

Machine Learning crash course

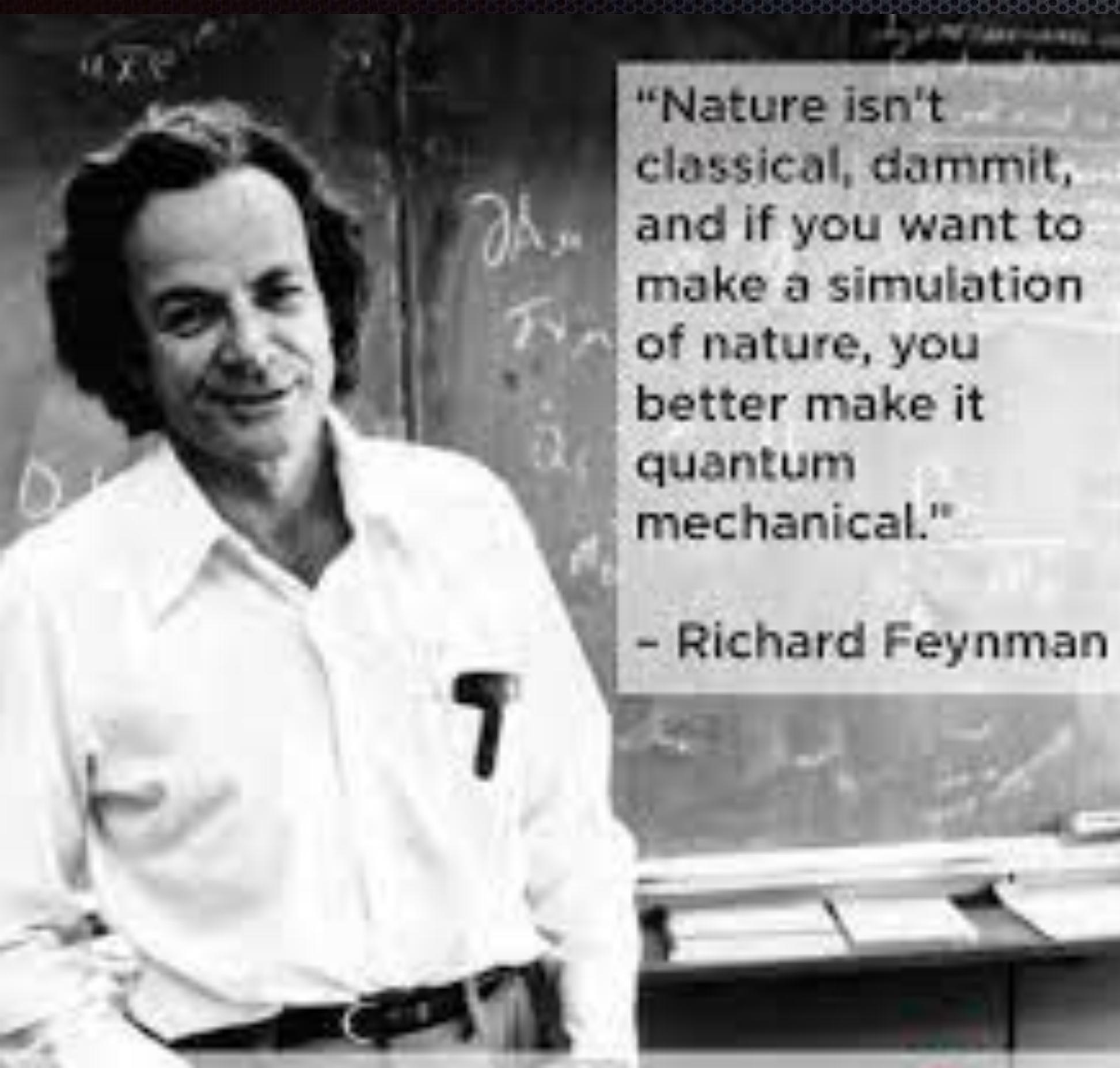
(Part-6)

Ahmed Hammad

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

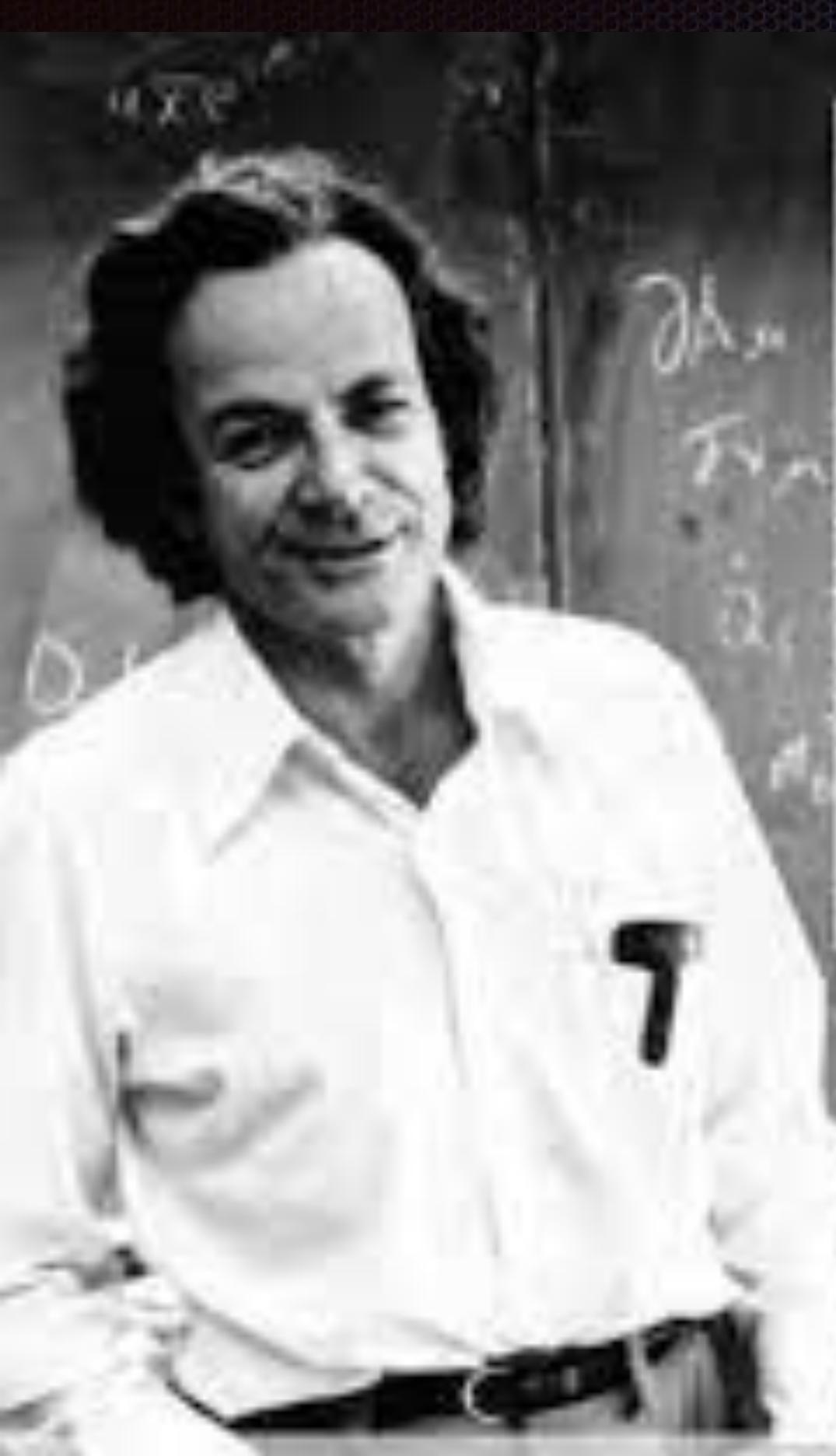
Introduction

*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 know



"Nature isn't
classical, dammit,
and if you want to
make a simulation
of nature, you
better make it
quantum
mechanical."

- Richard Feynman

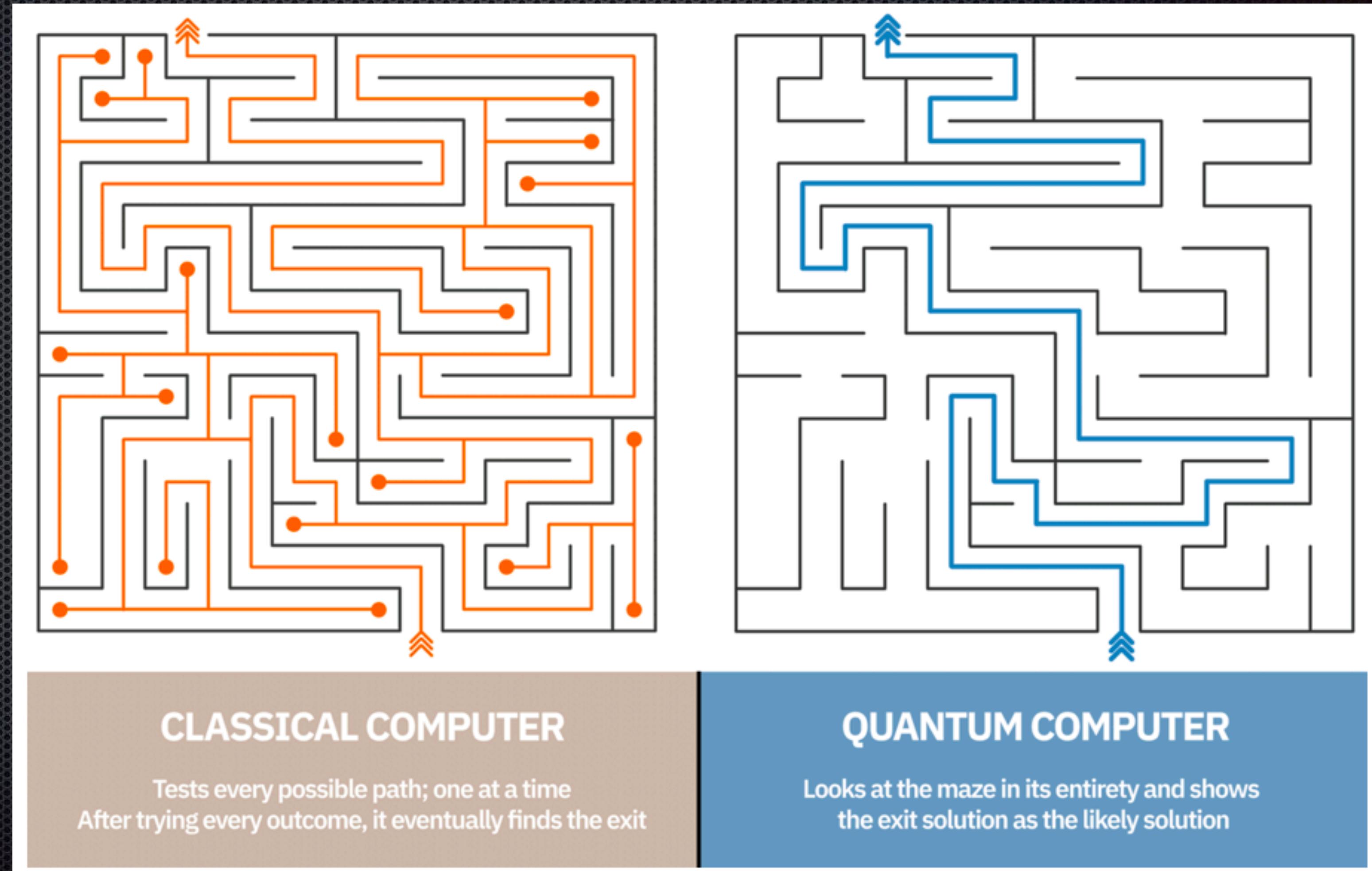
Now we know



Introduction

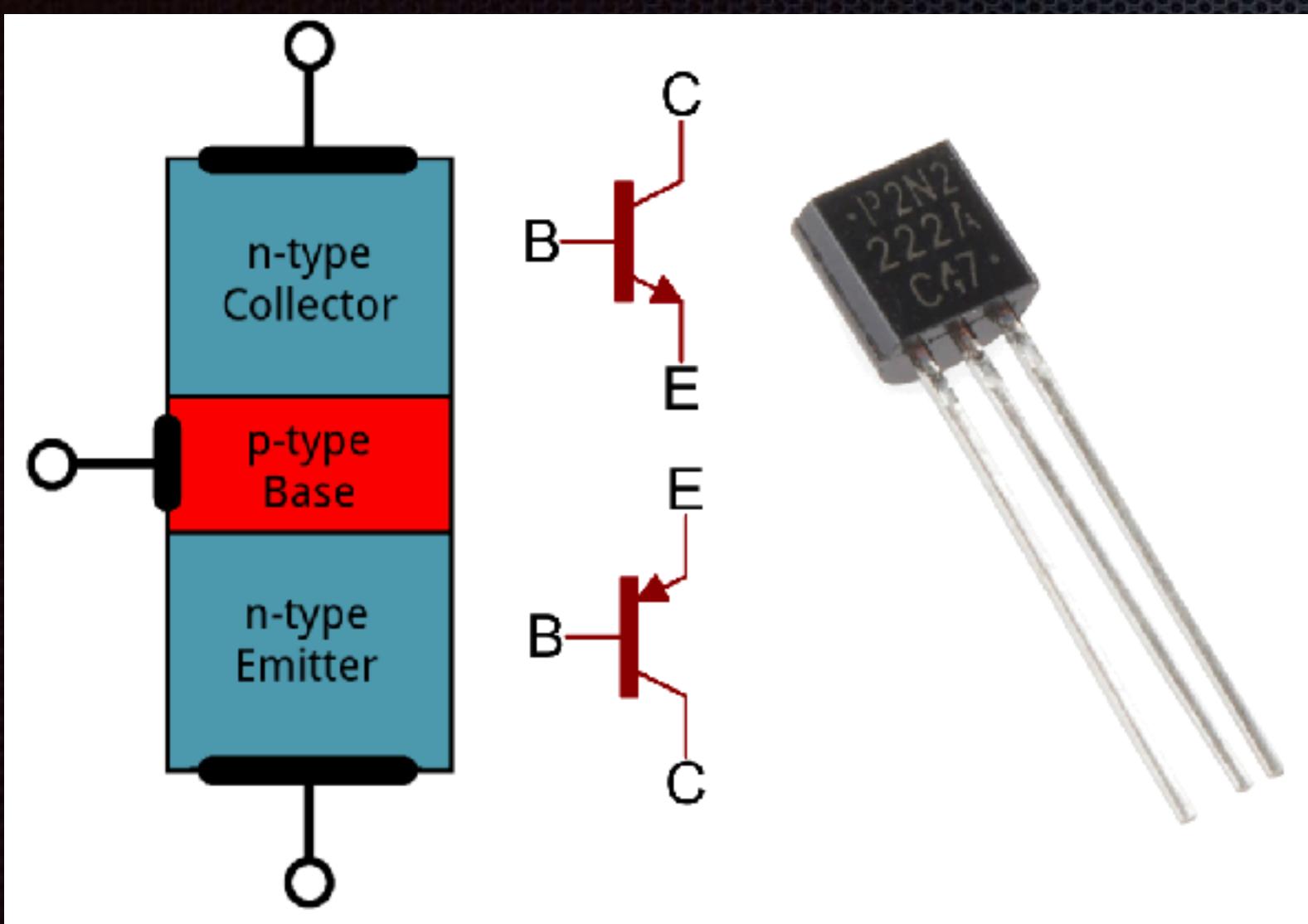
Using classical and quantum computers to search for unstructured data to find the exit of a maze

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

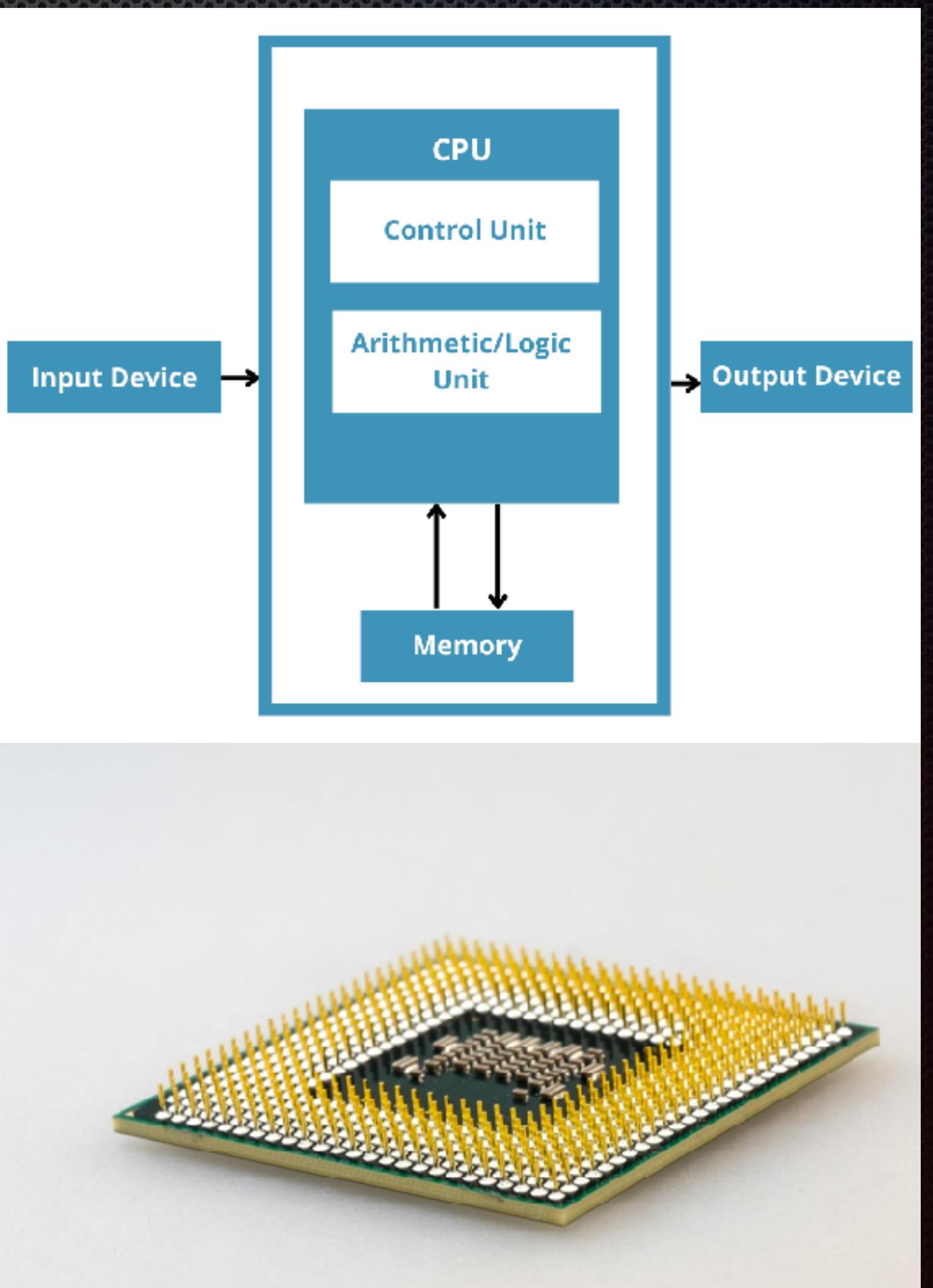
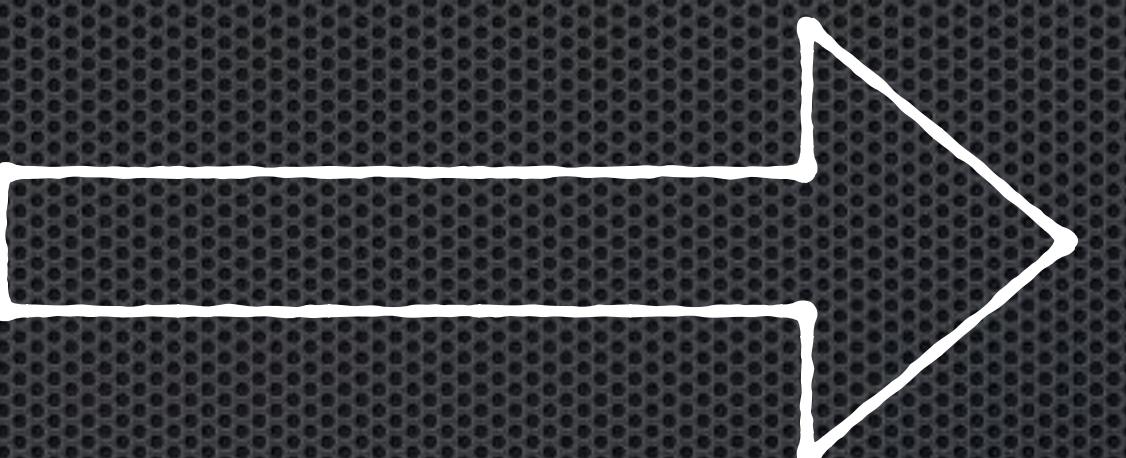


Introduction

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

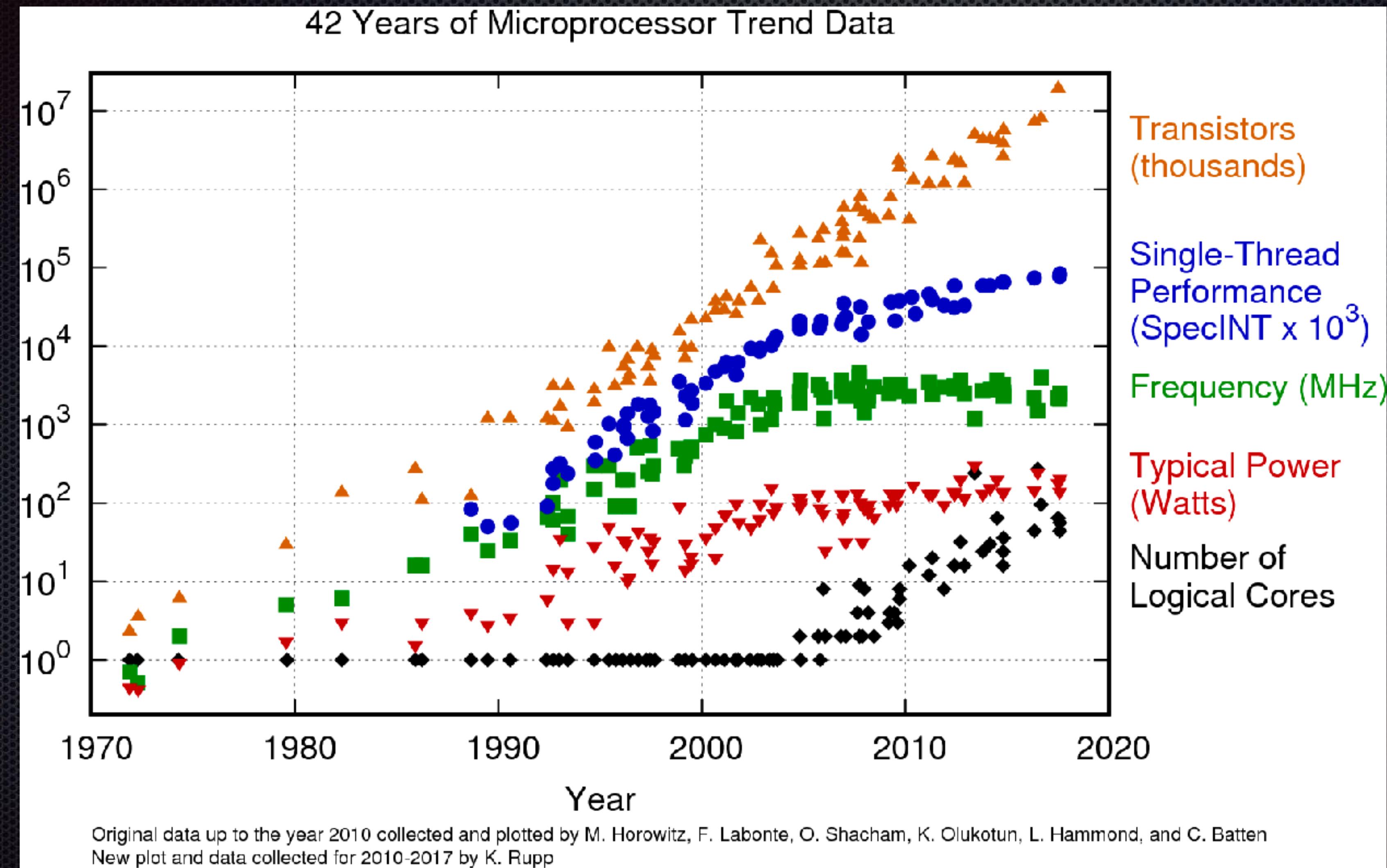


More and more gates
to construct a CPU



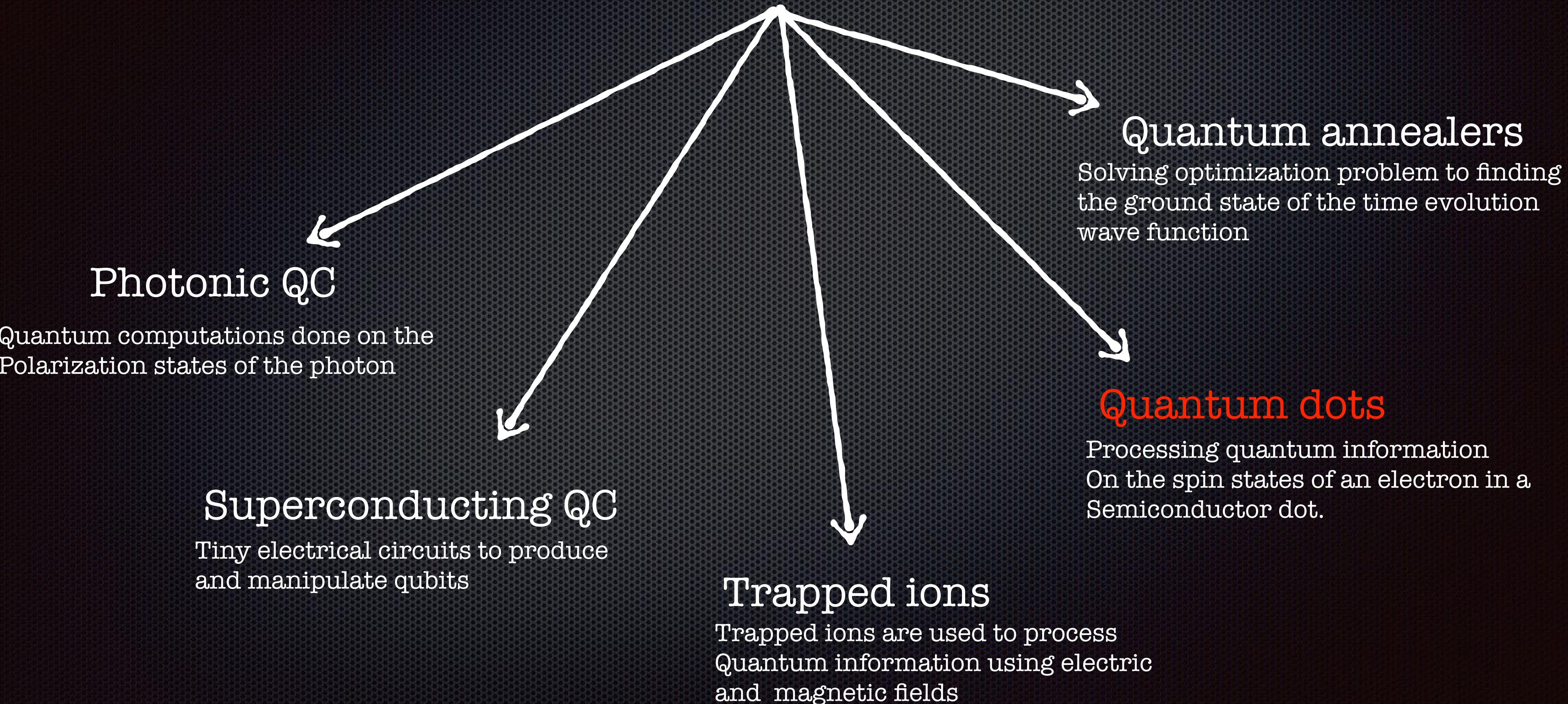
Introduction

Why do we need quantum computation



Introduction

Examples of quantum computers

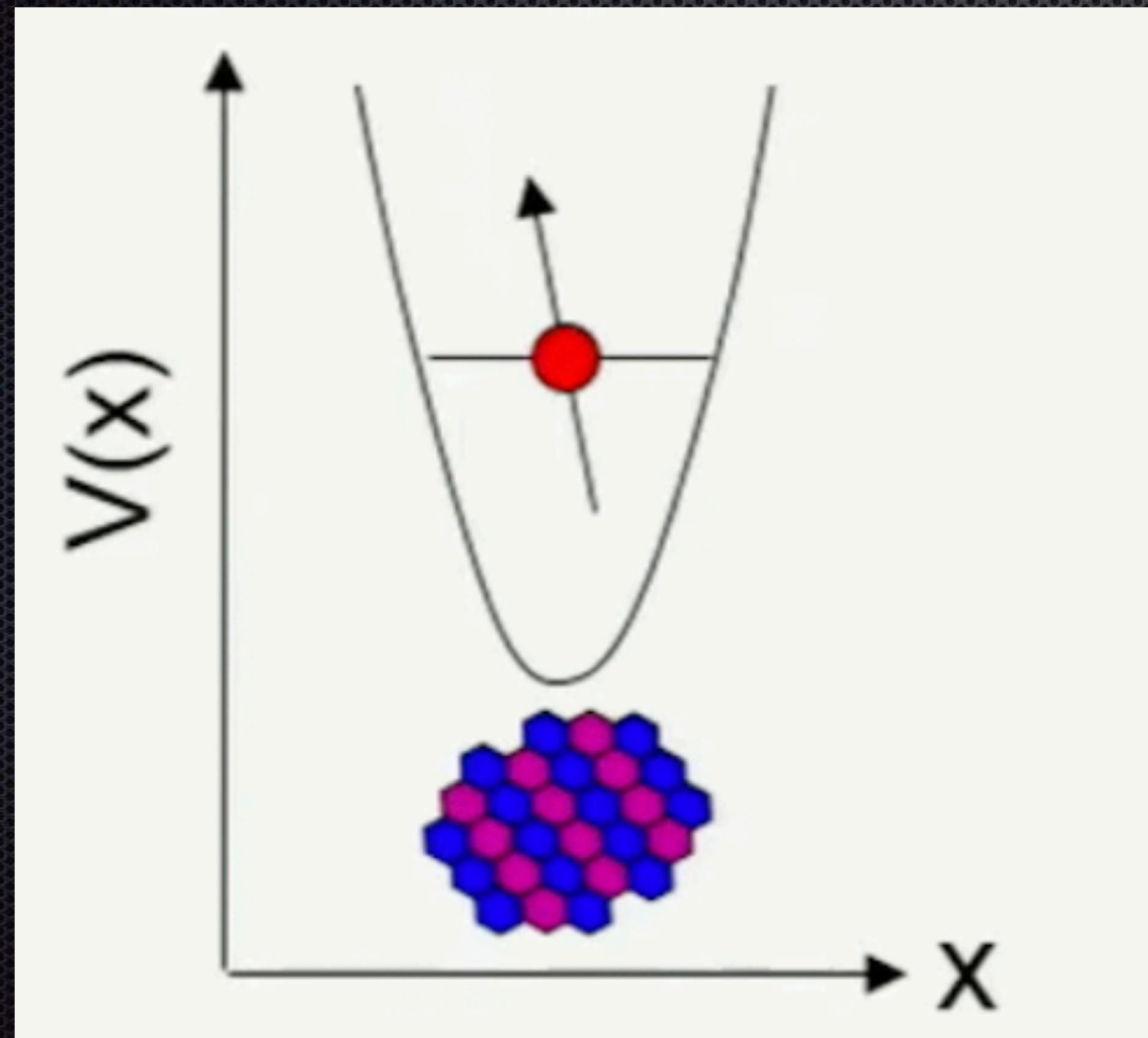


Quantum dot

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?

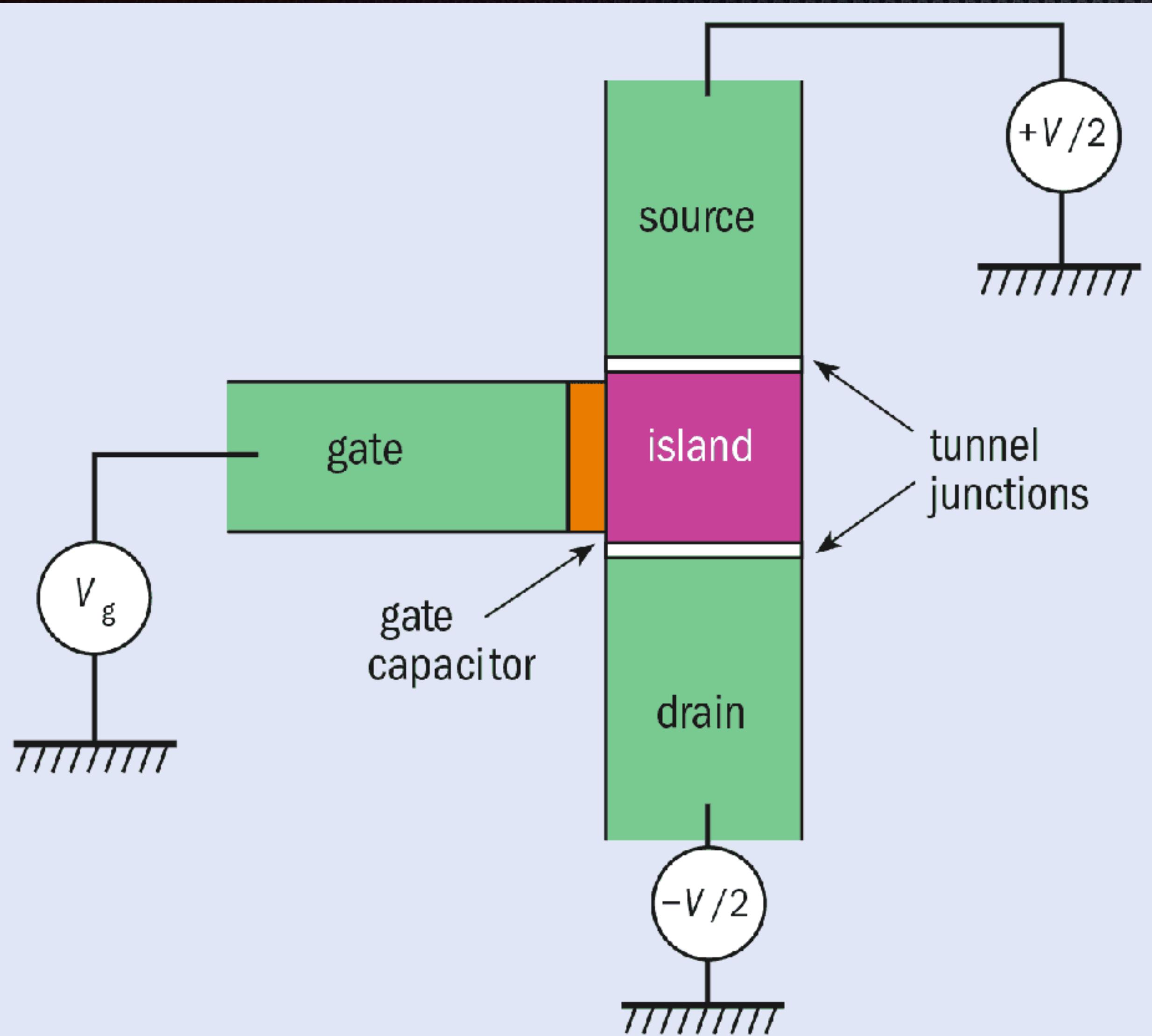
A How to cook a quantum dot at home? answer precisely

 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.

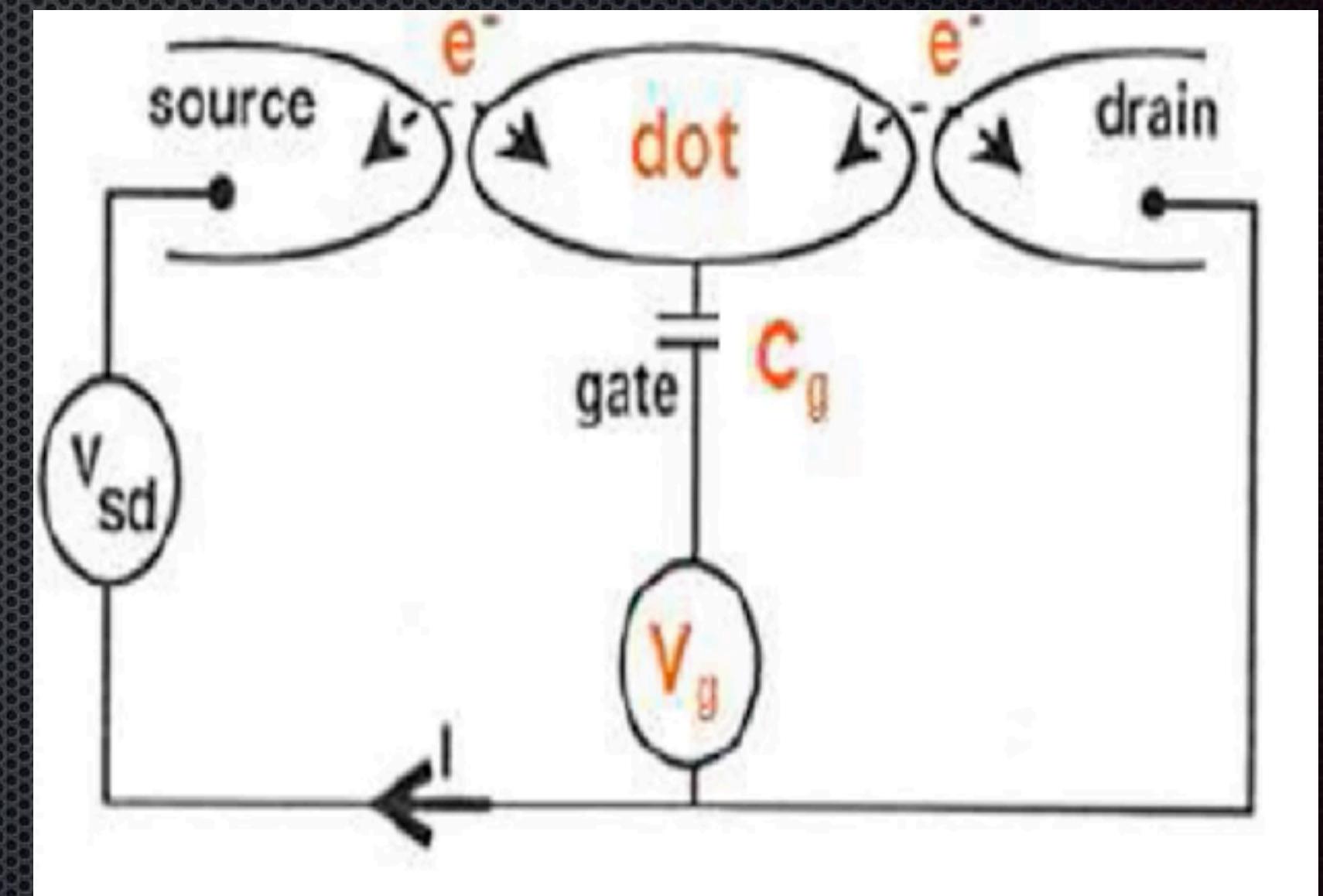
Furthermore, working with quantum dots typically requires a controlled environment, such as a laboratory setting, due to the potential health risks associated with handling certain chemicals and nanoparticles. It's important to prioritize safety and leave the synthesis of quantum dots to professionals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

Quantum dot

Single electron box



Electrons can tunnel to the island by controlling the **gate voltage**



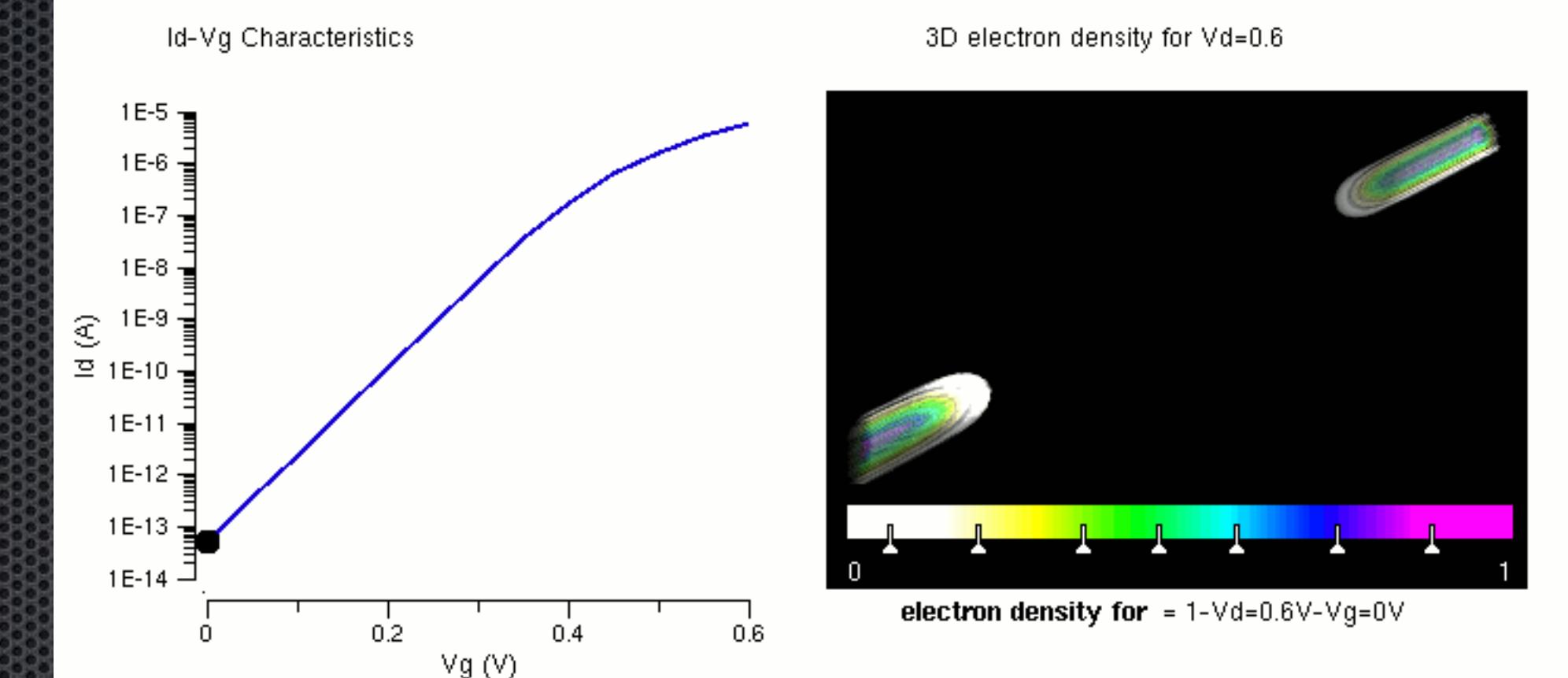
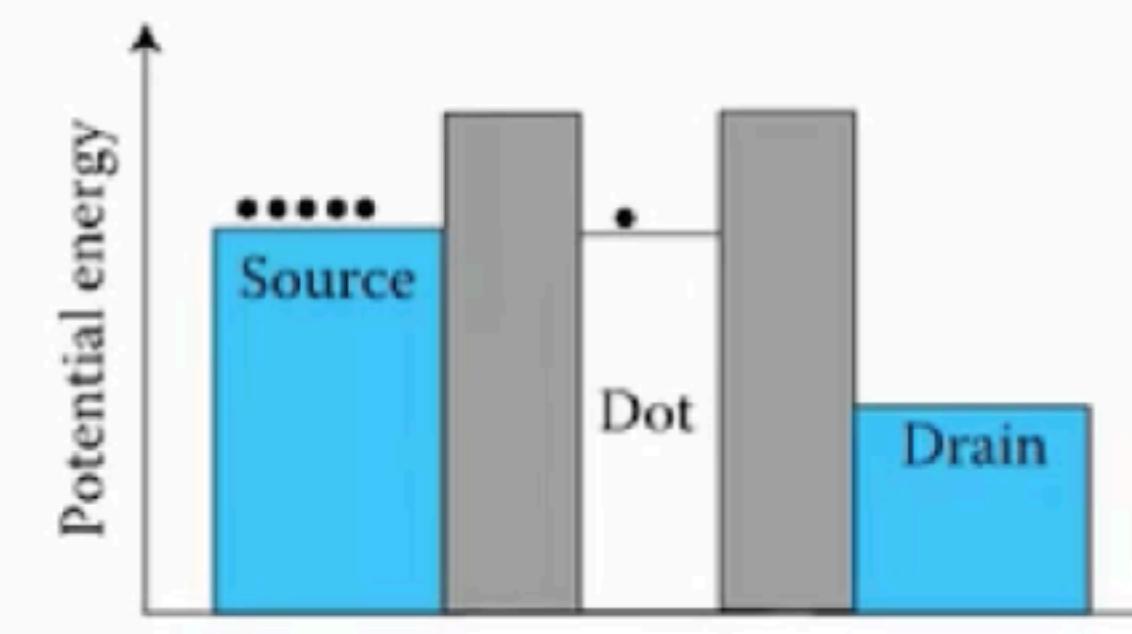
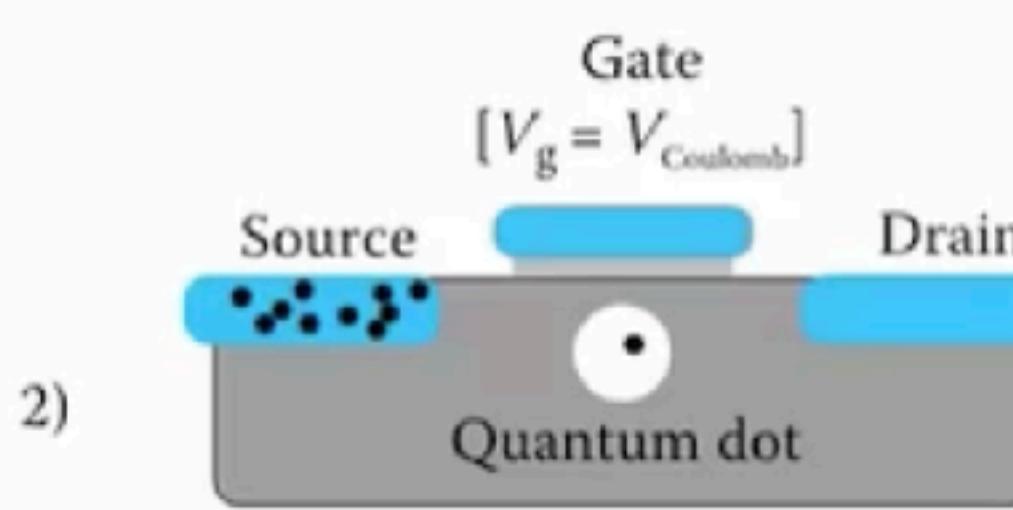
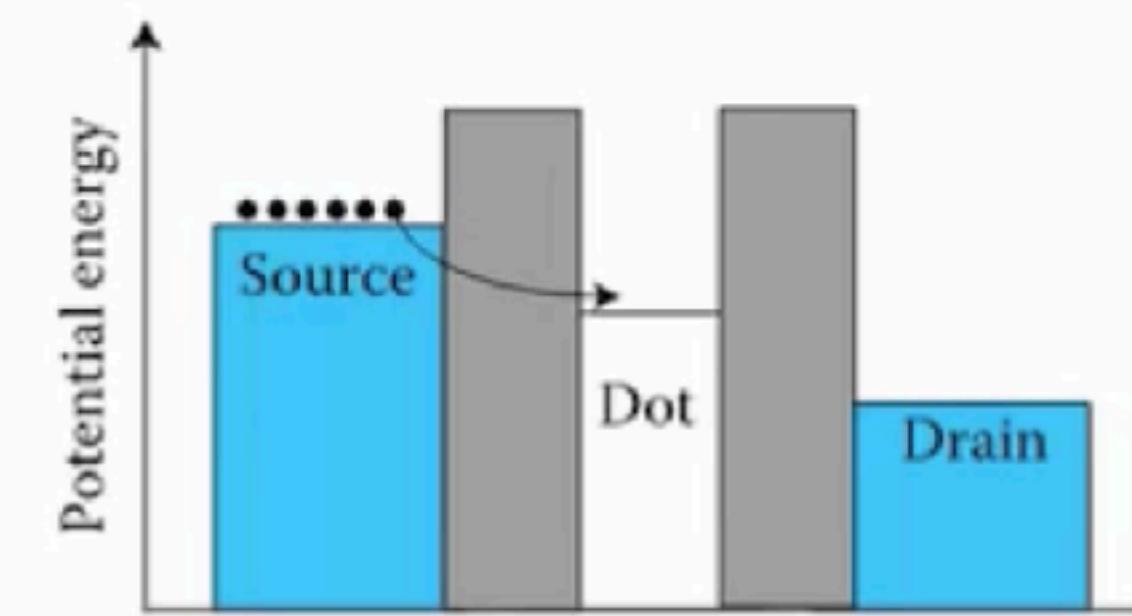
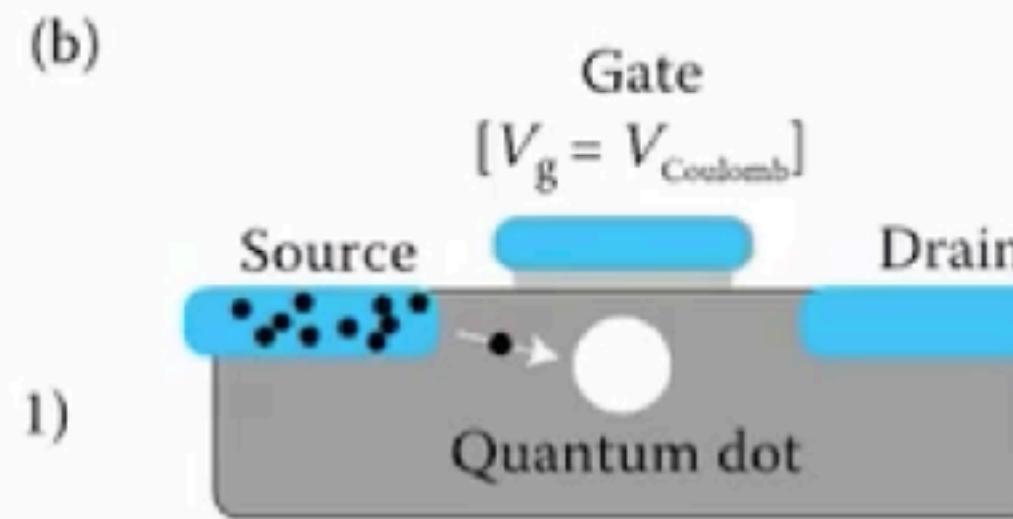
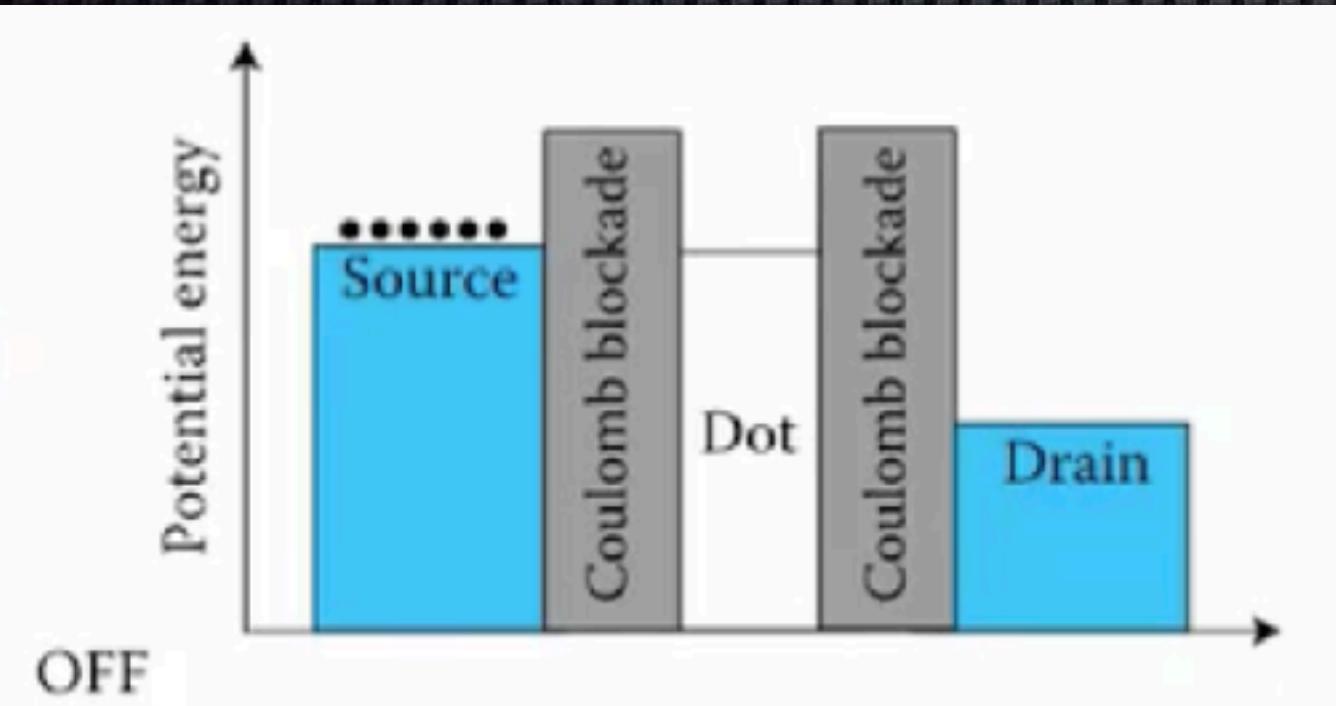
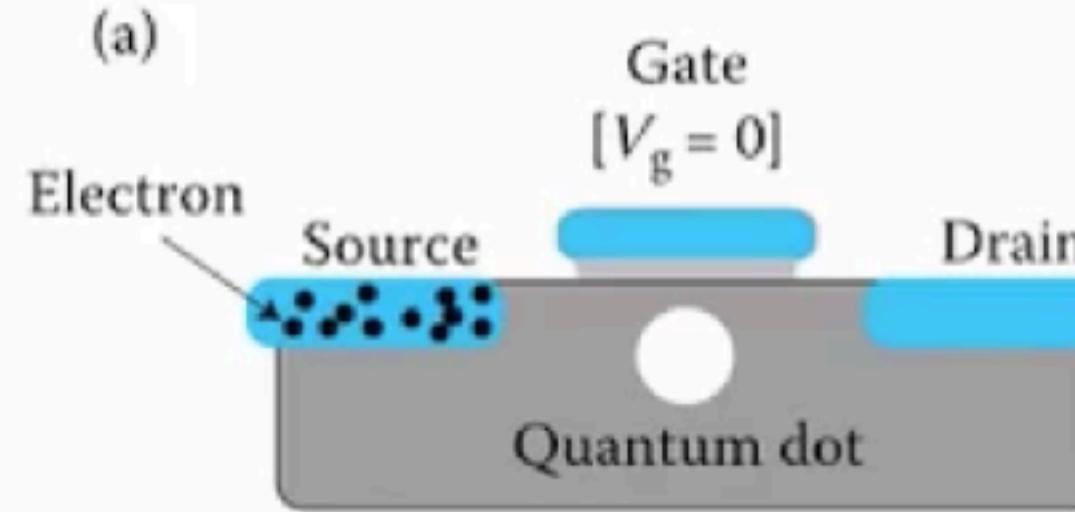
Due to Pauli exclusion principle, only a single electron can occupy the dot at a time. Once the dot is empty another electron can jump into the dot

Quantum dot

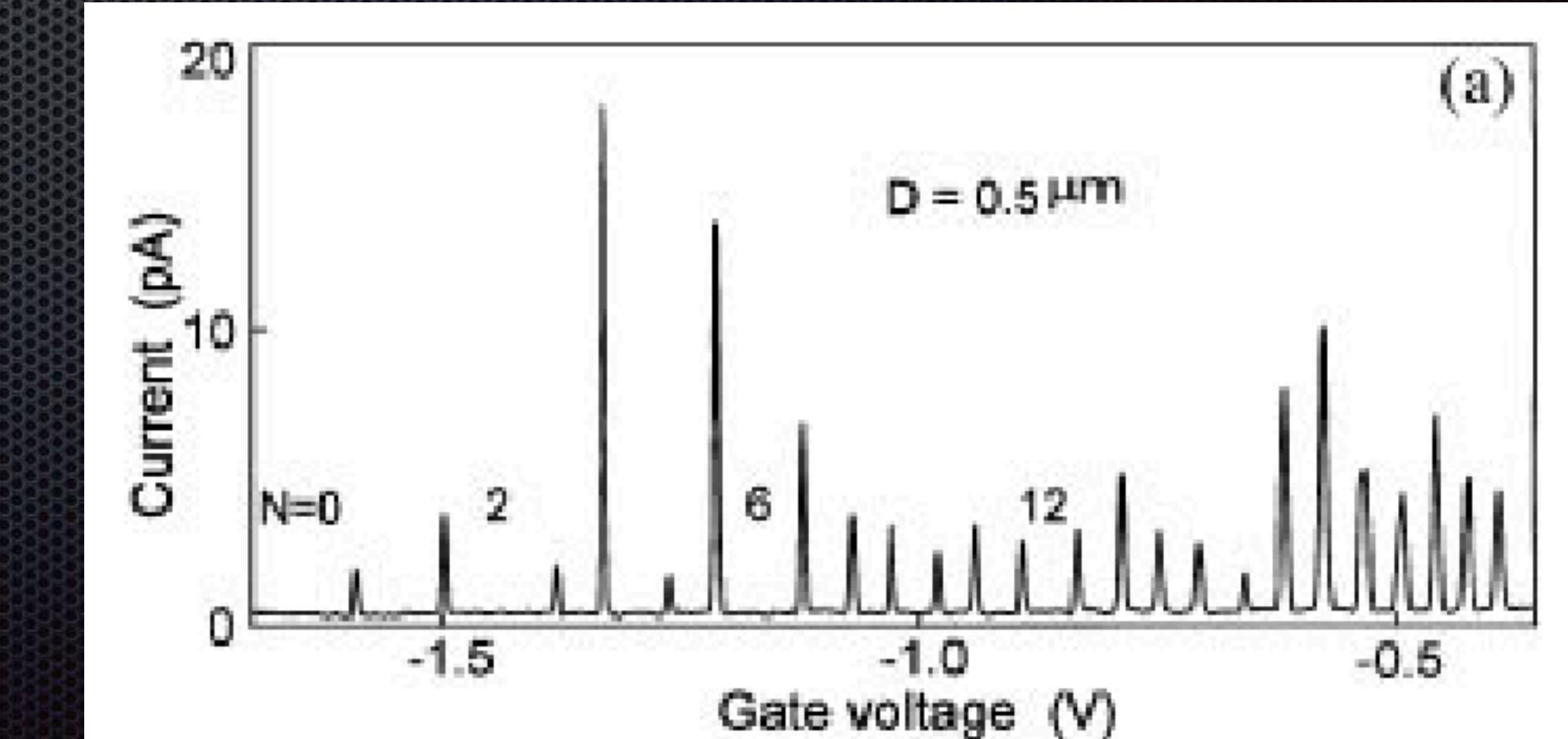
By controlling the gate voltage we can control the electron in the dot

Single electron box

Single-Electron Transistor (SET)



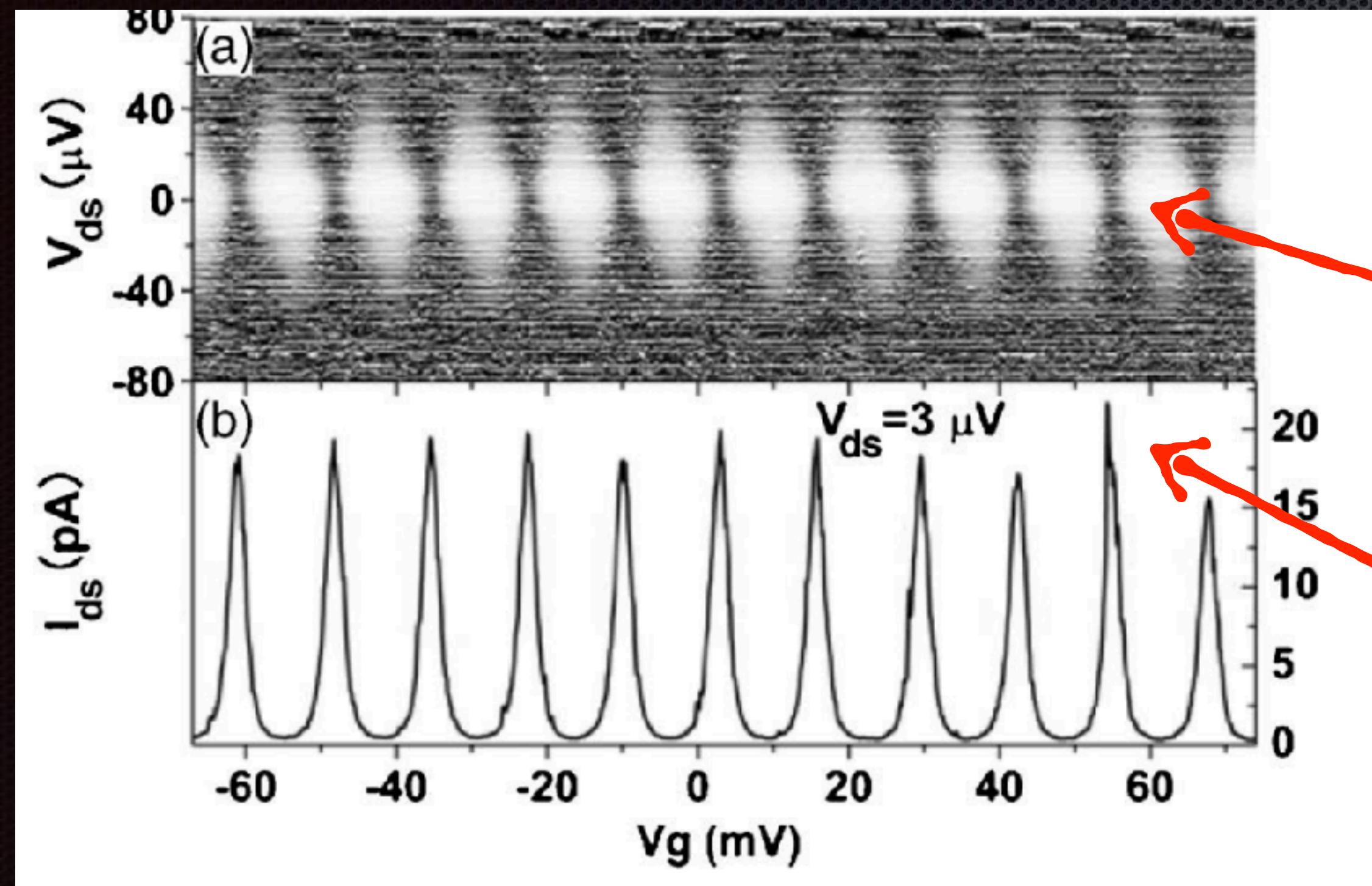
https://en.wikipedia.org/wiki/Threshold_voltage#/media/File:ThresholdFormationNowatermark.gif



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



We can control the current flow by controlling the gate voltage (V_g) and the drain-source voltage V_{sd}

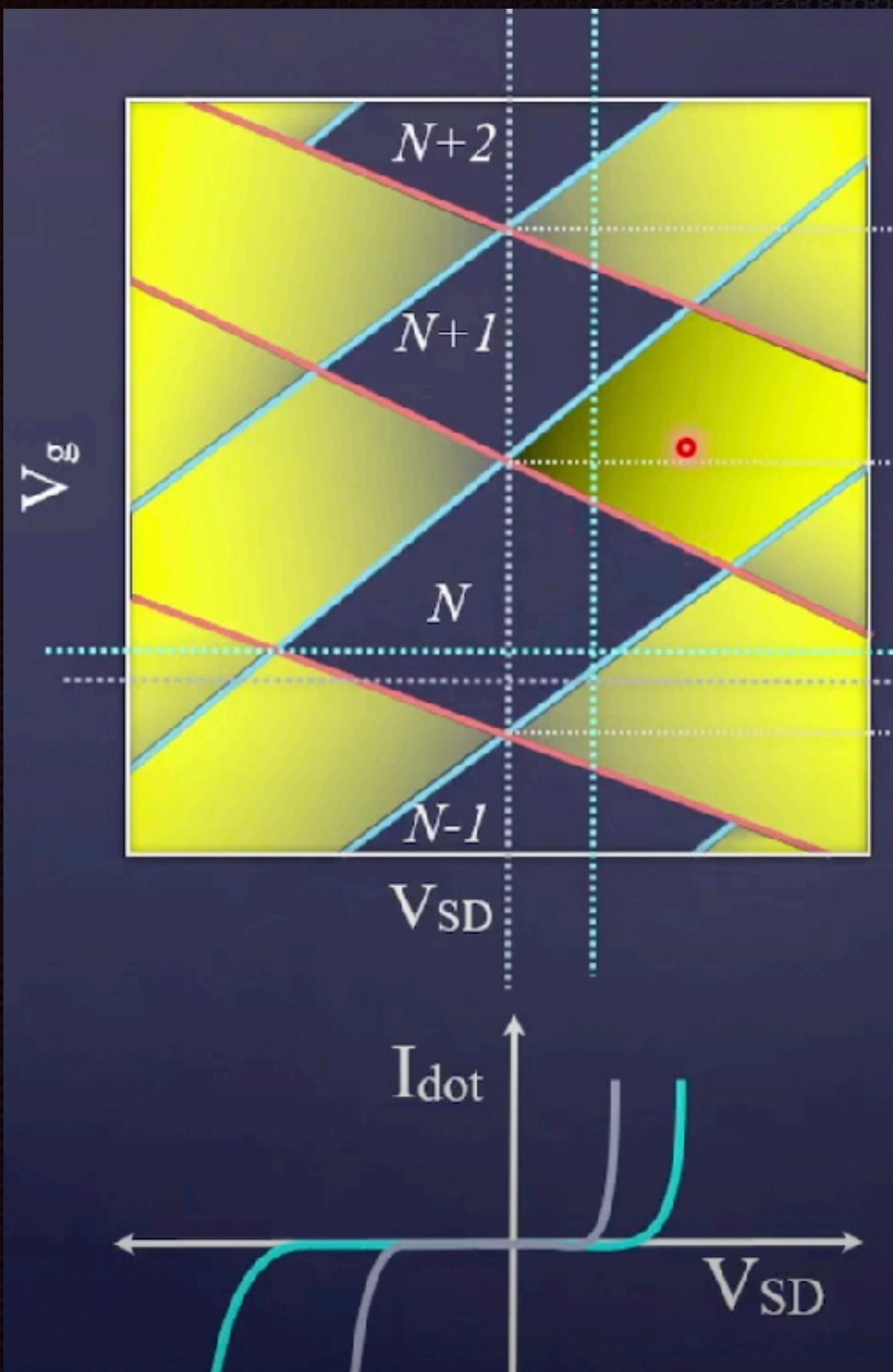
Diamond shape with no current flows inside
(Electron cage)

Current flows as pulses

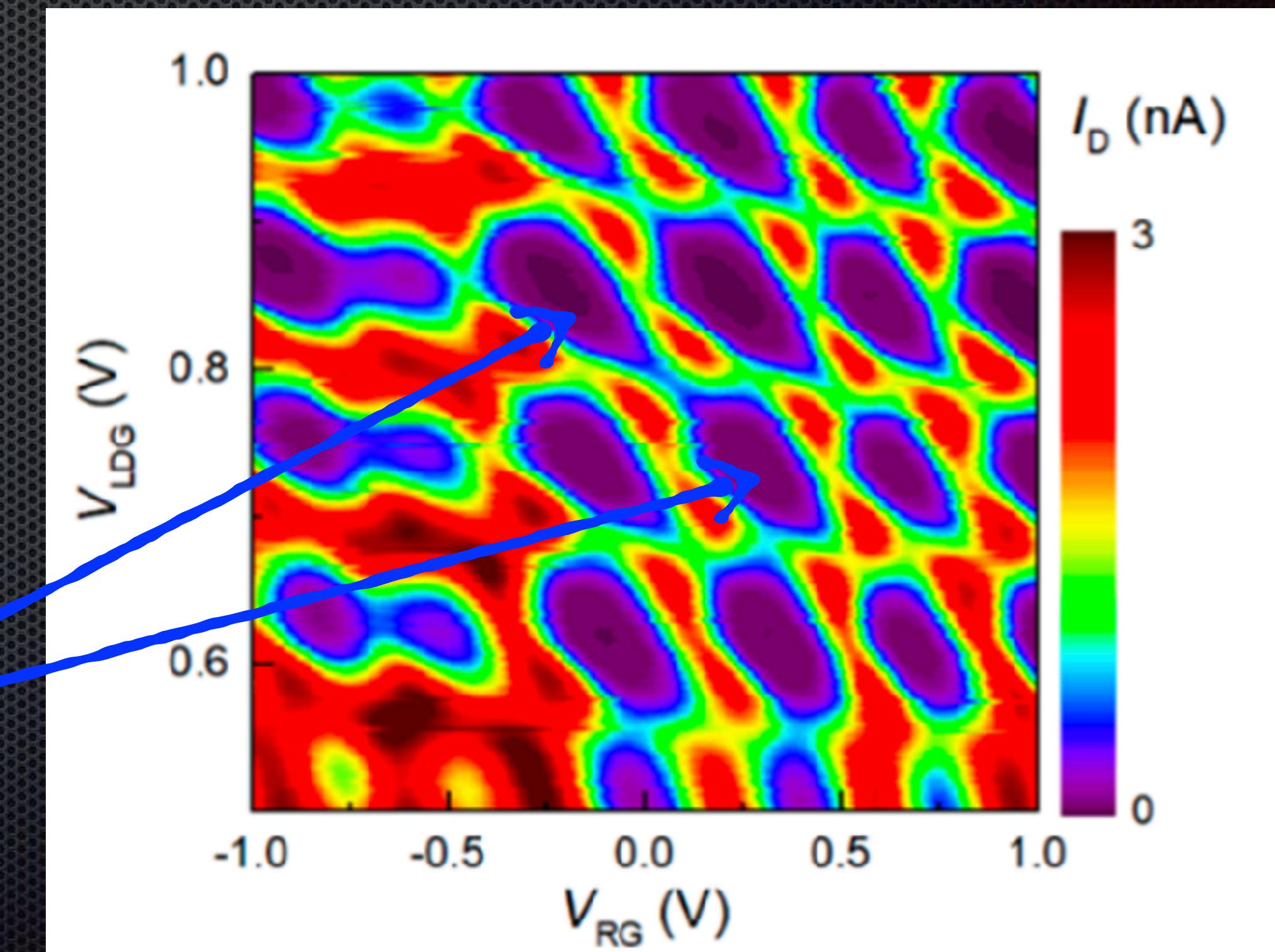
Quantum dot

Coulomb diamonds

Coulomb diamonds can act as traps for the electrons

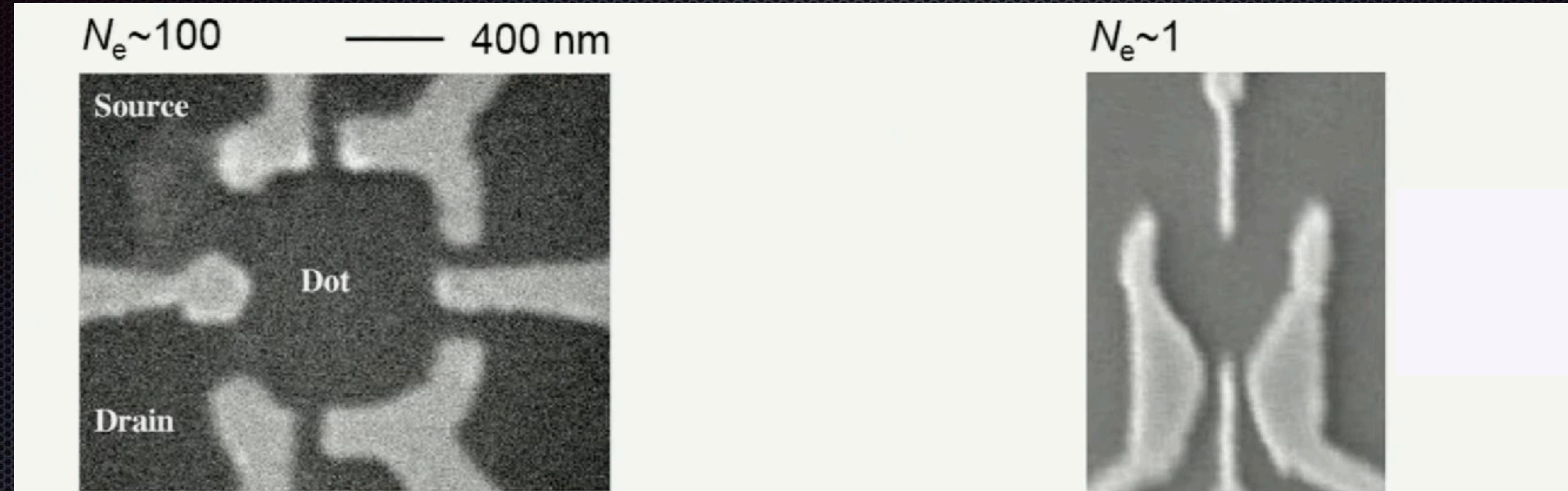


Quantum dots



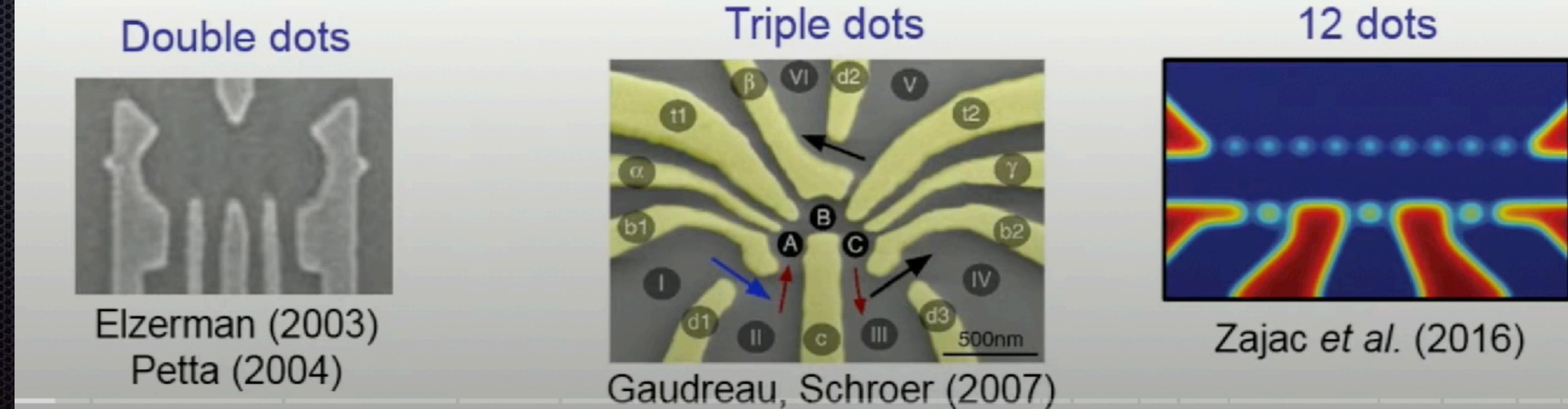
Quantum dot

Quantum dots example



Marcus group (1996)

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



Elzerman (2003)
Petta (2004)

Zajac et al. (2016)

Gaudreau, Schroer (2007)

Qubit dynamics

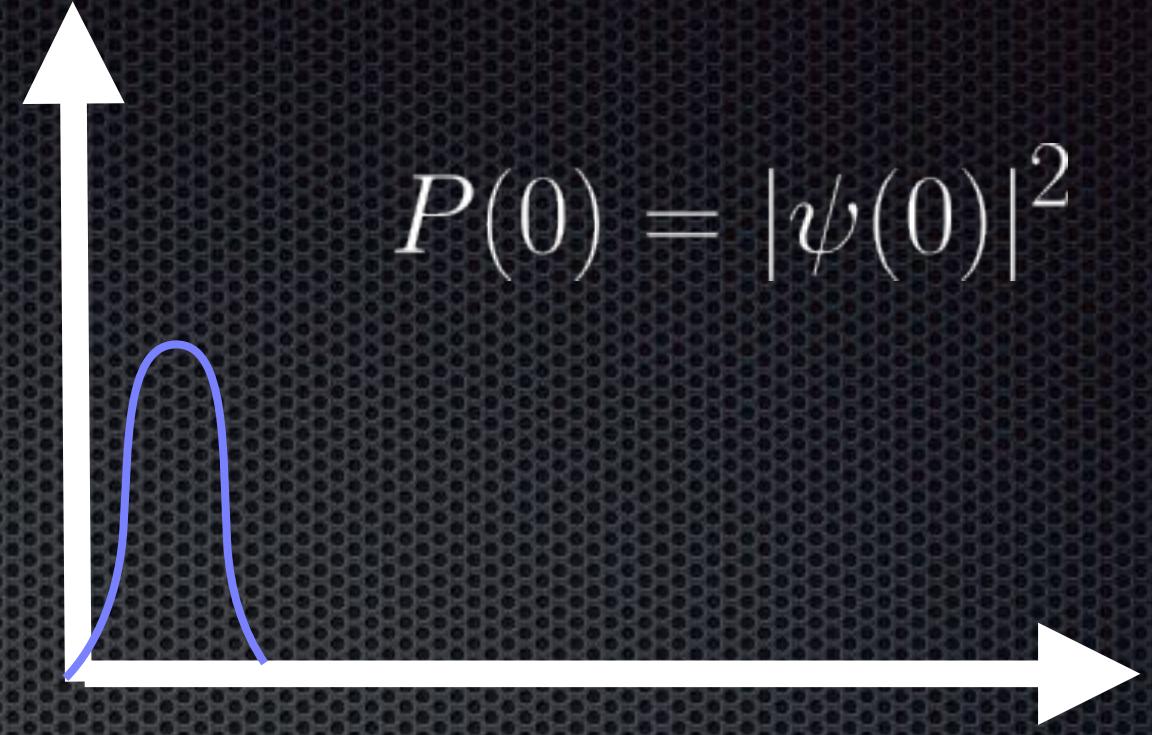
Well, now we know how to cook a quantum dot.
How to do computations on a qubit in a quantum dot?



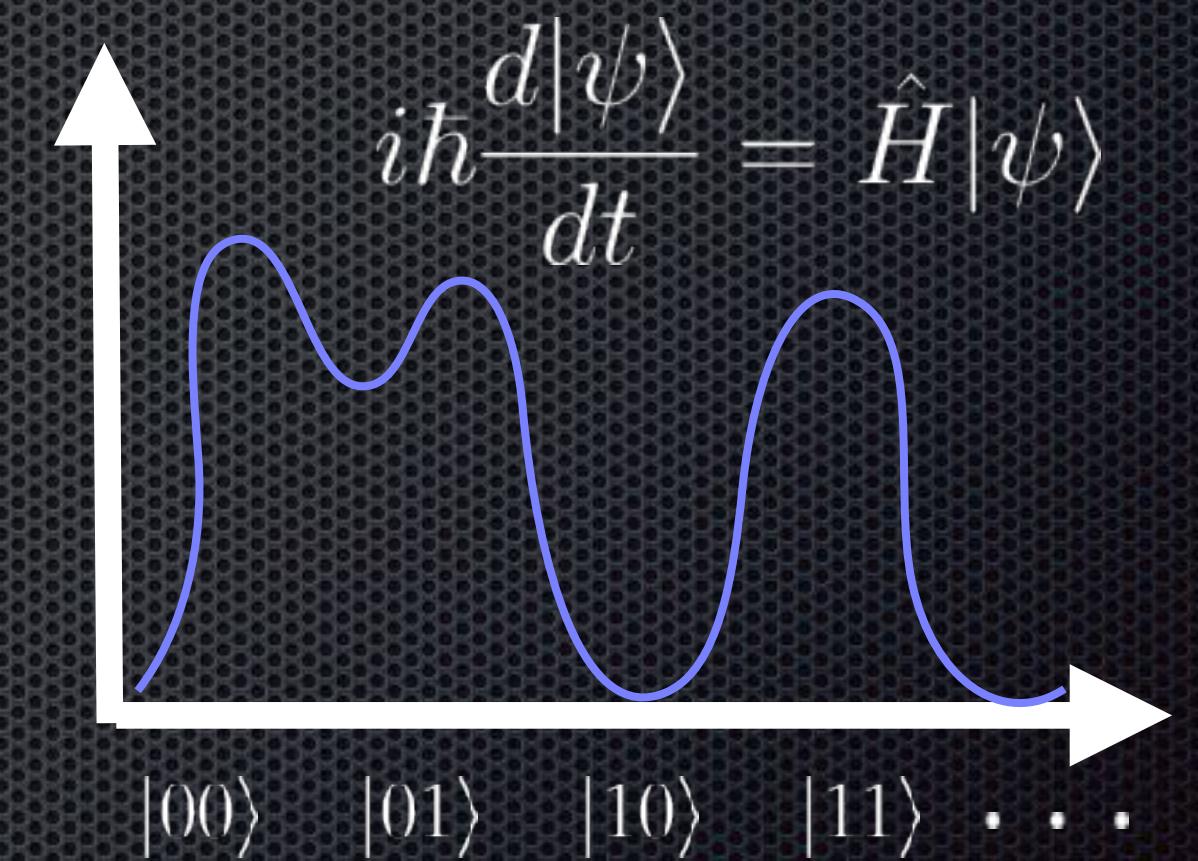
Qubit dynamics

Quantum computation

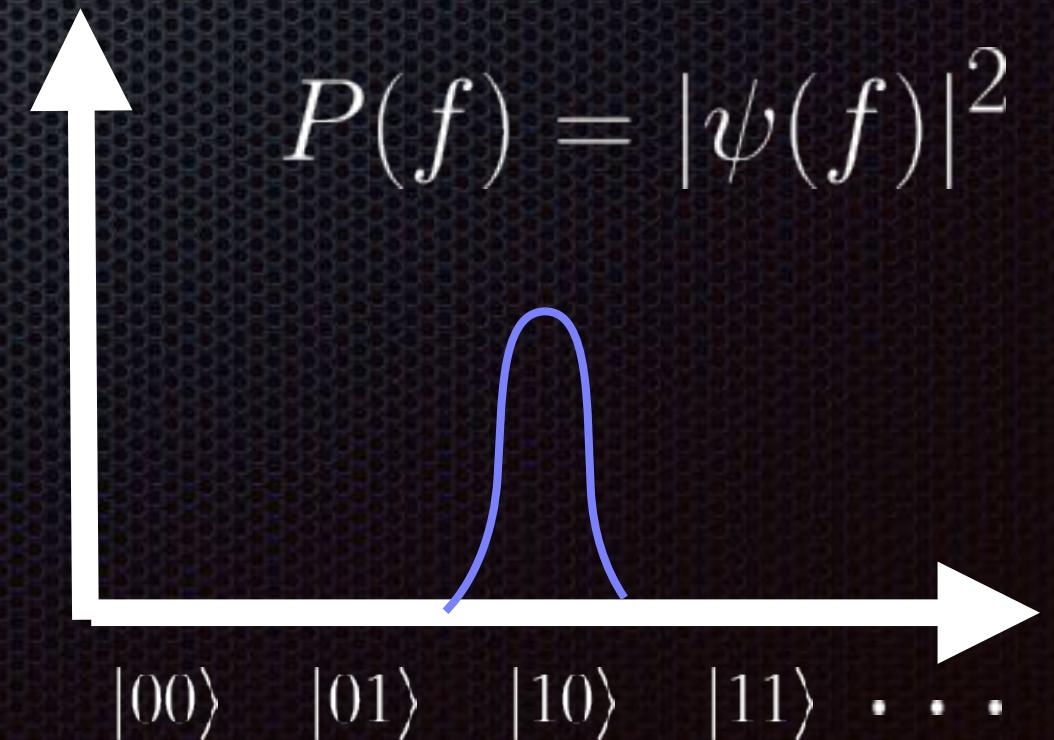
1- Initialize the qubits



2- Processing the qubits

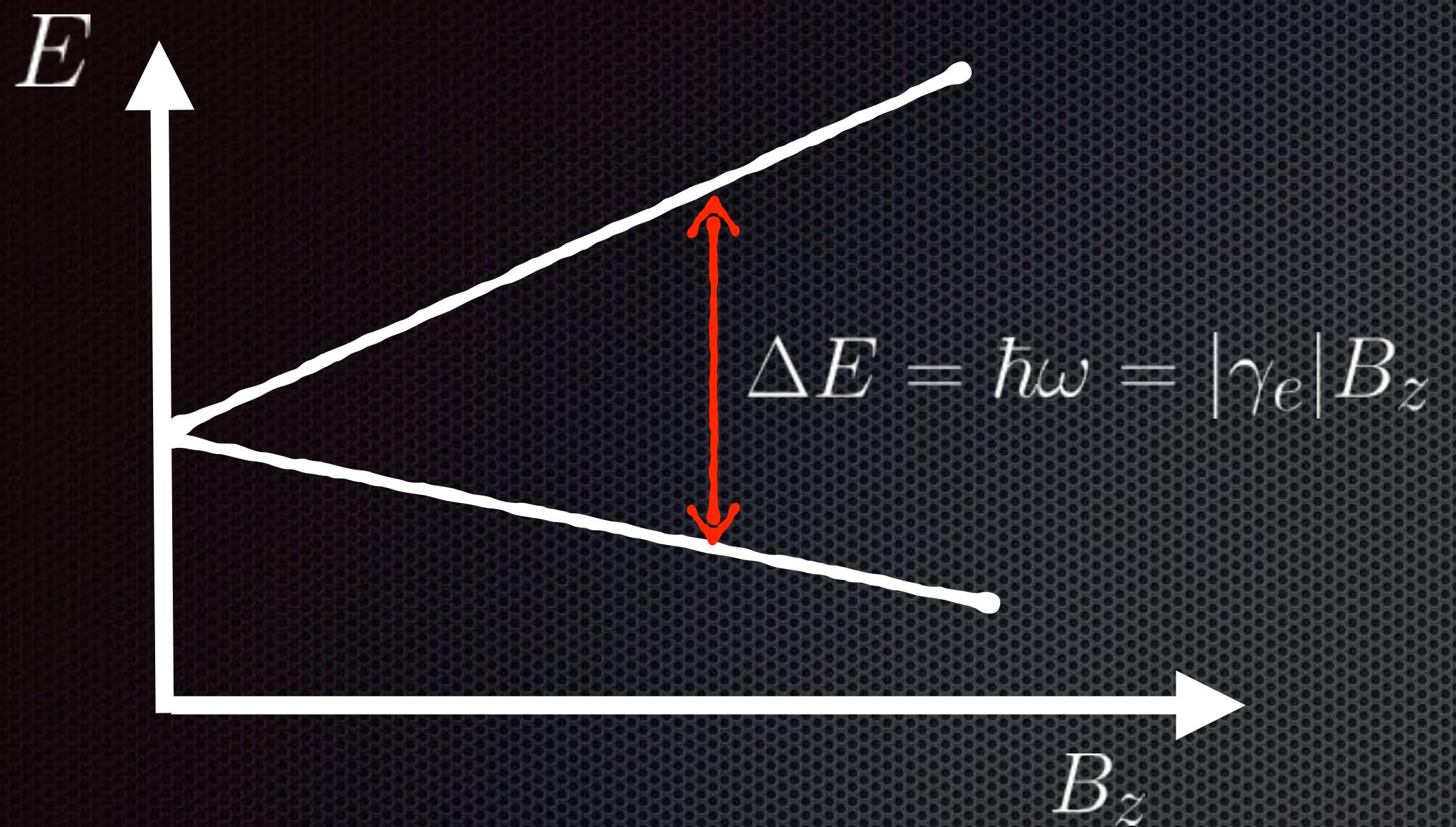


3- Measure the expectation value



Qubit dynamics

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



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

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

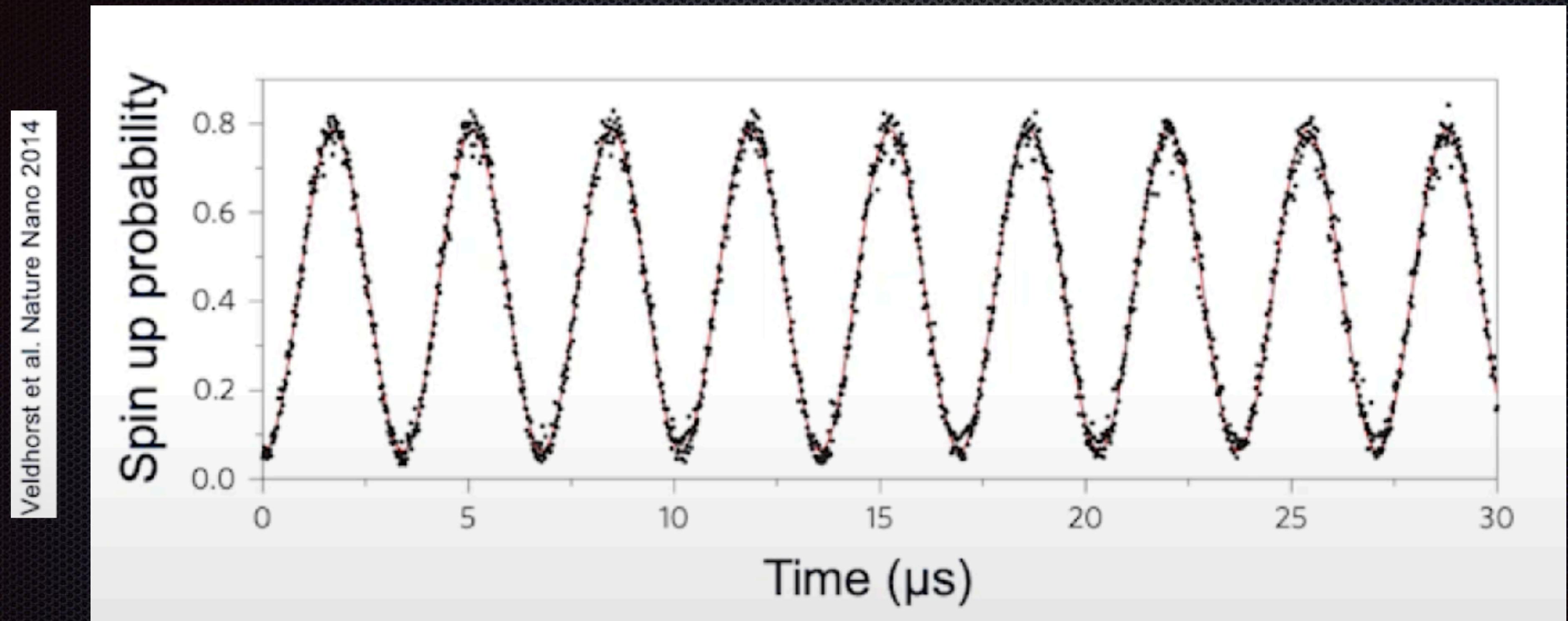
In the presence of magnetic field the electron spin will be randomly in any of the two states.
In the case of static magnetic field the spin states of the electron splits with energy difference.
We can initialize the electron in the zero state by lowering the energy of the quantum dot.

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

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

Qubit dynamics

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**"



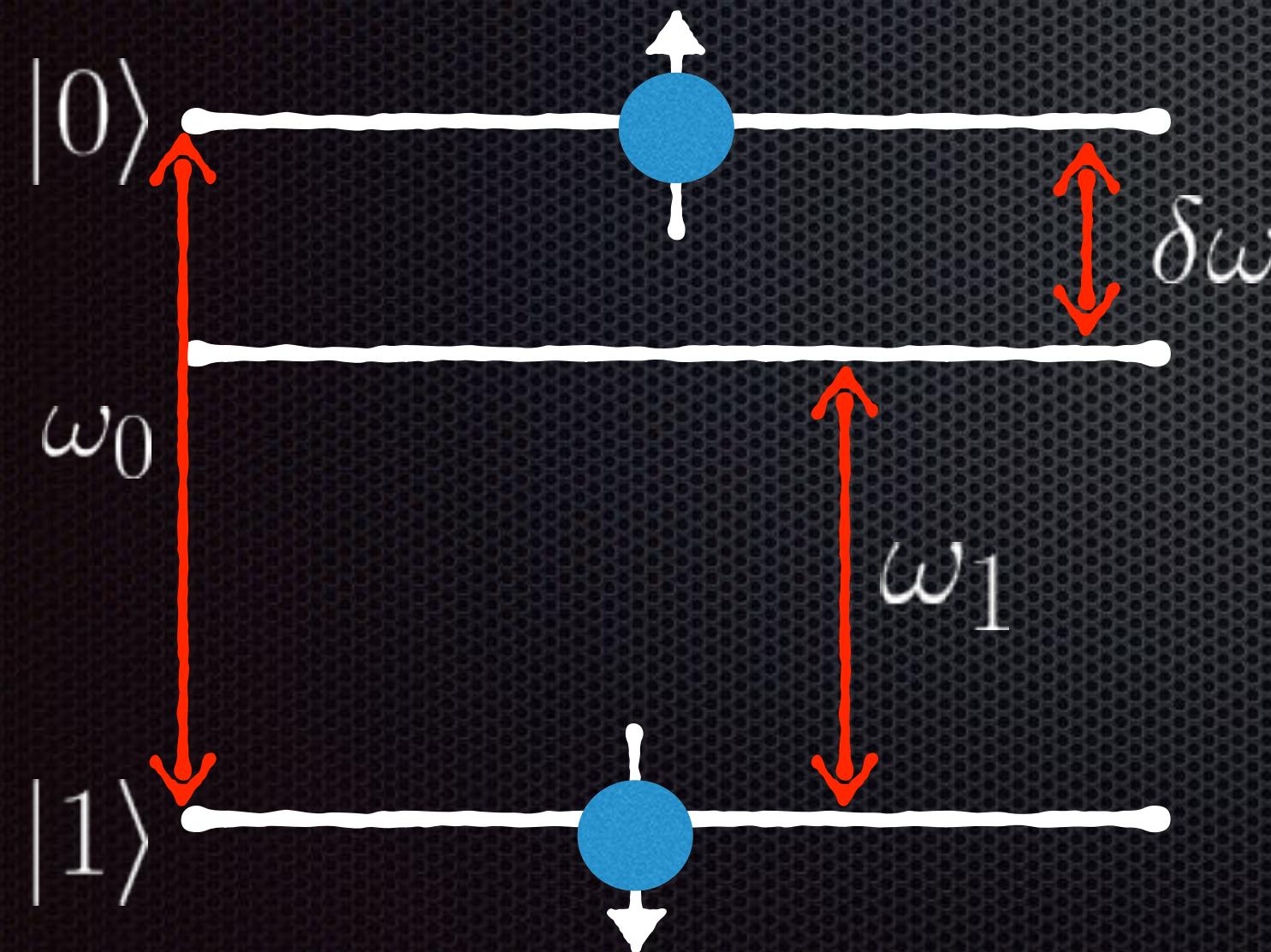
To understand the qubit dynamics we need to realize Rabi oscillations

Qubit dynamics

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

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

$$\hat{H}_{\text{Lab}} = \hat{H}_0 + \hat{H}_1 = \frac{\omega_0}{2} \sigma_z + \frac{\omega_1}{2} (\cos \omega t + \phi) \sigma_x \quad \omega_0 = |\gamma_e| B_z \quad \omega_1 = |\gamma_e| B_1$$



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

Qubit dynamics

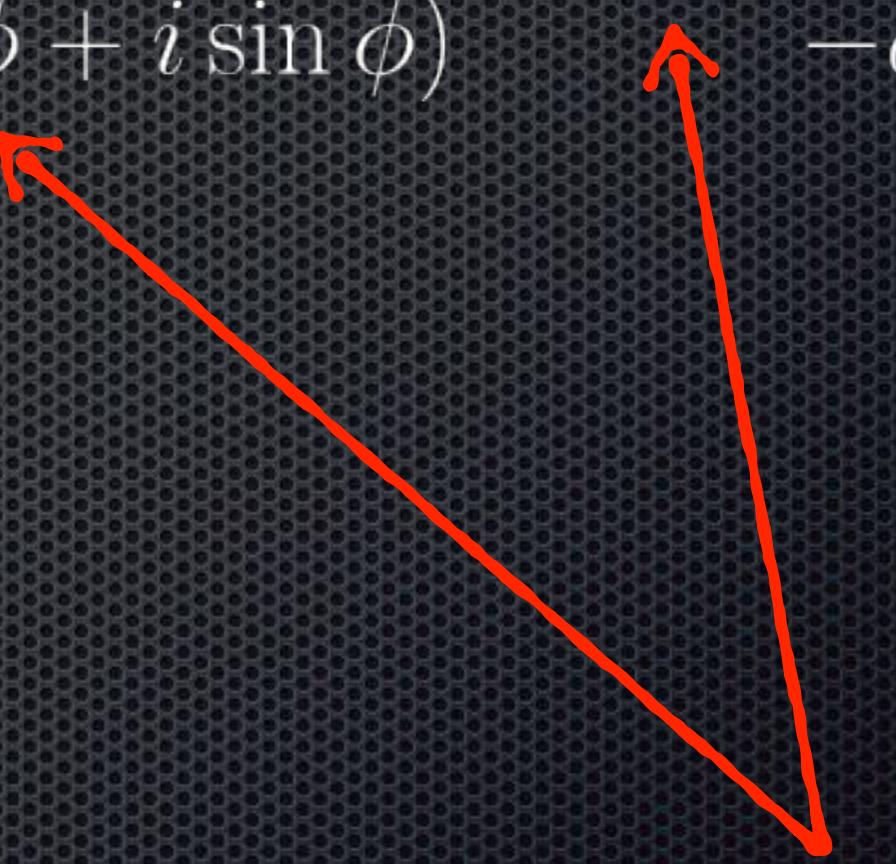
After tedious calculations, the Hamiltonian in the rotating frame

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

Generic form of the Hamiltonian in a rotating frames

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

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



Off-diagonal terms that
Couples the two spin states

Qubit dynamics

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

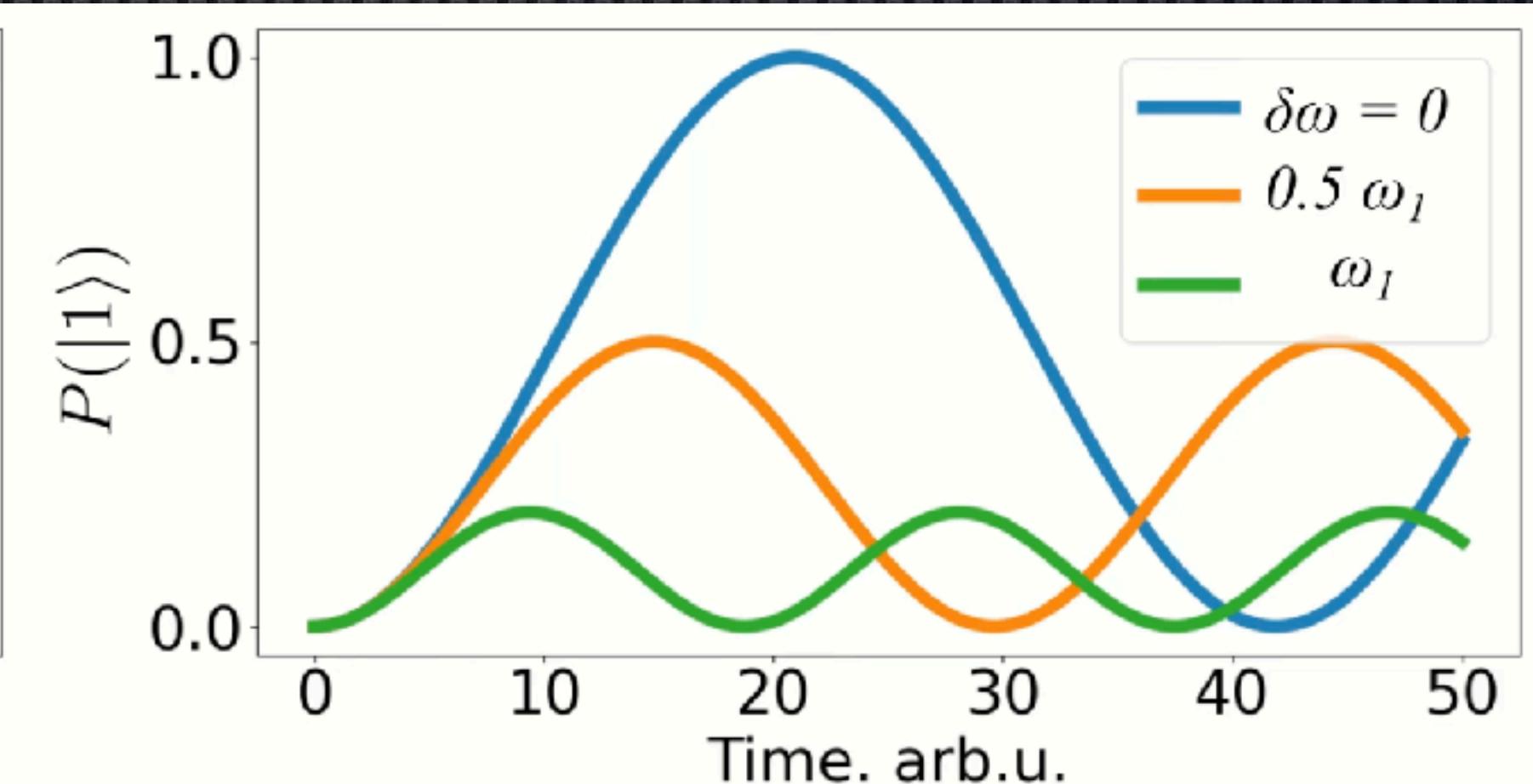
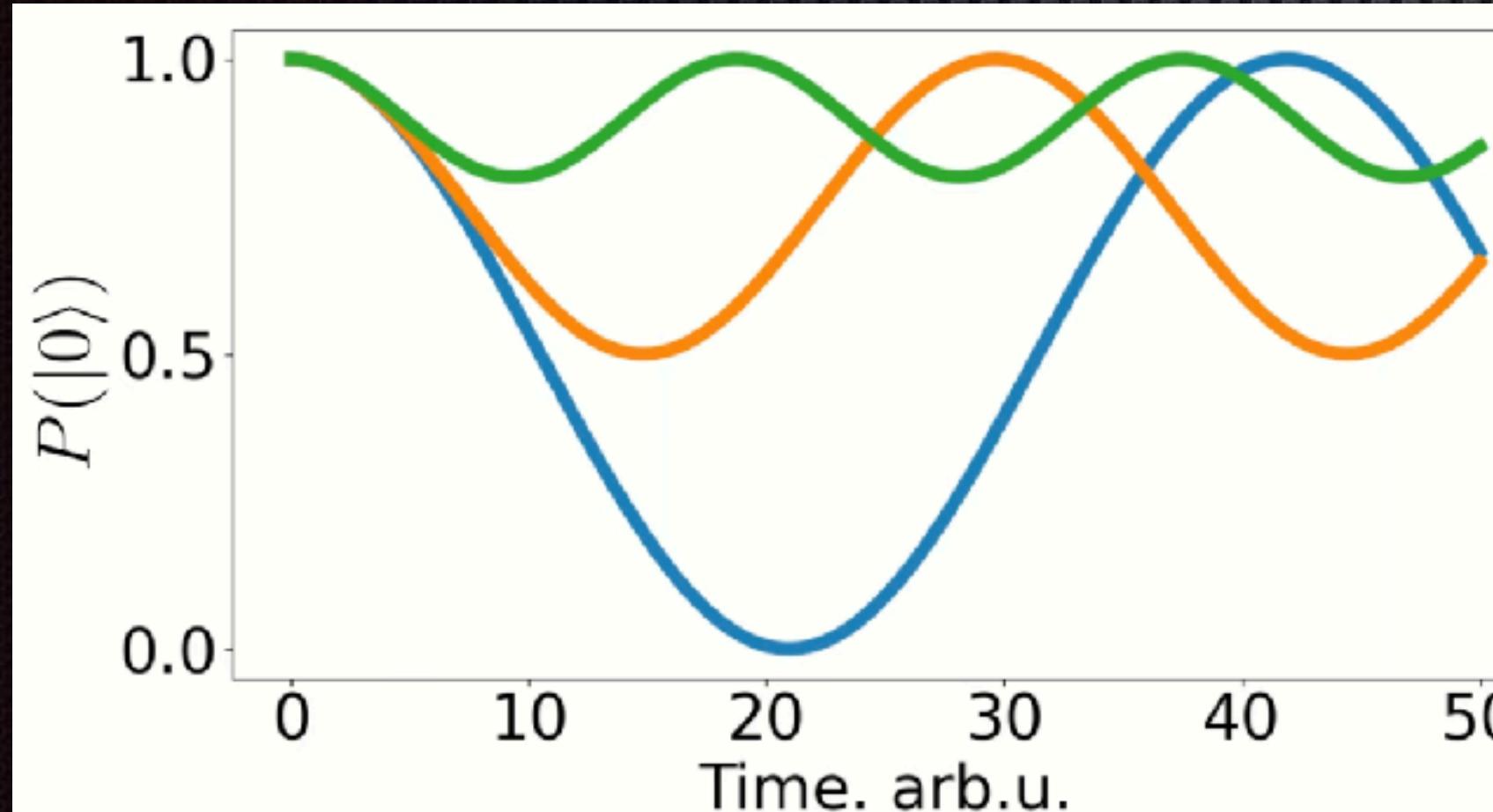
$$|\psi_{\text{rot}}(t)\rangle = \left(\cos \frac{\Omega_t}{2} - i \sin \frac{\Omega_t \delta\omega}{2} \right) |0\rangle - i \sin \frac{\Omega_t \omega_1}{4} e^{-i\phi} |1\rangle$$

With the probability of measuring the electron in state 1

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

With Rabi frequency

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



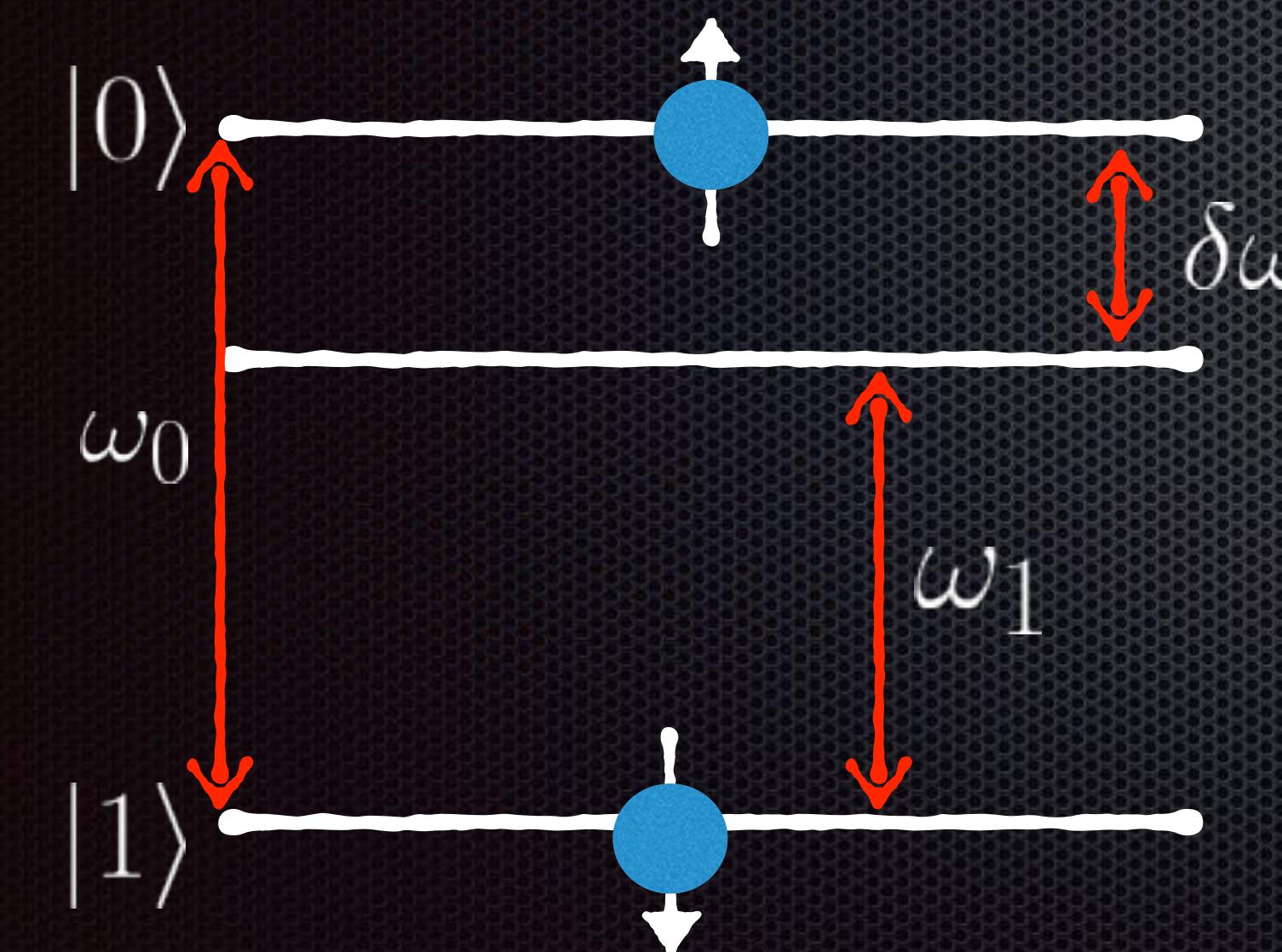
In the non-resonance case
the oscillation never reach
the state 1 or zero

Qubit dynamics

In the resonance case:

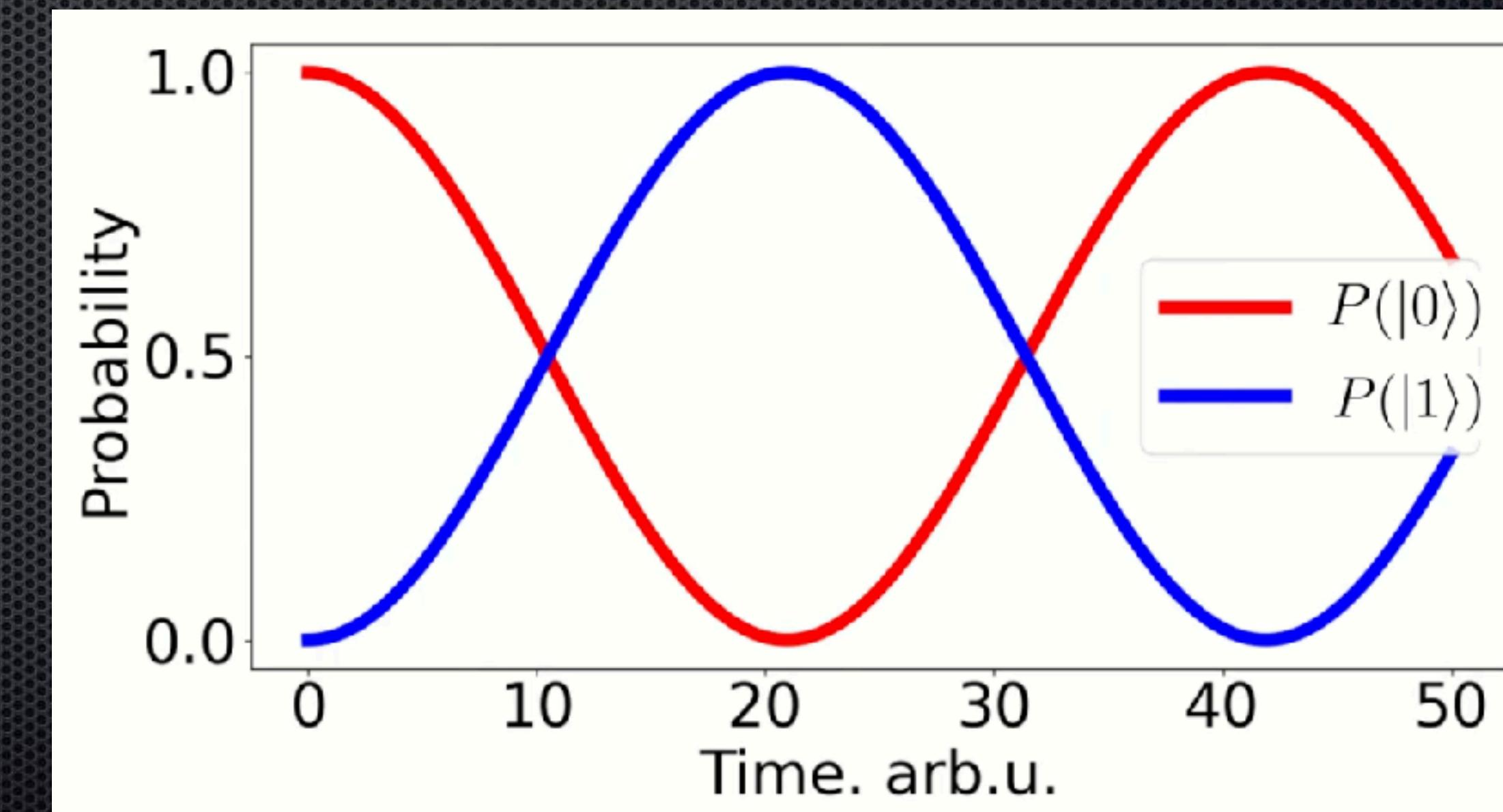
$$\delta\omega = 0$$

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



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

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

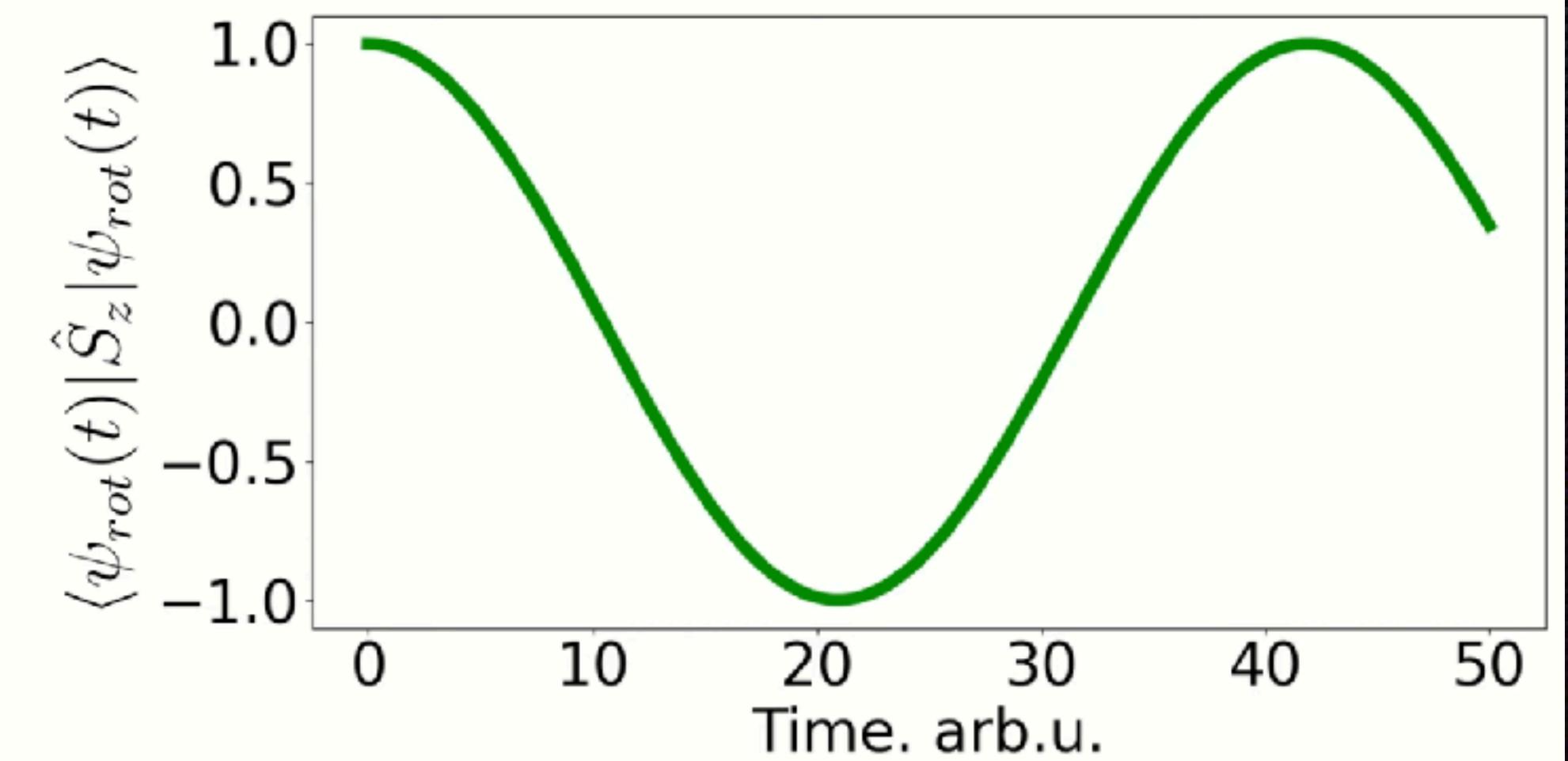
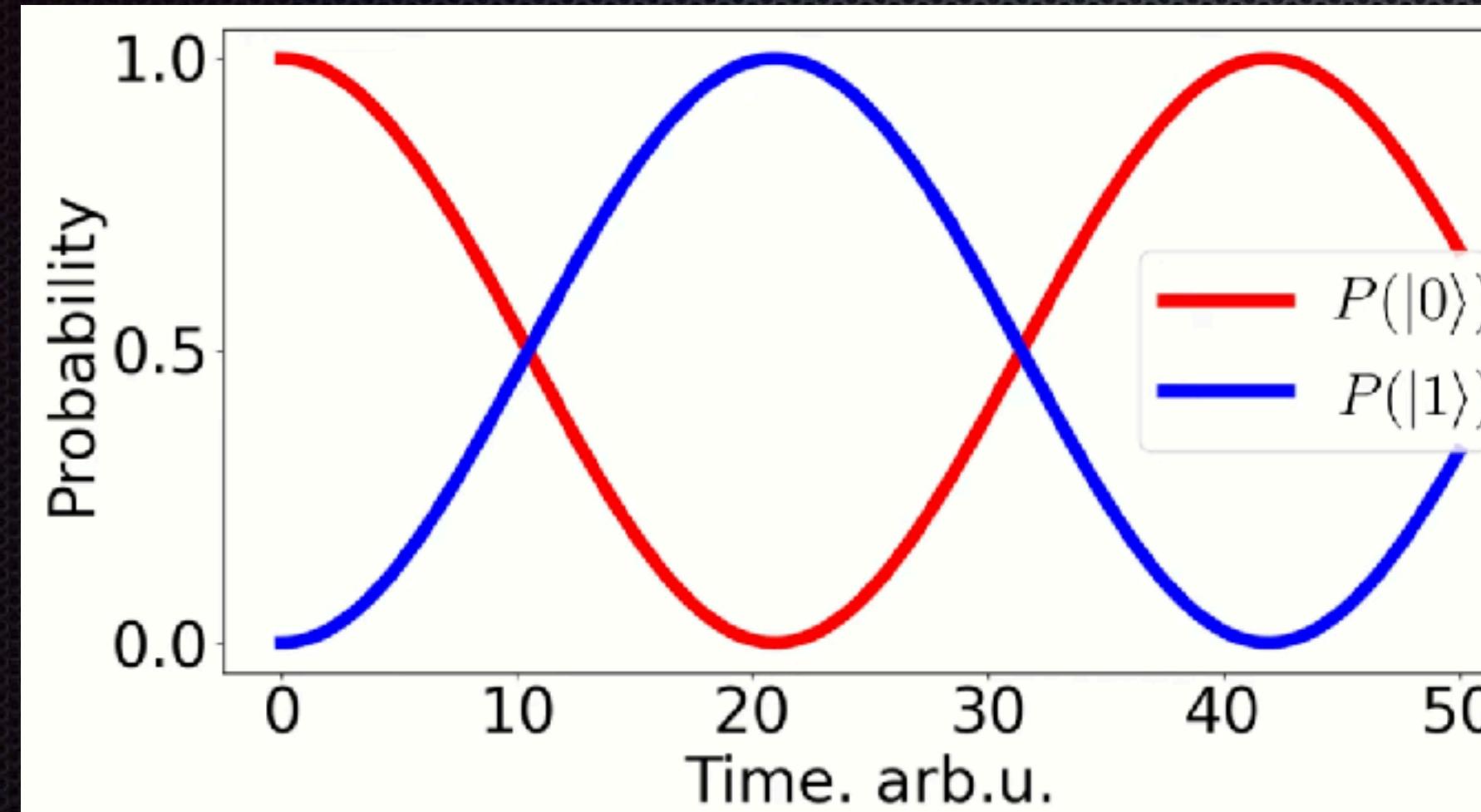


Maximal Rabi
Oscillations

Qubit dynamics

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 dynamics

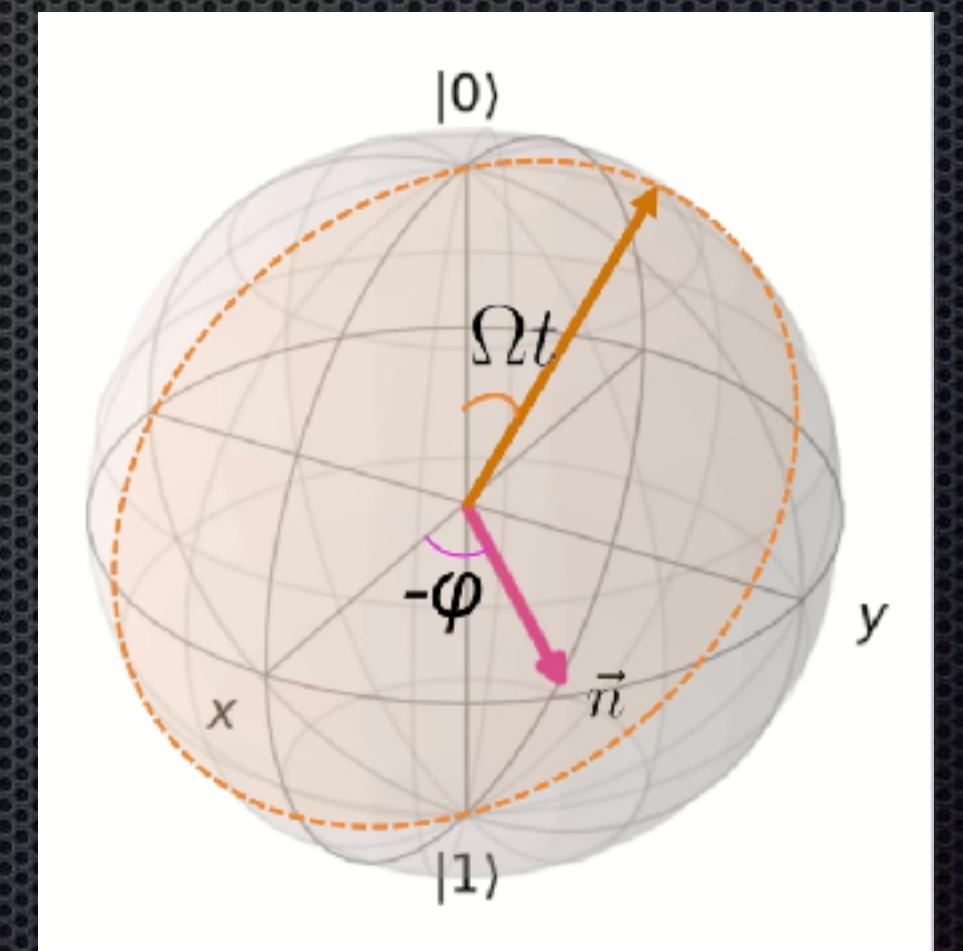
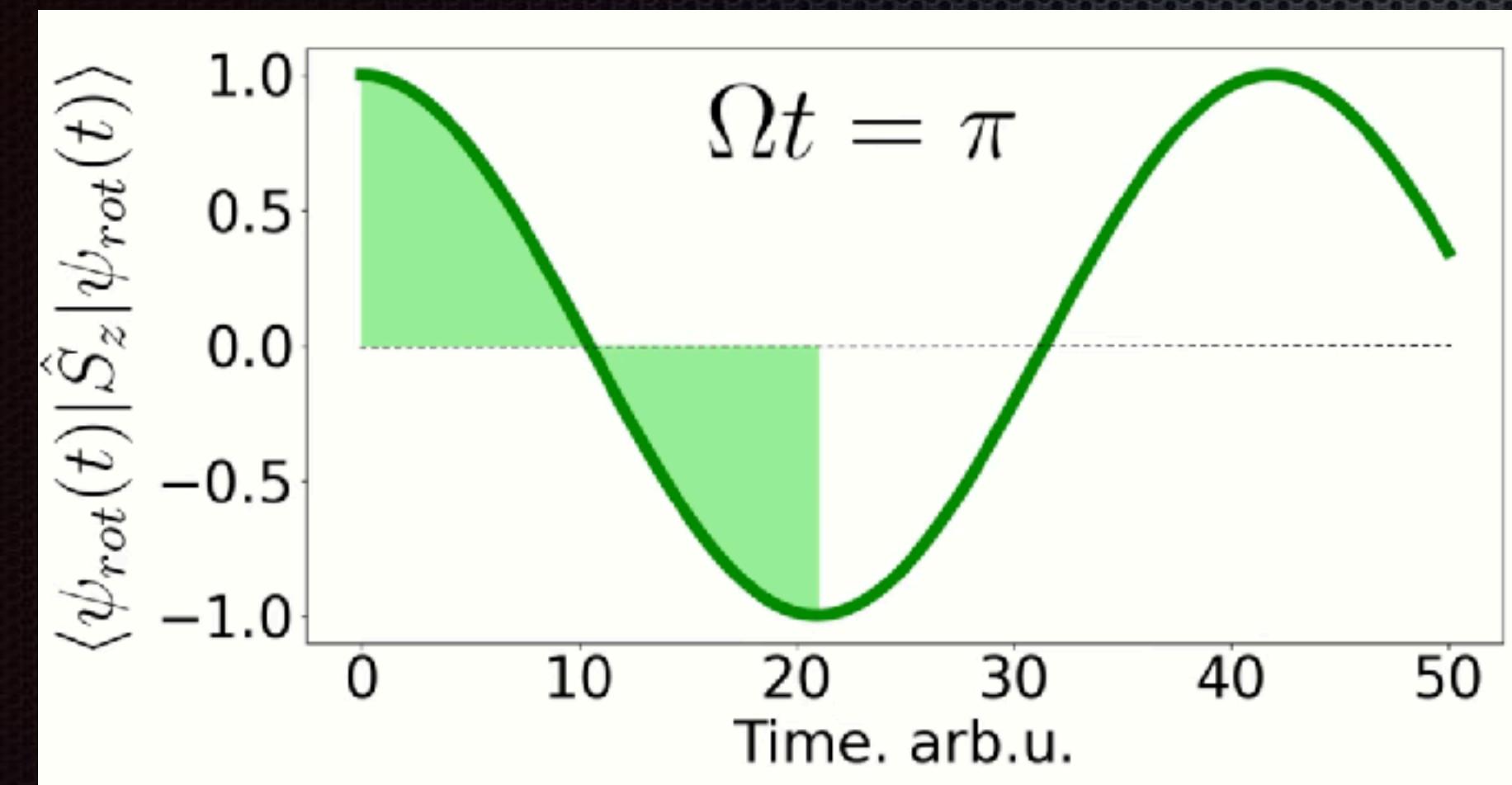
Both static and dynamic magnetic fields define the rotation of the qubit

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

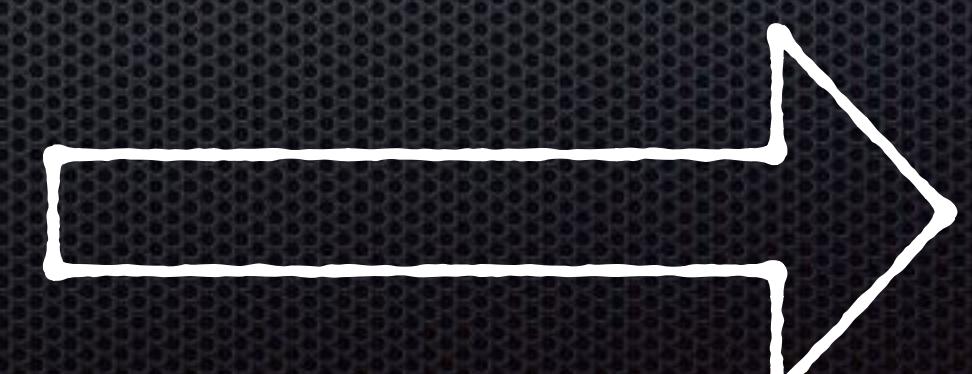
$$\delta\omega = 0$$

$$\vec{n} = (\cos \phi; -\sin \phi, 0)$$

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



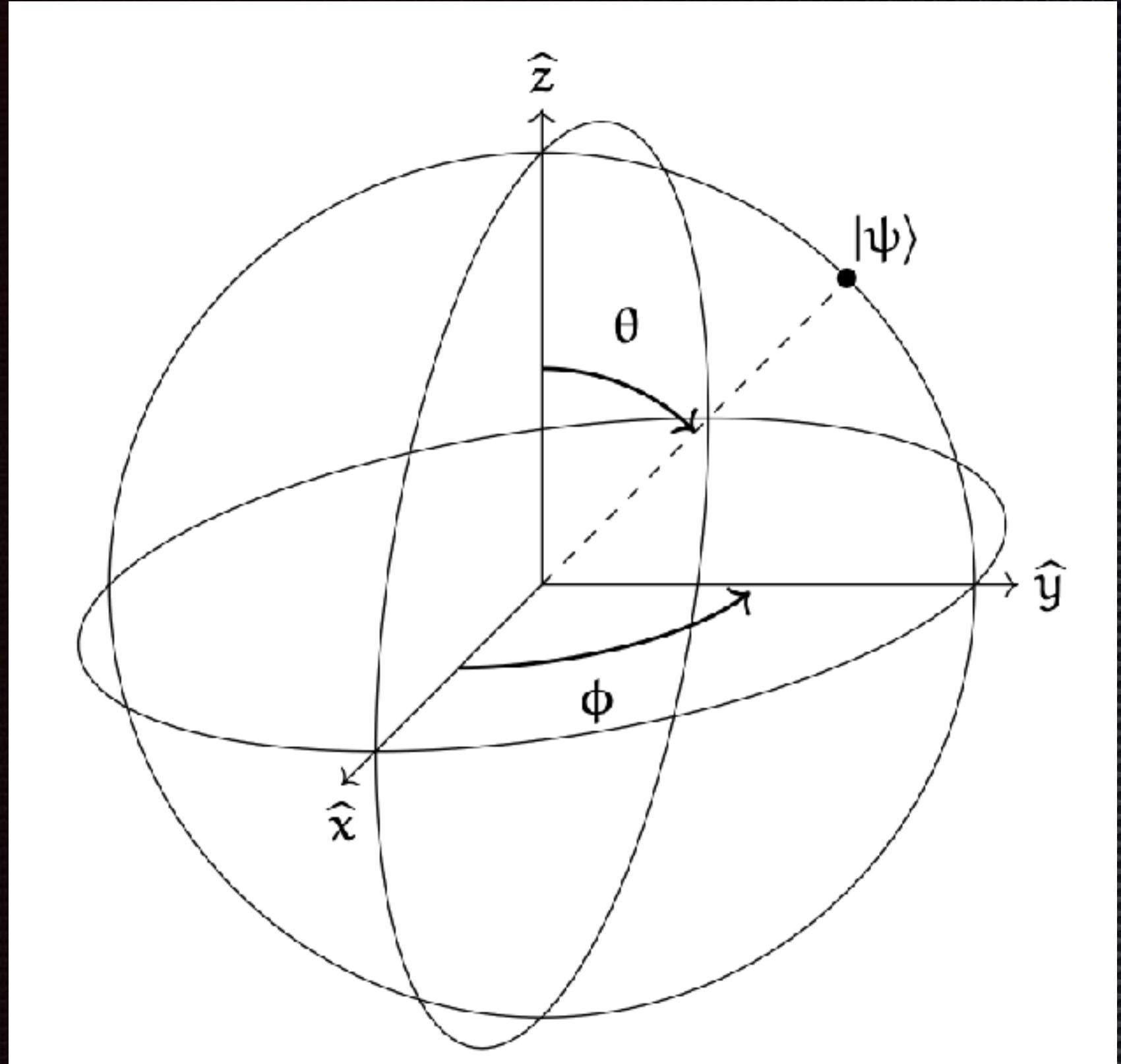
Pi pulses lead to the quantum gates



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

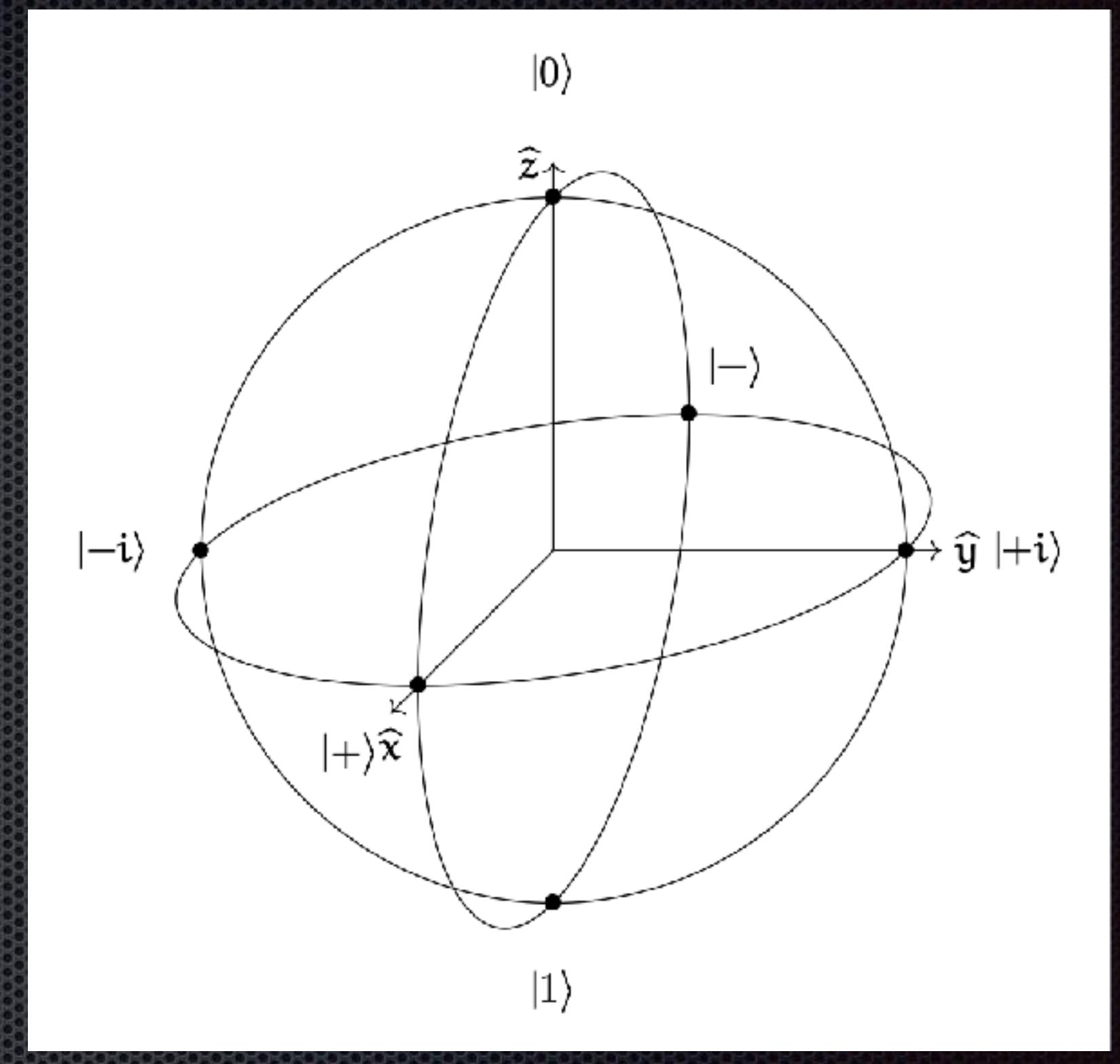


<http://threeplusone.com/gates>

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

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

Location of the orthogonal qubit states



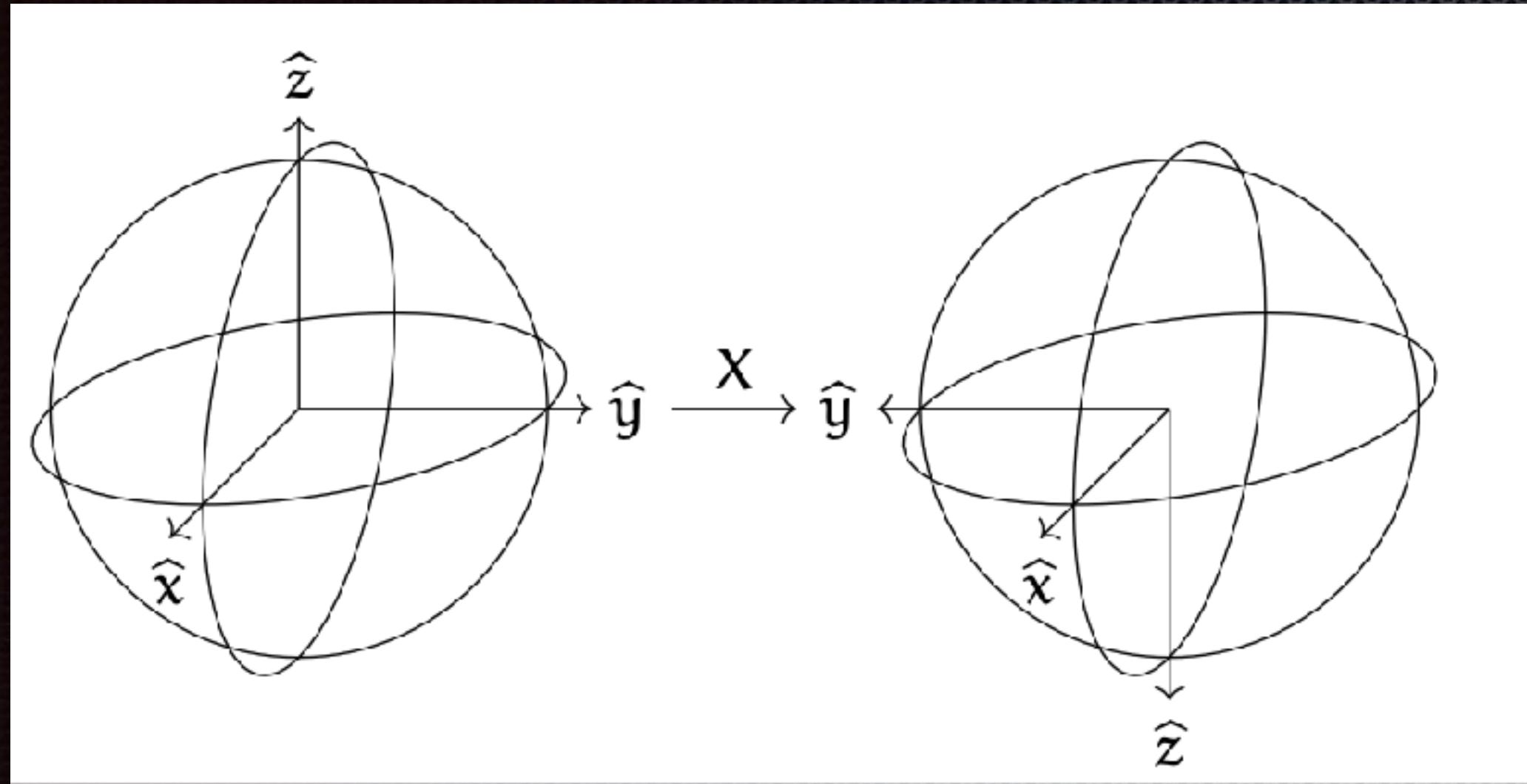
X basis	$ +\rangle = \frac{1}{\sqrt{2}}(0\rangle + 1\rangle)$	$\hat{n} = (+1, 0, 0)$
	$ -\rangle = \frac{1}{\sqrt{2}}(0\rangle - 1\rangle)$	$\hat{n} = (-1, 0, 0)$
Y basis	$ +i\rangle = \frac{1}{\sqrt{2}}(0\rangle + i 1\rangle)$	$\hat{n} = (0, +1, 0)$
	$ -i\rangle = \frac{1}{\sqrt{2}}(0\rangle - i 1\rangle)$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

Single qubit gates

<http://threeplusone.com/gates>

Pauli-X gate (bit flip)

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



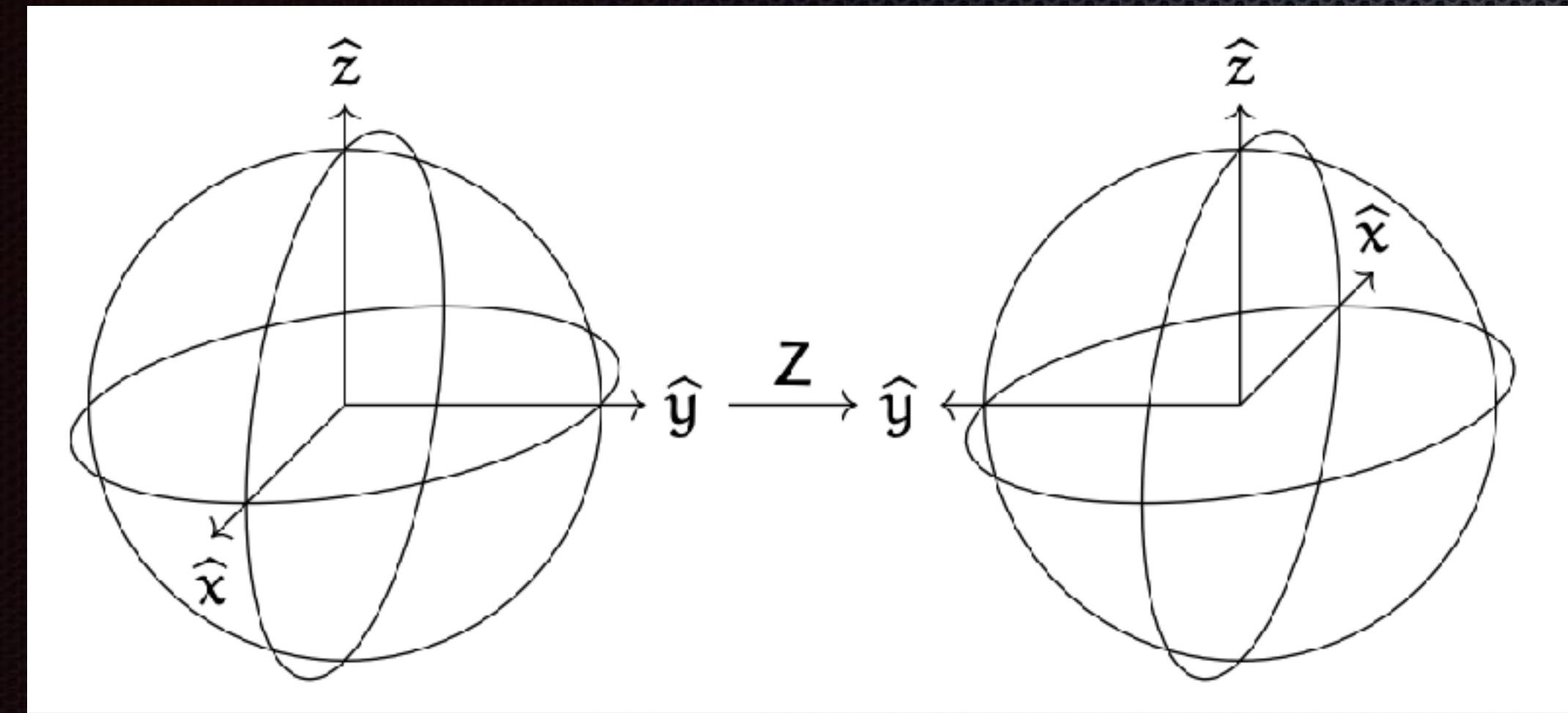
$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
A quantum circuit diagram showing a single horizontal line representing a qubit. The line passes through a square box labeled 'X', which represents the Pauli-X gate.

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

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

Pauli-Z gate (phase flip)

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



$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
A quantum circuit diagram consisting of a single horizontal line representing a qubit. In the center of this line is a small square box with the letter 'Z' written inside, representing the Pauli-Z gate.

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

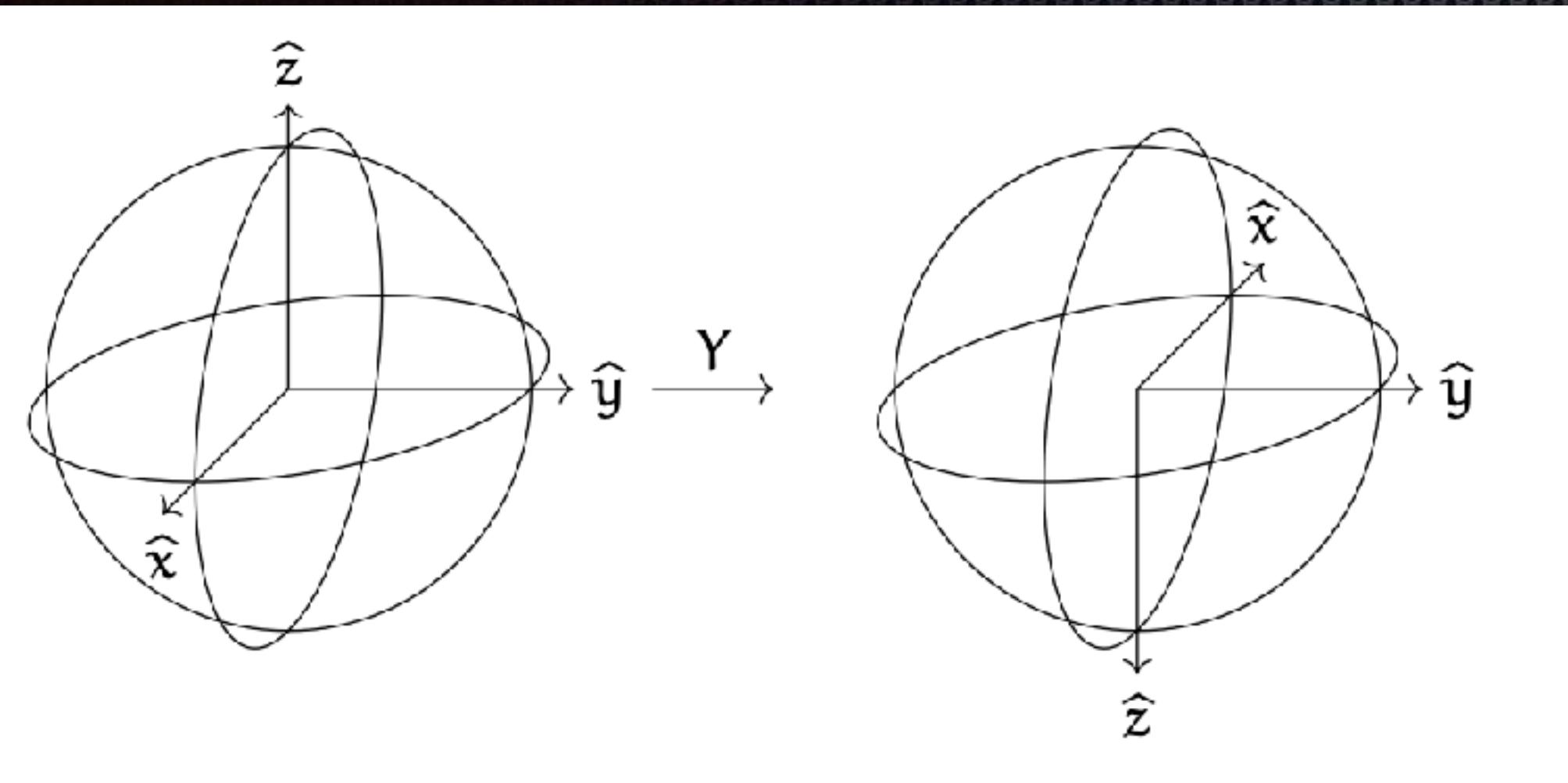
$$Z|1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} = -|1\rangle$$

Single qubit gates

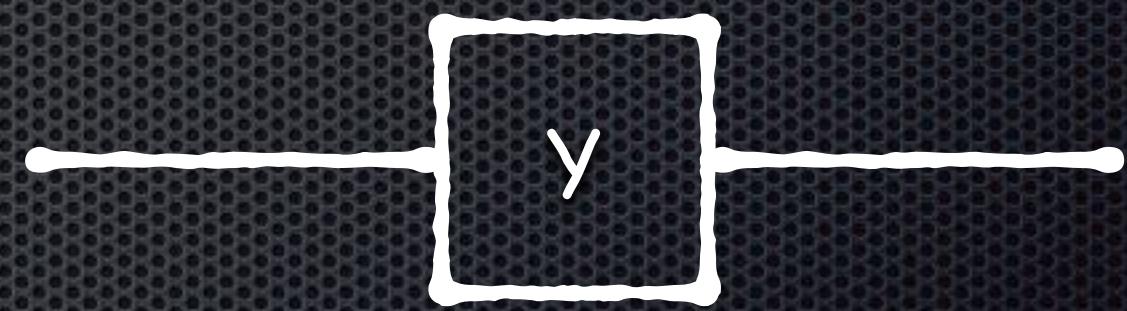
<http://threeplusone.com/gates>

Pauli-Y gate

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



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



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

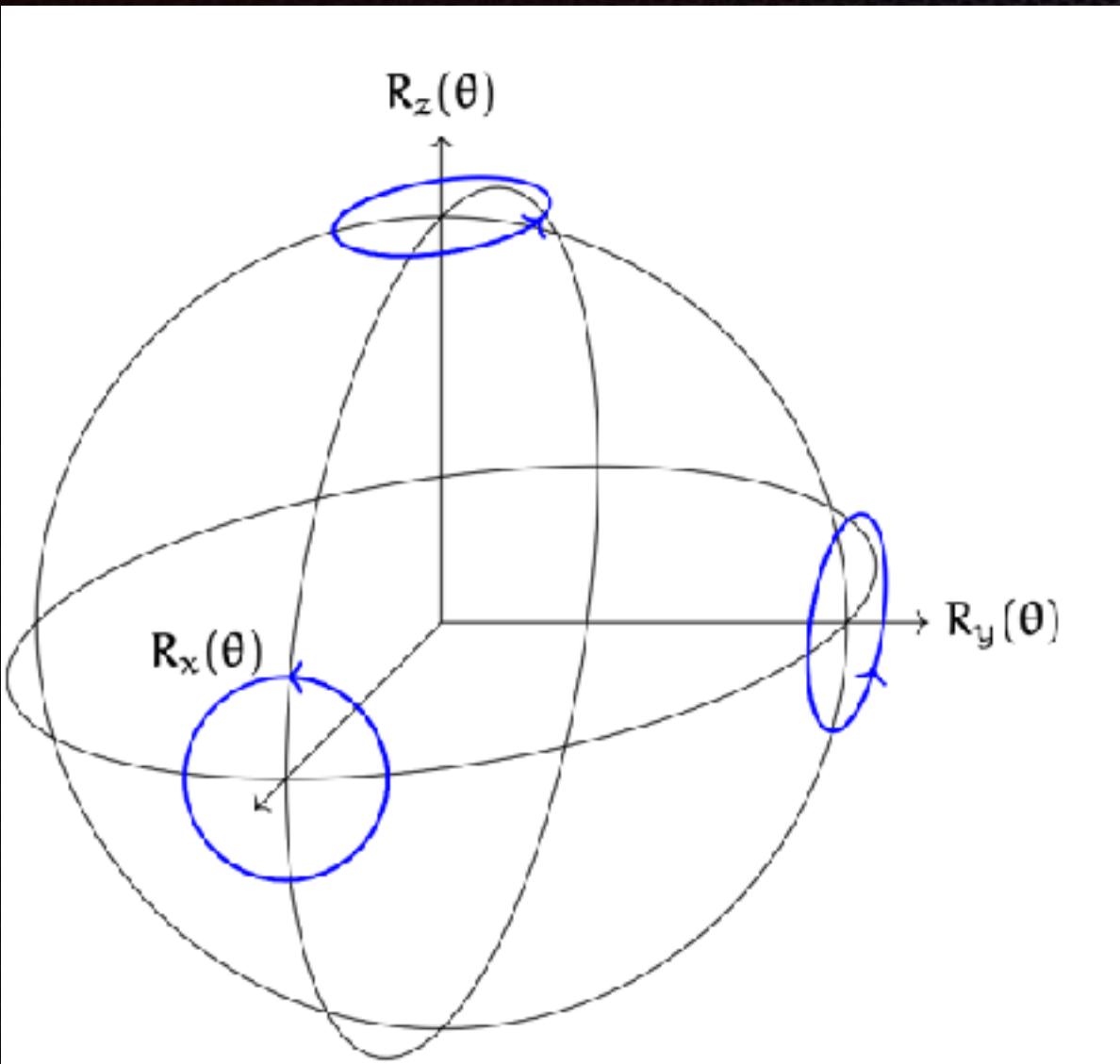
$$Y|1\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -i \\ 0 \end{pmatrix} = -i|0\rangle$$

Single qubit gates

<http://threeplusone.com/gates>

Pauli Rotation gate

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



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

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

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

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

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

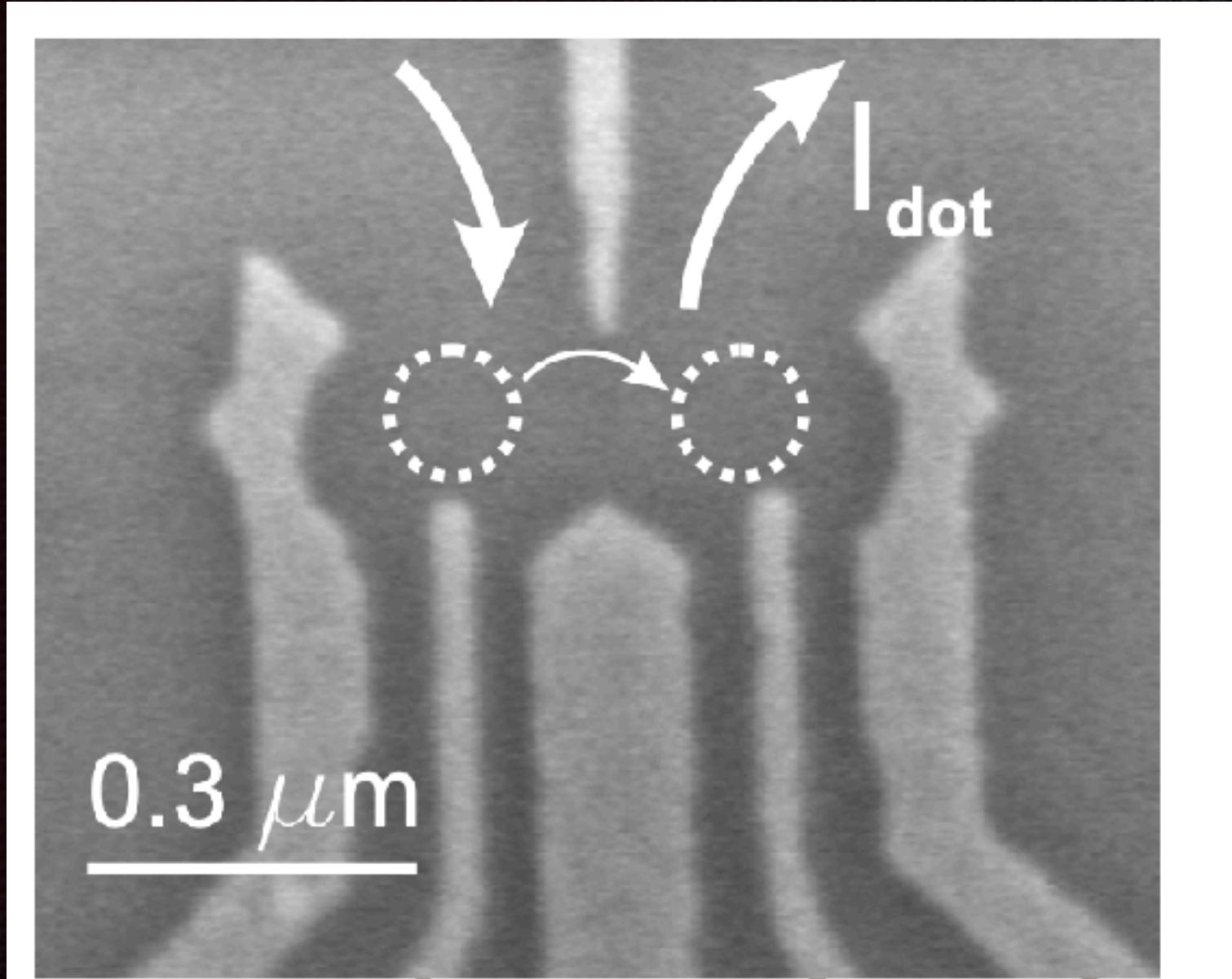


$$H|0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$$

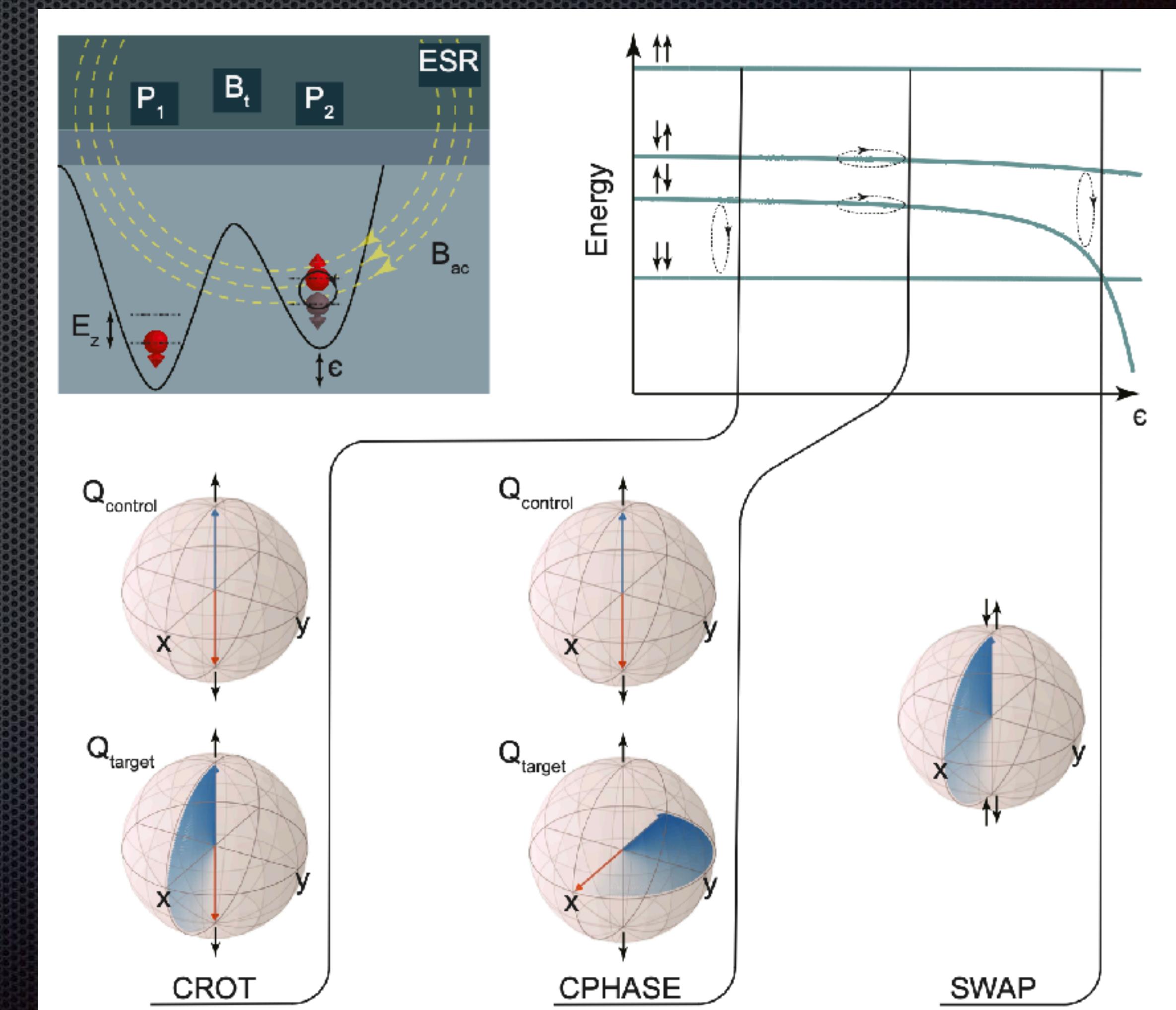
$$H|1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$$

Two qubit gates

Double quantum dot



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

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

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

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

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

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

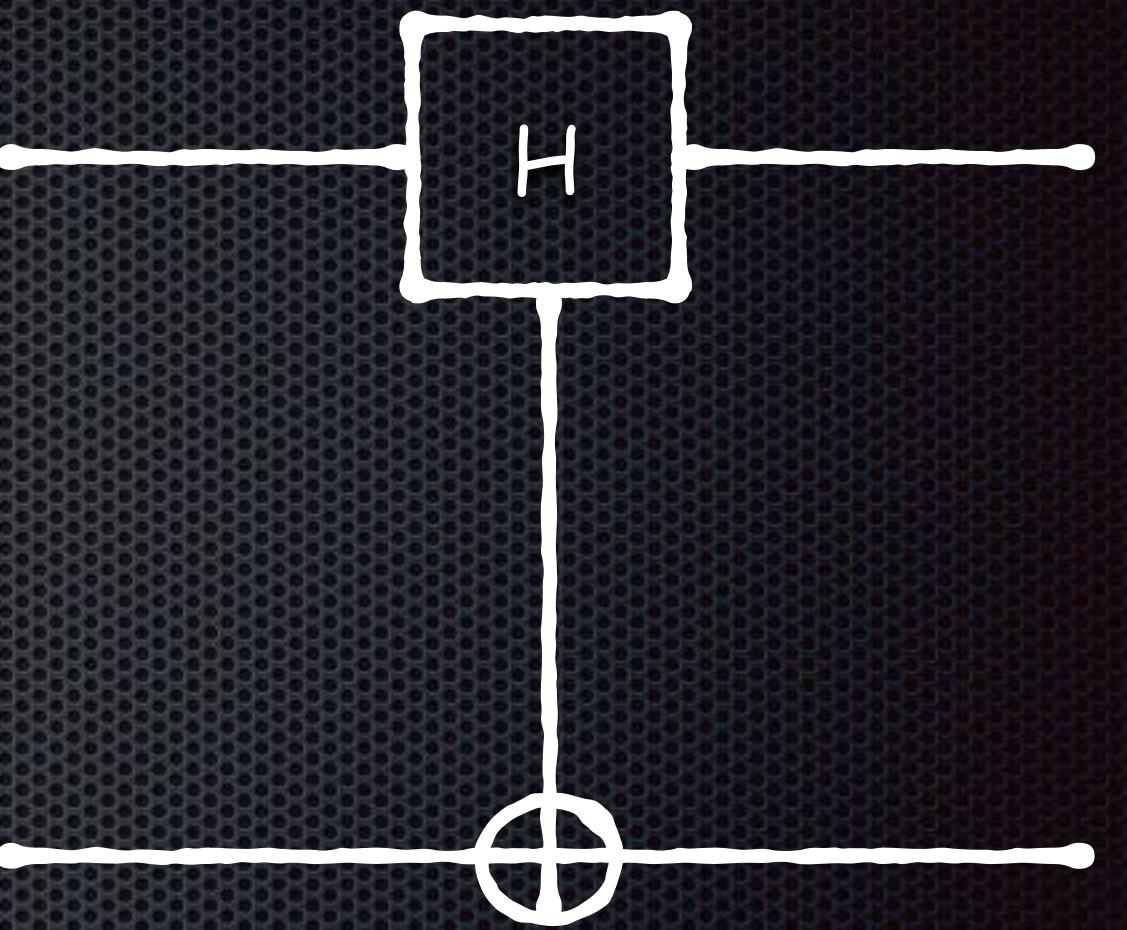
Two qubit gates

Control Not gate

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

Control qubit

Target qubit



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

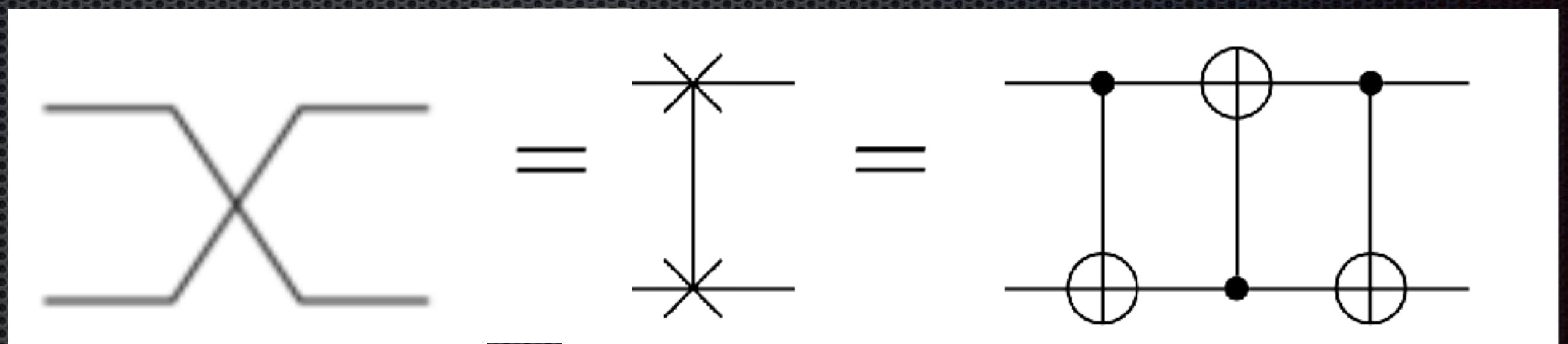
$$\text{CNOT}|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|11\rangle + \alpha_{11}|10\rangle$$

Two qubit gates

Swap gate

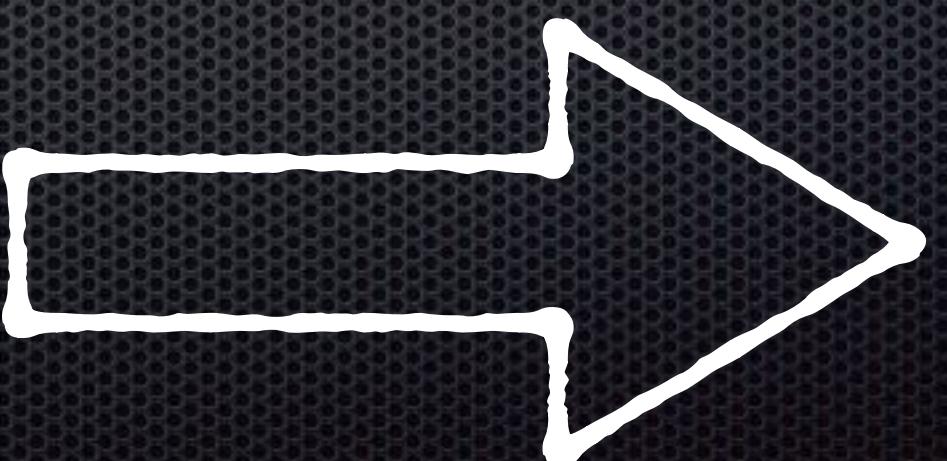
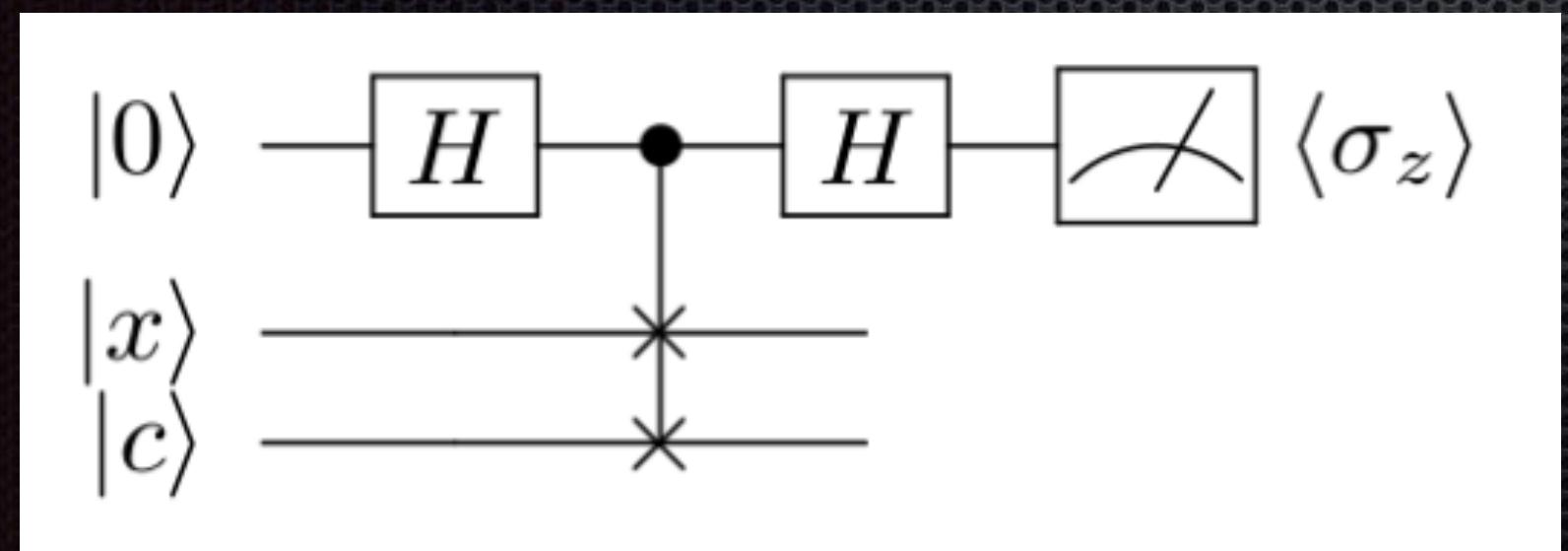
Swap gate flips the state of the qubits $|a, b\rangle \rightarrow |b, a\rangle$

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



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

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



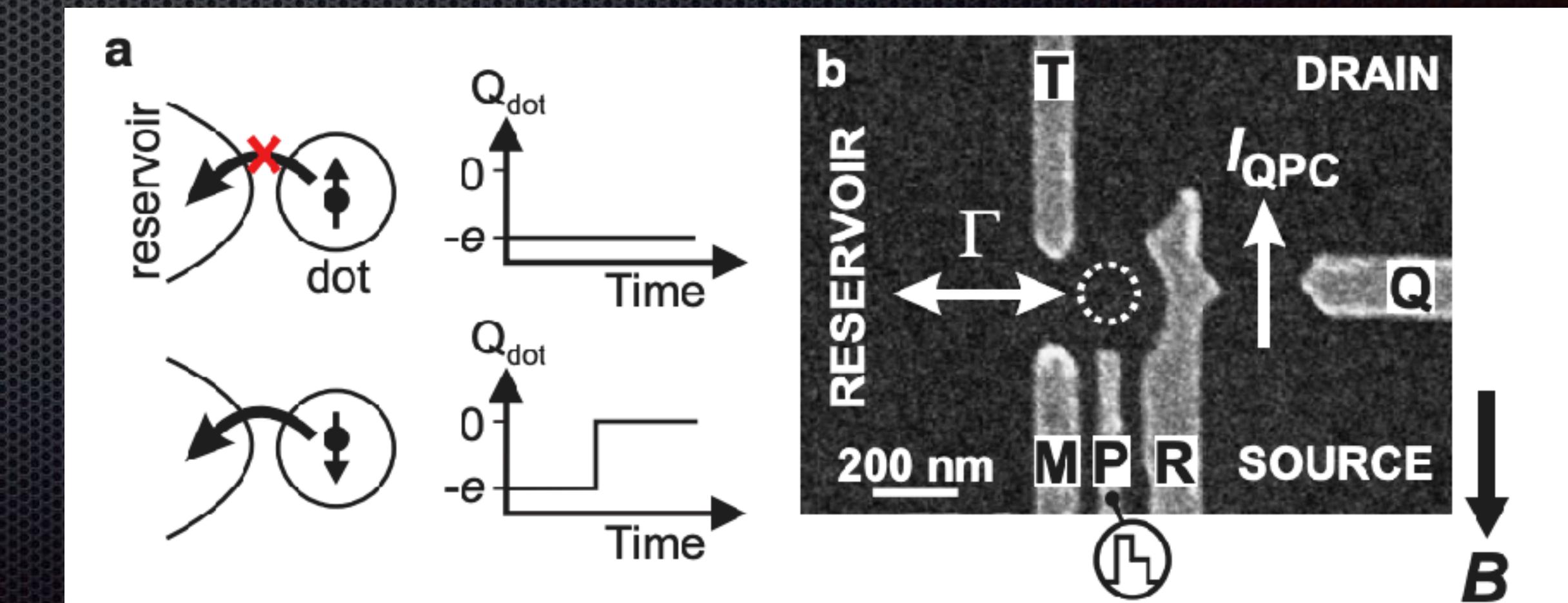
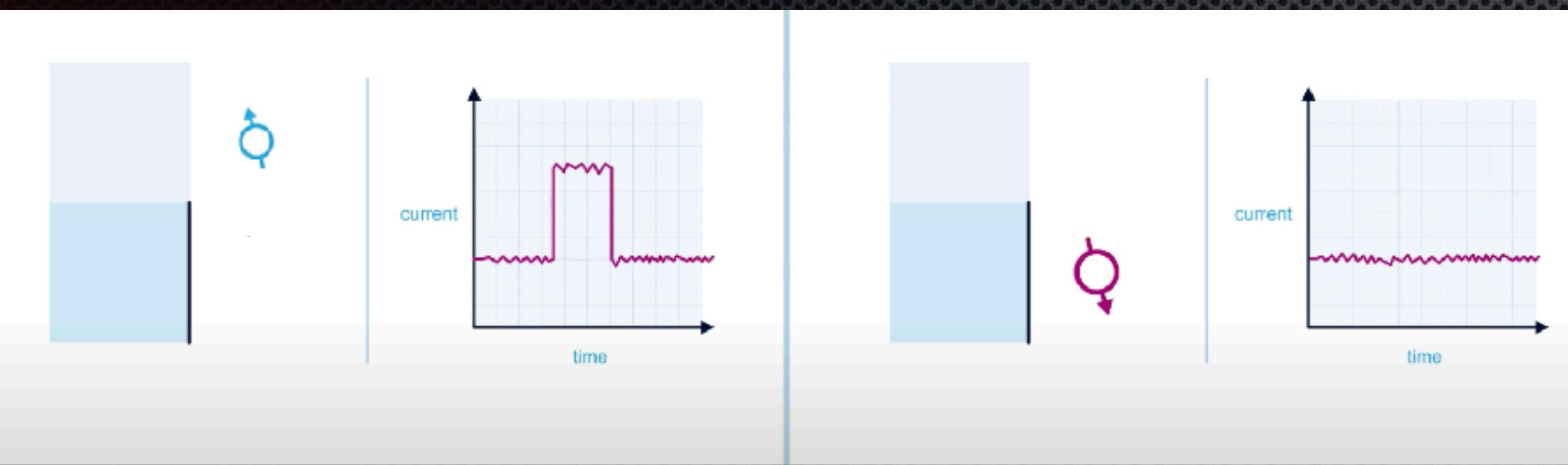
$$\text{Fid} = \langle \psi | \psi \rangle$$

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

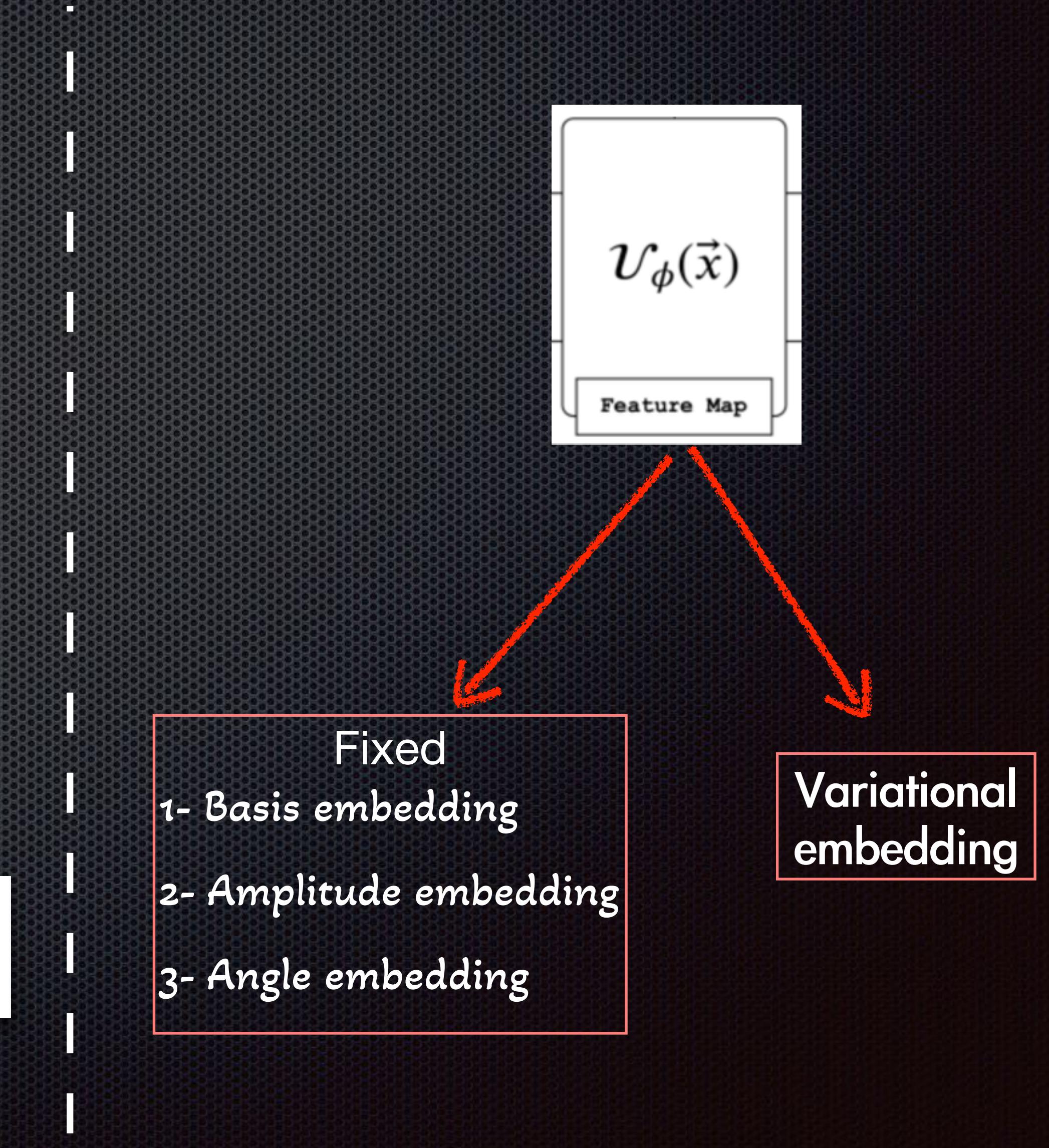
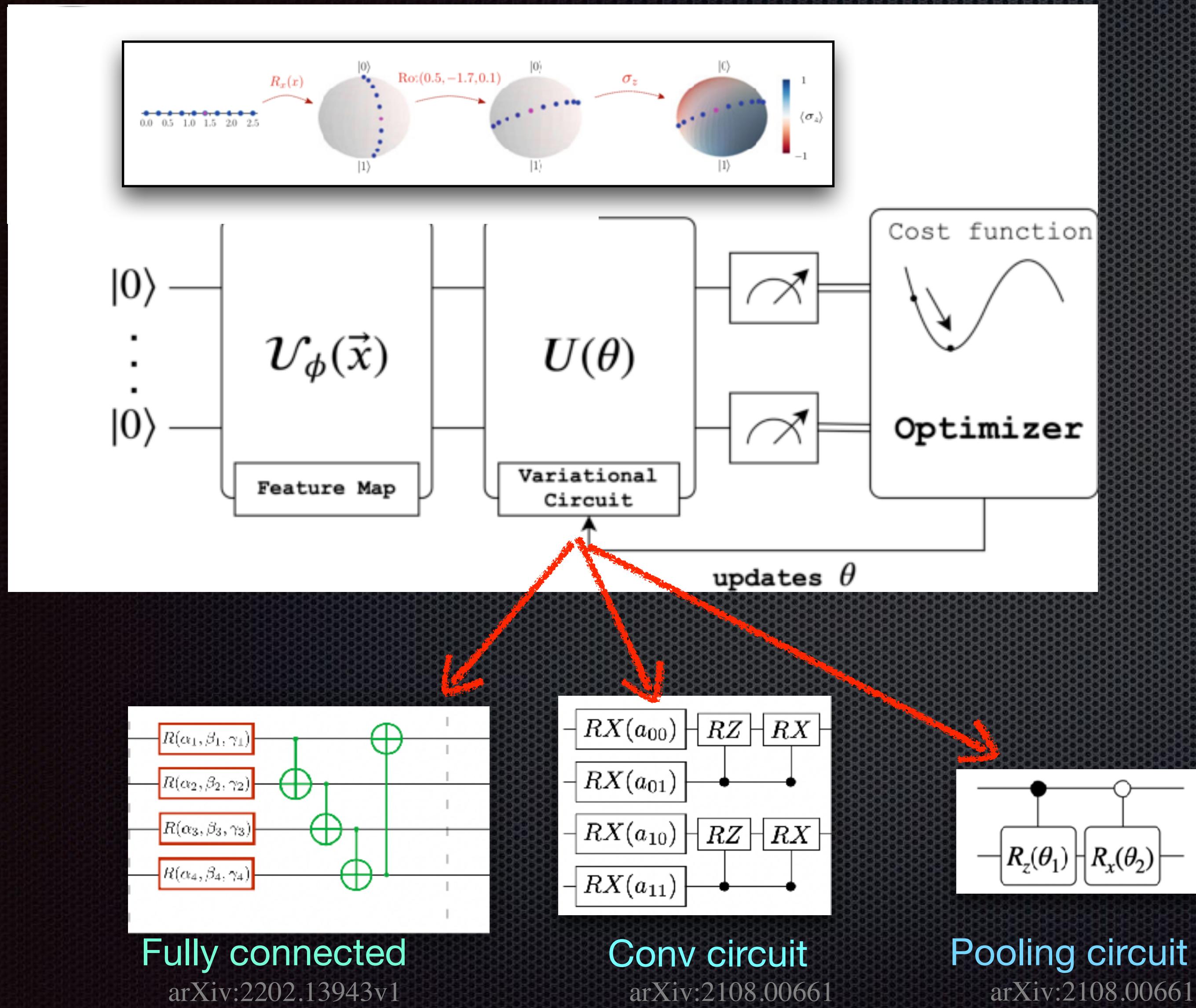
Kavli Institute of Nanoscience Delft and ERATO Mesoscopic Correlation Project, Delft University of Technology, PO Box 5046, 2600 GA Delft, The Netherlands

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

Variational quantum circuit

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

Variational quantum circuit



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

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

3- Angle encoding

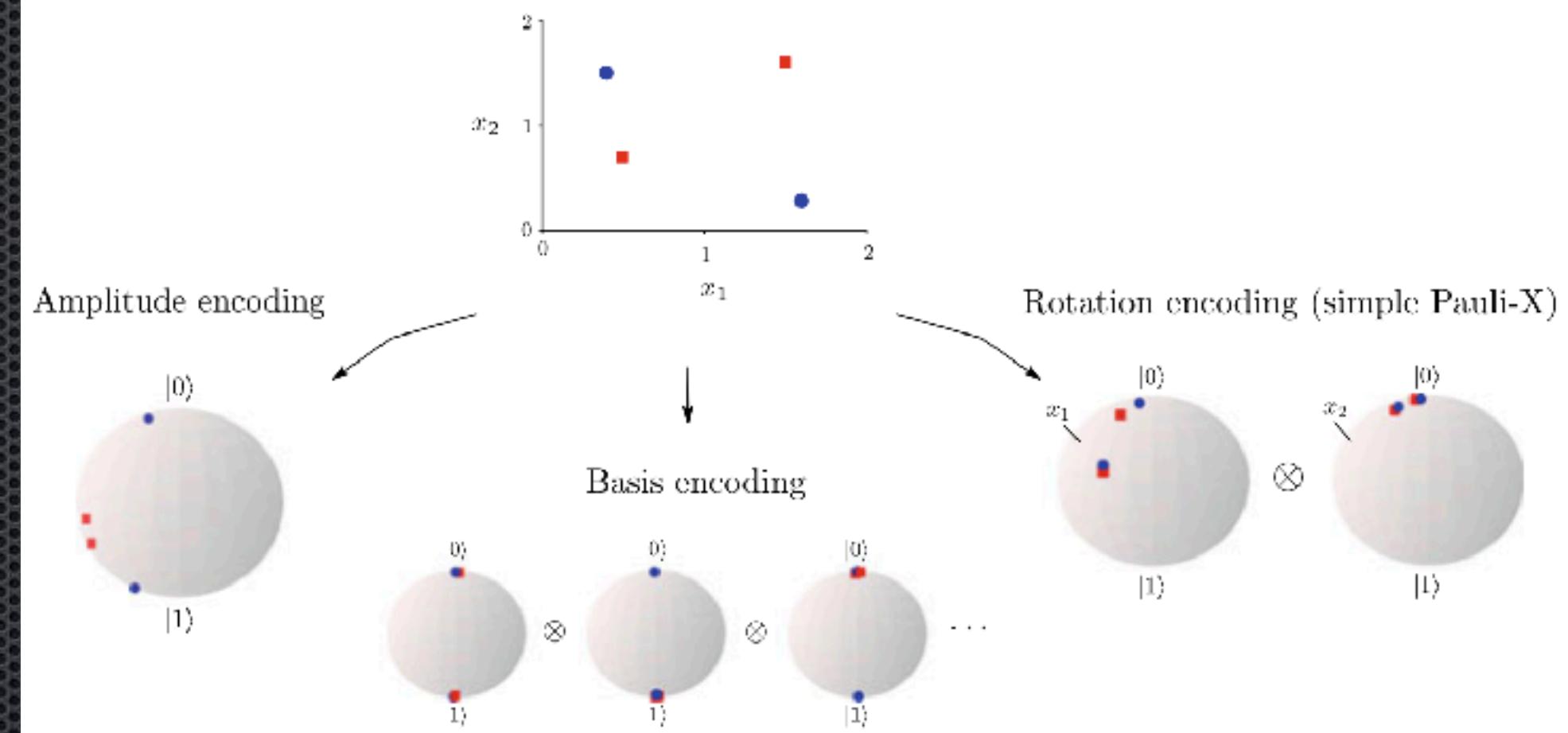
Associates the classical data the quantum states rotating angles

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

basis encoding of binary string (1, 0),
i.e. representing integer 2

$$|\psi\rangle = \alpha_0|00\rangle + \alpha_1|01\rangle + \alpha_2|10\rangle + \alpha_3|11\rangle$$

amplitude encoding of unit-length complex vector $(\alpha_0, \alpha_1, \alpha_2, \alpha_3)$



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?**

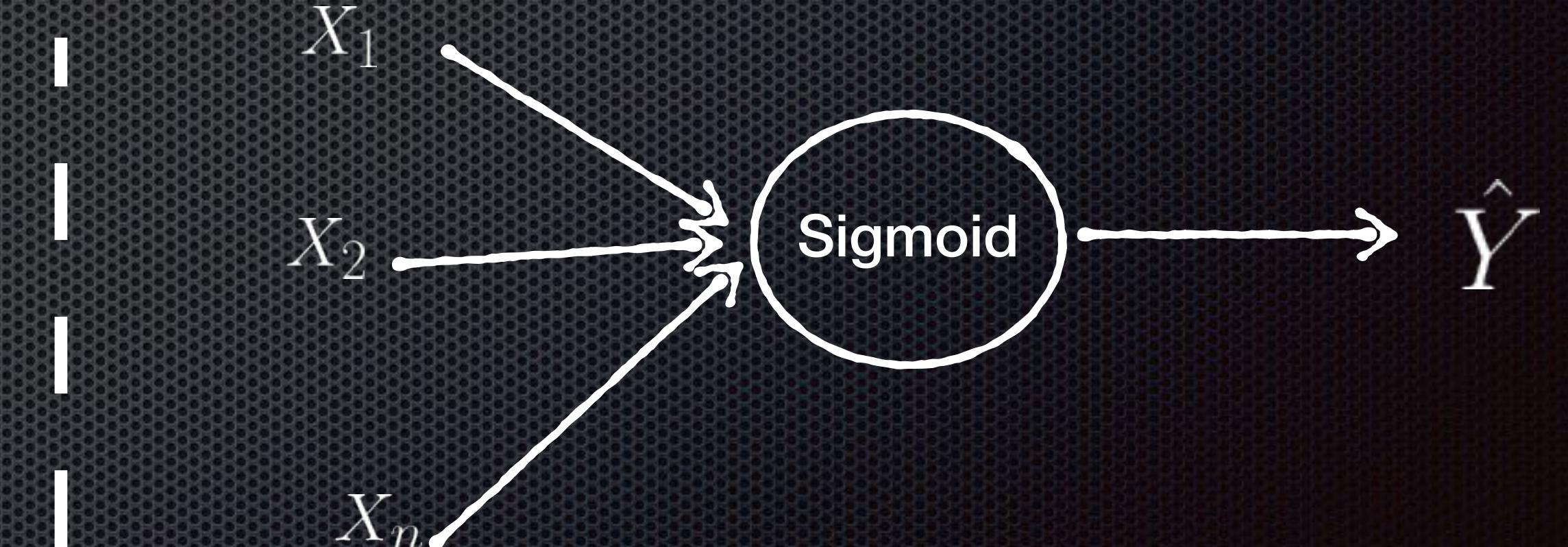
$$\nabla_{\theta} f(x; \theta_i) = \frac{1}{2} [f(x; \theta_i + \delta) - f(x; \theta_i - \delta)]$$

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

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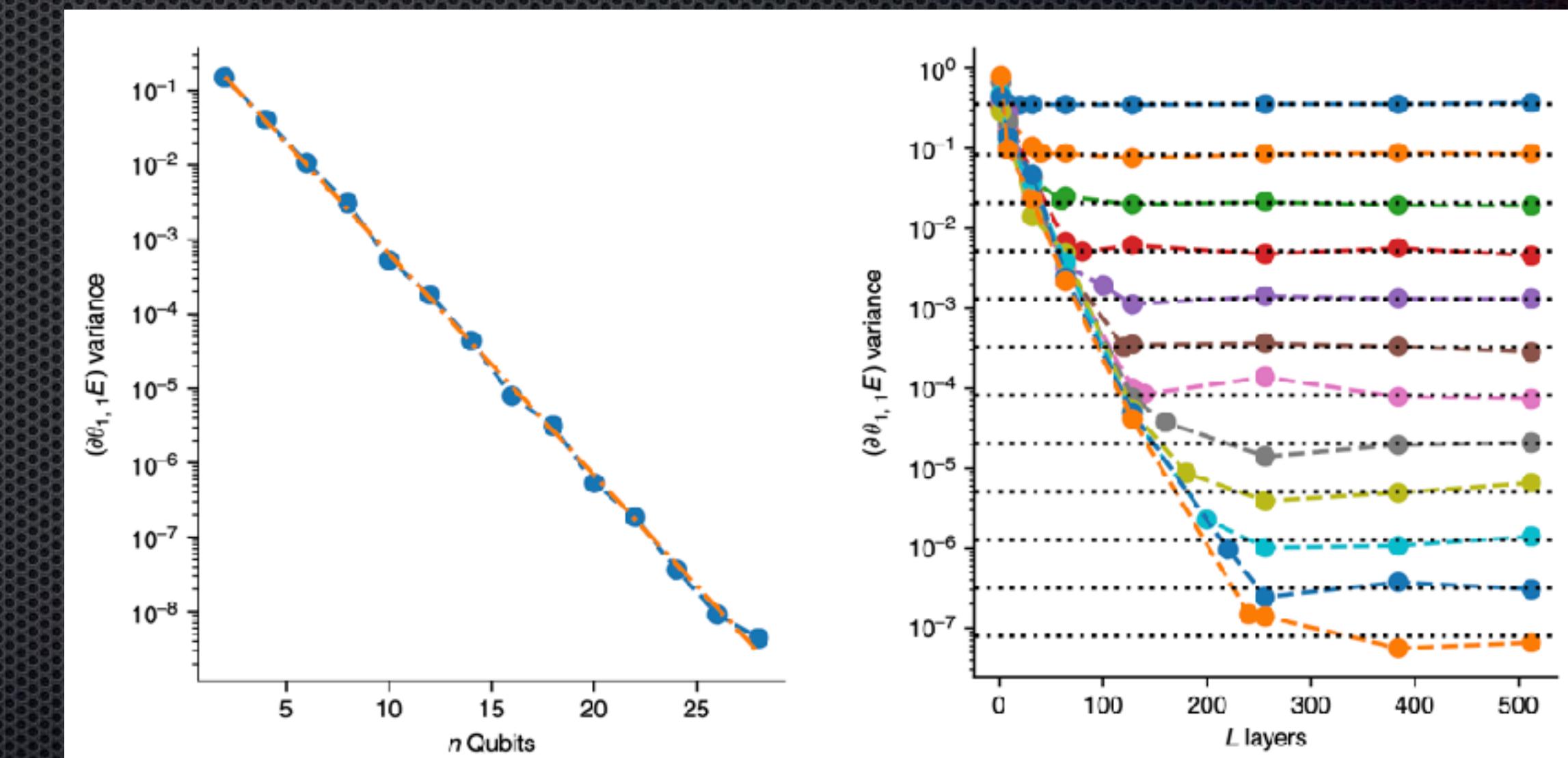
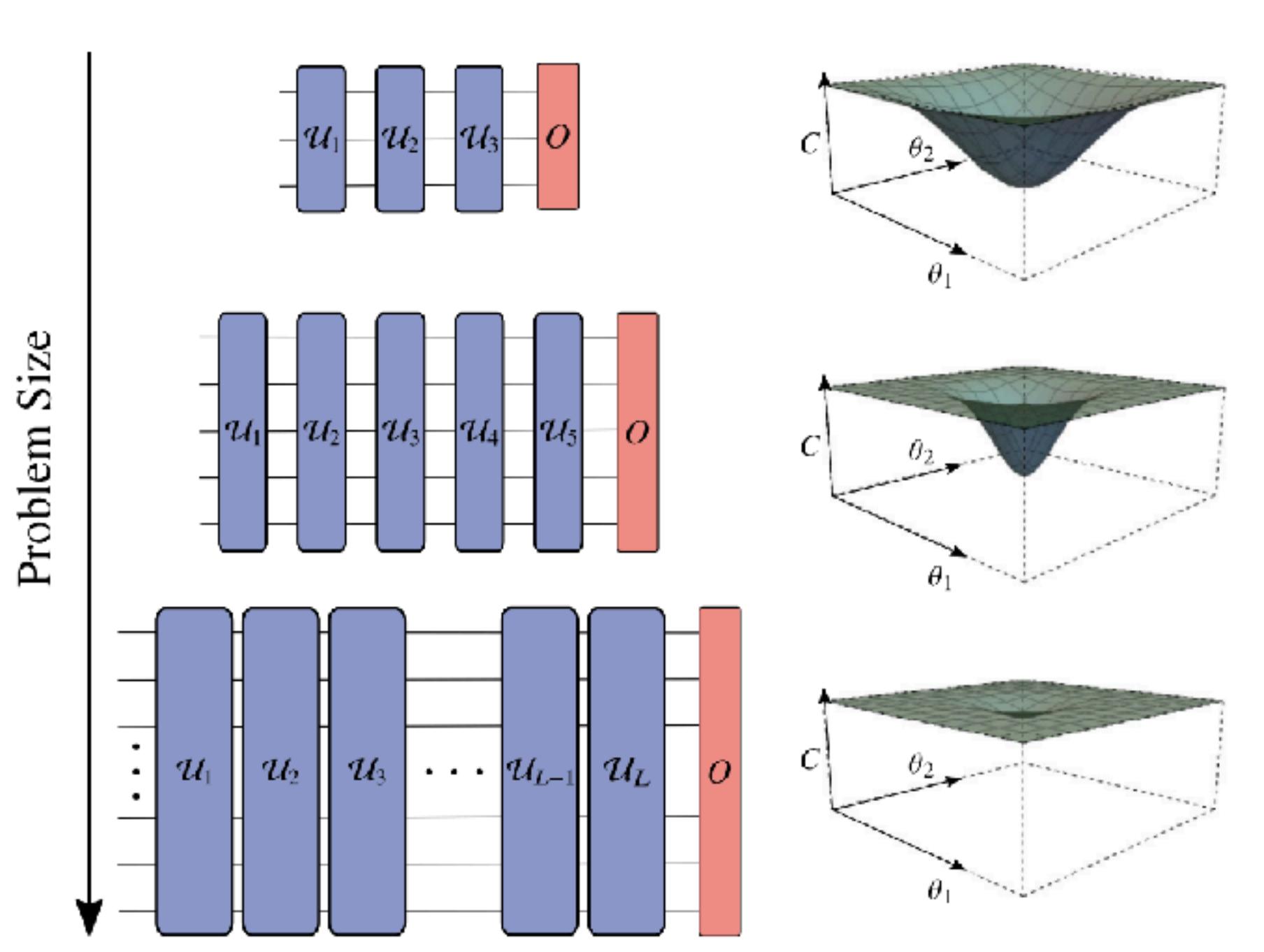
OPEN

Barren plateaus in quantum neural network training landscapes

Jarrod R. McClean¹, Sergio Boixo¹, Vadim N. Smelyanskiy¹, Ryan Babbush¹ & Hartmut Neven¹

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 proposed as initial guesses for exploring the space of quantum states. We show that the

<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!!