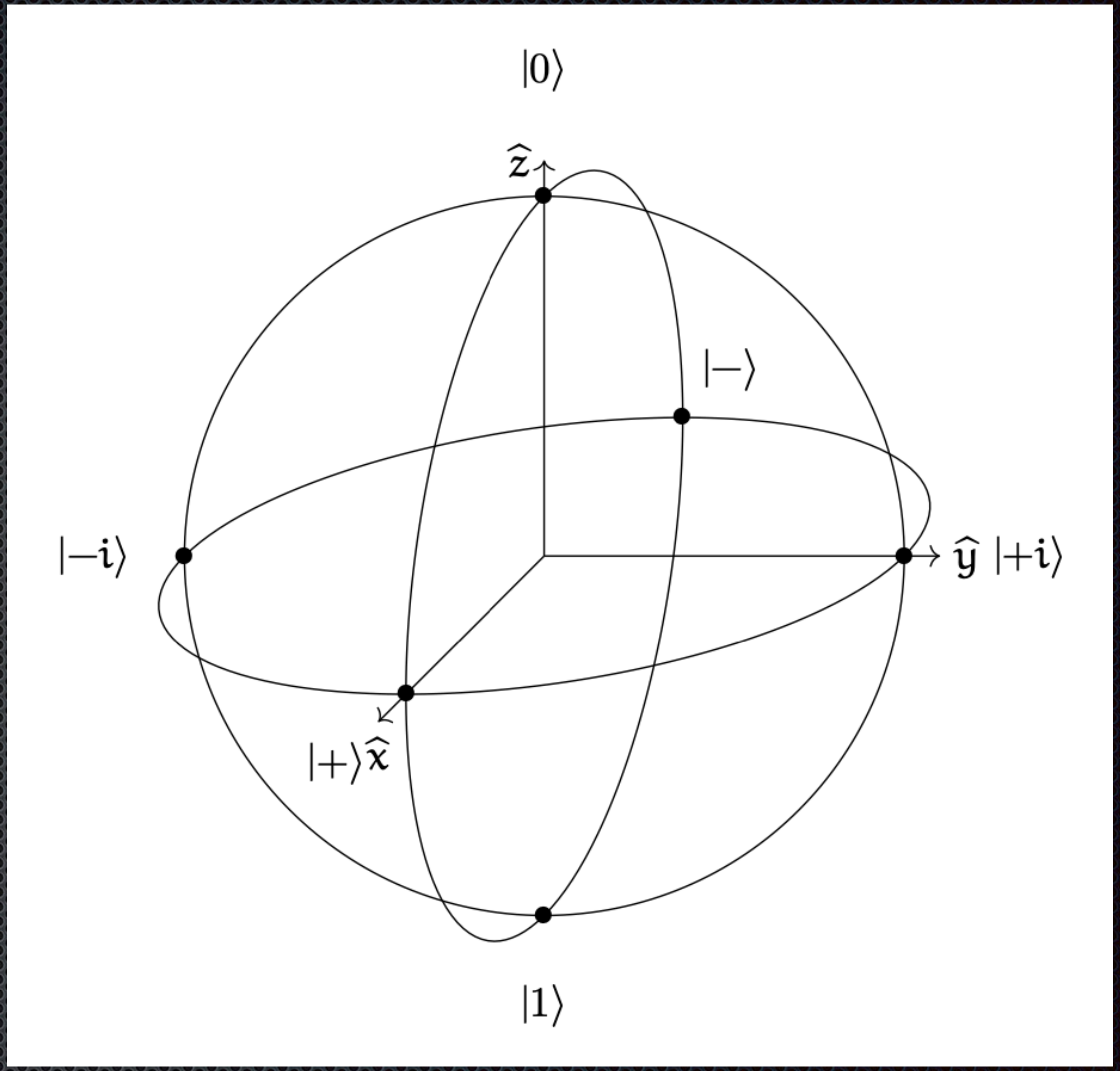


$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$

$$\vec{n} = (sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

http://threeplusone.com/gates

Location of the orthogonal qubit states



X basis	$\lvert+\rangle = \frac{1}{\sqrt{2}}(\lvert 0\rangle + \lvert 1\rangle)$	$\hat{n} = (+1, 0, 0)$
	$\lvert-\rangle = \frac{1}{\sqrt{2}}(\lvert 0\rangle - \lvert 1\rangle)$	$\hat{n} = (-1, 0, 0)$
Y basis	$\lvert+i\rangle = \frac{1}{\sqrt{2}}(\lvert 0\rangle + i\lvert 1\rangle)$	$\hat{n} = (0, +1, 0)$
	$\lvert-i\rangle = \frac{1}{\sqrt{2}}(\lvert 0\rangle - i\lvert 1\rangle)$	$\hat{n} = (0, -1, 0)$
Z basis	$\lvert 0\rangle$	$\hat{n} = (0, 0, +1)$
	$\lvert 1\rangle$	$\hat{n} = (0, 0, -1)$

Single qubit gates

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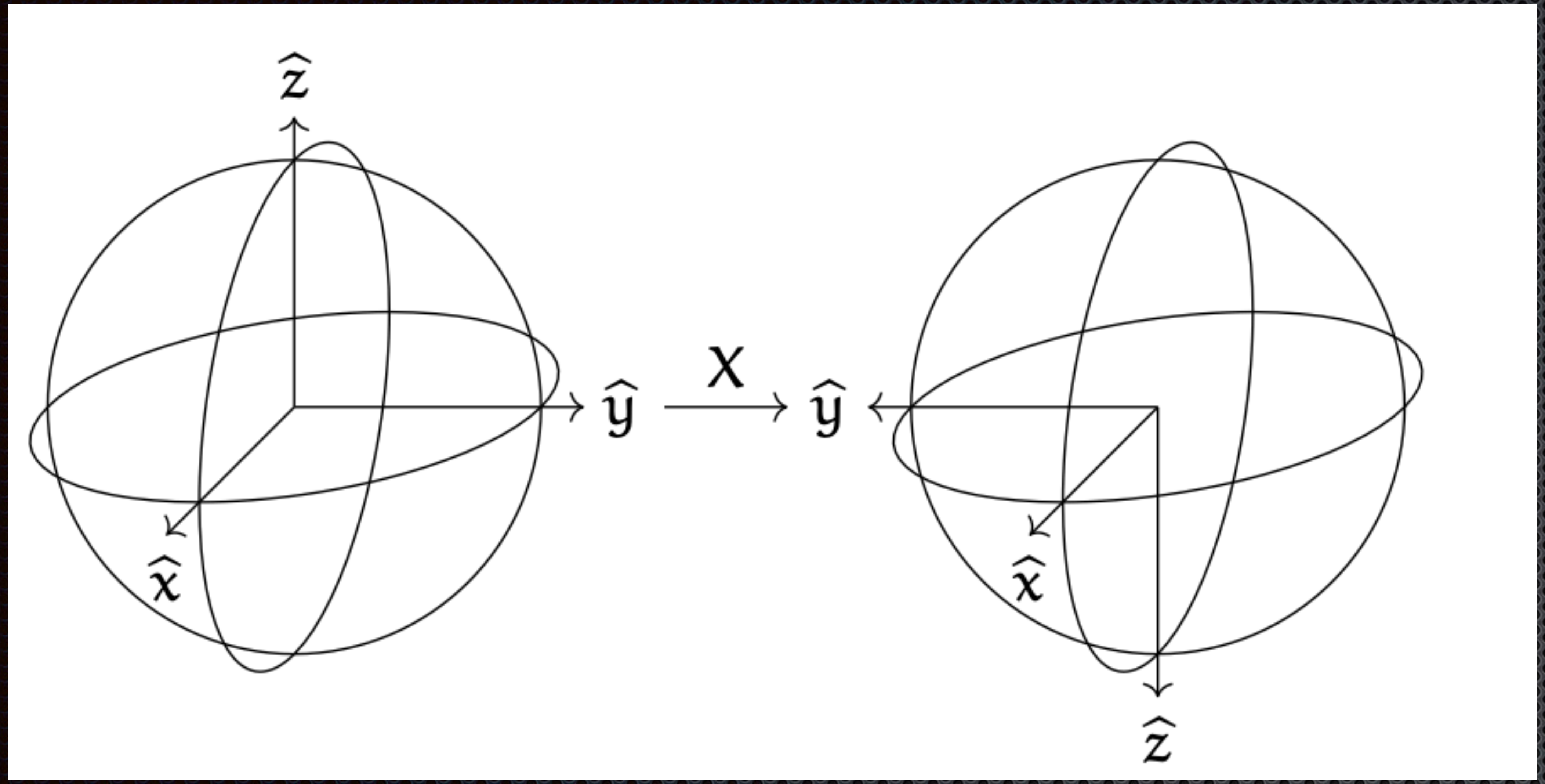
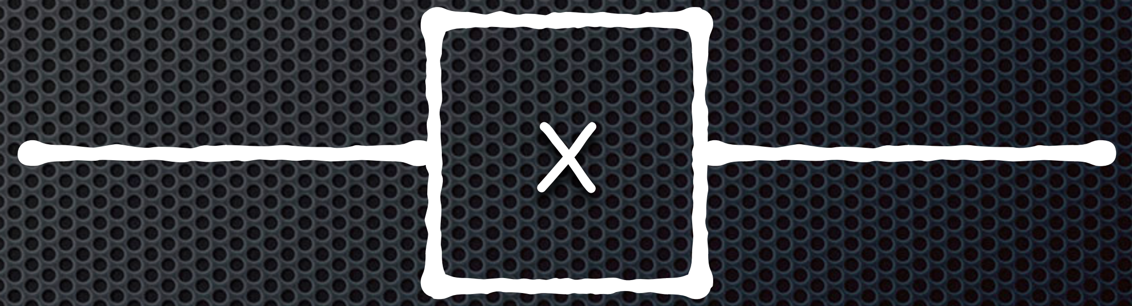
Pauli-X gate (bit flip)

The X-gate generates a half-turn in the Bloch sphere about the x axis



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



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

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

Single qubit gates

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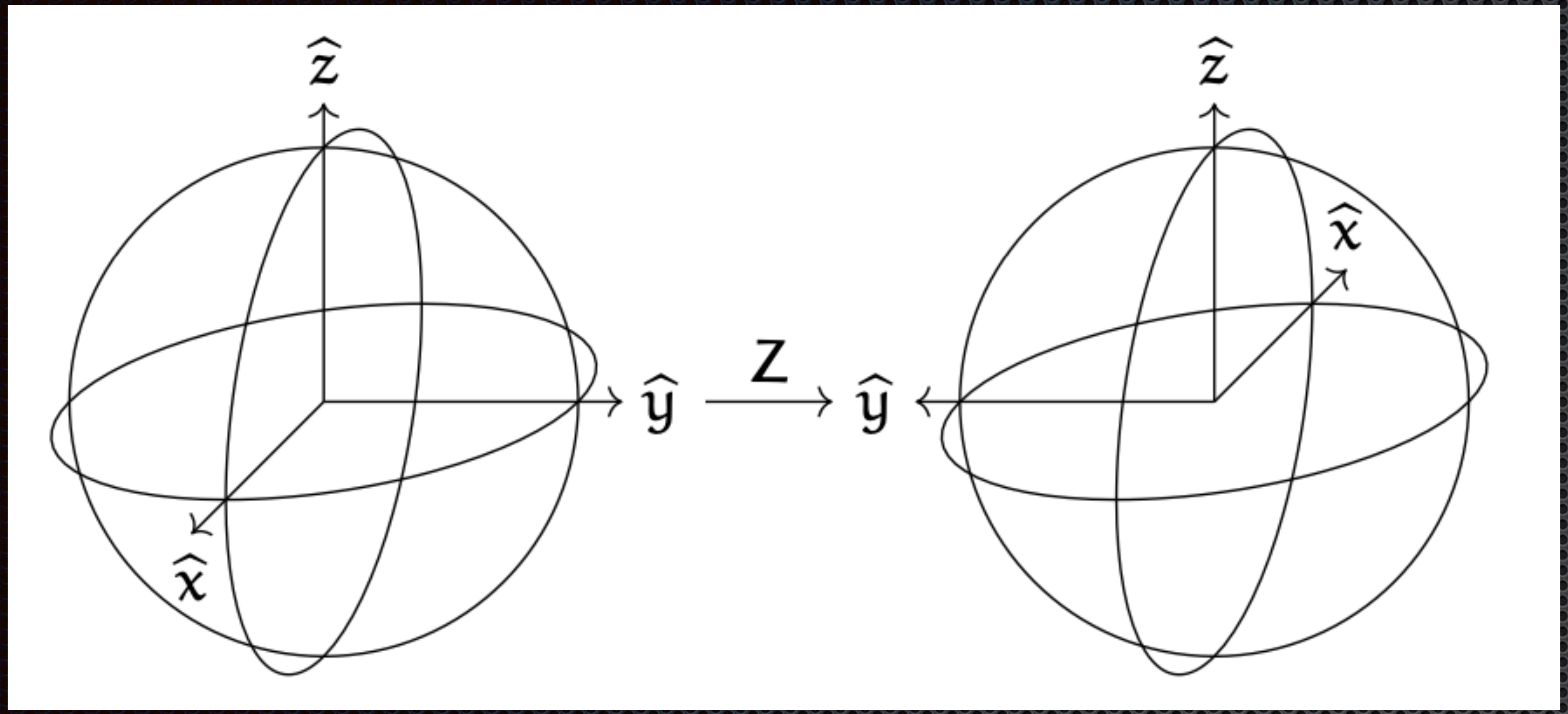
Pauli-Z gate (phase flip)

The Z-gate generates a half-turn in the Bloch sphere about the z axis



$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$-\boxed{Z}-$$

$$Z|0\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle$$

$$Z|1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} = -|1\rangle$$

Single qubit gates

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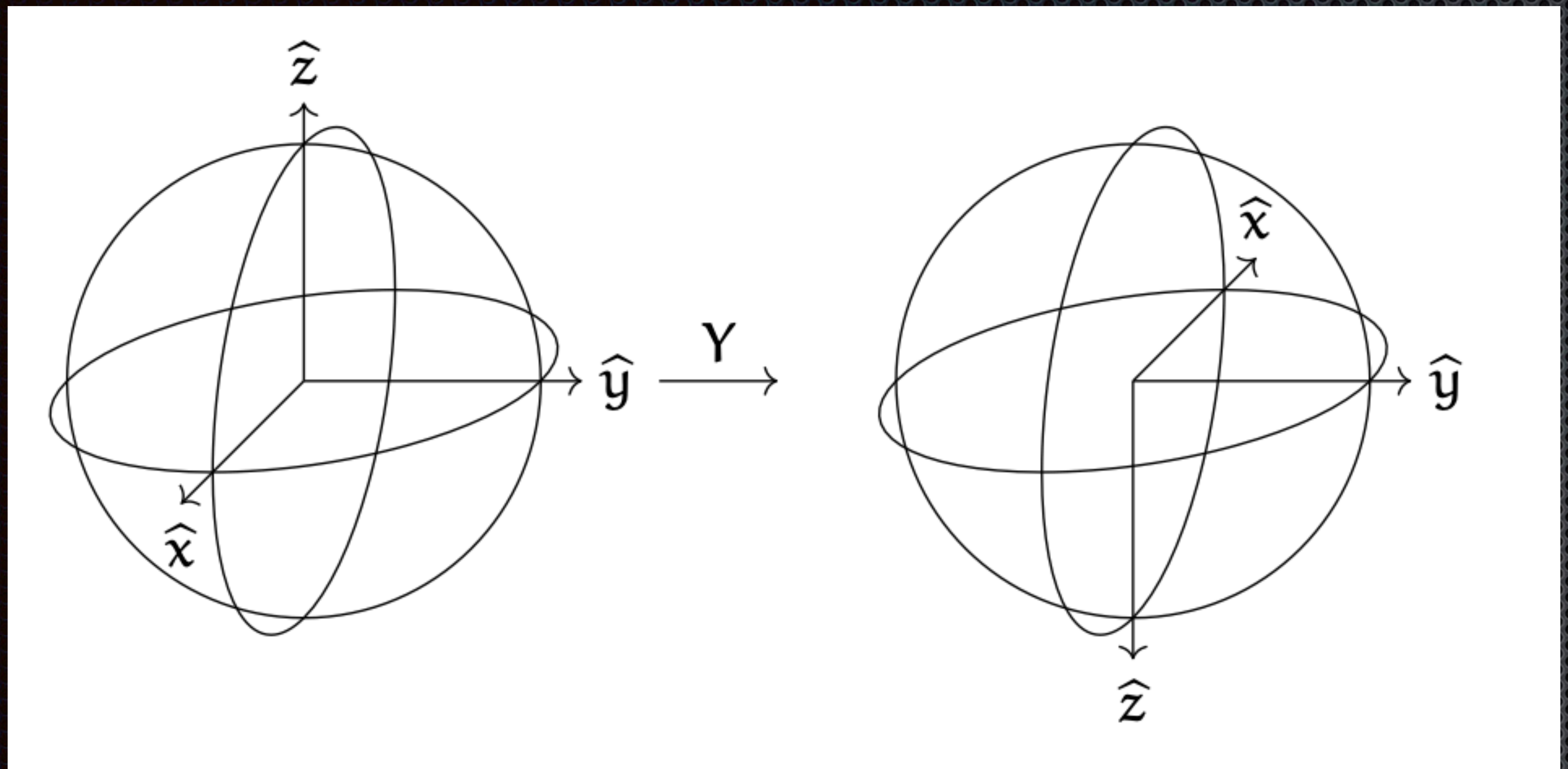
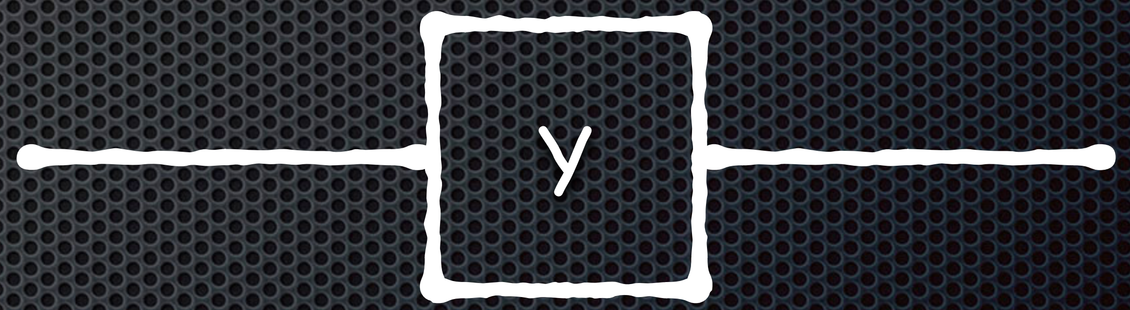
Pauli-Y gate

The Y-gate generates a half-turn in the Bloch sphere about the y axis



$$Y = -iZX = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$



$$Y|0\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ i \end{pmatrix} = i|1\rangle$$

$$Y|1\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -i \\ 0 \end{pmatrix} = -i|0\rangle$$

Single qubit gates

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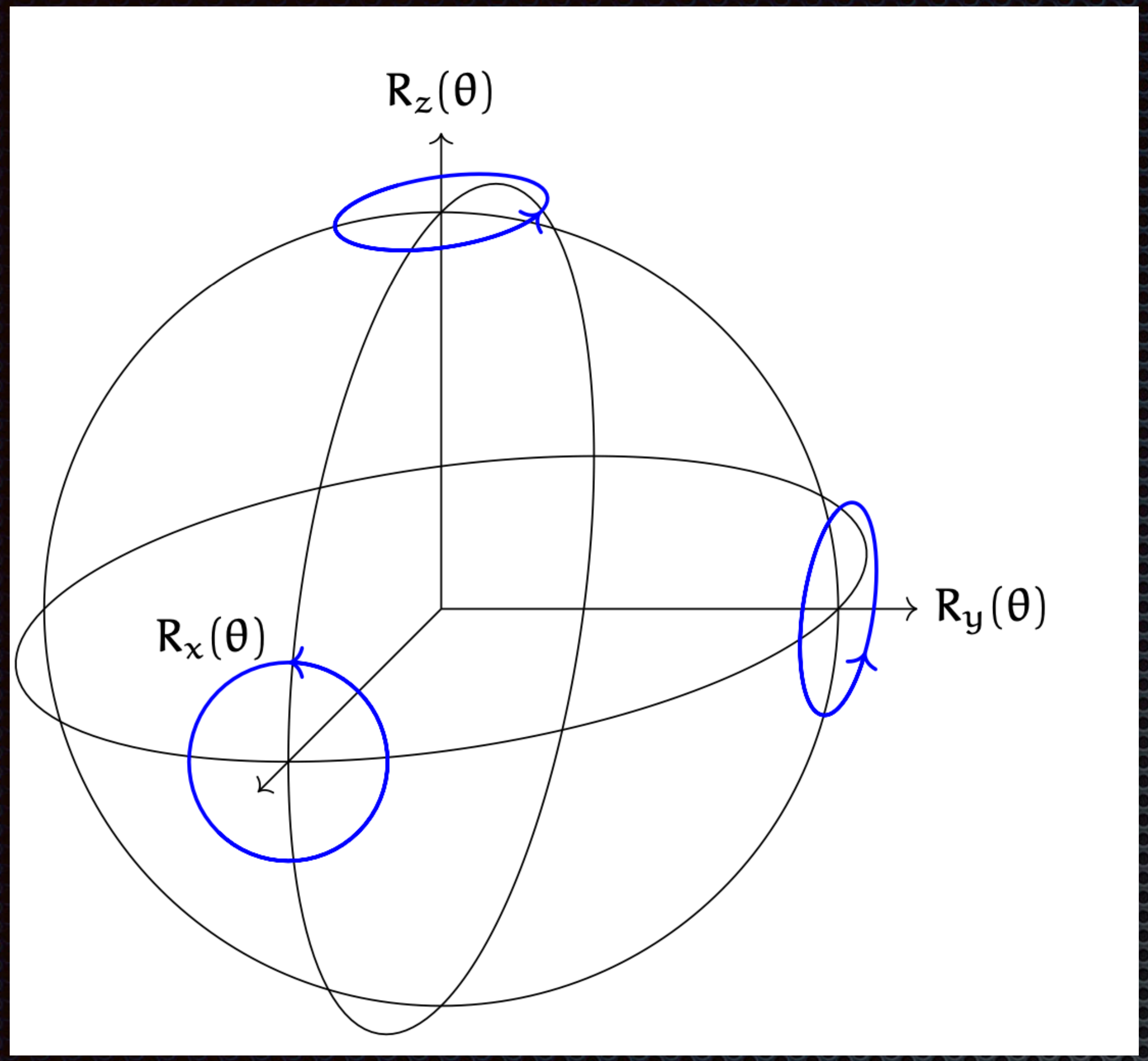
Pauli Rotation gate

The rotation of θ radians anti-clockwise about an arbitrary axis in the Bloch sphere



$$
\begin{aligned}
R_{\vec{n}}(\theta) &= e^{-i\frac{1}{2}\theta(n_x X + n_y Y + n_z Z)} \\
&= \cos(\tfrac{1}{2}\theta) I - i \sin(\tfrac{1}{2}\theta)(n_x X + n_y Y + n_z Z) \\
&= \begin{bmatrix} \cos(\frac{1}{2}\theta) - i n_z \sin(\frac{1}{2}\theta) & -n_y \sin(\frac{1}{2}\theta) - i n_x \sin(\frac{1}{2}\theta) \\ n_y \sin(\frac{1}{2}\theta) - i n_x \sin(\frac{1}{2}\theta) & \cos(\frac{1}{2}\theta) + i n_z \sin(\frac{1}{2}\theta) \end{bmatrix}
\end{aligned}
$$

$$
e^{i\theta A} = I + i\theta A - I\frac{\theta^2}{2!} - i\frac{\theta^3}{3!}A + I\frac{\theta^4}{4!}\ldots
$$

$$
= \left(1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4!}\right) I + iA\left(\theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!}\right) = \cos(\theta) I + i\sin(\theta) A
$$

Single qubit gates

http://threeplusone.com/gates

Hadamard gate

The Hadamard gate is so useful is that it acts on the computation basis states to create superpositions of zero and one states

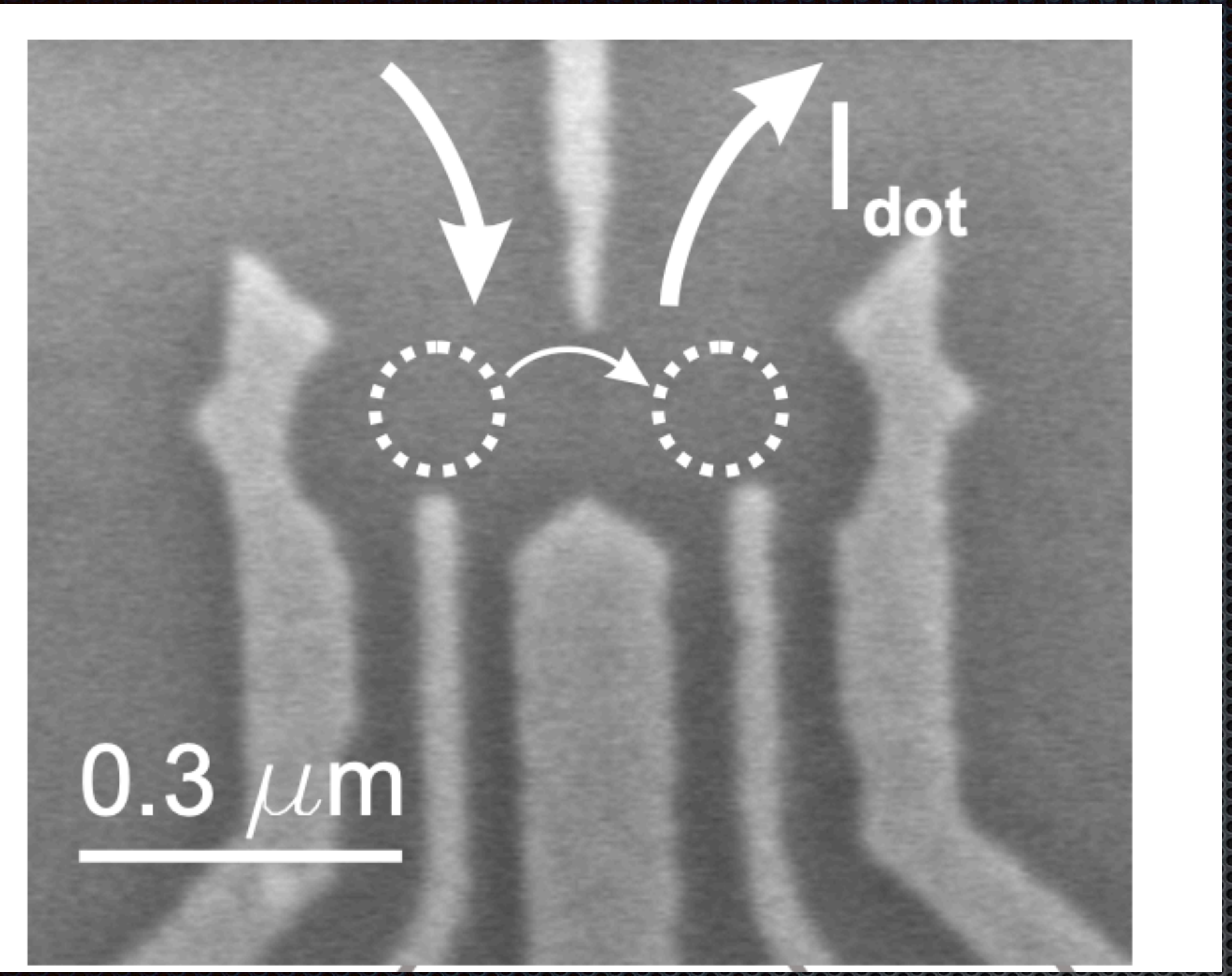
$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

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

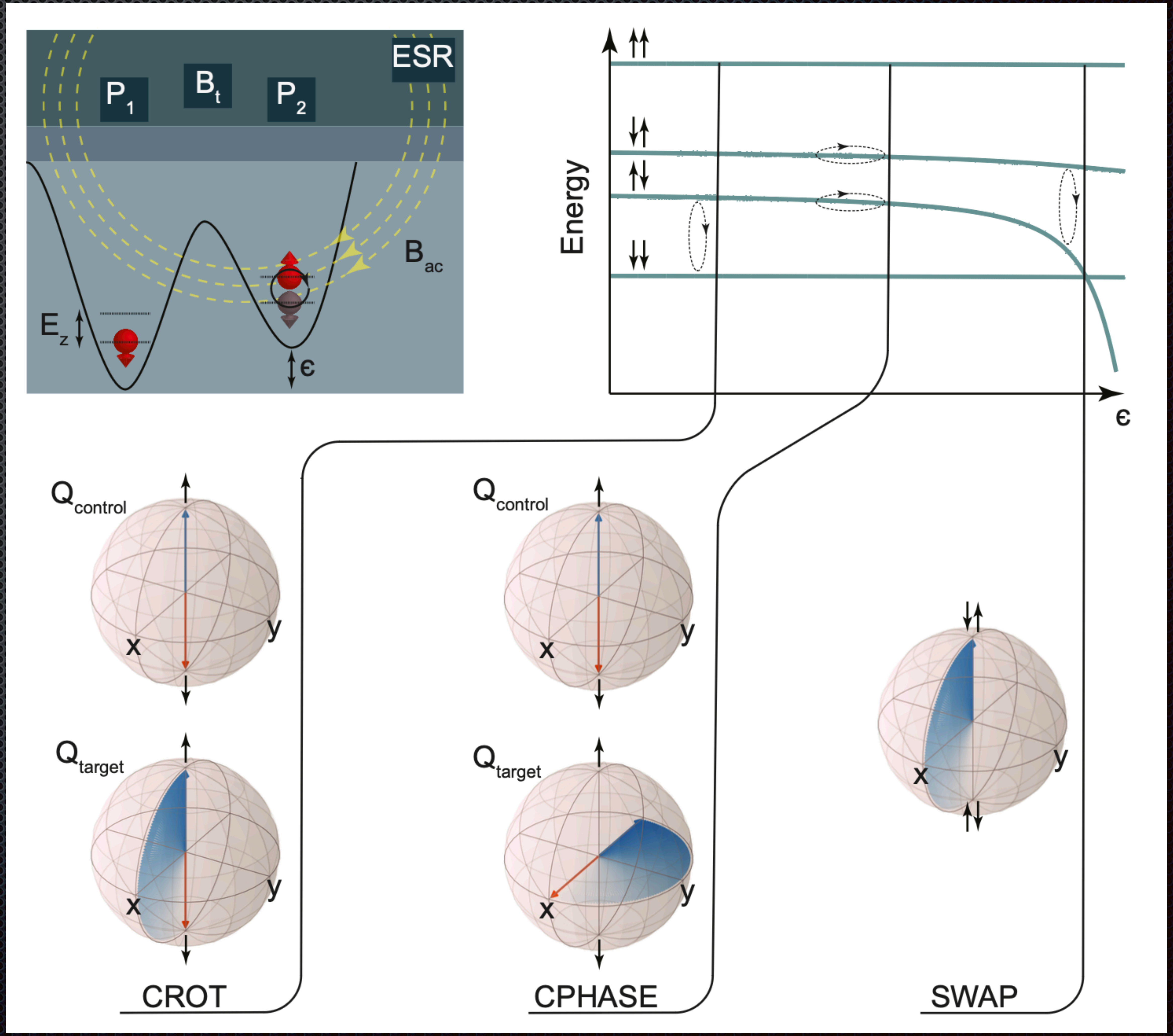
$$H|1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

Two qubit gates

Double quantum dot



arXiv:2007.09034v1



For the two qubit gate we can control the target qubit via the spin state of a control qubit

Two qubit gates

Two qubit system

$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

$$|00\rangle = |0\rangle \otimes |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$|01\rangle = |0\rangle \otimes |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

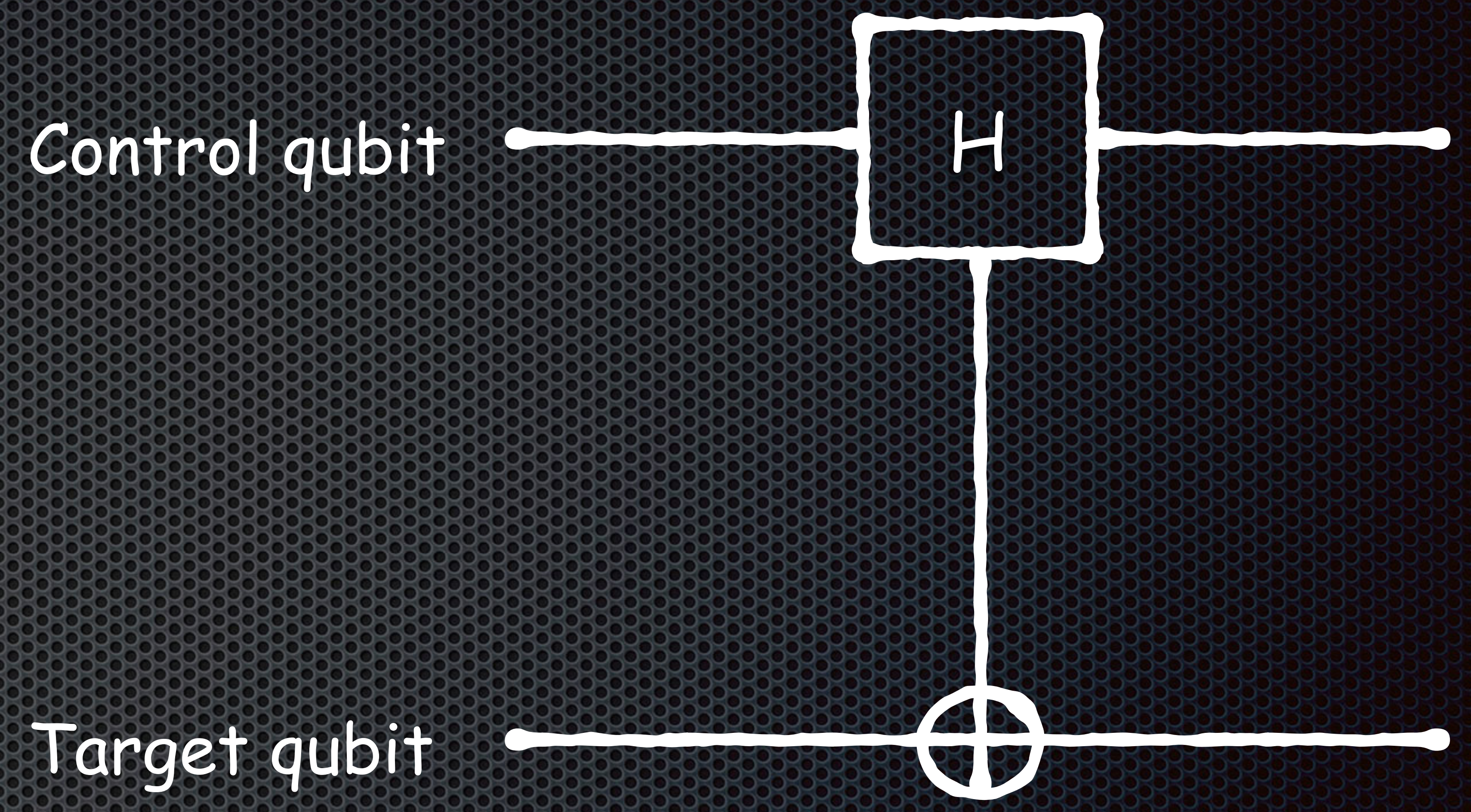
$$|10\rangle = |1\rangle \otimes |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$|11\rangle = |1\rangle \otimes |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Two qubit gates

Control Not gate

$$\text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$



$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

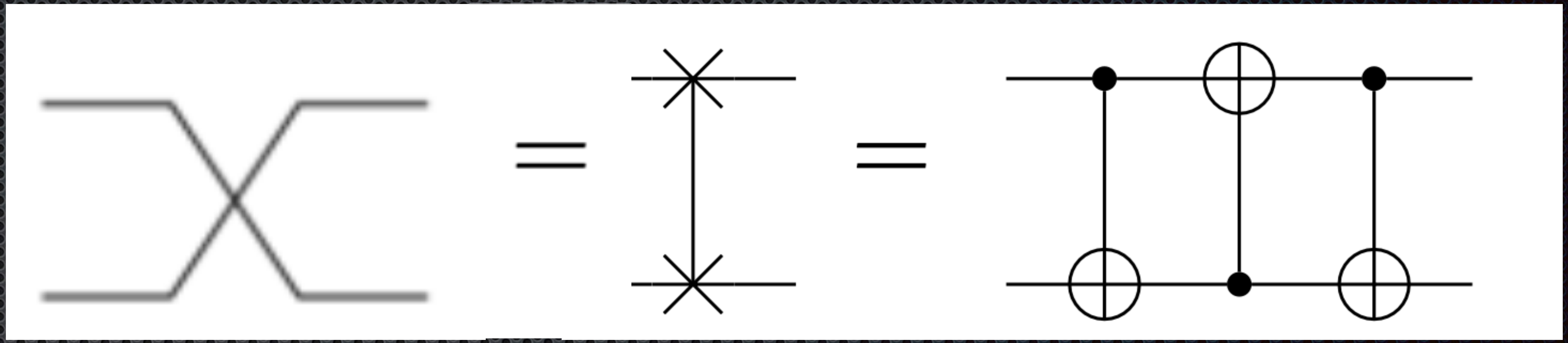
$$\text{CNOT}|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|11\rangle + \alpha_{11}|10\rangle$$

Two qubit gates

Swap gate

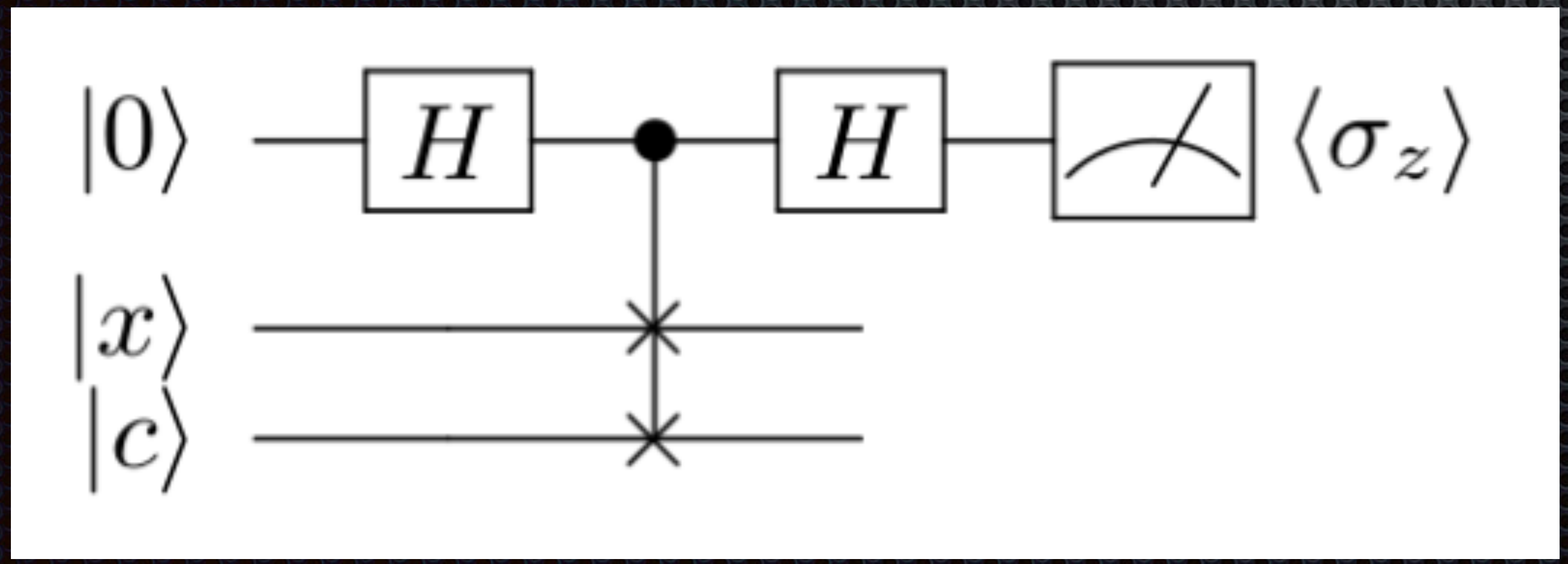
Swap gate flips the state of the qubits $|a, b\rangle \rightarrow |b, a\rangle$

$$\mathrm{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$



$$\mathrm{SWAP}|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|10\rangle + \alpha_{10}|01\rangle + \alpha_{11}|11\rangle$$

Swap gate is used to measure the fidelity of the two quantum states



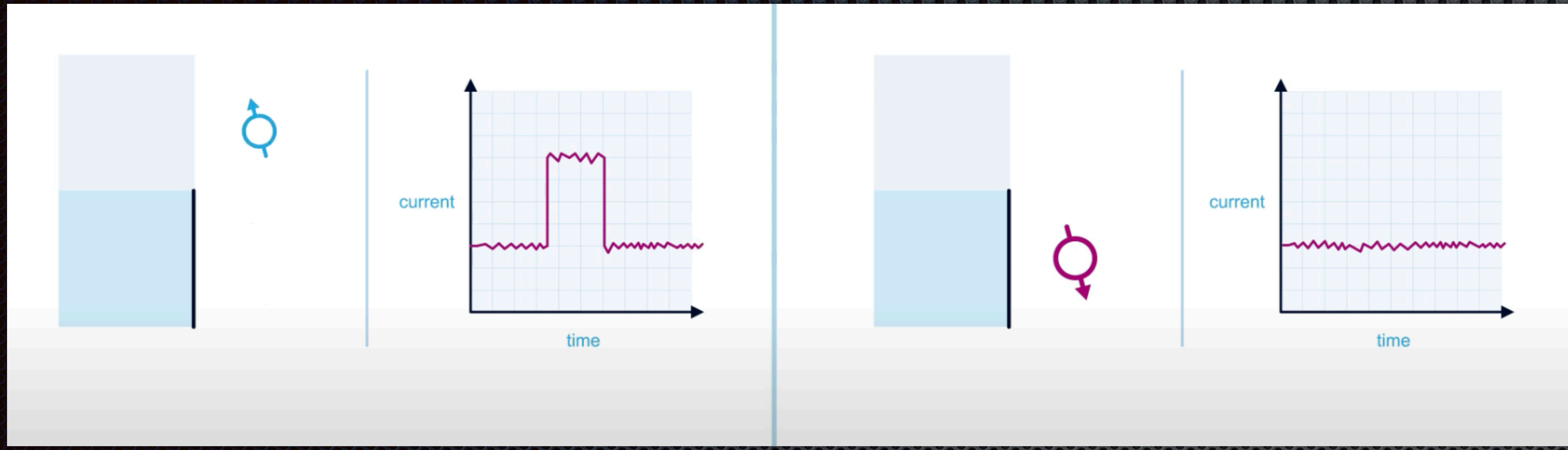
$$\mathrm{Fid} = \langle\psi|\psi\rangle$$

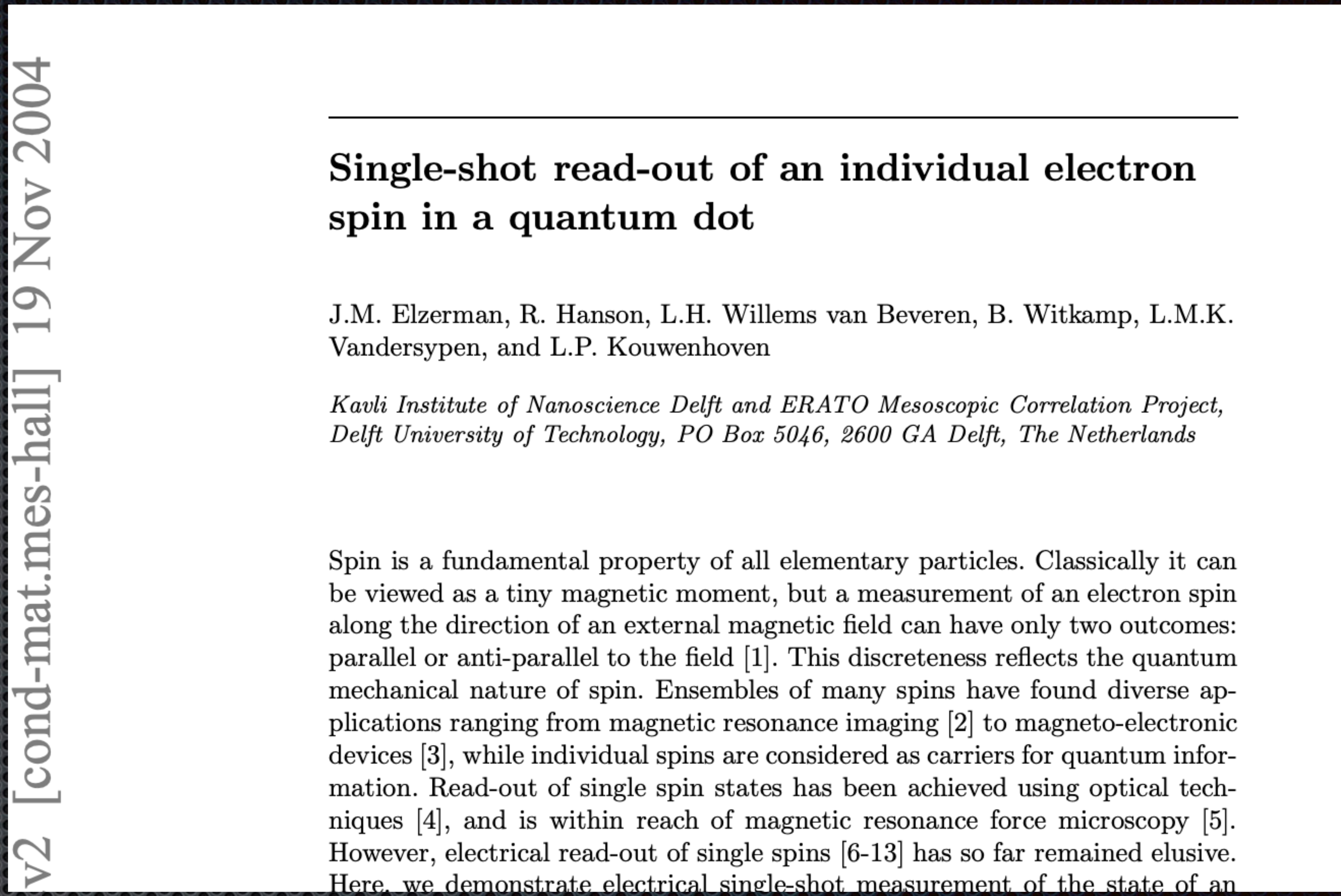
If the two states are similar states, F =1
If the two states are different, F=0

Measurement

Elzerman measurement

Measuring the spin state of the electron via the current measurement





v2 [cond-mat.mes-hall] 19 Nov 2004

Single-shot read-out of an individual electron spin in a quantum dot

J.M. Elzerman, R. Hanson, L.H. Willems van Beveren, B. Witkamp, L.M.K. Vandersypen, and L.P. Kouwenhoven

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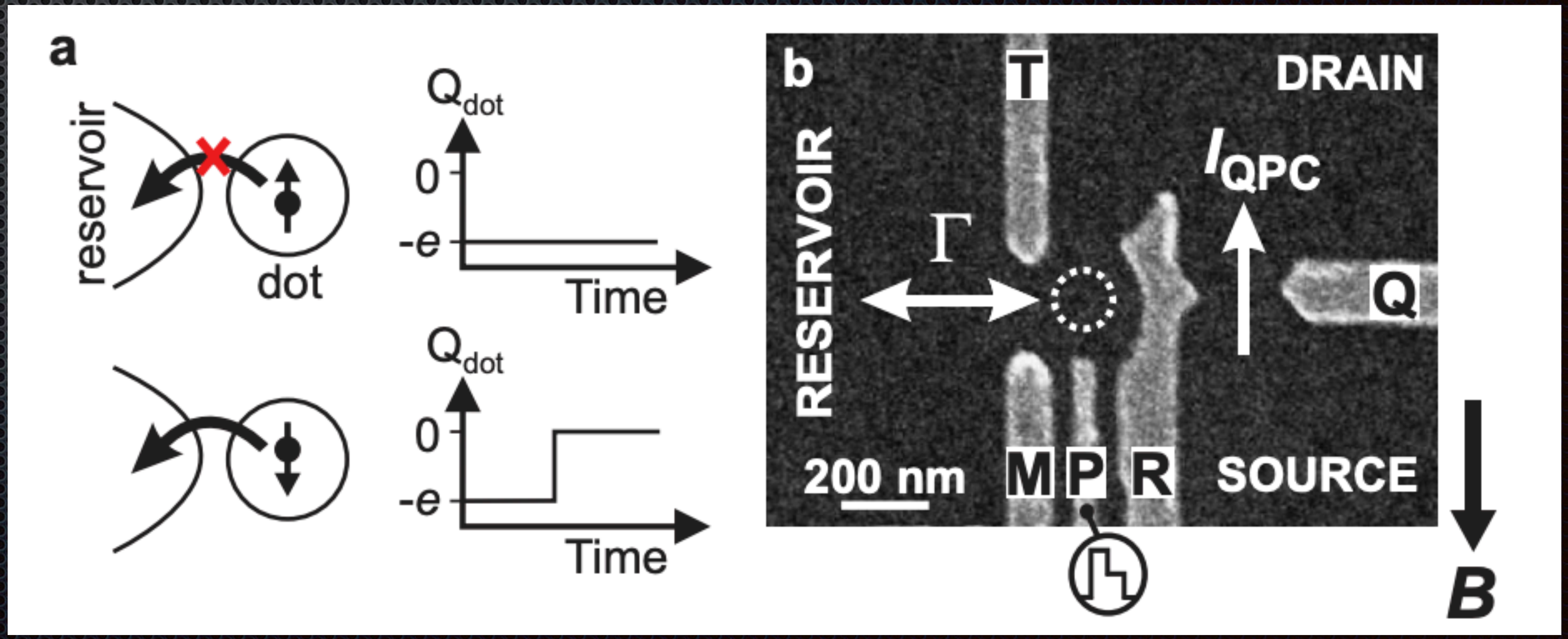
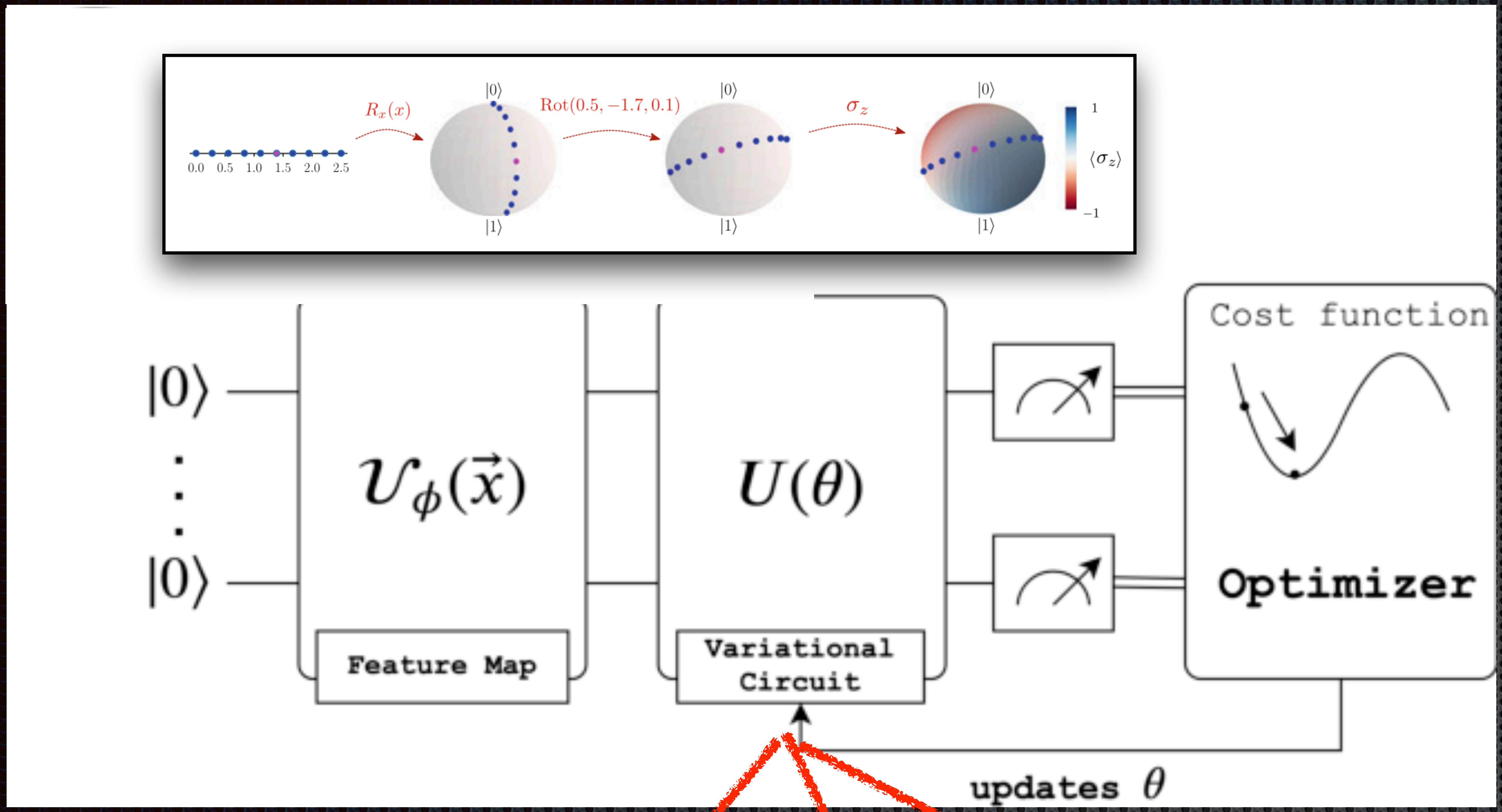
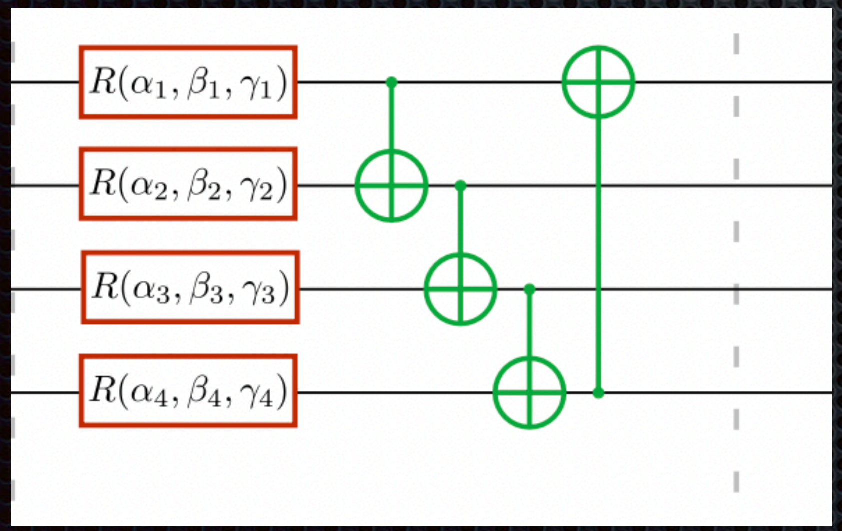
Spin is a fundamental property of all elementary particles. Classically it can be viewed as a tiny magnetic moment, but a measurement of an electron spin along the direction of an external magnetic field can have only two outcomes: parallel or anti-parallel to the field [1]. This discreteness reflects the quantum mechanical nature of spin. Ensembles of many spins have found diverse applications ranging from magnetic resonance imaging [2] to magneto-electronic devices [3], while individual spins are considered as carriers for quantum information. Read-out of single spin states has been achieved using optical techniques [4], and is within reach of magnetic resonance force microscopy [5]. However, electrical read-out of single spins [6-13] has so far remained elusive. Here, we demonstrate electrical single-shot measurement of the state of an



Now, lets add all what we learnt together to construct the variational quantum circuit

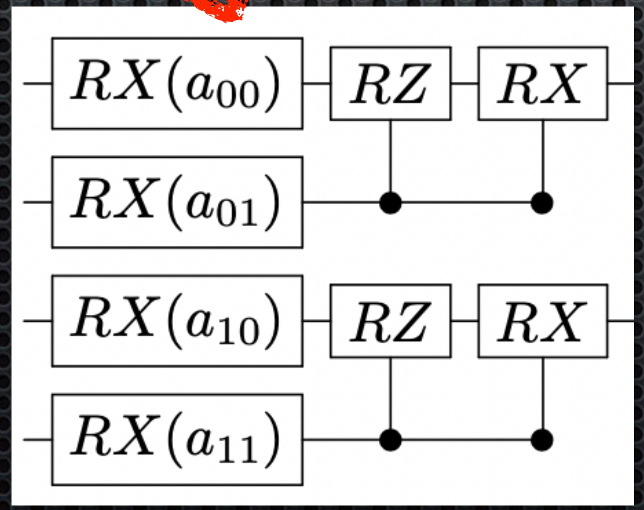
Variational quantum circuit





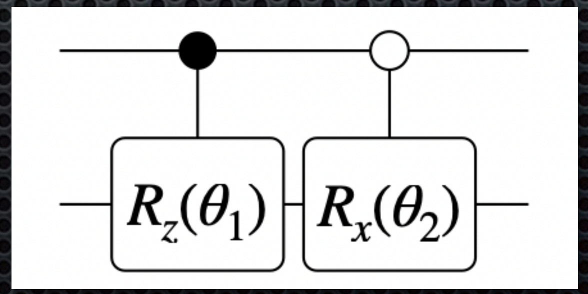
Fully connected

arXiv:2202.13943v1



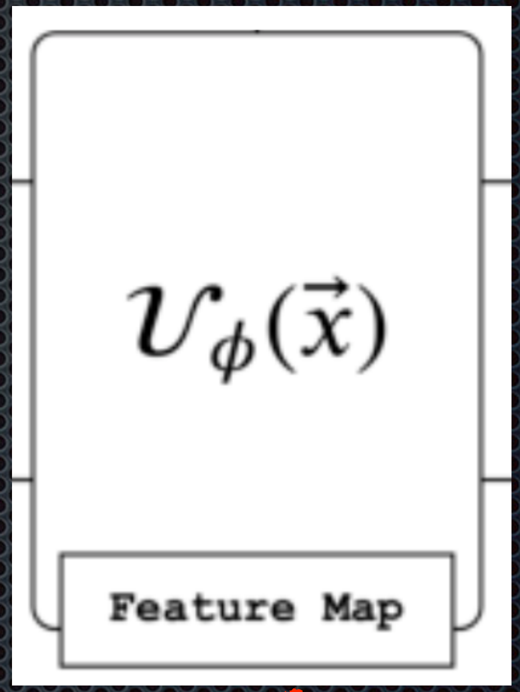
Conv circuit

arXiv:2108.00661



Pooling circuit

arXiv:2108.00661



Fixed

1- Basis embedding

2- Amplitude embedding

3- Angle embedding

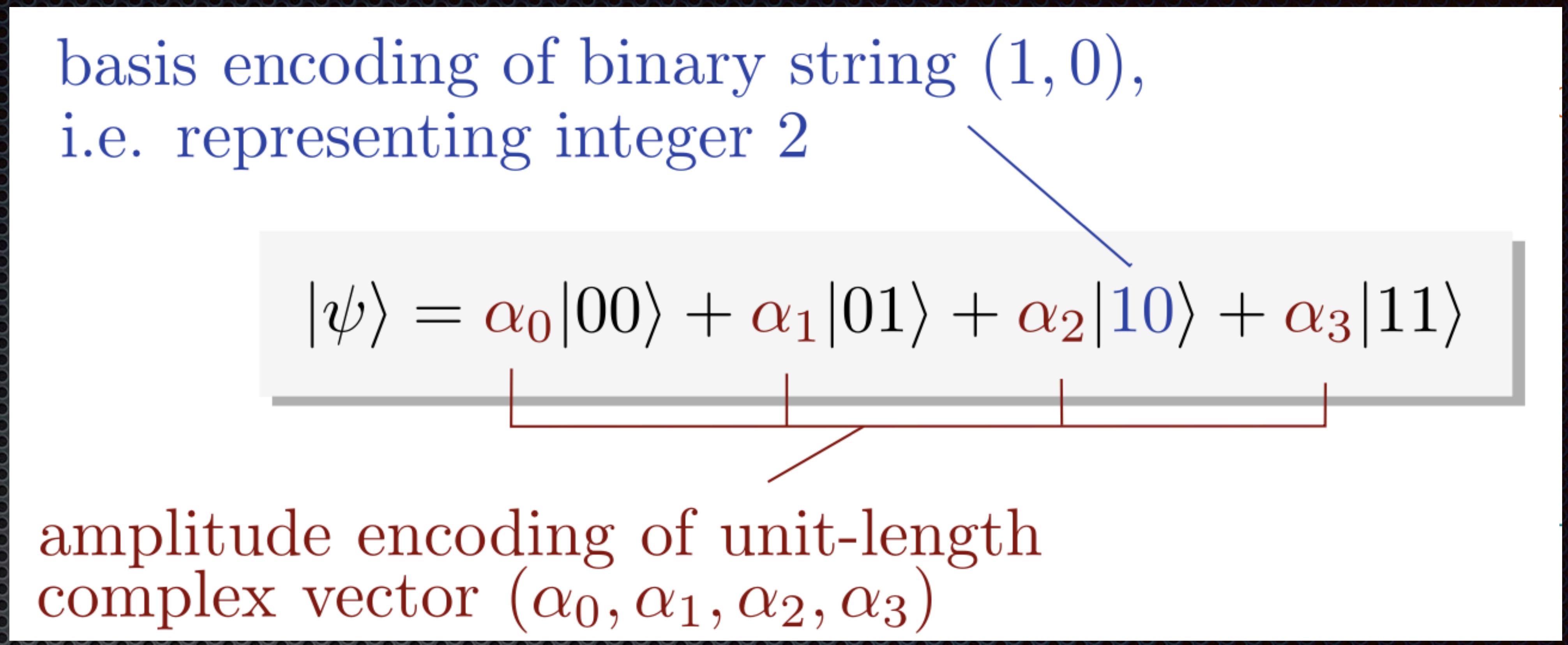
Variational embedding

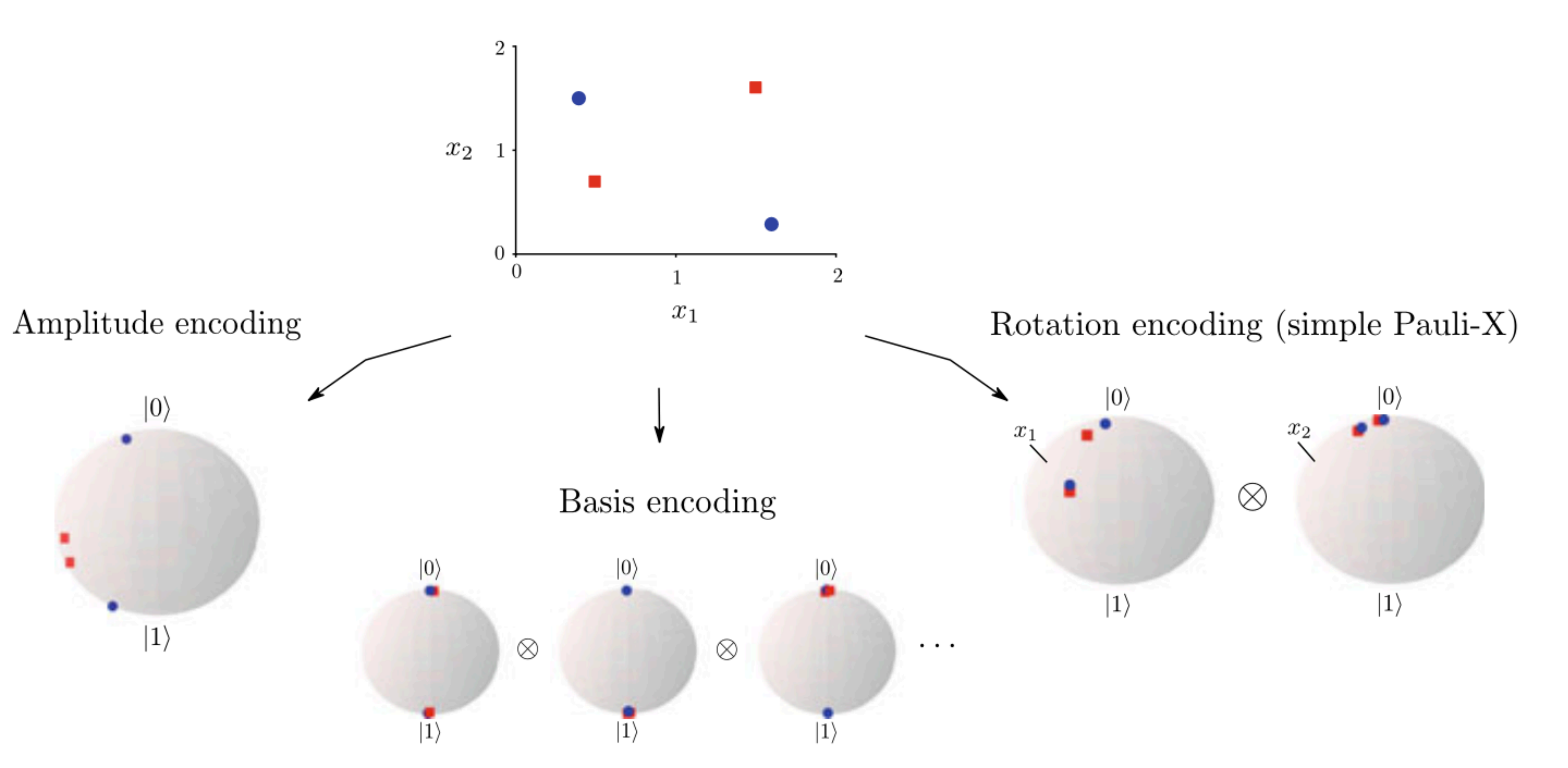
Variational quantum circuit

Classical data encoding on quantum computers

1- Basis encoding

Associates a computational basis state of an n-qubit system with Classical n-bit string





2- Amplitude encoding

Associates the classical data the quantum states amplitudes

$$X = (0.1, 0.2.0.3) \longmapsto |\psi\rangle = 0.1|00\rangle + 0.2|01\rangle + 0.3|10\rangle + 0.0|11\rangle$$

3- Angle encoding

Associates the classical data the quantum states rotating angles

$$R_y(0.1)|\psi\rangle = \cos(0.1)|0\rangle + \sin(0.1)|1\rangle$$

Variational quantum circuit

Back propagation in QML

For back propagation optimization using gradient descent method we need to compute the gradient

$$f(x;\theta_i) = \langle x|U^{\dagger}(\theta_i)\sigma_Z U(\theta_i)|x\rangle$$

The gradient can be computed using parameter shift rule, why not the chain rule as in classical ML?

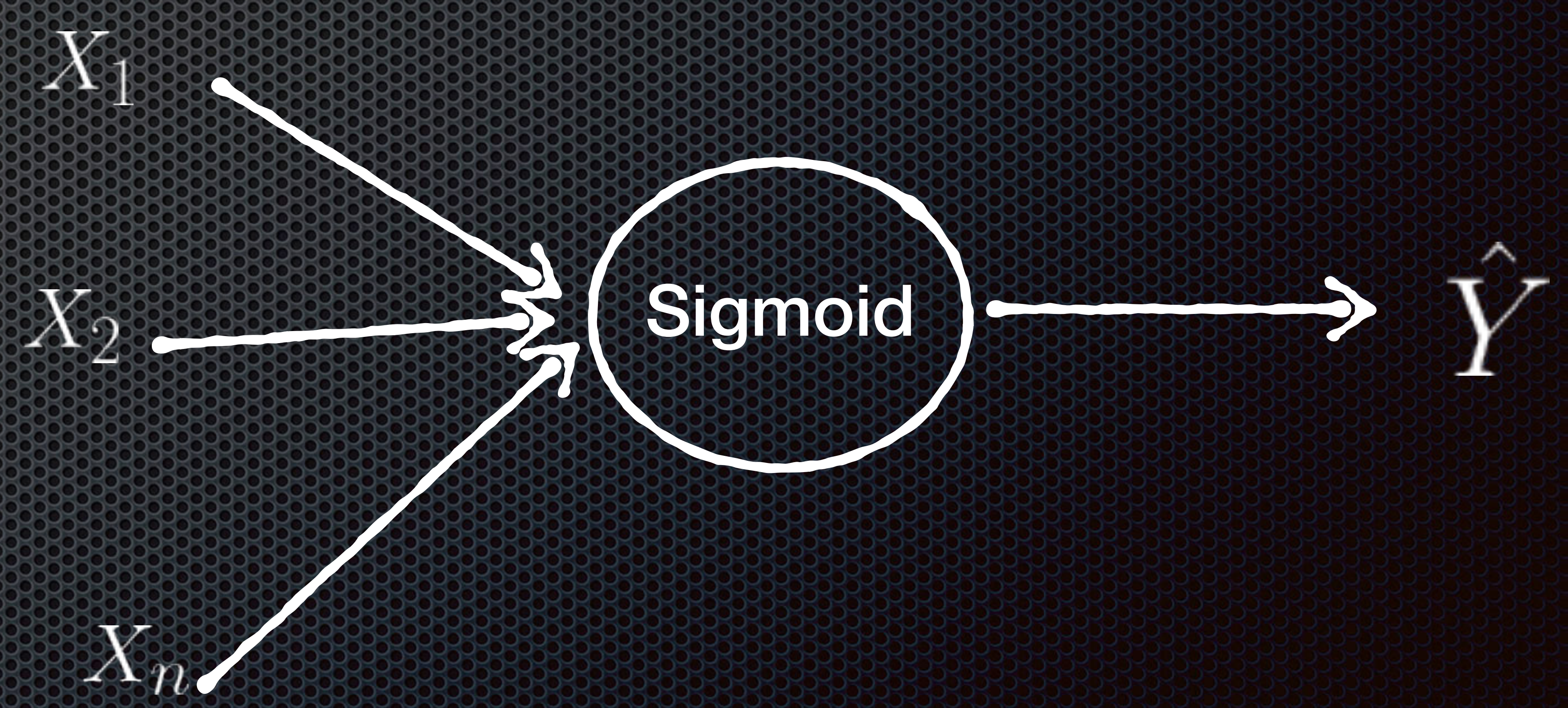
$$\nabla_\theta f(x;\theta_i) = \frac{1}{2}[f(x;\theta_i+\delta) - f(x;\theta_i-\delta)]$$

Binary classification in QML

$$\hat{Y} = \frac{1}{M_A}\sum_{a\in A}|\langle x|a\rangle|^2 - \frac{1}{M_B}\sum_{b\in B}|\langle x|b\rangle|^2$$

Most likely class A if $\hat{Y} > 0$

Most likely class B if $\hat{Y} \leq 0$



Most likely class A if $\hat{Y} > 0.5$

Most likely class B if $\hat{Y} \leq 0.5$

Barren Plateau

ARTICLE

DOI: 10.1038/s41467-018-07090-4

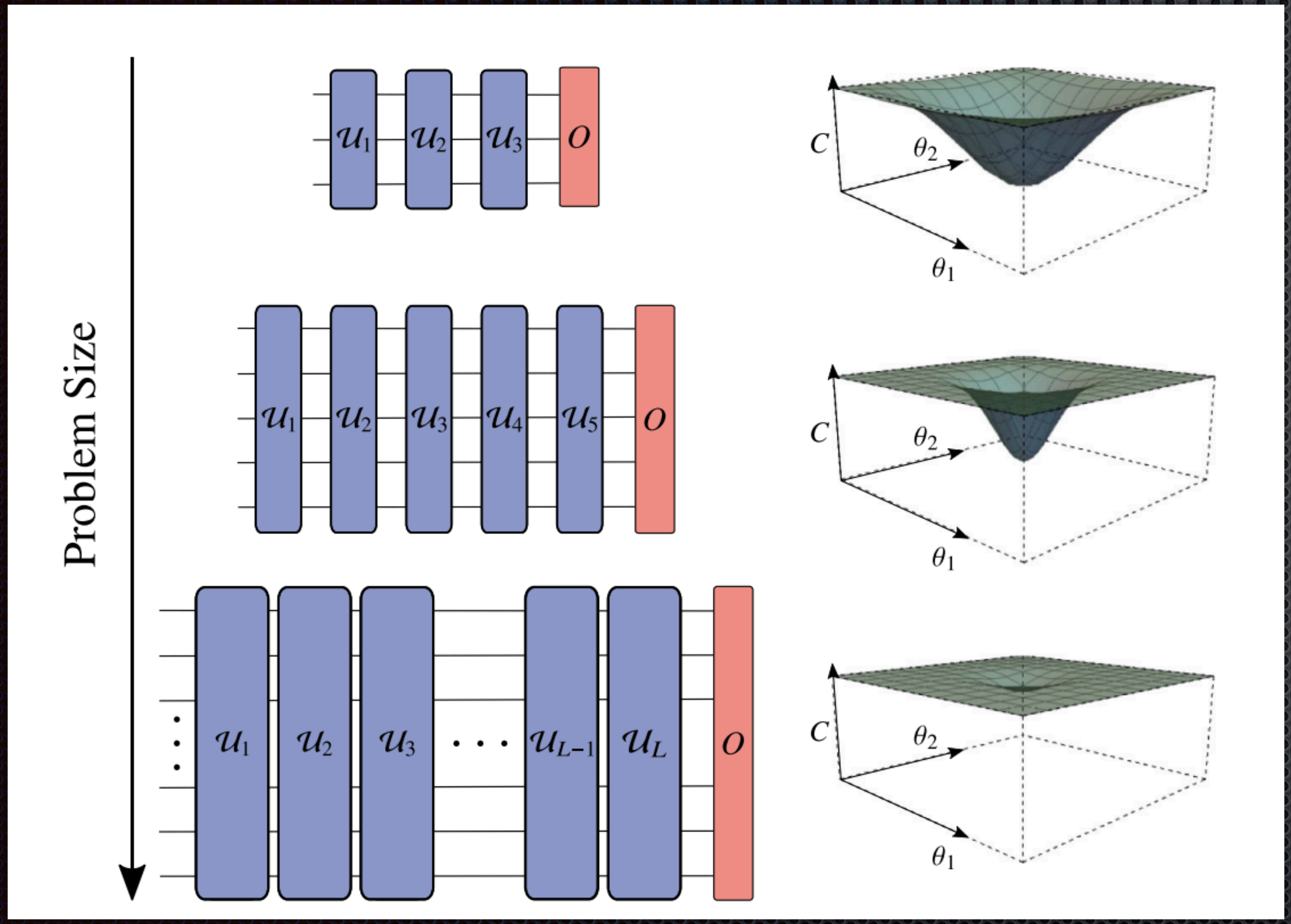
OPEN

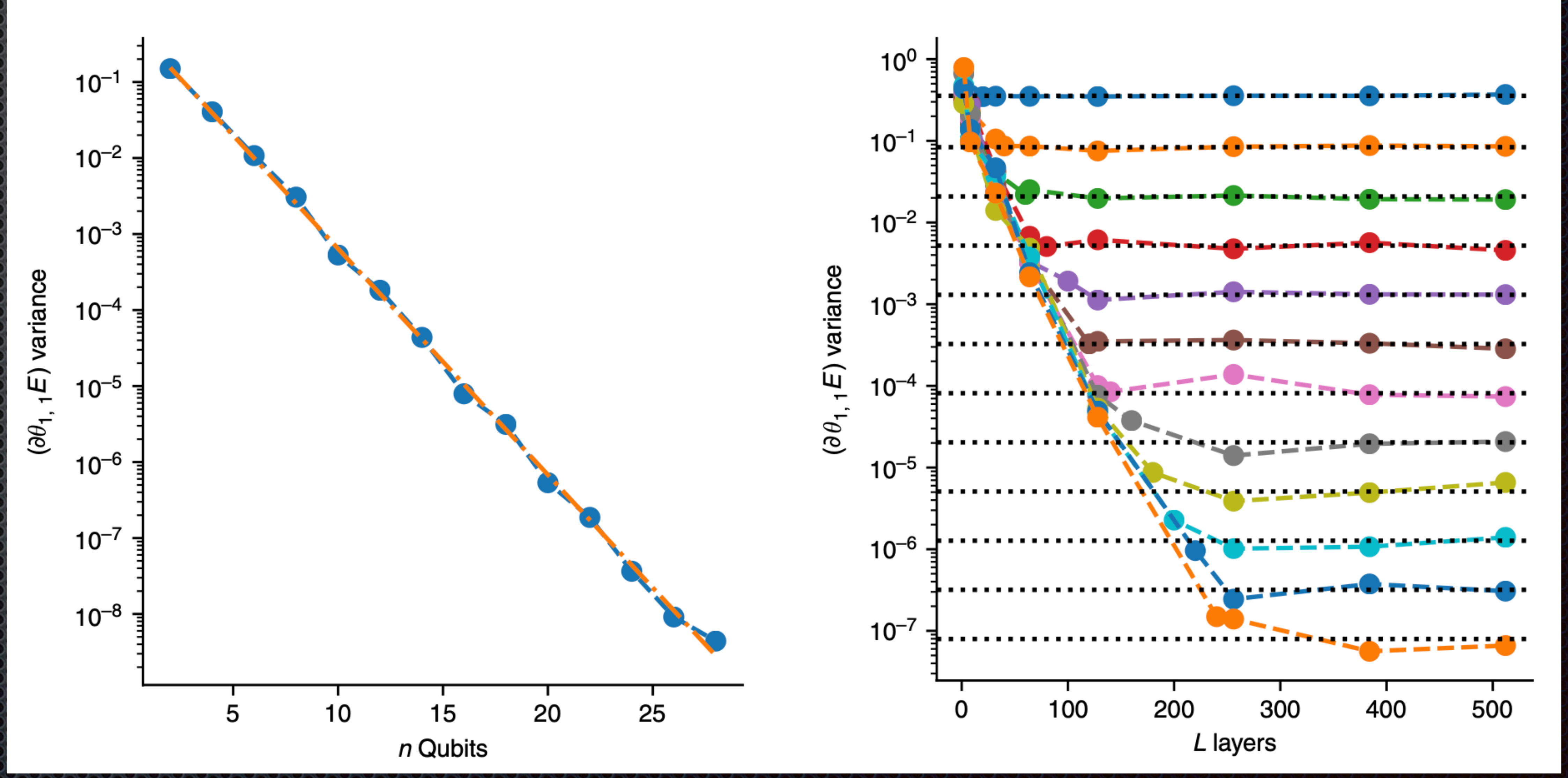
Barren plateaus in quantum neural network training landscapes

Jarrod R. McClean[1], Sergio Boixo[1], Vadim N. Smelyanskiy[1], Ryan Babbush[1] & Hartmut Neven[1]

Many experimental proposals for noisy intermediate scale quantum devices involve training a parameterized quantum circuit with a classical optimization loop. Such hybrid quantum-classical algorithms are popular for applications in quantum simulation, optimization, and machine learning. Due to its simplicity and hardware efficiency, random circuits are often

https://doi.org/10.1038/s41467-021-27045-6





Evenly increasing qubits

Now, lets go coding!!

Thank You for attending the lectures...

See you next time!!