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Quantum Computing

From Fundamentals to first Quantum Algorithms

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Agenda

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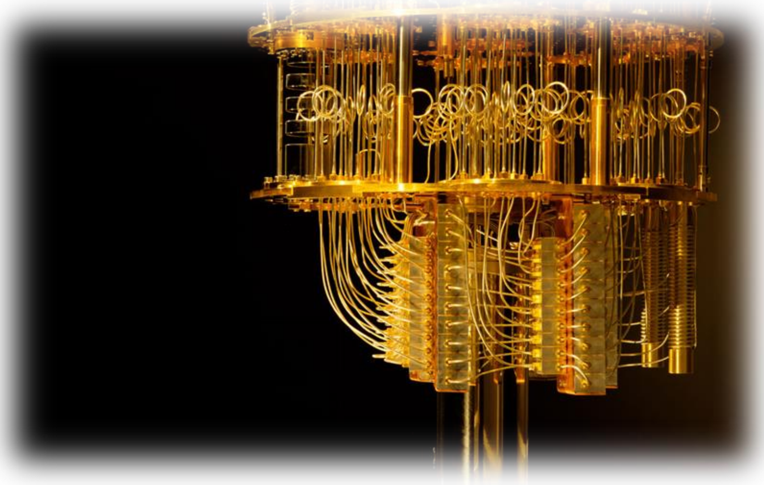
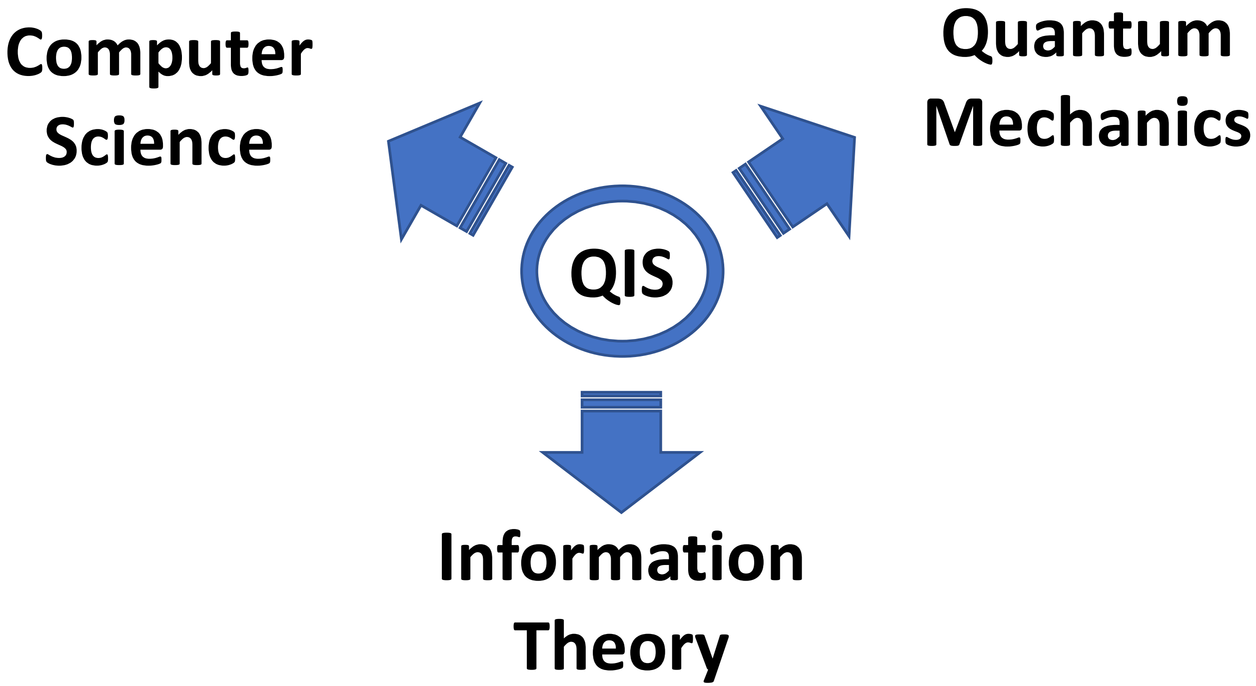
Goal: holistic picture and basic understanding of working principles

1. **Motivation** and Overview
2. Basic **Working Principles**
3. **Near-term** Applications
4. Simple Quantum **Algorithms**
5. **Challenges** and Limitations

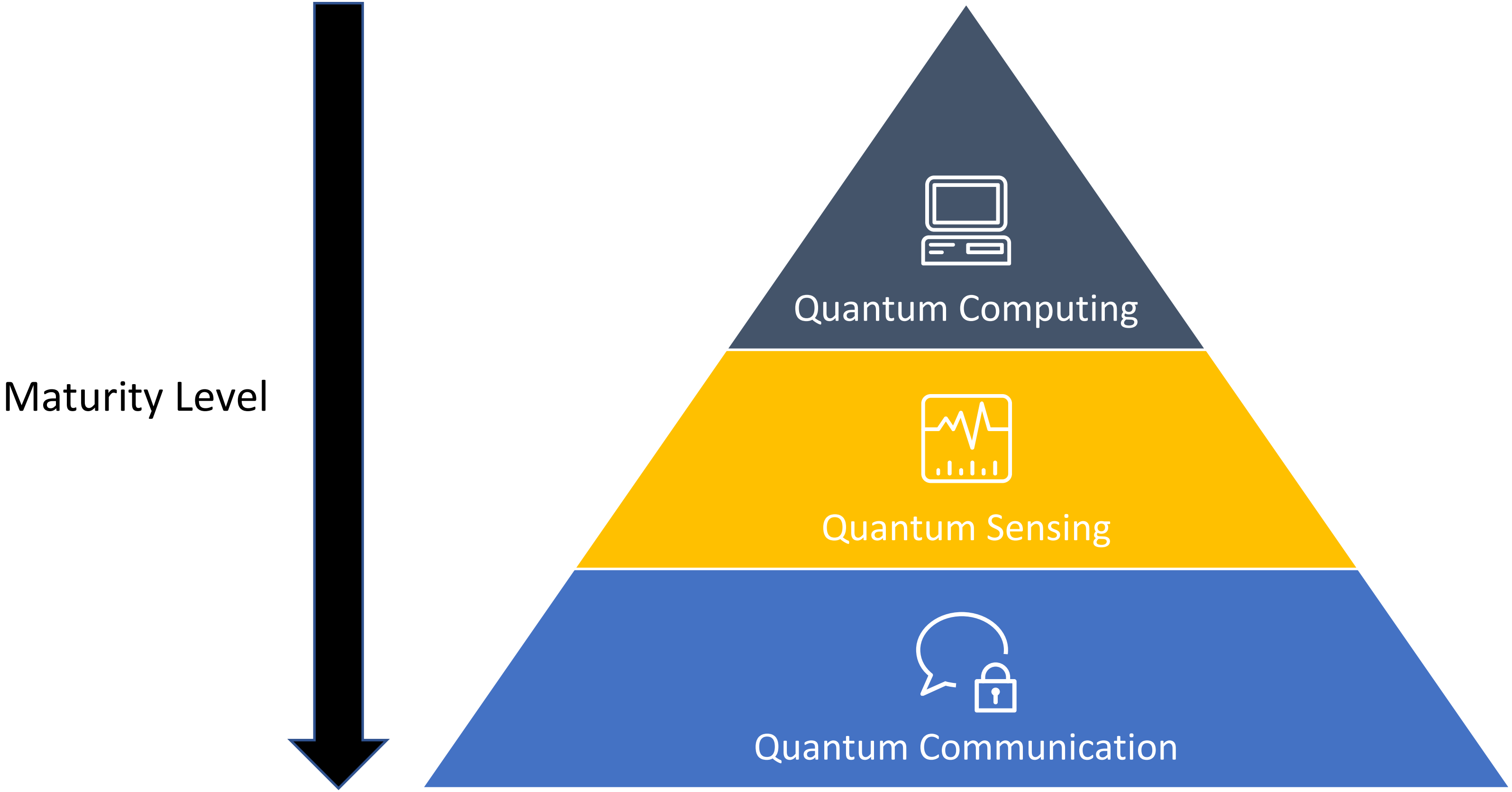


Overview and Motivation

Quantum Information Science (QIS)

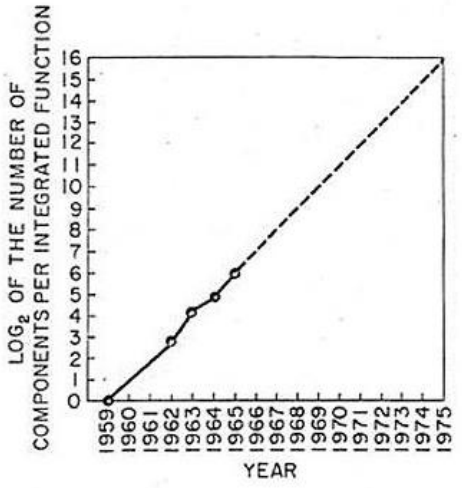


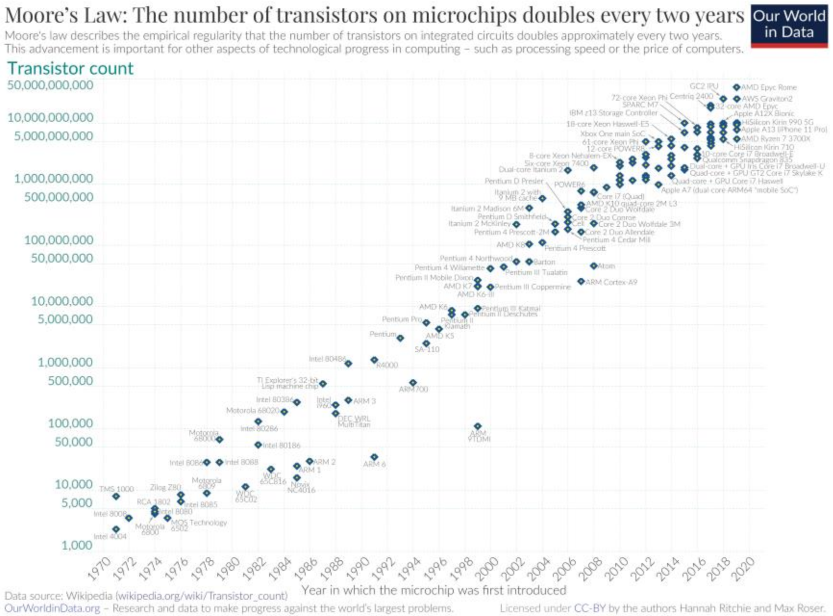
Quantum Technologies



Classical Computing: Limitations - Hardware

- **Limits of Moore´s law**
  - Doubling of transistor counts on microchips every 12-24 months
  - Physical limitations





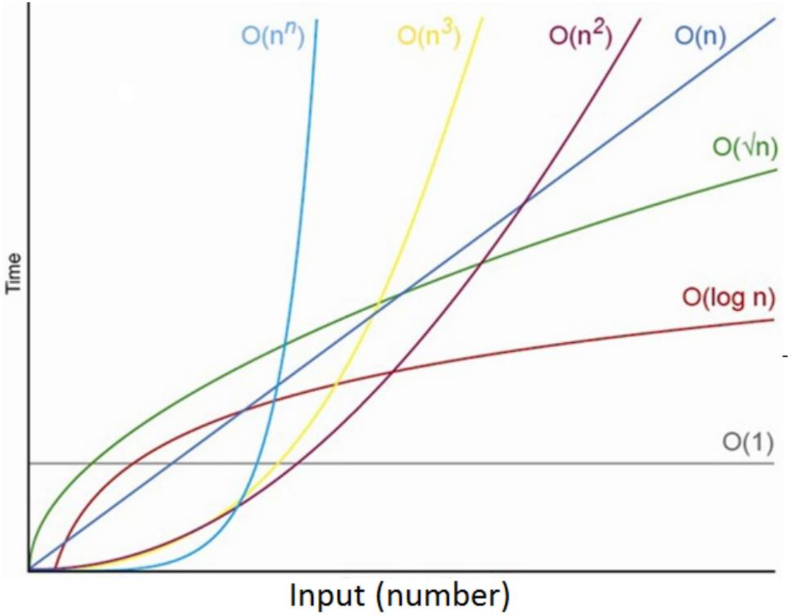
Source: https://web.archive.org/web/20211221191600/https://www.intel.com/pressroom/kits/events/moores_law_40th/index.htm?iid=tech_mooreslaw+body_presskit

Source: https://ourworldindata.org/technological-progress

Classical Computing: Limitations – Algorithms

- **Many complex problems are intractable for classical computing, e.g.:**
  - Exponentially growing search spaces
  - Simulation of quantum processes

- **Best case:**
  - From O(n^n) to O(n^1)



Source: Hidary (2019). Quantum Computing: An Applied Approach

Applications – from research to operations

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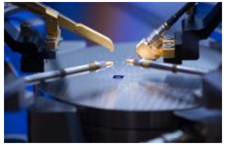
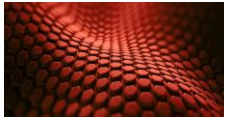
Research applications

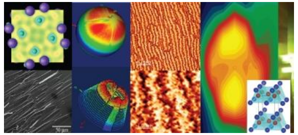

Batteries

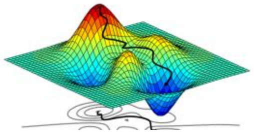

Drug discovery

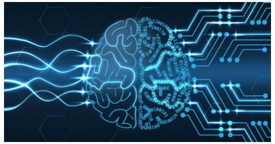

Semiconductors


Fertilizer production


Materials design


Condensed matter physics


Optimization


Machine Learning

Operations applications


Transportation


Finance


Energy utilities


Telecoms


Manufacturing


Marketing

Current Limitations of Quantum Computing

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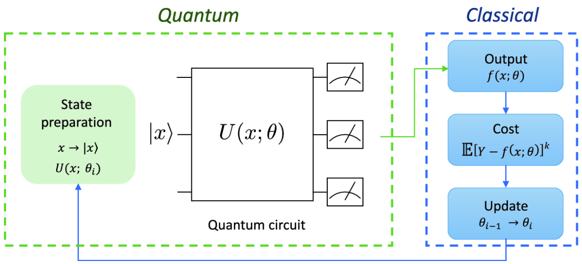
- **Technical Challenges:**
  - Sensitivity to environment
  - Accuracy of quantum operations
  - Scaling of quantum computers
  - …
- **Regimes**
  - Noisy Intermediate Scale Quantum (NISQ-era)
  - Fault-tolerant Quantum Computing

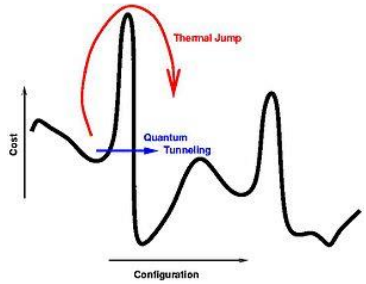
Preskill, J., 2018. Quantum computing in the NISQ era and beyond. *Quantum, 2,* p.79.

NISQ-Era Approaches to QC

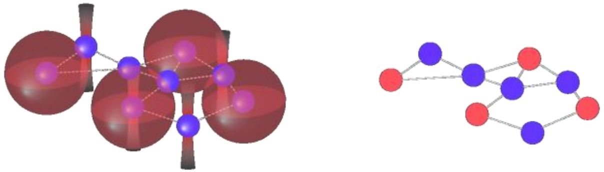
- **Variational Quantum Algorithms**
  - Similar to neural nets in ML
  - Gate-based → sequential programming



- **Quantum Annealing**
  - Encode optimization problem into energy of quantum system
  - System "wants" to stay in minimum



- **Quantum Simulators**
  - Encode problem into energy of quantum system
  - Different quantum phenomena



Quantum Computer – Hardware Architectures (1)

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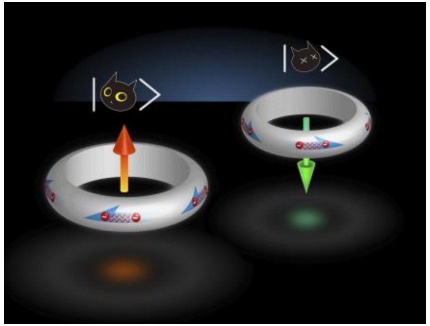
- **Photonics**
  - Photons are information carrier
  - Optical elements (mirrors, phase shifters) for manipulation
- **Superconductors**
  - Google, IBM,…
  - Electric current produces magnetic moment (spin)
  - Temperatures: mK
  - Microwave pulses for manipulation



Source: Johnston et. al (2019). Programming Quantum Computers

Quantum Computer – Hardware Architectures (2)

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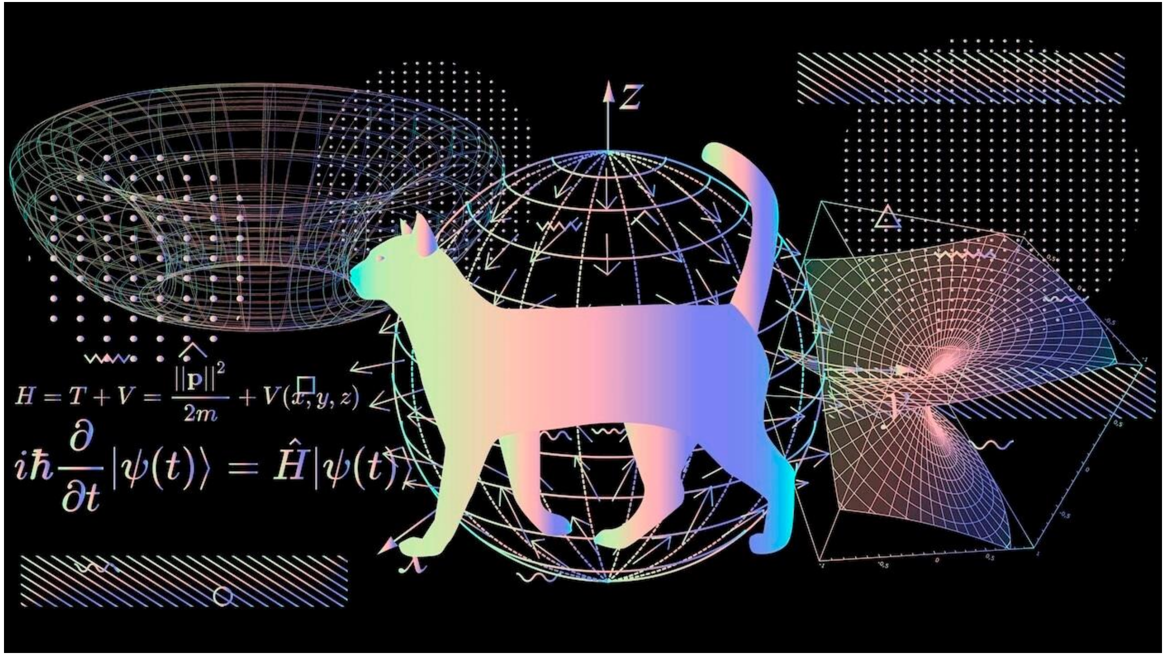
- **Trapped Ion**
  - Ions in electromagnetic field
  - Lasers for manipulation
- **And many more:**
  - Topological Quantum Computation
  - Neutral Atom Quantum Computation
  - …

All these approaches seek to make the jump to the next regime. To do this, they try to better model a Qubit.

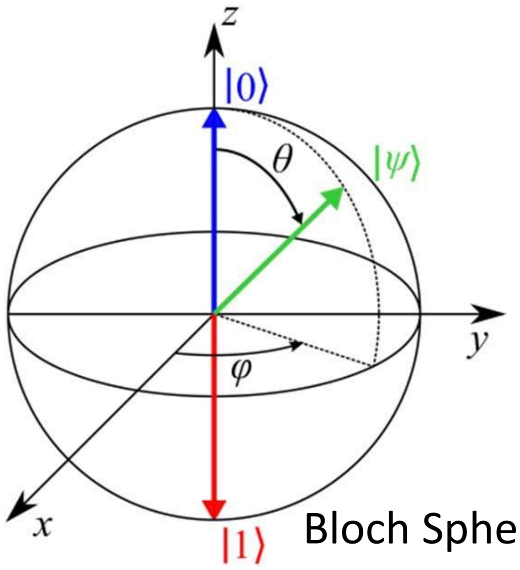
Basic Working Principles



Basic Concepts – From Bits to Qubits

- A qubit is a **two-level** quantum mechanical system
- The **state** of the qubit can be represented by a **vector**

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



Bloch Sphere

- Similar to classical bit 0,1 → $|0\rangle$, $|1\rangle$
- Can also be a mixture → **superposition**

Phase

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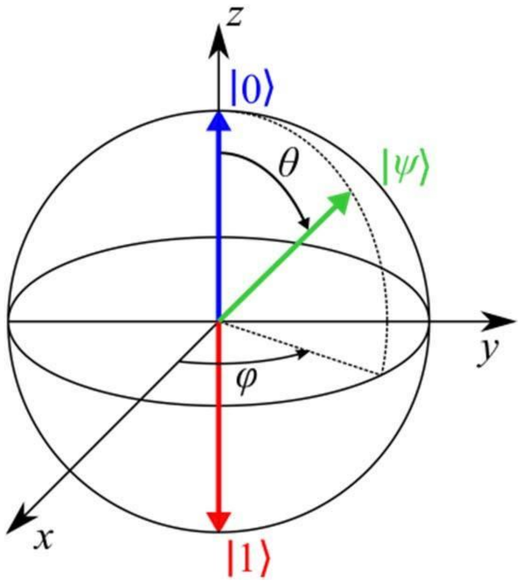
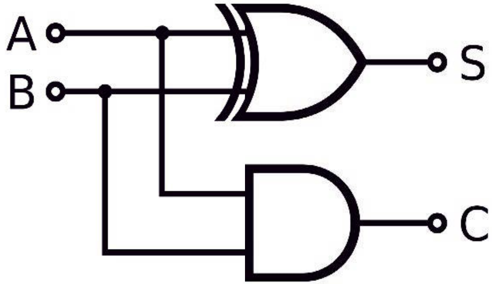
- Additional **degree of freedom** in quantum systems
- State as **complex** valued vector
- Often useful to **encode information** in the phase

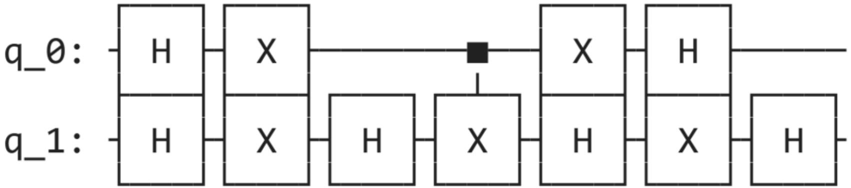


Basic Concepts – From Classical to Quantum Circuits

- **Classical Computing Circuit**

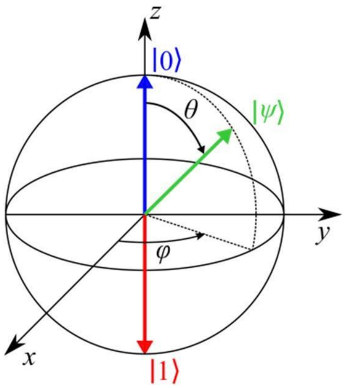


- **Quantum Computing Circuit**
  - Construct and read these diagrams from left to right
  - Input and output space are the same



Quantum Operator - Reversibility

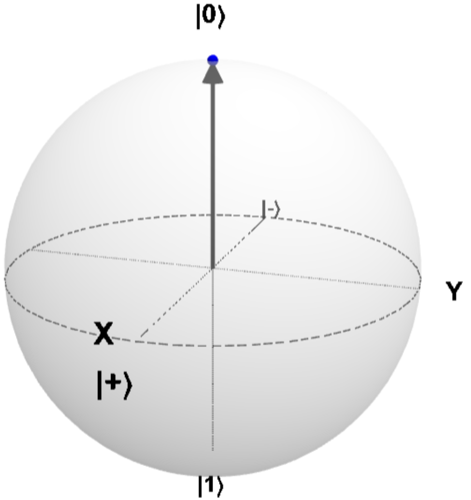
- **Isolated quantum system**
  - Every quantum operation is reversible
  - Every quantum operation is unitary
    → describes rotation but no change in vector length

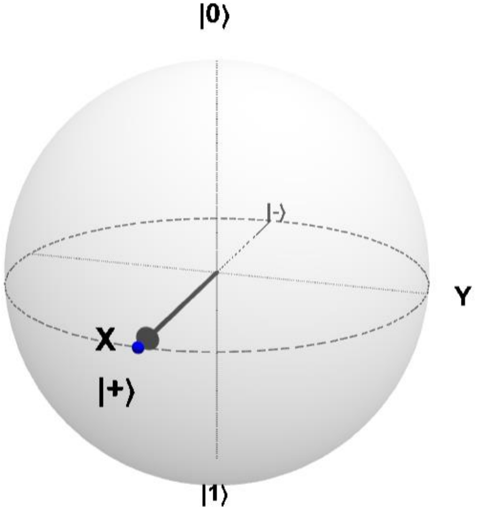


- Quantum operations **are matrices**
- **Reversibility**
  - $\boldsymbol{U}^{-1}\boldsymbol{U}|\Psi\rangle = \boldsymbol{U}^{\dagger}\boldsymbol{U}|\Psi\rangle = |\Psi\rangle$
  - $\boldsymbol{U}^{\dagger}$ is U transposed and complex conjugated

Quantum Operations – Hadamard

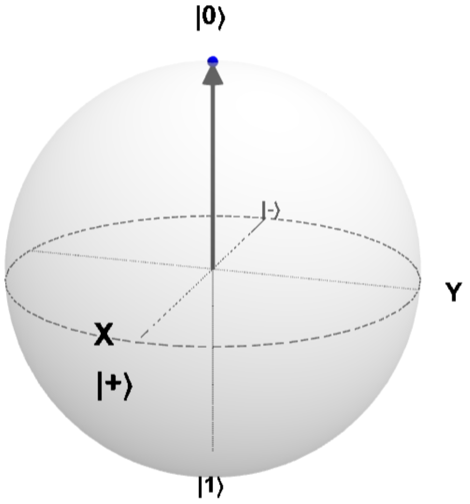
- Hadamard operator is *crucial* in quantum computing
- Takes a qubit into an equal superposition of two states

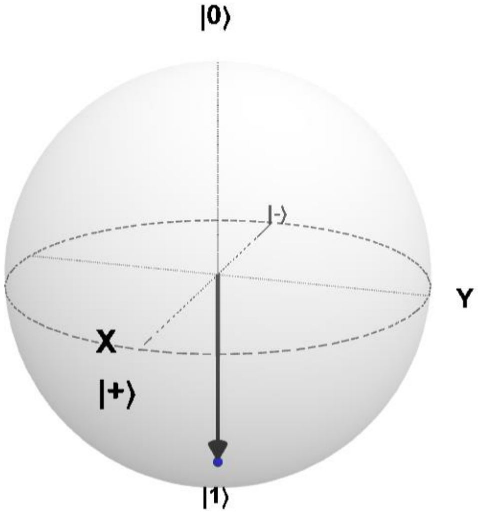




Quantum Operations – Pauli X

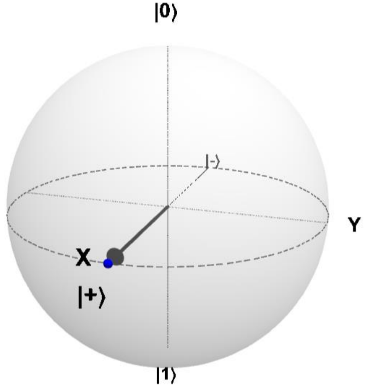
- Similar behavior like *Not* in classical computing
- Also known as *Not Gate*

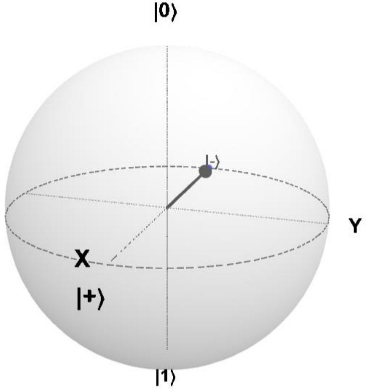




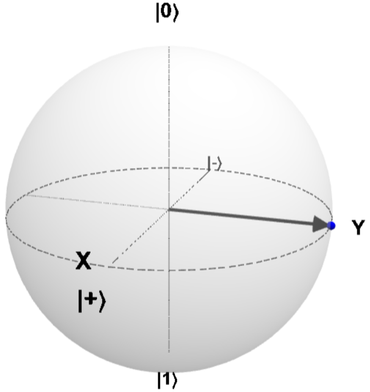
Quantum Operations – Pauli Y & Z

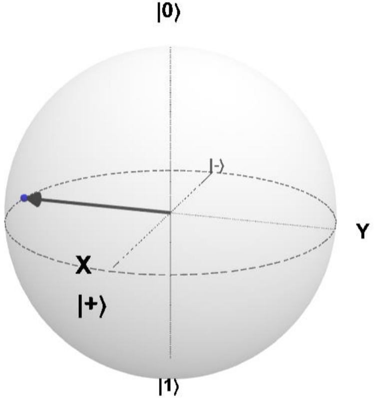
- Pauli Y





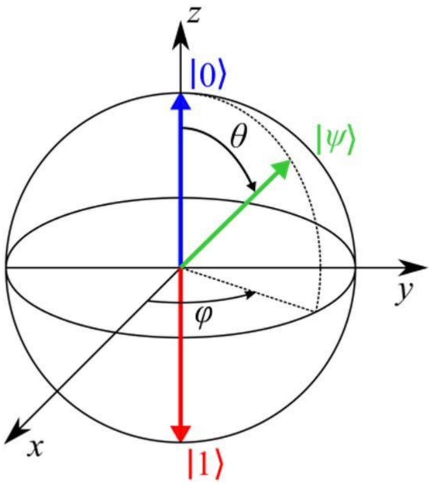
- Pauli Z





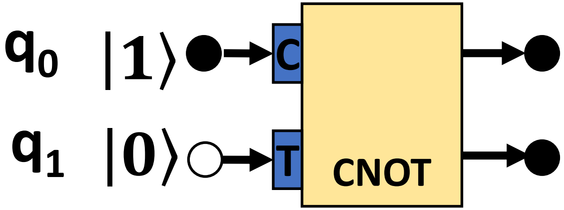
Single Qubit Gates – Parameterized Gates

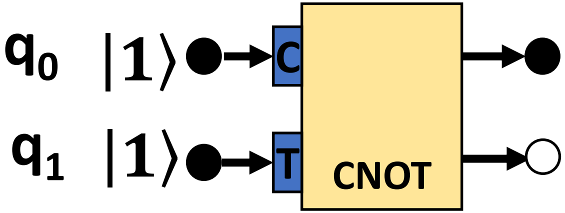
- **Bloch sphere rotations can be parametrized**
  - E.g., rotation of φ around z-axis
- **3 angles for any arbitrary rotation**
  - Euler's rotation theorem
- **Examples:**
  - RX, RY, RZ



Quantum Operations – CNOT

- Controlled-NOT (CNOT)
- First Qubit is the *control qubit*
- Second Qubit is the *target* qubit
- Examples

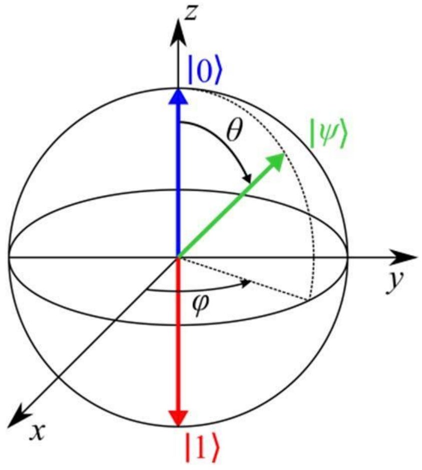




Basic Concepts - Measurement

- **Measurement destroys superposition**
  - Non-reversible quantum operation
  - What was state before measurement?
- Probability distribution → Quantum state
- No-cloning theorem

  → Repeated computation and measurement
- **Intermediate states** of the quantum system are **not accessible**



Tensor Product

- Description of space for 2 (or multiple) qubits
- Notation $\otimes$
- 2-qubit-state example

Product state: $$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} \otimes \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \begin{pmatrix} a_1 * \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} \\ b_1 * \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} a_1 a_2 \\ a_1 b_2 \\ b_1 a_2 \\ b_1 b_2 \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$$

In general : $|\psi\rangle = \boldsymbol{a}|\mathbf{00}\rangle + \boldsymbol{b}|\mathbf{01}\rangle + \boldsymbol{c}|\mathbf{10}\rangle + \boldsymbol{d}|\mathbf{11}\rangle$

Condition for separability: $\frac{a}{b} = \frac{c}{d}$, otherwise: „**entangled**“

n qubits → length of vector: 2^n

Basic Concepts – Entanglement

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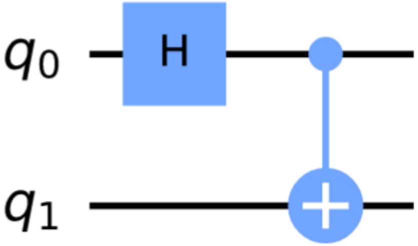
- **Correlation between states of qubits**
  - One can gain information about a qubits state by knowing the states of the other qubits
  - Non-entangled states can be simulated efficiently by classical computers → power of QC comes (a.o.) from entanglement
- **E.g.,: Bell States (completely entangled):**
  - $|\Psi_+\rangle = \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}|\mathbf{00}\rangle + \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}|\mathbf{11}\rangle$
  - $|\Psi_-\rangle = \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}|\mathbf{00}\rangle - \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}|\mathbf{11}\rangle$
  - $|\Phi_+\rangle = \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}|\mathbf{01}\rangle + \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}|\mathbf{10}\rangle$
  - $|\Phi_-\rangle = \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}|\mathbf{01}\rangle - \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}|\mathbf{10}\rangle$

Multi-qubit gates – Entangled states

- **Consider the following example:**



- **H** $|00\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |01\rangle) = |0+\rangle$
- **CNOT** $|0+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ → **Bell-state**

Quantum Circuits

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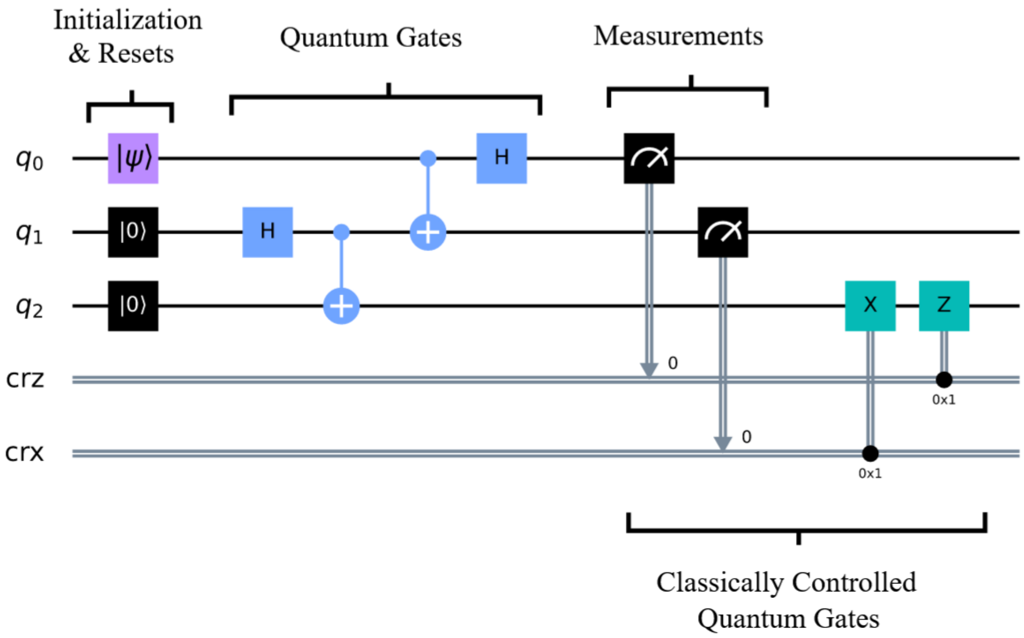
- **Qiskit definition:**

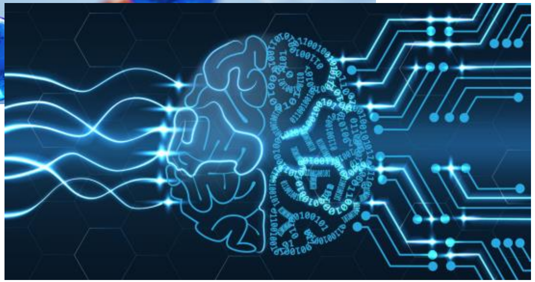
*„A **quantum circuit** is a computational routine consisting of coherent **quantum operations** on **quantum data**, such as qubits. It is an **ordered sequence** of quantum gates, measurements and resets, which **may be conditioned on real-time classical computation**.”*



Source: https://qiskit.org/documentation/apidoc/circuit.html

Algorithms & Application Areas






Regimes of Quantum Computing

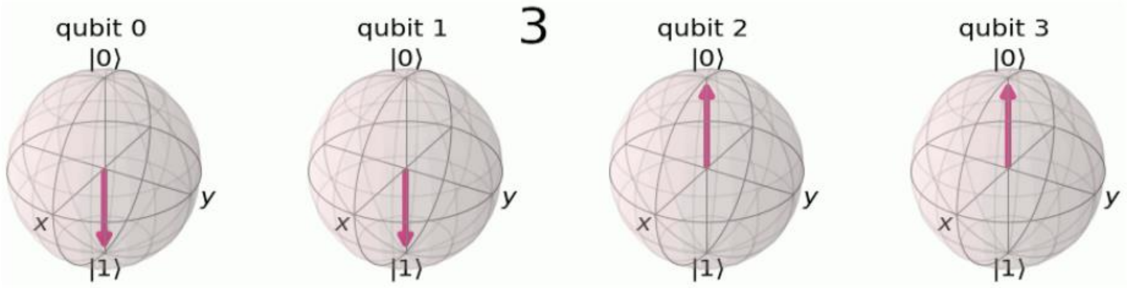
- **Fault-tolerant QC → broad application, provable advantage**
  - Quantum Fourier Transform
  - Grover Search Algorithm

- **NISQ-era QC → niche applications, probably better heuristic**
  - Quantum Chemistry → VQE
  - Optimization → QAOA
  - Quantum Machine Learning → QNN, QTDA

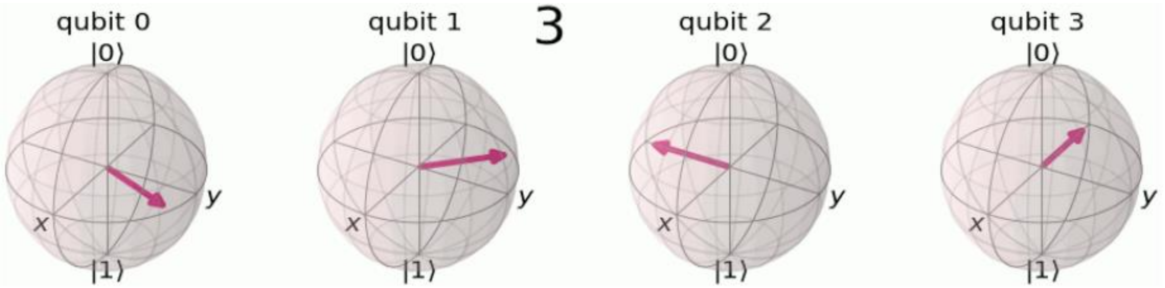
Quantum Fourier Transform

- **Quantum** implementation of **discrete Fourier transform**
- **Part** of many **quantum algorithms** (Shor,…)

Computational basis

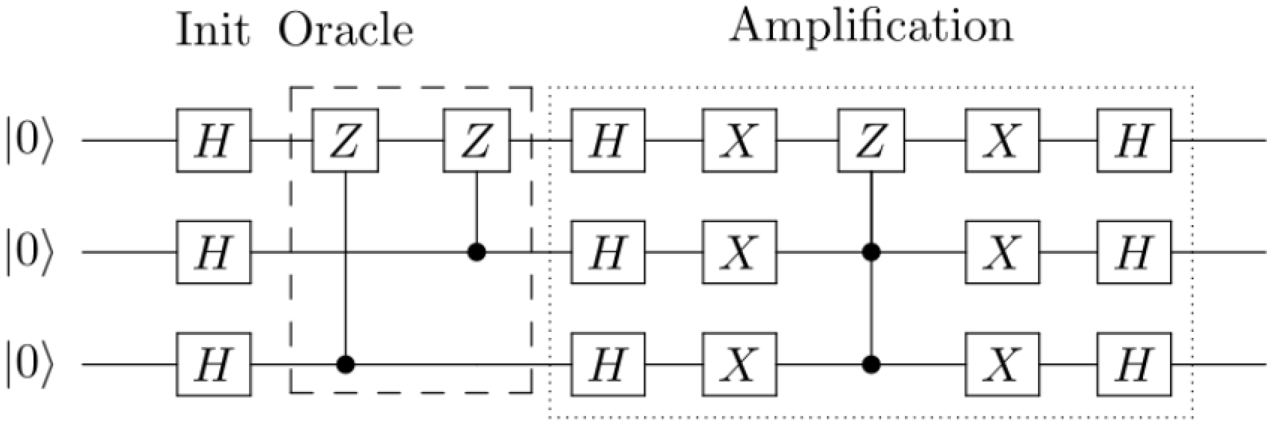


Fourier basis



Grover-search algorithm

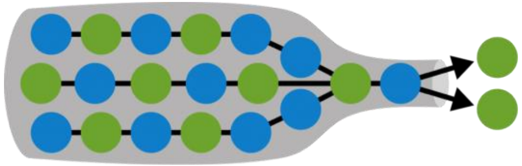
- **Database searches**, subroutine in other algorithms,…
- **Quadratic** speed-up



Quantum Algorithms – Requirements

Solve useful problem

Speed-up or other advantage



Relatively small data

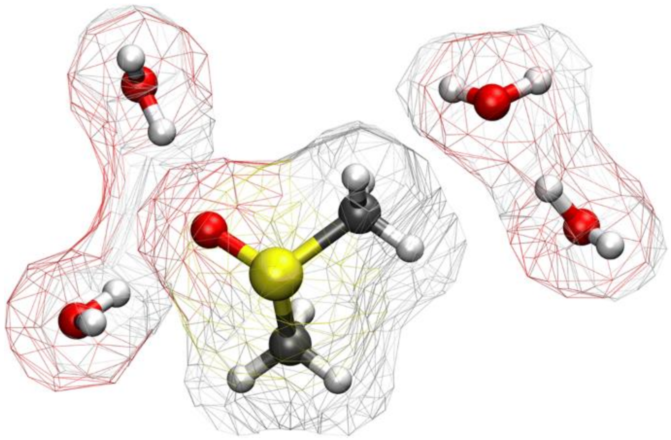
Correctness guarantees

Resources can be estimated

→ goal today: find promising problem where hybrid algorithm is better heuristic than purely classical approach

Application Areas – Quantum Chemistry

- **Closest to idea of Feynman 1981:**
  - ➢ Simulate quantum systems (molecules) with quantum systems (QC)



- **Scientific insights**
  - ➢ Quantum mechanical properties of molecular systems
  - ➢ Physiological processes (e.g., photosynthesis, DNA mutation)

Application Areas – Quantum Chemistry

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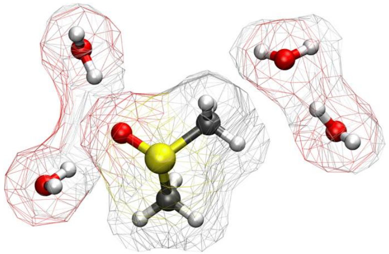
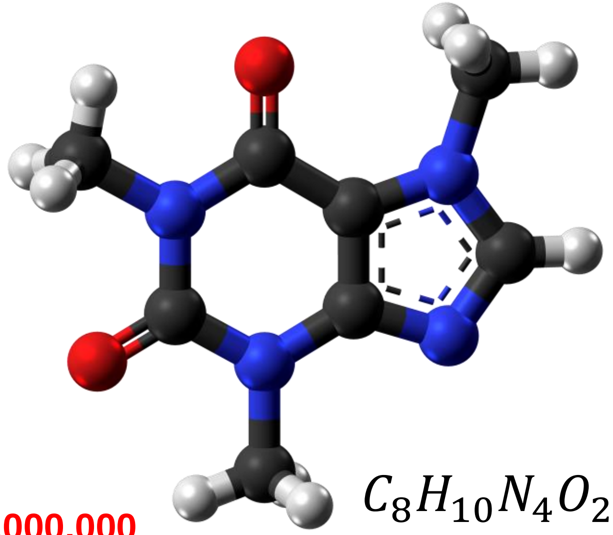
- **Simulation of molecular behaviour at quantum level:**
  - Drug design
  - Materials design
  - Development of new chemicals (e.g. catalyst in agriculture)

- **Classical approach:**
  - Calculations based on simplified model of molecule
  - Check a posteriori validity of the model



Quantum Chemistry- Example

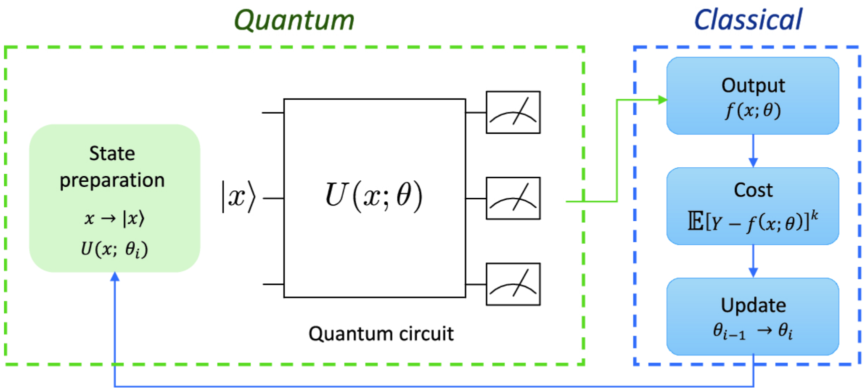
- **Molecule as quantum object:**
  - Many particles (e.g., nuclei, electrons)
  - Many-body problem
  - Highly interacting
- **Caffeine: 24 atoms**
- **Classical computation: 10^{48} bits**
  - **10,000,000,000,000,000,000,000,000,000,000,000,000,000,000,000,000,000**
- **Quantum computation: 160 qubits**



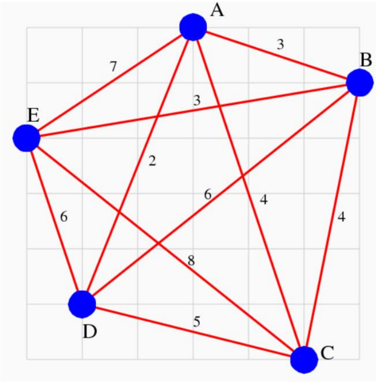
$C_8H_{10}N_4O_2$

Variational Quantum Eigensolver – VQE

- Computes **ground state energy**
- Makes use of **parameterized gates (VQA)**
- **Procedure:**
  - Generate trial state with U(θ)
  - Measure in computational basis
  - Calculate cost function: energy
  - Update parameters classically (e.g. gradient descent)



Application Areas – Quantum Optimization

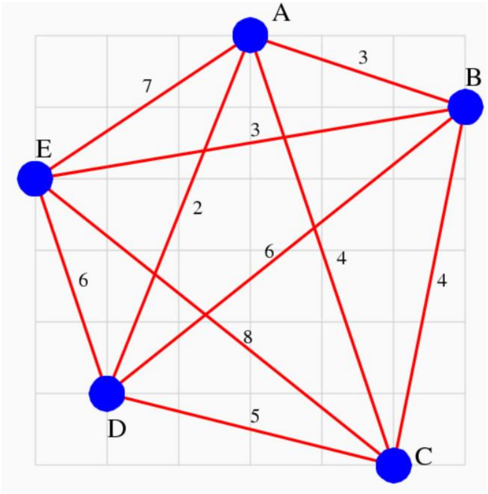


- **Industrial relevance**
  - Logistics,
  - Manufacturing,
  - …
- **Examples:** graph optimization, routing, scheduling
  - Usually exponentially growing search space
- **Classical computation**
  - Expensive algorithms (e.g., brute force algorithms)
  - Use of approximative heuristics (e.g., genetic algorithms)

Quantum Optimization – Example

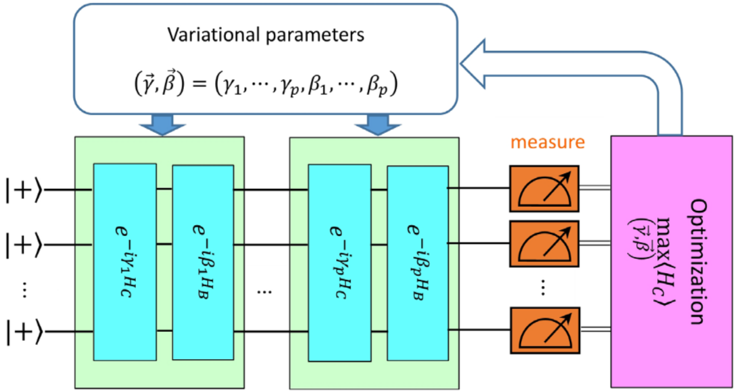
Travelling Salesman Problem

- ➢ Visit all cities → shortest route?
- ➢ E.g., 20 cities: 20x19x18x..x2x1= 2,430,000,000,000,000,000 combinations



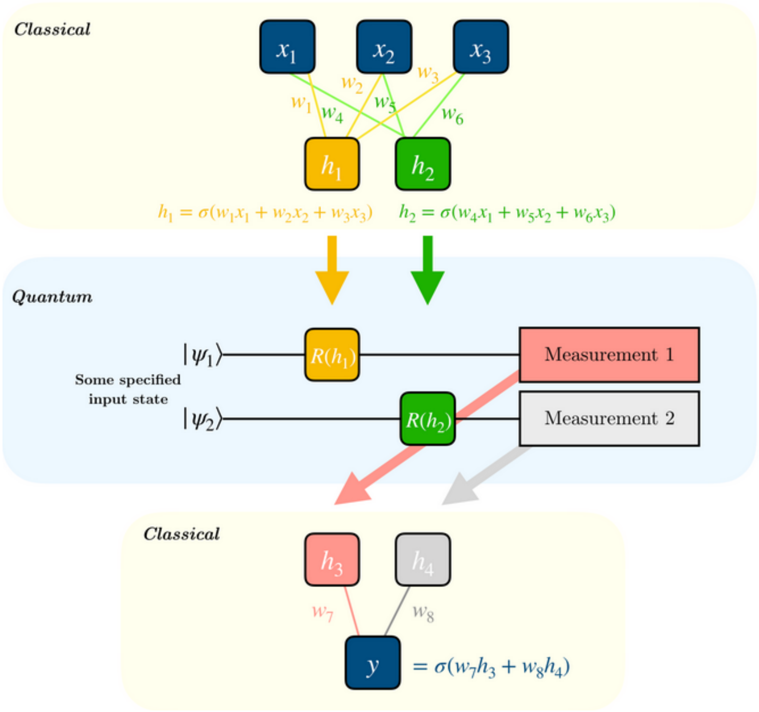
Quantum Approximate Optimization Algorithm – QAOA

- Algorithm for **combinatorial optimization** problems
- Very **similar to VQE** but with a defined ansatz
- **Procedure:**
  - Generate trial state with $U_C(\gamma), U_B(\beta)$
    - $U_C(\gamma)$: problem unitary
    - $U_B(\beta)$: mixing unitary
  - Measure in computational basis
  - Calculate cost function
  - Update parameters classically
- **Discrete** form of **Quantum Annealing**



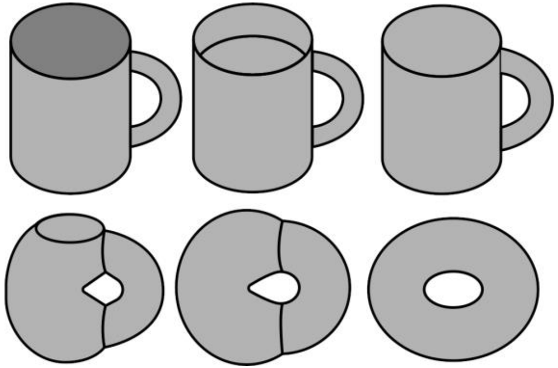
Application Areas – Quantum Machine Learning

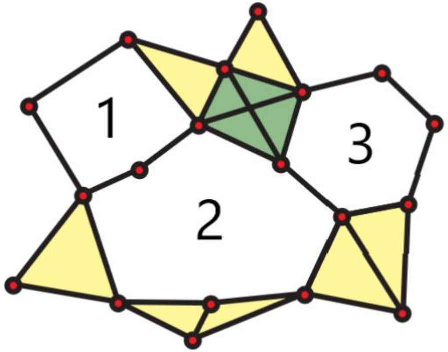
- **Mostly quantum-enhanced ML**
  - ➢ Hybrid nature
  - ➢ E.g., Quantum GAN
- **Idea:**
  - ➢ Work in large space
  - ➢ Harness non-determinism
- **Quantum Topology Analysis**
- **Quantum Neural Networks**
  - ➢ Variational Quantum Algorithms
- And many more (Q-SVM, etc.)



Quantum Topological Data Analysis

- **Procedure**
  - Radius around data points
  - If touch → edge on graph
  - Graph → topological object
- **E.g., Betti numbers:**
  - number of k-dimensional holes
  - E.g., torus → b0: 1, b1: 2, b2: 1
- **Provable superpolynomial speedup for:**
  - Betti-dense (lot of holes) AND
  - Large in clique numbers (lot of edges)



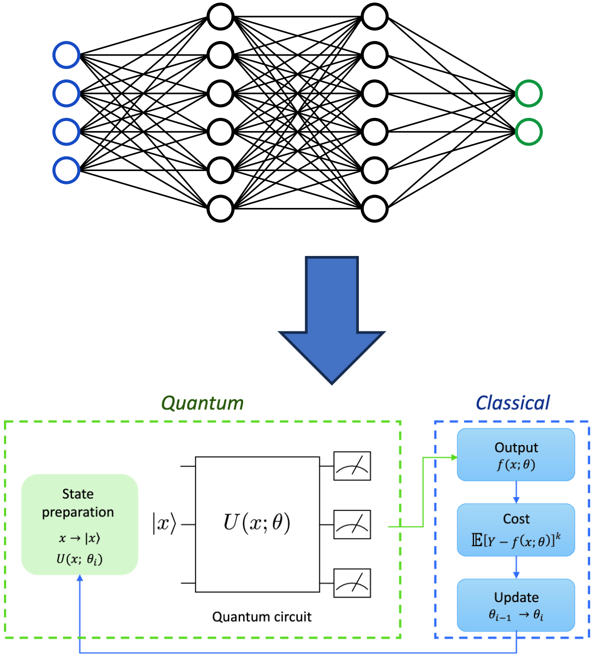


Gyurik, C., Cade, C., & Dunjko, V. (2022). Towards quantum advantage via topological data analysis. *Quantum*, *6*, 855.

Quantum Neural Nets

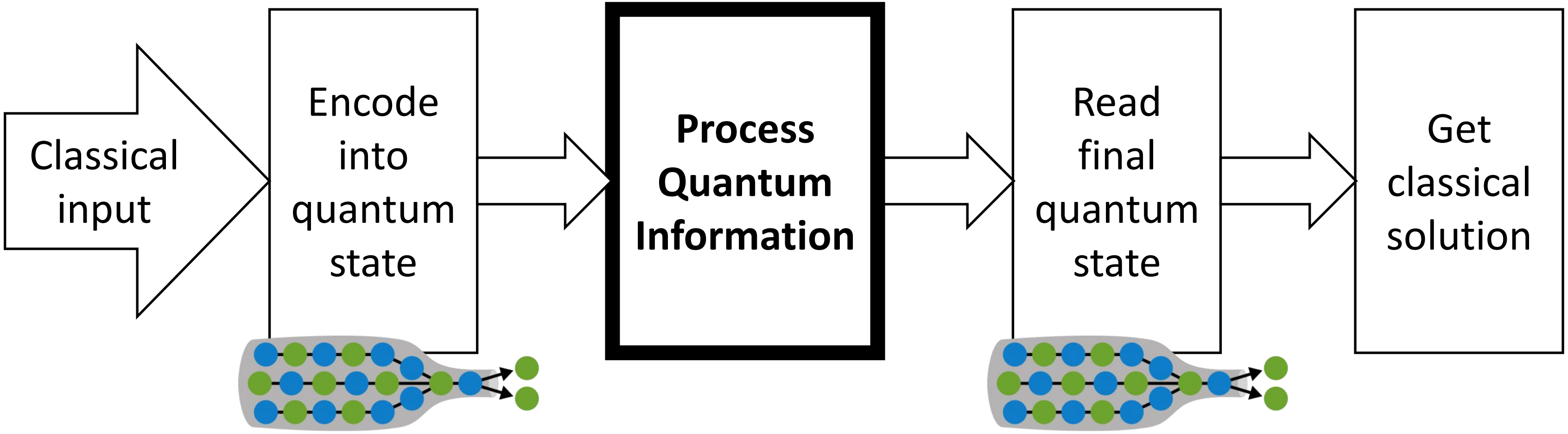
JOHANNES KEPLER UNIVERSITY LINZ

- **Advantages supposed esp. for quantum data**
  - Material science,
  - Drug design,…
- **Quantum often part of hybrid model**
  - Before, after, parallel, etc. to classical NN
- **Challenges**
  - Abundance of local minima
  - Barren plateau
  - Noise → erase landscape features
  - Required: classically hard to simulate
  - Input / output problem



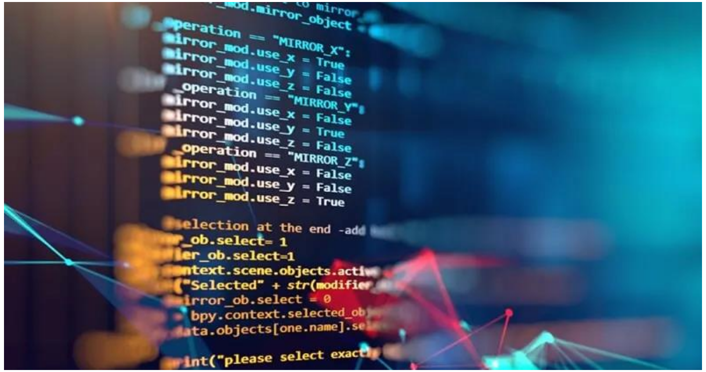
Challenges & Limitations

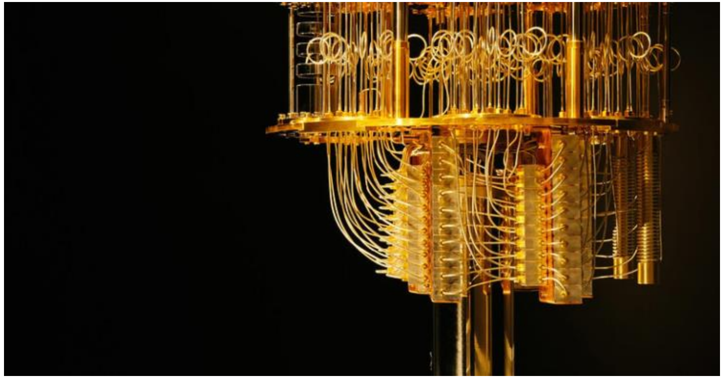
Quantum Information Processing – Bottlenecks




Ewin Tang
Quantum Recommendation Systems
arXiv:1807.0427
1
arXiv:1811.00414
Ewin Tang
Quantum PCA
Ewin Tang
arXiv:1811.04909
Low rank HHL

Challenges and Limitations





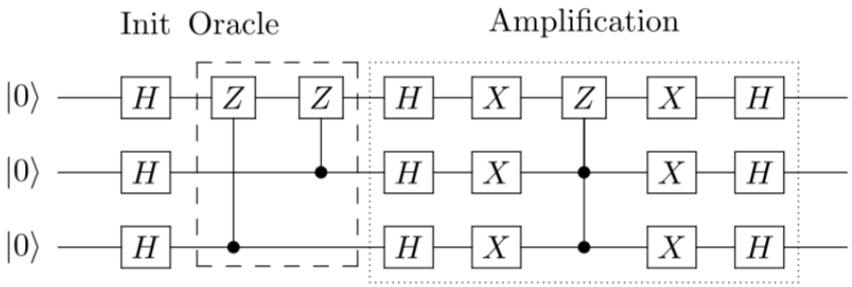
Algorithms & Software

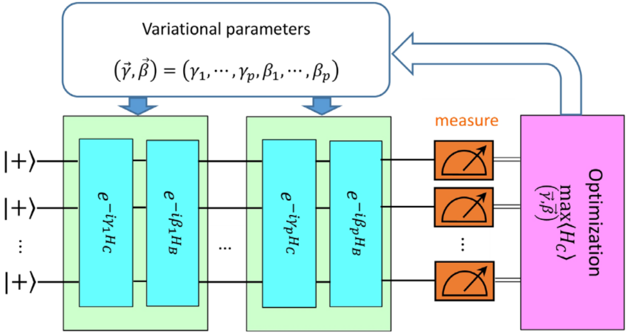
- Dequantization
- Error correction
- Compilers
- …

Hardware

- Fidelity
- Error correction
- Scalability
- …

Challenges and Limitations





Fundamental

- No copies
- No assessment of intermediate states
- Decoherence
- …

Variational Quantum Algorithms

- Abundance of local minima
- Barren plateau
- Require a LOT of runs
- …

Summary of Challenges

Fault-tolerant Quantum Computing:

- Provable improvement for some applications
- Requires a lot of research

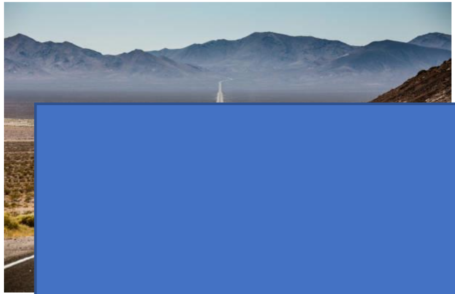
NISQ-era:

- No provable improvement
- Maybe still better heuristic especially in combination with classical computing

---

- **Fidelity** has to improve drastically
- QCs will **NEVER replace** classical ones!!!

Summary of Challenges



BUT:

QC has **immense transformative potential**

→ rather time scale is questionable

→ topics still requires a lot of fundamental and applied research

→ interesting to bring in ideas from various disciplines

Fault-toleran

- Provable i
  some app ... cially in
- Requires a ... uting

- **Fidelity** has to improve drastically
- QCs will **NEVER replace** classical ones!!!

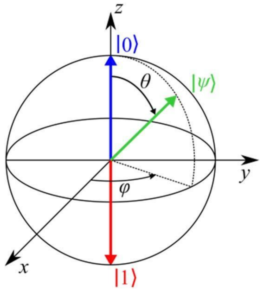
Wrap-Up

1. Motivation and Overview

- Classical computing faces severe scaling issues
- QC is applicable to a variety of computational problems
- There are diverse approaches to quantum computing

2. Basic Working Principles

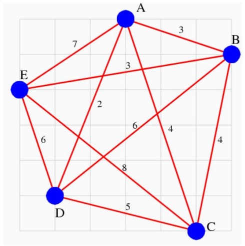
- QC harnesses quantum mechanical phenomena
- Mathematically its linear algebra



Wrap-Up

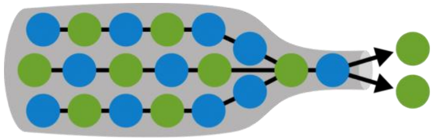
3. Near-term Applications are

- Quantum chemistry
- Quantum optimization
- Quantum machine learning



4. Challenges and Limitations

- Interesting challenges remain
- Quantum computers are (universal) special purpose machines
- The potential is worth the effort




HOW'S YOUR QUANTUM COMPUTER PROTOTYPE COMING ALONG?
GREAT!
Dilbert.com DilbertCartoonist@gmail.com
THE PROJECT EXISTS IN A SIMULTANEOUS STATE OF BEING BOTH TOTALLY SUCCESSFUL AND NOT EVEN STARTED.
4-17-12 ©2012 Scott Adams, Inc./Dist. by Universal Uclick
CAN I OBSERVE IT?
THAT'S A TRICKY QUESTION.