Advanced Computational Methods in Condensed Matter Physics

Lecture 11

Introduction to Quantum Computing

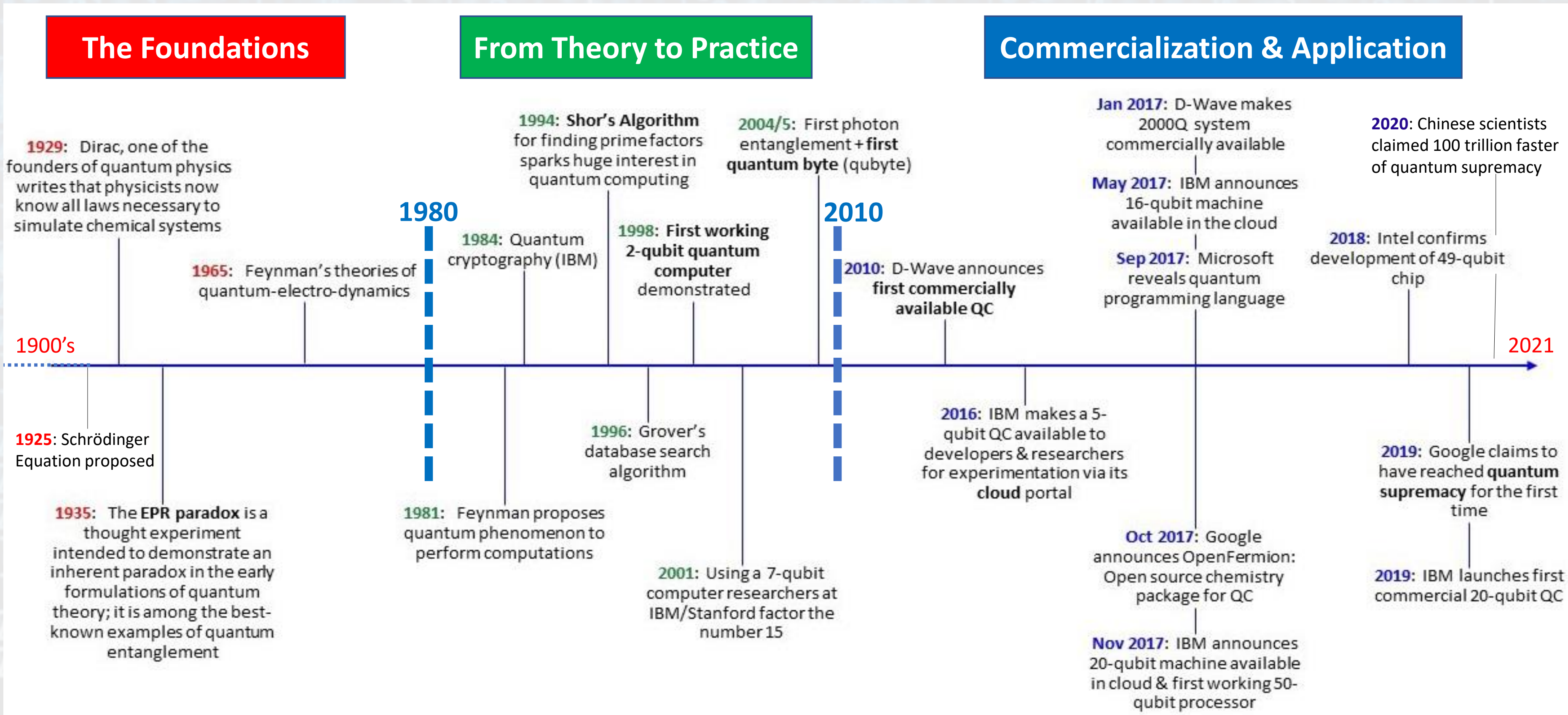
- Qiskit

What is Quantum Computing?

- **Quantum Computer**
  A computer that uses laws of quantum mechanics to perform massively parallel computing through superposition, entanglement, and decoherence

- **Classical Computer**
  A computer that uses voltages flowing through circuits and gates, which can be controlled and manipulated entirely by classical physics

Evolution of Quantum Theory & Quantum Technology



Quantum Mechanics

Quantum mechanics is the theory that describes the behavior of microscopic systems, such as photons, electrons, atoms, molecules, etc.

Nobody understands quantum mechanics!

"No, you're not going to be able to understand it.... You see, my physics students don't understand it either. That is because I don't understand it. Nobody does. ... The theory of quantum electrodynamics describes nature as absurd from the point of view of common sense. And it agrees fully with an experiment. So, I hope that you can accept nature as she is – absurd"

--Richard Feynman

…

- Quantum states, represented by Dirac's ket, | ψ >, evolve in time according to the Schrödinger equation:

$$d|\psi\rangle/dt = -i\hat{H}(t)|\psi\rangle/\hbar,$$

- which implies that time evolution is described by unitary transformations:

$$|\psi\rangle \to \hat{U}|\psi\rangle.$$

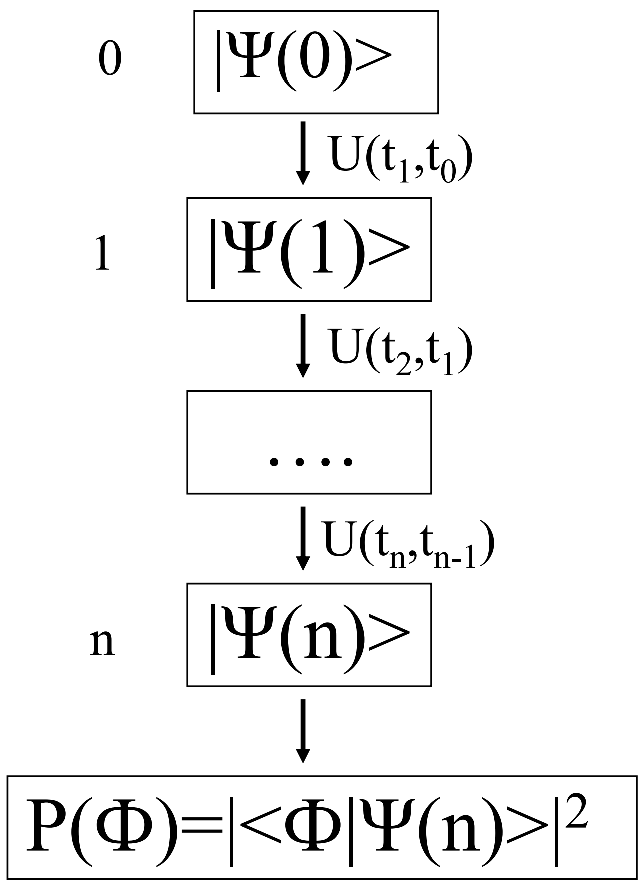
$$d\hat{U}(t)/dt = -i\hat{H}(t)\hat{U}(t)/\hbar.$$

- where | ψ> is the quantum state (wavefunction) and H is Hamiltonian

- This theory, which has been extensively tested by experiments, is probabilistic in nature. The outcomes of measurements on quantum systems are not deterministic.

- Between measurements, quantum systems evolve according to linear equations (the Schrödinger equation). This means that solutions to the equations obey a superposition principle: *linear combinations of solutions are still solutions*.

Quantum Computing Approach using Flow Chart



PREPARATION:

The initial preparation of the state defines a wave function at time $t_0=0$.

STATE EVOLUTION:

Evolved by a sequence of unitary operations

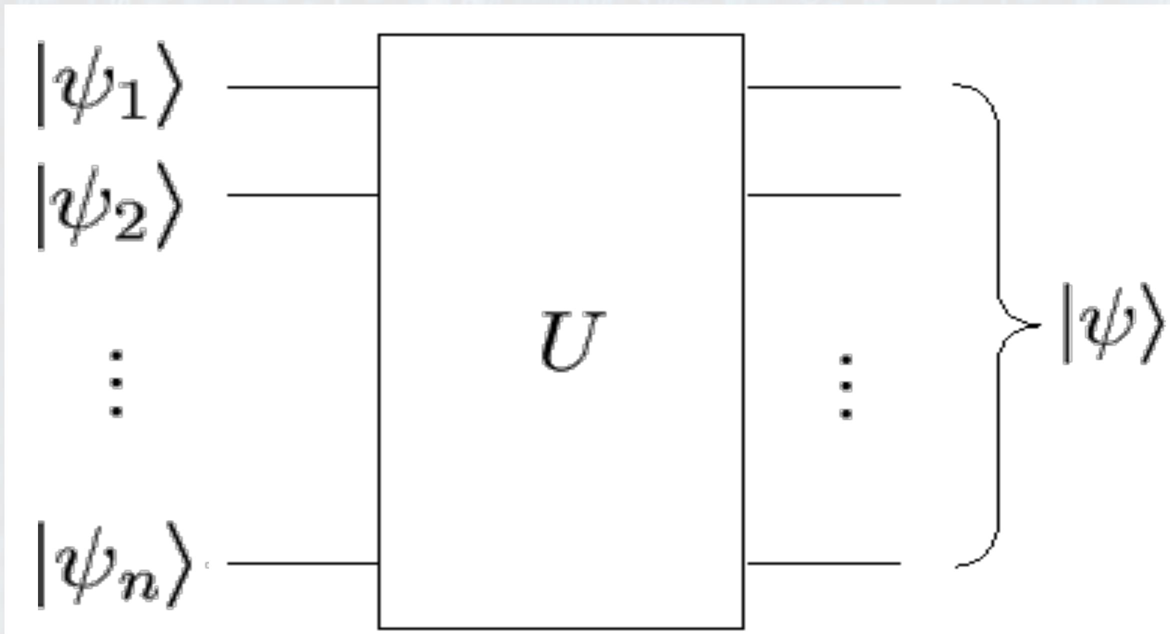
....

MEASUREMENT:

Quantum measurement is projective.

Collapsed by measurement of the state

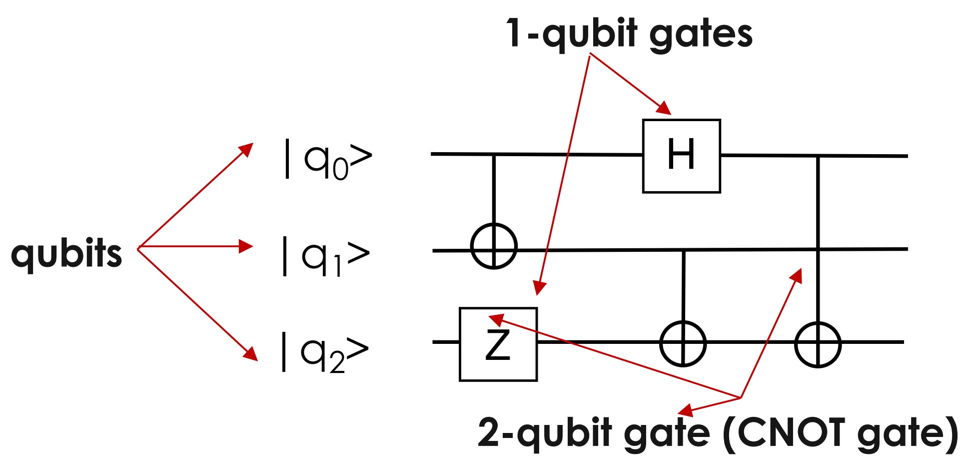
Quantum Computing using Quantum Circuits



On a quantum computer, programs are executed by unitary evolution of an input that is given by the state of the system, $|\psi_n>$, which can in either 0 or 1 state → qu**bit**. (for n-level states: ***qudits)***
Since all unitary operators are invertible, we can always reverse or 'uncompute' a computation on a quantum computer.

Concrete Example

Abstract Quantum Computing with **Gate-based Computing Model**



1-qubit gate (2 x 2 matrix)

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

2-qubit gate (4 x 4 matrix)

$$CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Why is programming with 1-qubit gates + CNOTs Popular?

- **Theoretical level**: **universal** quantum computation model.
- **Hardware level**: good abstraction for getting **high-fidelity hardware implementation**

Continued next week…

Tasks:

- create account on ibm.com/quantum
- Install qiskit (python)

More information:

https://github.com/hywong2/Intro_to_Quantum_Computing

Quantum Registers

Value can be stored in a classical register	Basis states in a quantum register
$(0000)_2 = 0$	$\|0\rangle \otimes \|0\rangle \otimes \|0\rangle \otimes \|0\rangle = \|0\rangle\,\|0\rangle\,\|0\rangle\,\|0\rangle = \|0000\rangle = \|0\rangle_{10}$
$(0001)_2 = 1$	$\|0\rangle \otimes \|0\rangle \otimes \|0\rangle \otimes \|1\rangle = \|0\rangle\,\|0\rangle\,\|0\rangle\,\|1\rangle = \|0001\rangle = \|1\rangle_{10}$
$(0010)_2 = 2$	$\|0\rangle \otimes \|0\rangle \otimes \|1\rangle \otimes \|0\rangle = \|0\rangle\,\|0\rangle\,\|1\rangle\,\|0\rangle = \|0010\rangle = \|2\rangle_{10}$
$\vdots$	$\vdots$
$(1111)_2 = 15$	$\|1\rangle \otimes \|1\rangle \otimes \|1\rangle \otimes \|1\rangle = \|1\rangle\,\|1\rangle\,\|1\rangle\,\|1\rangle = \|1111\rangle = \|15\rangle_{10}$

Superposition of basis states of multiple qubits

$$\begin{aligned} |\Psi\rangle &= a_0\,|00\cdots0\rangle + a_1\,|00\cdots1\rangle + \cdots + a_{2^n-1}\,|11\cdots1\rangle \\ &= a_0\,|0\rangle_{10} + a_1\,|1\rangle_{10} + \cdots + a_{2^n-1}\,|2^n-1\rangle_{10} \end{aligned}$$

Superposition

$$|\Psi\rangle = a_0|00\cdots0\rangle + a_1|00\cdots1\rangle + \cdots + a_{2^n-1}|11\cdots1\rangle$$
$$= a_0|0\rangle_{10} + a_1|1\rangle_{10} + \cdots + a_{2^n-1}|2^n-1\rangle_{10}$$

n = 300 (e.g. electrons)
$2^{300} = 10^{90}$ complex coefficients, a_i

Number of atoms in the universe < 10^{82}

Total number of storage in the world < 10^{21} bytes

Quantum parallelism & measurement

Linear Quantum mechanics

$$
\begin{aligned}
f(|\Psi\rangle) &= f(0.5|0\rangle + 0.5|1\rangle + 0.5|2\rangle + 0.5|3\rangle) \\
&= 0.5 f(|0\rangle) + 0.5 f(|1\rangle) + 0.5 f(|2\rangle) + 0.5 f(|3\rangle)
\end{aligned}
$$

$f(|\Psi\rangle)$ → $f(|0\rangle)$, $f(|1\rangle)$, $f(|2\rangle)$, $f(|3\rangle)$

Measurement

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

$|\alpha|^2$ → $|0\rangle$

$|\beta|^2$ → $|1\rangle$

Quantum gates

- Quantum gates rotate the vector (state) in the corresponding hyperspace
- *Very often, a gate is just a laser or microwave pulse*
- Some gates have classical counterparts
  - NOT gate (1-qubit)
  - CNOT gate (2-qubit)

$$U_{XOR}\,|ab\rangle = |a a \oplus b\rangle$$

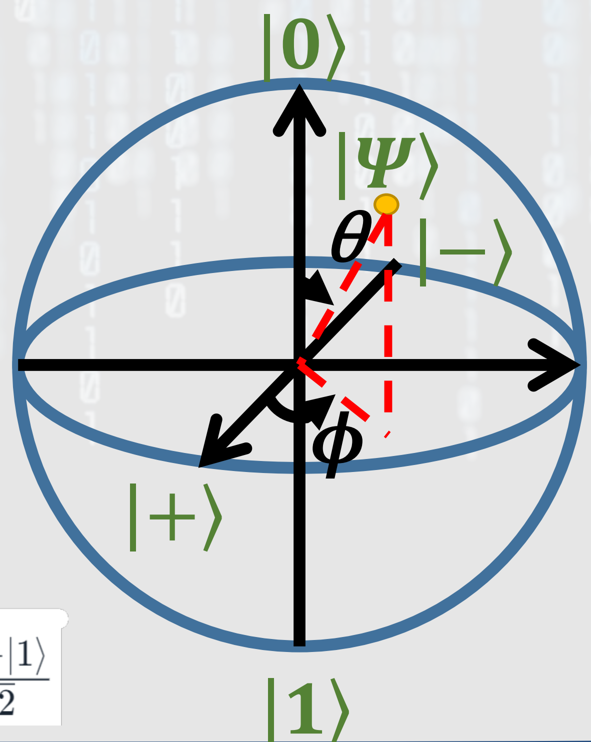
- Some gates have no classical counterparts
  - Hadamard gate

$$H\,|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

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

$$|+\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}} \quad |-\rangle = \frac{|0\rangle-|1\rangle}{\sqrt{2}}$$

Bloch Sphere



The H-Gate

- After a qubit in state |0> or |1> has been acted upon by a H gate, the state of
- the qubit is an equal superposition of |0> and |1>. Thus, the qubit goes from a deterministic state to a truly random state, i.e., if the qubit is now measured, we will measure |0> or |1> with equal probability.
- We see that H is its own inverse, that is, $H^{-1} = H$ or $H^2 = I$. Therefore, by applying H twice to a qubit we change nothing. This is amazing!
- By applying a randomizing operation to a random state produces a deterministic outcome!
- One of the most important gates in quantum computing!

CNOT Gate

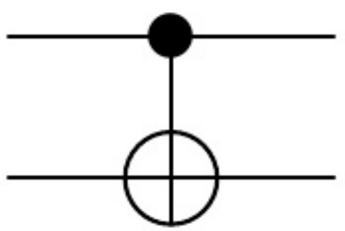
- ***Controlled NOT*** gate
- Acts on two qubits
  - If the control qubit is set to 0, target qubit is the same
  - If the control qubit is set to 1, target qubit is flipped

$$|00\rangle \rightarrow |00\rangle, \quad |01\rangle \rightarrow |01\rangle$$
$$|10\rangle \rightarrow |11\rangle, \quad |11\rangle \rightarrow |10\rangle$$

Matrix representation

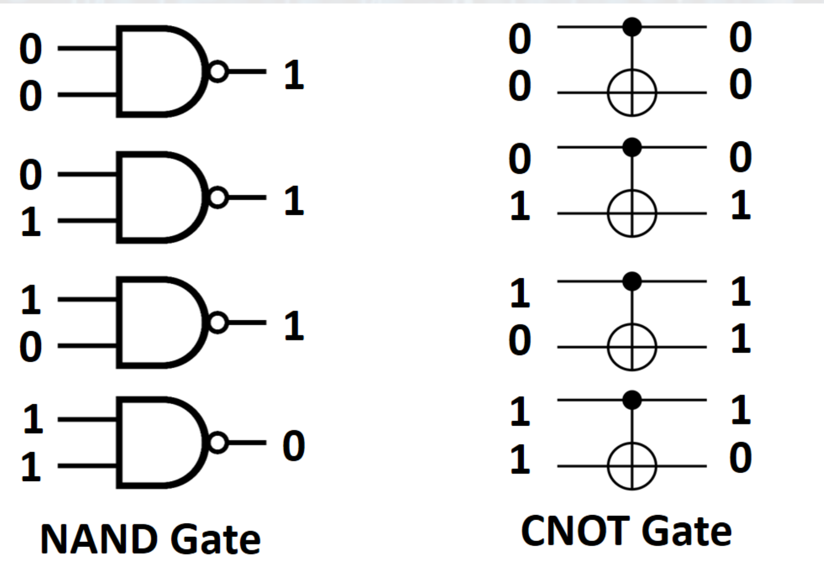
$$CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Circuit representation



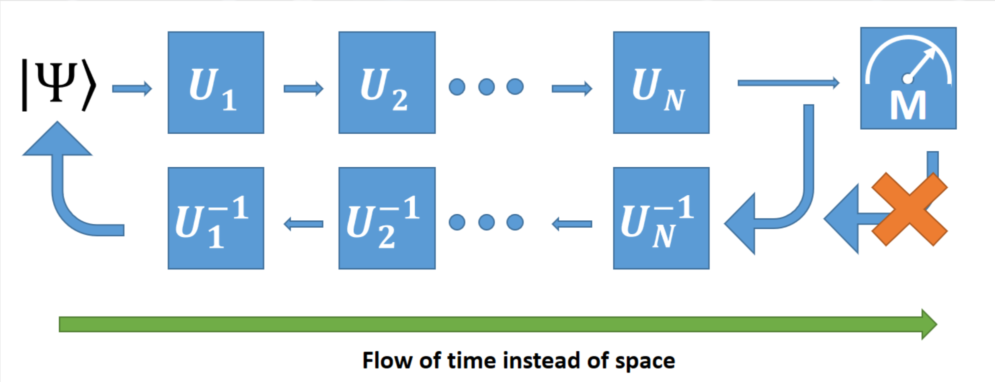
Equivalent to classical gate operation XOR

Quantum Gates and Circuits

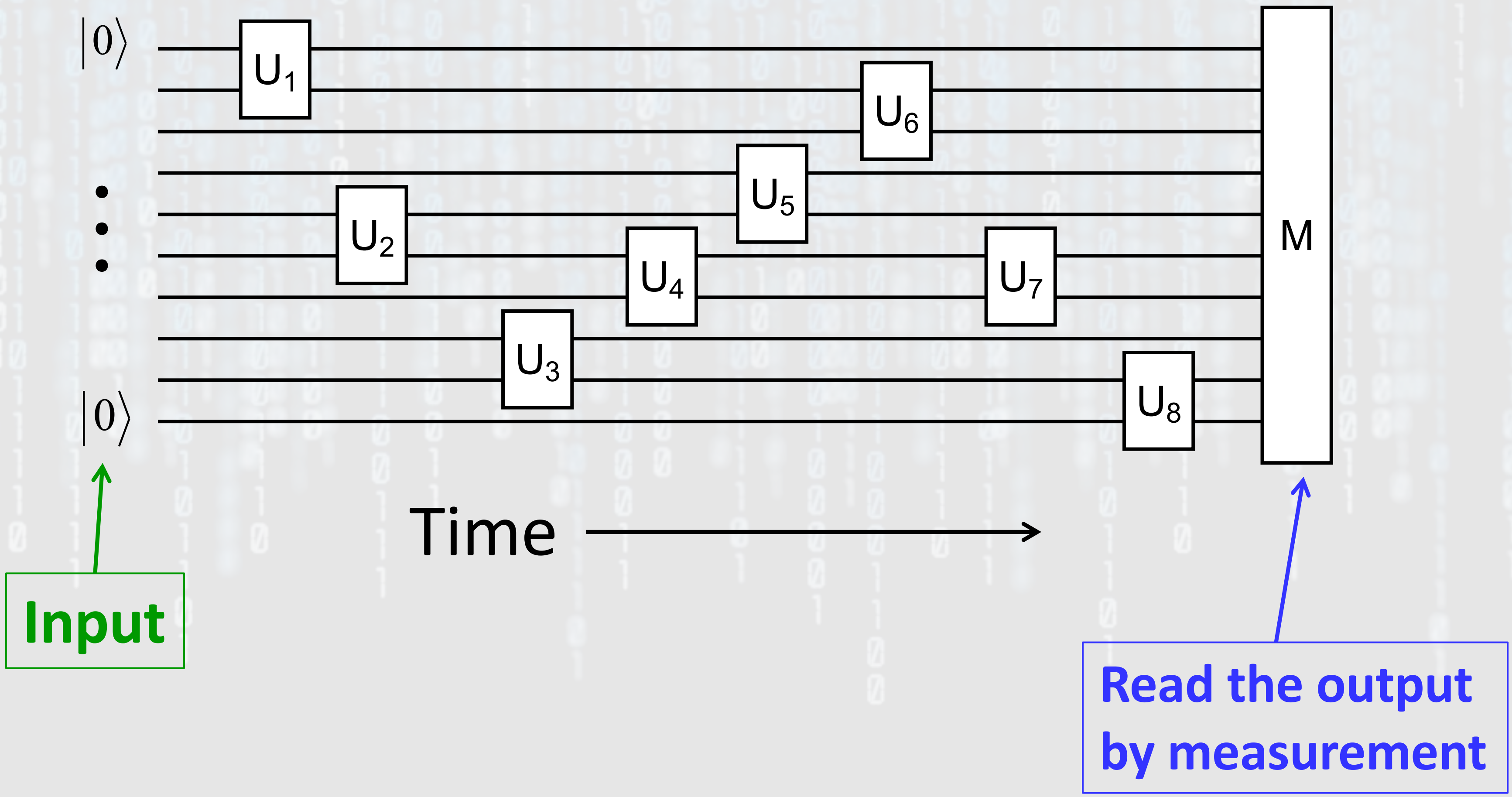


Quantum gates must be reversible

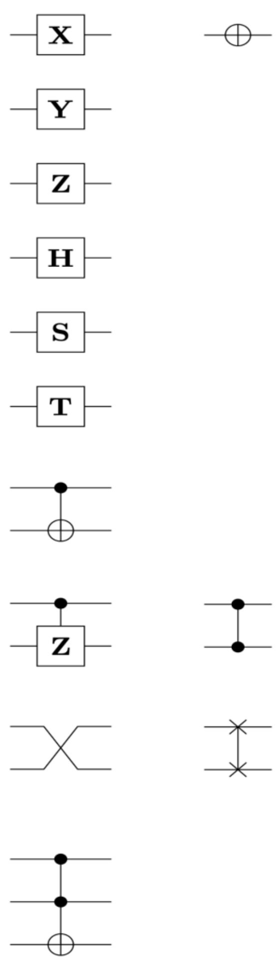
Quantum circuit is the application of operations (microwave/laser pulses) to usually stationary qubit carriers.



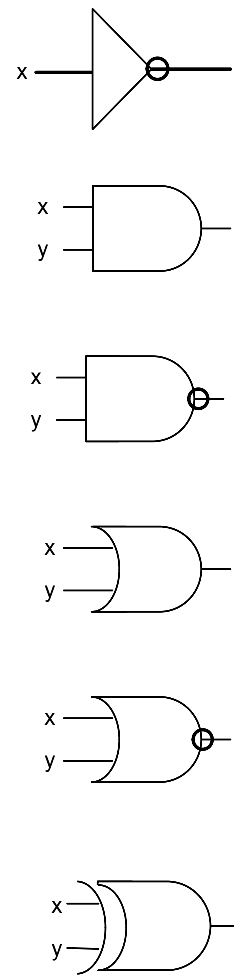
Larger Quantum Circuit



Quantum vs. Classical Gates



Operator	Gate(s)	Matrix
Pauli-X (X)	X	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	Y	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	Z	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	H	$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	S	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	T	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)	Z	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)		$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$



NOT gate: y = NOT(x)

x	y
0	1
1	0

AND gate: z = (x) AND (y)

x	y	z
0	0	0
0	1	0
1	0	0
1	1	1

NAND gate: z = (x) NAND (y)

x	y	z
0	0	1
0	1	1
1	0	1
1	1	0

OR gate: z = (x) OR (y)

x	y	z
0	0	0
0	1	1
1	0	1
1	1	1

NOR gate: z = (x) NOR (y)

x	y	z
0	0	1
0	1	0
1	0	0
1	1	0

XOR gate: z = (x) XOR (y)

x	y	z
0	0	0
0	1	1
1	0	1
1	1	0

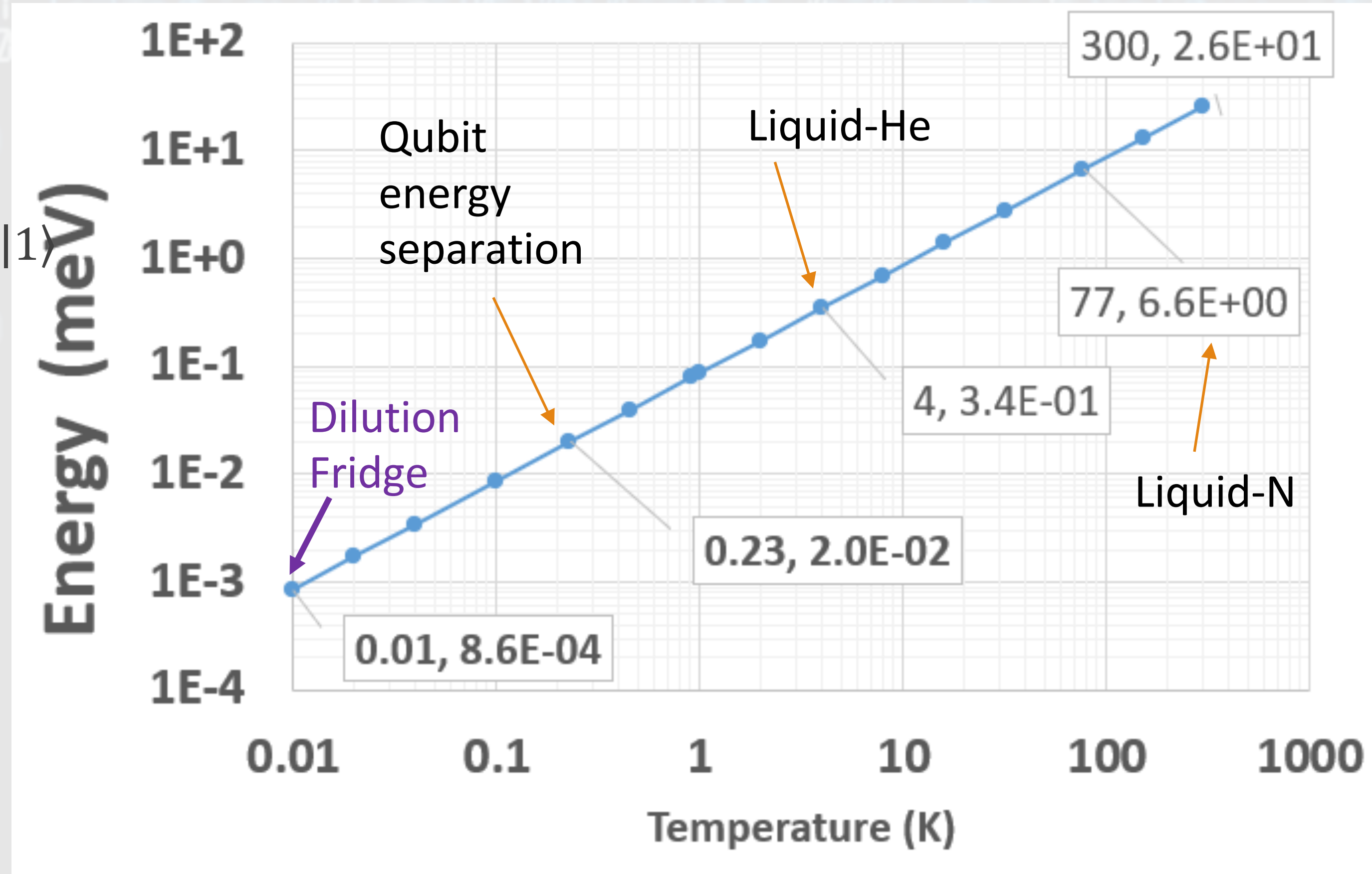
Noise, De-coherence Time and Energy Scale

Qubit loses its state due to noise

Need ultra-low temperature to avoid thermal noise

Decoherence time:

- $T_1: |1\rangle \Rightarrow |0\rangle$
- $T_2: |0\rangle + |1\rangle \Rightarrow ?|0\rangle ?|1\rangle$



Other quantum gates

1-Bit Phase Shift Gate

Definition

The matrix of $U_{PS,\Phi}$ is $U_{PS,\Phi} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\Phi} \end{pmatrix}$

$$U_{PS,\Phi}\,|1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\Phi} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ e^{i\Phi} \end{pmatrix} = e^{i\Phi} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = e^{i\Phi}\,|1\rangle$$

When $\Phi = \pi$ $\begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ because $e^{i\pi} = \cos\pi + i\sin\pi = -1.$

And this is just the $\boldsymbol{\sigma}_z$ matrix, one of the important Pauli matrices. And it is also called the **Z-gate**.

Z-gate behaves as a NOT gate in the $|+\rangle$ / $|-\rangle$ basis →

$$U_{PS,\pi}\,|+\rangle = U_Z\,|+\rangle = U_Z \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

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

2-Bit Phase Shift Gate (Controlled-PS)

Definition →

$$U_{CPS,\Phi}\,|ab\rangle = e^{i(a\cdot b)\Phi}\,|ab\rangle$$

$$U_{CPS,\Phi}\,|00\rangle = e^{i(0\cdot 0)\Phi}\,|00\rangle = |00\rangle$$

$$U_{CPS,\Phi}\,|01\rangle = e^{i(0\cdot 1)\Phi}\,|01\rangle = |01\rangle$$

$$U_{CPS,\Phi}\,|10\rangle = e^{i(1\cdot 0)\Phi}\,|10\rangle = |10\rangle$$

$$U_{CPS,\Phi}\,|11\rangle = e^{i(1\cdot 1)\Phi}\,|11\rangle = e^{i\Phi}\,|11\rangle$$

$$U_{CPS,\Phi} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\Phi} \end{pmatrix}$$

$$U_{CPS,\Phi}\,|\Psi\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\Phi} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ e^{i\Phi}\delta \end{pmatrix}$$

$$= \alpha\,|00\rangle + \beta\,|01\rangle + \gamma\,|10\rangle + e^{i\Phi}\delta\,|11\rangle$$

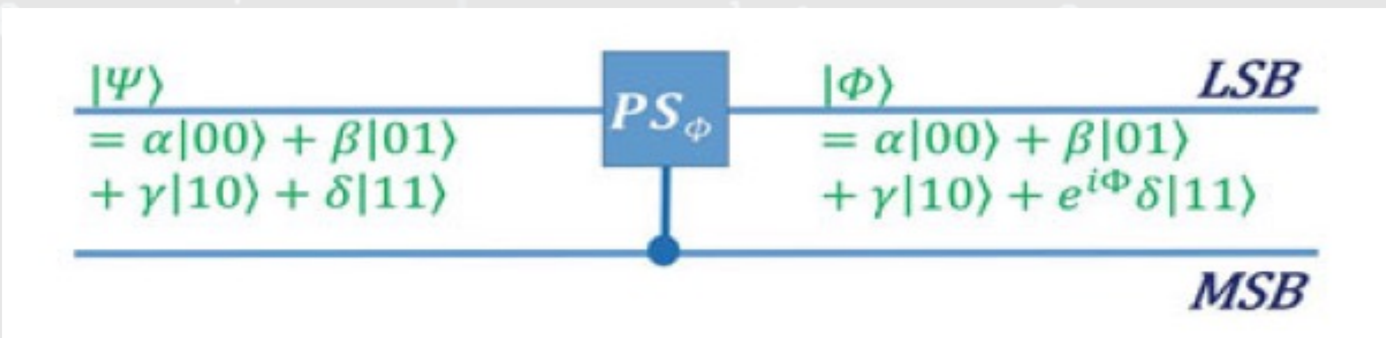
…

$$U_{CPS,\Phi} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\Phi} \end{pmatrix}$$

$$U_{CPS,\Phi}\,|ab\rangle = e^{i(a\cdot b)\Phi}\,|ab\rangle$$

- A is Control Qubit
- B is Target Qubit

$$U_{CPS,\Phi}\,|11\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\Phi} \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ e^{i\Phi} \end{pmatrix} = e^{i\Phi}\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = e^{i\Phi}\,|11\rangle$$



Toffoli (Controlled-Controlled NOT, CCNOT) Gate (3-qubit)

$$\boldsymbol{T}\,|abc\rangle = \boldsymbol{T}\,|a\rangle \otimes |b\rangle \otimes |c\rangle = \boldsymbol{T}\,|a, b, c\rangle = |a, b, (a \cdot b) \oplus c\rangle$$

$$\boldsymbol{T}\,|0, 0, 0\rangle = |0, 0, (0 \cdot 0) \oplus 0\rangle = |0, 0, 0\rangle$$

$$\boldsymbol{T}\,|0, 0, 1\rangle = |0, 0, (0 \cdot 0) \oplus 1\rangle = |0, 0, 1\rangle$$

Toffoli gate can be used as universal gate in classical circuit

$$\boldsymbol{T} = \begin{pmatrix} 1&0&0&0&0&0&0&0\\ 0&1&0&0&0&0&0&0\\ 0&0&1&0&0&0&0&0\\ 0&0&0&1&0&0&0&0\\ 0&0&0&0&1&0&0&0\\ 0&0&0&0&0&1&0&0\\ 0&0&0&0&0&0&0&1\\ 0&0&0&0&0&0&1&0 \end{pmatrix}$$

$$\boldsymbol{T}\,|111\rangle = \begin{pmatrix} 1&0&0&0&0&0&0&0\\ 0&1&0&0&0&0&0&0\\ 0&0&1&0&0&0&0&0\\ 0&0&0&1&0&0&0&0\\ 0&0&0&0&1&0&0&0\\ 0&0&0&0&0&1&0&0\\ 0&0&0&0&0&0&0&1\\ 0&0&0&0&0&0&1&0 \end{pmatrix} \begin{pmatrix} 0\\0\\0\\0\\0\\0\\0\\1 \end{pmatrix} = \begin{pmatrix} 0\\0\\0\\0\\0\\0\\1\\0 \end{pmatrix} = |110\rangle$$

Qiskit Demos: Decoherence times

Use Qiskit to characterize the coherence lifetimes of an IBM quantum computer

Coherence ⇔ how long a qubit reliably retains both its population information and its phase

timescales characterizing qubit behavior:

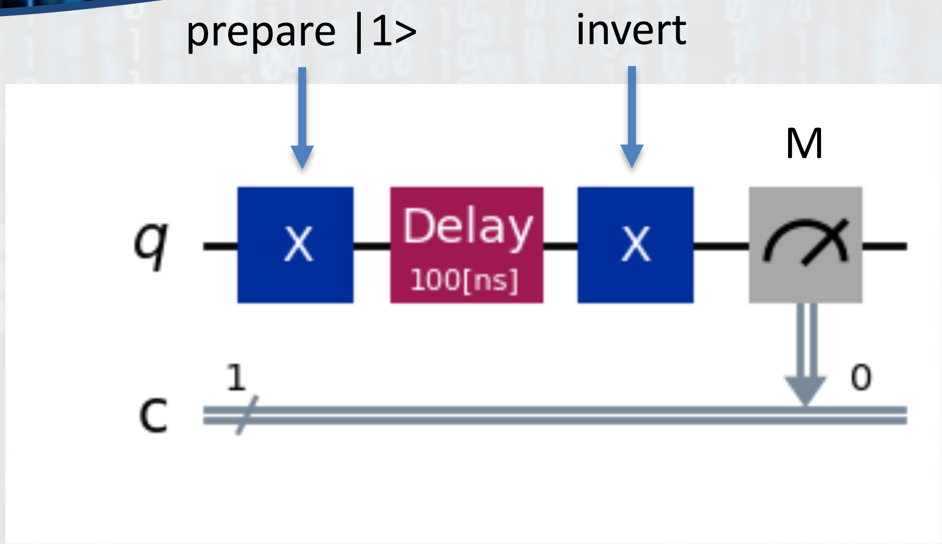
- T_1: energy relaxation time (decay from $|1\rangle$ to $|0\rangle$)

> The standard sequence for measuring the relaxation time is
>
> $$X \rightarrow \tau \rightarrow M$$
>
> Start with $|0\rangle \rightarrow$ X gate prepares $|1\rangle \rightarrow$ delay $\tau \rightarrow$ measure
> If qubit relaxes during τ, probability of measuring $|1\rangle$ decreases exponentially.
> Repeat experiment for many τ, average over many shots, then fit
>
> $$P_1(\tau) \approx \exp(-\tau/T_1)$$
>
> from which T_1 can be extracted

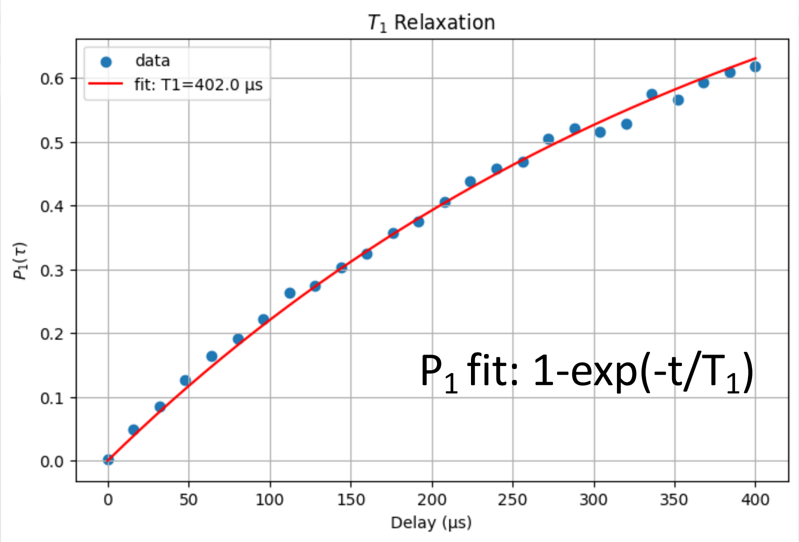
- T^*_2 : ensemble dephasing time arising from slow, shot-to-shot fluctuations in the qubit frequency
- T_2: true irreversible dephasing time obtained from a Hahn-echo sequence

T_1

We implement:
(here 100ns delay)




```
qc = QuantumCircuit(1,1)
qc.x(0)                    # prepare |1>
qc.delay(100, 0, 'ns')     # use 100ns
qc.x(0)                    # flip back
qc.measure(0, 0)
```

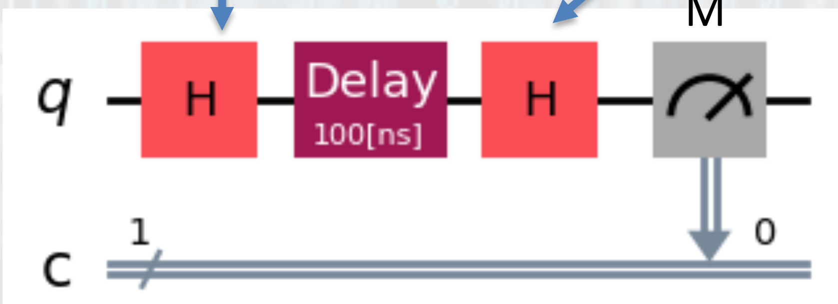


T^*_2

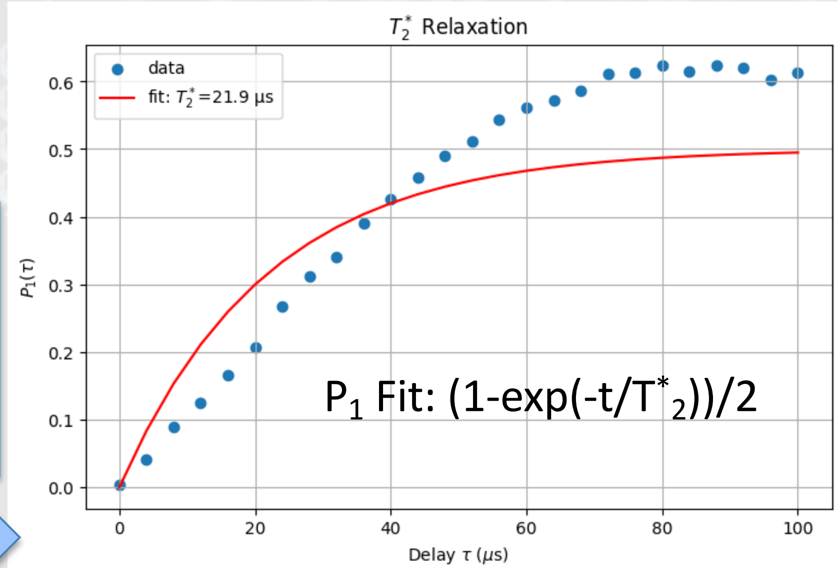
For T^*_2 we use the Ramsay sequence: H -> τ -> H -> M
This is the single-qubit analog of an NMR free-induction decay (FID) measurement

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

Should revert to |0>, if decayed, only with 50% probability




```
qc = QuantumCircuit(1,1)
qc.h(0)                    # prepare |+>
qc.delay(100, 0, 'ns')     # use 100ns
qc.h(0)                    # map back
qc.measure(0, 0)
```



T_2

For T_2 we use the Hahn echo sequence: H -> τ/2 -> X -> τ/2 -> H -> M
This is analogous to the NMR spin-echo experiment.


```
qc = QuantumCircuit(1,1)
qc.h(0)                # prepare |+>
qc.delay(50, 0, 'ns’)  # use 50ns
qc.x(0)                # invert
qc.delay(50, 0, 'ns’)  # use 50ns
qc.h(0)                # map back
qc.measure(0, 0)
```