HPS

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Quantum Computing

A brief introduction for the curious

Learning Objectives

- The state of quantum computing
- What are qubits and quantum circuits?
- The cool phrases: superposition and entanglement
- How does quantum computing physically even work?
- The Deutsch-Josza algorithm

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What is Quantum Computing?

"Quantum computation ... will be the first technology that allows ... distributing components of a complex task among vast numbers of parallel universes, and then sharing the results."
- Deutsch, *The Fabric of Reality* (1997)

Okay, still… what is Quantum Computing?

- Quantum computers utilizes quantum mechanics to solve complex problems
- From the ground up, it uses different physical representations to operate
    - ✗Bits   ⟶   ✓Qubits
    - ✗Transistors   ⟶   ✓e.g. Ions, photons
    - ✗Voltage   ⟶   ✓LASERS!
    - ✗Linear power   ⟶   ✓Exponential power
- QC **may** be superior to classical computing in
    - Simulating Quantum systems (highly probable)
    - Combinatorial optimization problems (probable)
    - Cryptography / prime factorization (probable)
    - Machine learning and other fields (unknown)

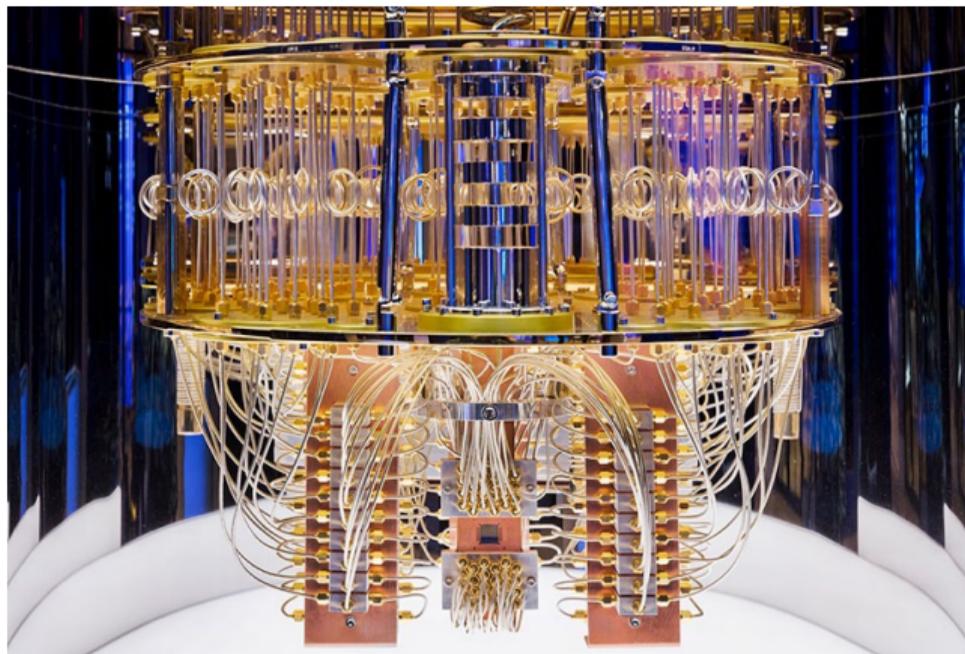# A superconducting quantum computer

Figure: Source: IBM

State of Quantum Computing

- Noisy, intermediate-size Quantum era (**NISQ**)
- Quantum Computers with hundreds of qubits
- High error rate (noise) due to external influences and imperfect control
- Full error tolerance in NISQ era unachievable due to overhead
- Quantum advantage attempts and disputes
  - ► Google in 2019 Kalai, Rinott, and Shoham, "Google's Quantum Supremacy Claim: Data, Documentation, and Discussion"
  - ► IBM in 2023 Patra et al., "Efficient tensor network simulation of IBM's largest quantum processors"
  - ► probably requires thousands or millions of qubits
- Great time to do basic research
  - ► ... if interested in algorithms and/or Quantum mechanics
  - ► Availability of accessible frameworks and learning material
- Promising fields are Quantum Chemistry, Combinatorial Optimization, Machine Learning
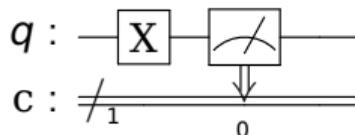
The qubit

- The smallest unit of information in QC is the **qubit**
- Qubits are represented as two-dimensional $\mathbb{C}$-vectors $\vec{q}$ which are unitary
- Below two states of a qubit form its **Computational Basis**:
  $$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ and } |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$
- $|\psi\rangle$ known as **ket** notation
- Computations with these states are similar to classical computing (bits 0 and 1)
- All quantum states are a linear combination (**superposition**) of $|0\rangle$ and $|1\rangle$
- $|\psi\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha |0\rangle + \beta |1\rangle$ where $\alpha, \beta \in \mathbb{C}$
- (Unitary implies $|\alpha|^2 + |\beta|^2 = 1$)

Gates: Operations on qubits

- **Quantum gates** do operations on qubits (cf. logic gates in classical computing)
- Gates apply linear transformations on the statevector of qubits, i.e. matrices
- (Since statevectors need to remain unitary, gates have determinant 1, always!)
- Important 1-qubit gates are the **NOT gate (X)** and the **Hadamard gate (H)**

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

- Other notable gates: Pauli $\{X, Y, Z\}$, Phase $P(\phi)$, and Universal $U(\theta, \phi, \lambda)$
- The inverse of any gate is shown with $\dagger$ e.g. $GG^{\dagger} = I = G^{\dagger}G$ for some gate G
- The Hadamard and Pauli gates are their own inverses, for example

Quantum Circuits and Measurement

- **Quantum Circuits** can represent quantum computations

$$q : \boxed{\text{X}} \rightarrow \boxed{\measuredangle}$$
$$c : \not{}_1 \qquad \downarrow \atop 0$$

- Contain the quantum & classical registers, gates and **measurements**
- Measuring qubits collapses them into computational bases i.e. $|0\rangle's$ and $|1\rangle's$
- These bases can then be turned into bits for classical computing
- Which one they collapse into depends on a probability distribution
- If $|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$, then prob. collapse to $|0\rangle : \mathbb{P}_{|\psi\rangle}(|0\rangle) = |\alpha|^2$
- (For greater detail on these probabilities, look at the *Comprehensive-Notes* pdf)
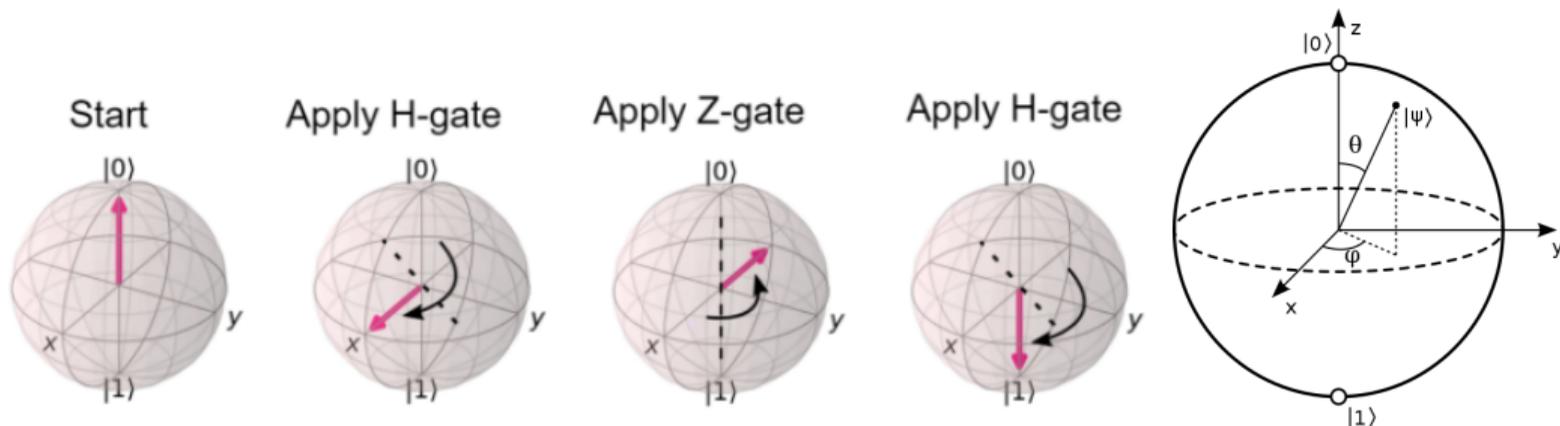
Superposition measurement

■ E.g: $|\psi\rangle = HX|0\rangle = H|1\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{-1}{\sqrt{2}}|1\rangle \Rightarrow$ Chances of $|0\rangle$ or $|1\rangle$ are 50\50
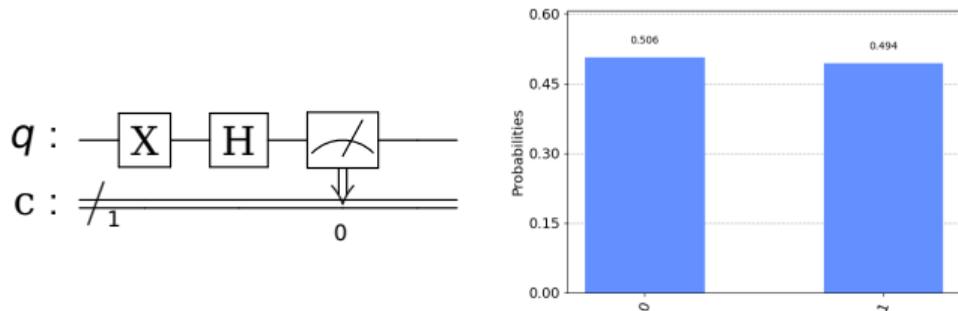
■ Even without X, we just made a coin toss
■ (This is Schrödinger's cat: We are officially Quantum now!)

Bloch Sphere

- **Bloch Sphere**: Useful representation of qubit statevectors (for our brains)
- Can represent any statevector with 2 angles: $0 \leq \theta \leq \pi$ and $0 \leq \varphi \leq 2\pi$

Multiple qubit states

- Qubit states are combined by tensor product, i.e. for two qubits:

$$|a\rangle \otimes |b\rangle = \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} \otimes \begin{bmatrix} b_0 \\ b_1 \end{bmatrix} = \begin{bmatrix} a_0 b_0 \\ a_0 b_1 \\ a_1 b_0 \\ a_1 b_1 \end{bmatrix}$$

$$= a_0 b_0 |00\rangle + a_0 b_1 |01\rangle + a_1 b_0 |10\rangle + a_1 b_1 |11\rangle$$

- Prob. distribution of measuring 2 qubits:
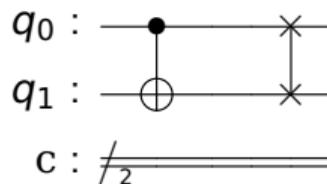$|a_0 b_0|^2 + |a_0 b_1|^2 + |a_1 b_0|^2 + |a_1 b_1|^2 = 1$

- For example: $|0\rangle \otimes |1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = |01\rangle$

- Can be extended to n qubits: $|q_1\rangle \otimes |q_2\rangle \otimes ... \otimes |q_n\rangle$
- Grows exponentially, only $\sim$30-40 qubits can be simulated classically

MORE gates: 2-qubit gates

- We got the **CNOT**(*controlled-not*) gate
- $\bigoplus$ is the **target** and • is the **control**
- Also got the **SWAP** gate (X−X)

$q_0 :$

$q_1 :$

$c : /_2$

$$CNOT = CX = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} I & \mathbf{0} \\ \mathbf{0} & X \end{bmatrix} \qquad SWAP = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- Note: Above form of CX only if applied to $|q_0 q_1\rangle$, depends on control and target
- ANOTHER note: *Qiskit's* qubit ordering of a circuit top-down: $|q_1 q_0\rangle$

SWAPs

- In QC, qubits aren't always connected; SWAPs let them be
- SWAPs are expensive $$$; want optimal connectivity (some QC have all-2-all)

IBM's 10 Quantum Device Lineup
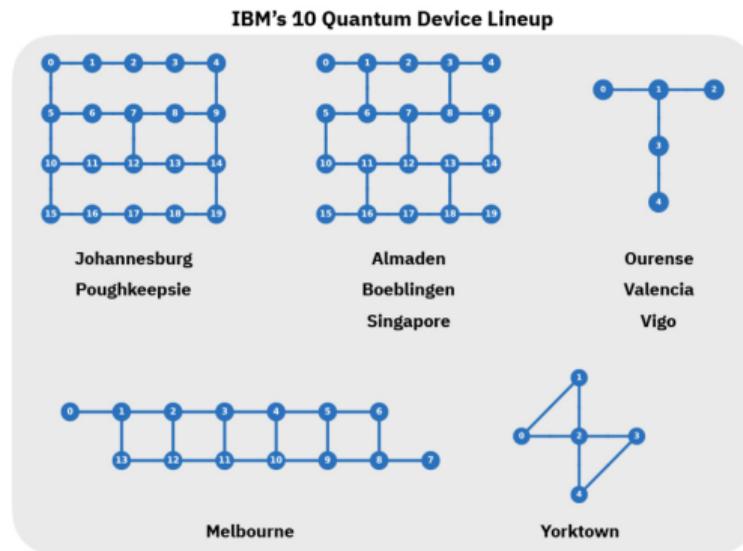
Qiskit model and OpenQASM

- Qiskit contributors, *Qiskit: An Open-source Framework for Quantum Computing* is the quantum toolkit developed by IBM
- Can be installed as package to Python
- Uses OpenQASM Cross et al., "OpenQASM 3: A broader and deeper quantum assembly language" as its Intermediate Represenation to communicate with the QPUs
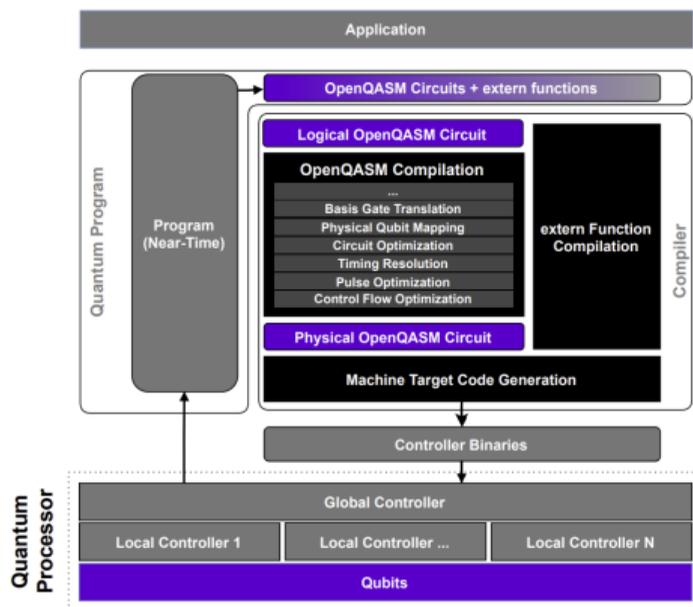

Figure: Compilation Model. Source: OpenQASM paper

Gate structure

- All n-qubit gates can be decomposed into 1- & 2-qubit gates (so stick to those)
- Thus 'n-qubit gates' in a circuit would refer to a subset of gates (for perspective)
- 2-qubit gates generally have the control\target form (except SWAPs)
- $\begin{bmatrix} I & \mathbf{0} \\ \mathbf{0} & G \end{bmatrix}$ with 1-qubit gate G
- Don't let names like control and target fool you; the control qubit can also be changed (this is called **phase kickback**)
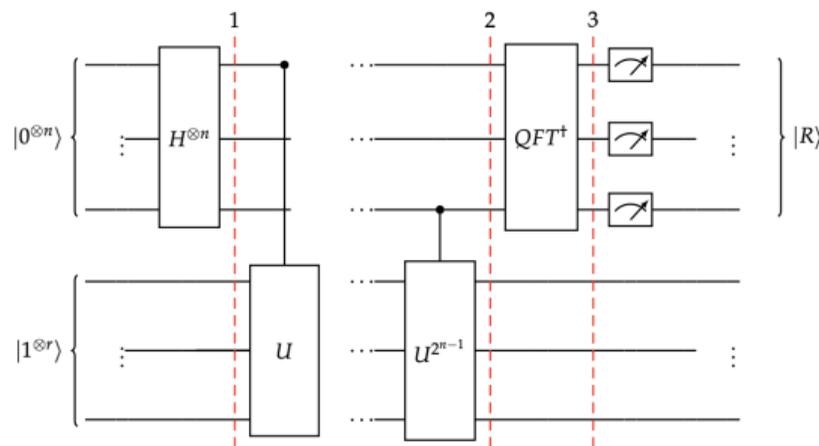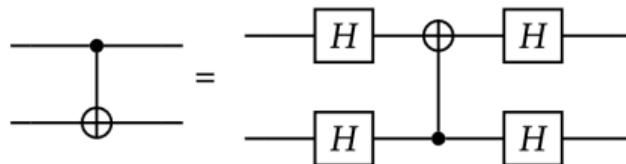

Figure: Shor's algorithm, for example

Phase kickback

- Important tool for algorithms, namely the quantum phase estimation
- Key attribute setting quantum apart from classical
- The beauty of many quantum algorithms lies in saving the solution in the phase of qubits via controlled-gates
- Represents a reverse of roles:

Phases

- You might wonder: 'if $\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ with $\alpha, \beta \in \mathbb{C}$, what about $\begin{bmatrix} -1 \\ 0 \end{bmatrix}$ or $\begin{bmatrix} i \\ 0 \end{bmatrix}$ or $\begin{bmatrix} \frac{1+i}{\sqrt{2}} \\ 0 \end{bmatrix}$?'
- Basically... look at the *Comprehensive Notes* (we don't care much about)
- Multiplying any $\mathbb{C}$-unit (a **global phase**) by a statevector, does not change it for our purposes
  - ▶ The Bloch sphere still looks the same
  - ▶ First entry in the statevector can be $\in \mathbb{R}$

- Some statevectors have same measurement prob. distribution

- They differ by a **relative phase** (comp. effect!)

- Purpose of phase gate $P(\phi) = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix}$
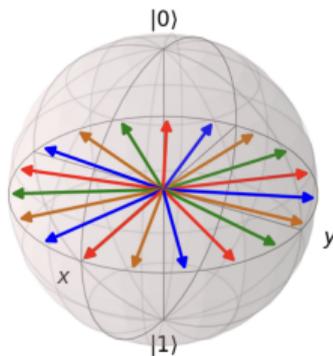
Entanglement

■ Consider the following circuit:
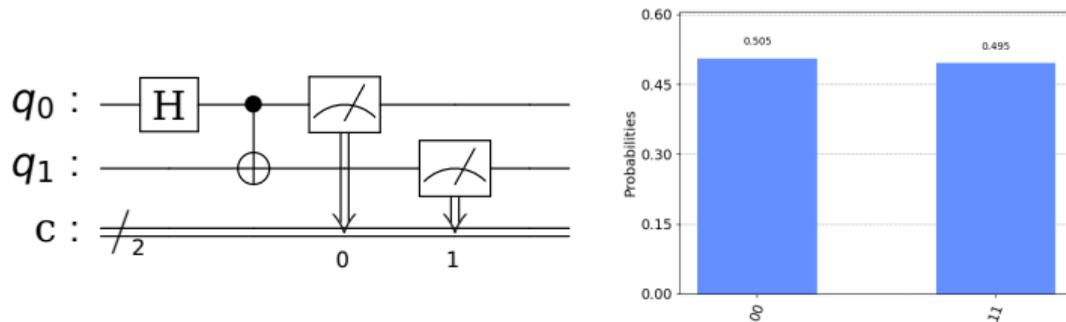
■ Each qubit is equally likely to be measured as $|0\rangle$ and as $|1\rangle$

■ However, both qubits will always be in the **same** state after measurement

■ This is called **entanglement**

■ Einstein's spooky action at a distance: More Quantum weirdness!

■ What happens: $CNOT(I \otimes H)|00\rangle = CNOT[\frac{1}{\sqrt{2}}(|00\rangle + |01\rangle)] = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

Deutsch-Josza algorithm overview

- First proposed by David Deutsch and Richard Josza in 1992 David Deutsch, "Rapid solution of problems by quantum computation"
- One of the first quantum algorithms that show quantum can trump classical
- Exponentially faster than any deterministic classical algorithm
- JUST LOOK AT THAT SMILE! SO PROUD

Deutsch's problem

- Consider an unknown function of a one bit input x
- The output $f(x)$ could either be **constant** 0 or 1 or depend on x (**balanced**)
- Two tests required classically to determine balanced vs. constant
- Quantum circuit for the generalised problem:
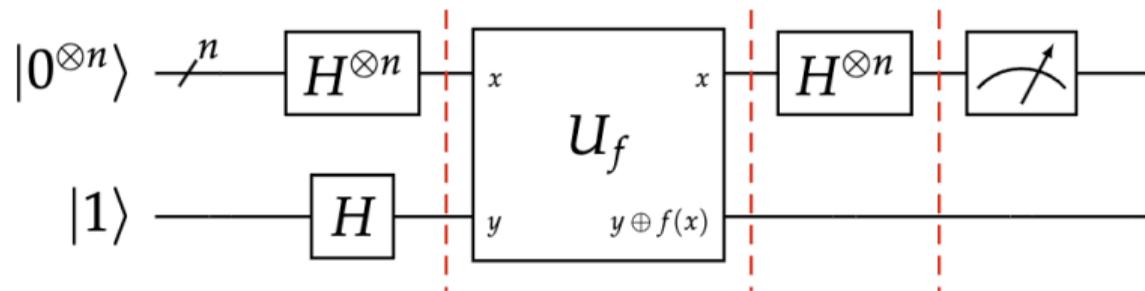
- Remember: Quantum gates must be reversible

Solution part 1: Phase kickback

- Our $U(f)$ gate transforms $|x\rangle |y\rangle$ to $|x\rangle |y \oplus f(x)\rangle$ ($\oplus$: plus, then modulo 2)
- Let's "cheat": Instead of using $|0\rangle$ for $|y\rangle$ we use $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$
- Then, if we apply our gate $U(f)$:
  $U(f) |x\rangle \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$
  $= |x\rangle \frac{1}{\sqrt{2}}(|f(x)\rangle - |1 \oplus f(x)\rangle)$
  $= (-1)^{f(x)} |x\rangle \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$
- Now we have encoded information in the sign (or phase) of the input qubit

Solution part 2: Input superposition

- We will now use the function information encoded in the phase
- We initialize $|x\rangle$ as superposition of both possible values: $|x\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$
- We can ignore the output Qubit and get, after applying $U(f)$:
  $(-1)^{f(x)} |x\rangle = \frac{1}{\sqrt{2}}((-1)^{f(|0\rangle)} |0\rangle + (-1)^{f(|1\rangle)} |1\rangle)$
- That means constant functions result in $|q_0\rangle = \pm\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$
- Balanced functions result in $|q_0\rangle = \pm\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$
- (Note that multiplying a Qubit state globally by -1 does not change it)
- Use the H gate and measure to get $|0\rangle$ for constant and $|1\rangle$ for balanced
- We have solved Deutsch's problem in one try!
- Deutsch-Josza extends this to input length n: One try vs. worst case $2^{n-1} + 1$

Implementing Deutsch-Josza extended algorithm

- Let's look again at Deutsch's algorithm:
    - Prepare (input) qubit-0 in $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ state
    - Prepare (output) qubit-1 in $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ state
    - Apply the oracle
    - Apply the Hadamard gate to qubit-0
    - Measure: If $|0\rangle$, the function is constant, else $|1\rangle$ if it is balanced
    - Oracles: constant implies 0 or 1. Balanced implies identity or negate

- Your job is to increase this to 3 or more input qubits (your job, not mine)

- The math of this general version can be found in the Comprehensive Notes

- Now balanced can be many more possibilities. Suppose 3 input qubits and 1 output qubit. Example balanced oracle:
    - $f(000) = f(101) = f(111) = f(100) = 0$
    - $f(110) = f(011) = f(010) = f(001) = 1$
    - You should measure $|000\rangle$ for constant, and anything else for balanced

What does GWDG offer?

- Our QC team provides HPC-QC software solutions, research and consulting
- SCC, Emmy and Grete have QC containers to run simulations on
  - ▶ Qiskit, Qulacs, Cirq, Qsim, Qibo, QuTip...
- Bachelors/Masters theses are available!
- We are engaged in publishing new research regarding NISQ software
- We provide courses and workshops (like this one!)
- We do not have our own quantum computer
- Our webpage is https://gwdg.de/en/community-pages/qc-intro/ for more info

Further reading

- Recap linear algebra:
  Essence of linear algebra on YouTube

- Deutsch's algorithm explained using a state machine:
  Quantum Computing for Computer Scientists on YouTube

- Introduction for self study:
  Quantum computing for the very curious

- Everything on Qiskit, lots of tutorials: https://qiskit.org/

- Good textbooks:
  - Quantum Computing: An Applied Approach by Jack D. Hidary
  - Quantum Computing verstehen von Matthias Homeister

- Brief overview of the field (link to arxiv.org):
  Quantum Computing in the NISQ era and beyond, John Preskill

References

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Exercises

Have fun with the exercises :)