Introduction for Quantum Algorithms for Scientific Computation: An Applied Math Perspective

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Outline

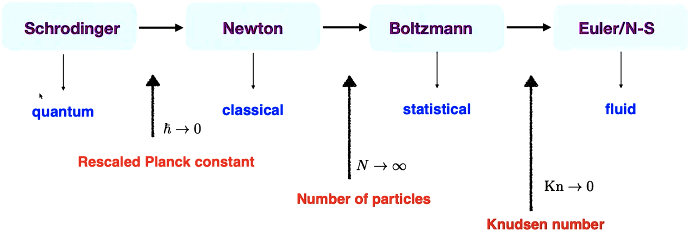
1. Intro to Quantum Computing
   - Motivations
   - Basics of QC
2. Block Encoding and Hamiltonian Simulation
3. Other advanced topics
   - General Differential Equations *(optional)*
   - Ham. Sim. with Unbounded Operators *(workshop talk)*

Part 1.1: Some **Motivations** for Quantum Computations

Different Levels of Physics

multiscale physics fig by Prof. Qin Li

Different Levels of Physics



multiscale physics fig by Prof. Qin Li

Different Levels of Physics

Schrodinger $\rightarrow$ Newton $\rightarrow$ Boltzmann $\rightarrow$ Euler/N-S

quantum classical statistical fluid

$\hbar \to 0$

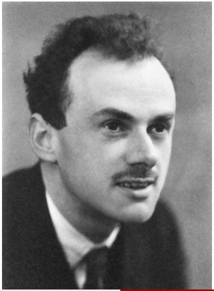
Rescaled Planck constant

$N \to \infty$

Number of particles

$\mathrm{Kn} \to 0$

Knudsen number



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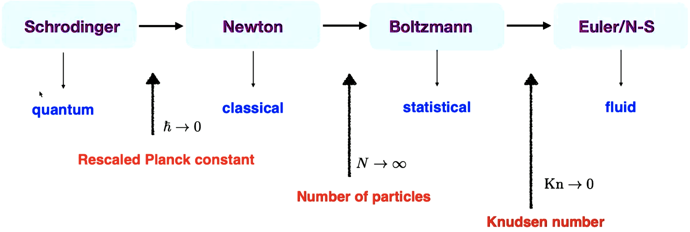

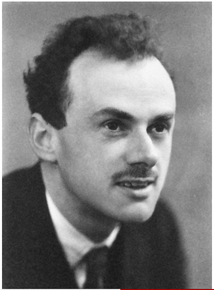

“the underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.”

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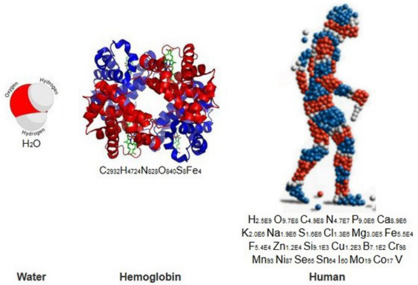
Schrödinger equation for Molecular Dynamics

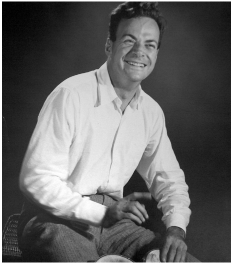


To describe its behaviour: (x: nuclei coordinates, y: electronic coordinates, M: mass of a nucleus, m: mass of an electron.)

$$\hat{H}_{\text{total}} = -\frac{\hbar^2}{2M}\Delta_x - \frac{\hbar^2}{2m}\Delta_y + V(x,y), \quad x \in \mathbb{R}^d, y \in \mathbb{R}^n$$

$$i\hbar\partial_t\psi = \hat{H}_{\text{total}}\psi$$

Quantum Computing 101



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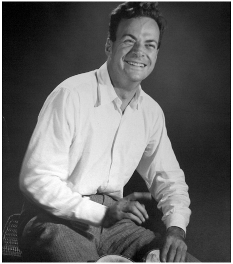

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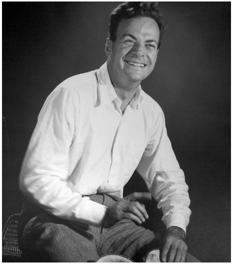

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$$\mathrm{i}\partial_t |\psi(t)\rangle = H(t) |\psi(t)\rangle , \quad |\psi(0)\rangle = |\psi_0\rangle .$$

$H(t) \equiv H,$ to simulate e^{-iHt} for H of very high dimension!.

Why on a Quantum Computer?

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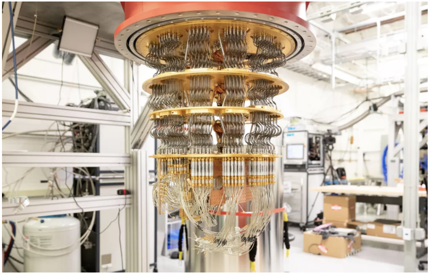

Left: Google; Picture by Stephen Shankland (CNET). Right: Ion-trap quantum computer at Duke quantum center.

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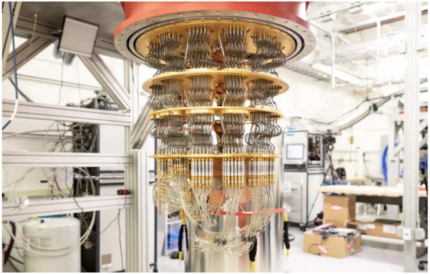

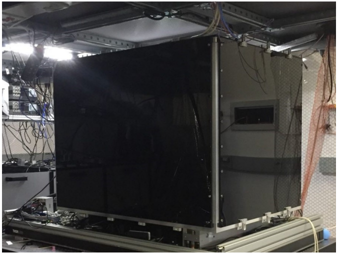

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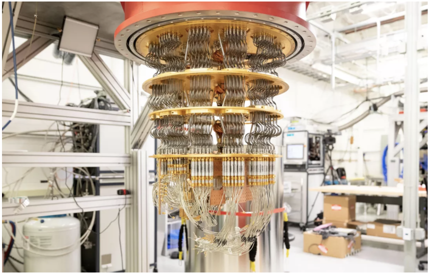

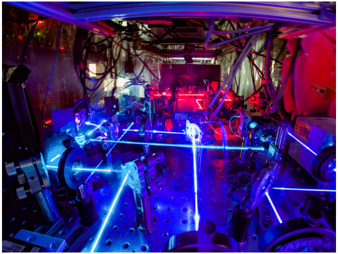

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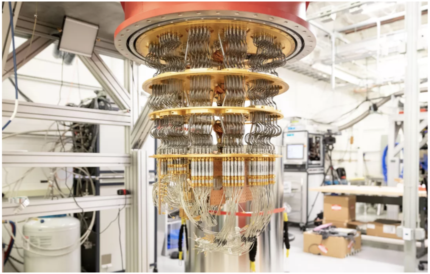

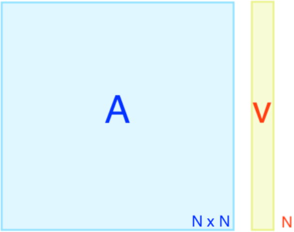

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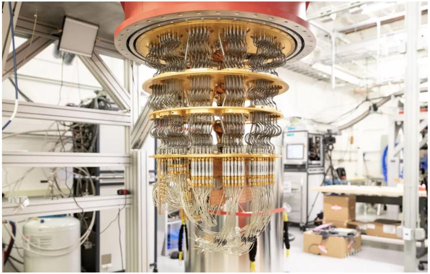

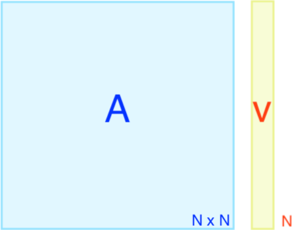

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Quantum Advantage:
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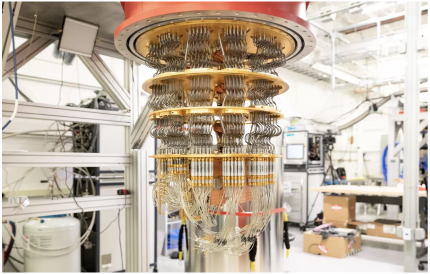

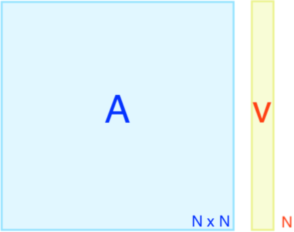

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Potential Applications: numerical algebra, numerical differential equations, and many more scientific computing topics

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Part 1.2: How? Some **Basics** of Quantum Computations

Basic QC Glossary

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- Braket Notations: For $\dim(\mathcal{H}) = N$,

$$|\psi\rangle := \psi = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{N-1} \end{pmatrix}, \ \langle\psi| := \psi^\dagger \text{ complex conjugate.}$$

  Inner product $\langle\psi|\phi\rangle := \langle\psi, \phi\rangle = \sum_{j\in[N]} \bar{\psi}_j \phi_j$.
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$\mathrm{Tr}(|x\rangle\langle y|) = \langle y|x\rangle$, $\quad |x\rangle\langle x|$ is a projection operator.

Basic QC Glossary – one qubit & superposition

- Simple example: 2 dimensional case

  Standard/ Computational Basis Vectors $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

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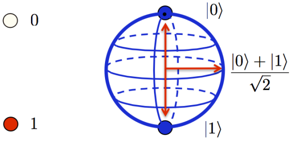

Classical Bit **Qubit**

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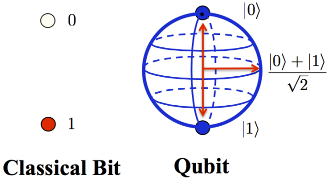

Geometry of a qubit: Bloch Sphere

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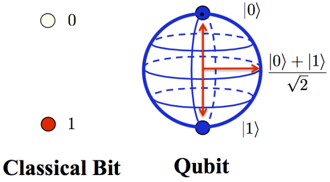

Geometry of a qubit: Bloch Sphere

Wait... Something is off?

Basic QC Glossary – one-qubit state

Quantum Principle: Physical properties remain unchanged w.r.t. a global phase.

$$|\psi\rangle \to e^{i\theta} |\psi\rangle, \quad \theta \in \mathbb{R}.$$

Undistinguishable under the laws of quantum mechanism.

fig from QuTech.

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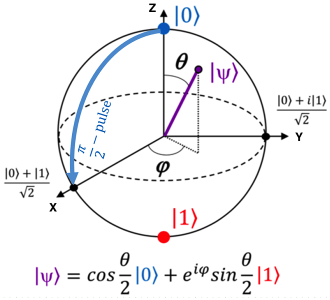

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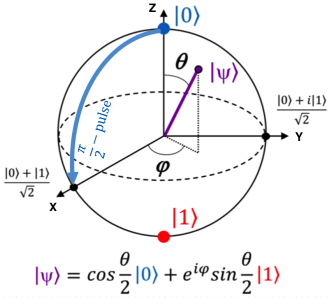

$|0\rangle, |1\rangle$ also called Z basis states.

When $\theta = \pi/2$, $\phi = 0$,
$|+\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$

When $\theta = \pi/2$, $\phi = \pi$,
$|-\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$

called the X basis states.

fig from QuTech.

Basic QC Glossary – multi-qubit state

- For general n-qubit system, $\mathcal{H} = \mathcal{B}^{\otimes n}$.

Basic QC Glossary – multi-qubit state

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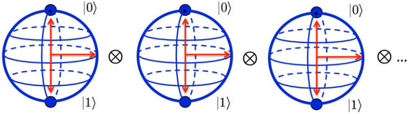
- Tensor Product



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E.g., $|00\rangle := |0\rangle \otimes |0\rangle =$, $|01\rangle := |0\rangle \otimes |1\rangle =$,
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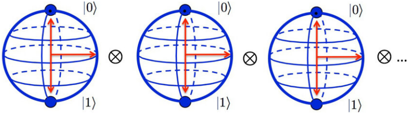

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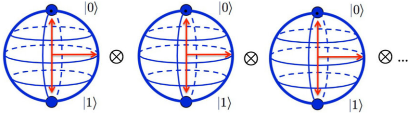

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In quantum braket notation,

$$\begin{aligned} |x\rangle \otimes |y\rangle :=& (x_0 |0\rangle + x_1 |1\rangle) \otimes (y_0 |0\rangle + y_1 |1\rangle) \\ =& x_0 y_0 |00\rangle + x_0 y_1 |01\rangle + x_1 y_0 |10\rangle + x_1 y_1 |11\rangle . \end{aligned}$$

What is the relationship with N and n?

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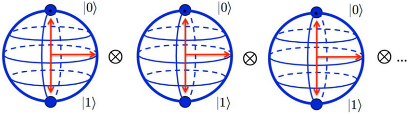

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What is the relationship with N and n? $\boxed{N = 2^n}$!

Basic QC Glossary – multi-qubit state & entanglement

- An n-qubit state is called a product state, if it can be represented as the tensor product of one-qubit states $|\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_n\rangle$. E.g., $|00\rangle$, $\frac{1}{2}\left(|00\rangle + |01\rangle + |10\rangle + |11\rangle\right)$

Basic QC Glossary – multi-qubit state & entanglement

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  Proof: Suppose $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = (a\,|0\rangle + b\,|1\rangle) \otimes (c\,|0\rangle + d\,|1\rangle)$
  $ac = bd = 1/\sqrt{2}, \quad ad = bc = 0$. Impossible. $\square$

Two important quantum features:

Superposition and Entanglement

Basic QC Glossary – operators: quantum gates

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Basic QC Glossary – common one-qubit gates cont'd

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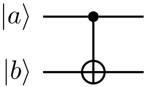
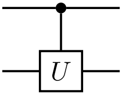
- Phase-shift Gate: $P(\phi) = P(\varphi) = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{bmatrix}$
  $Z = P(\pi)$, $S = P(\pi/2) = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$, $T = P(\pi/4) = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{bmatrix}$

Common two-qubit gates

- CNOT (controlled-NOT)



- controlled-U gate



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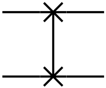

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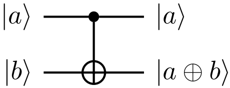

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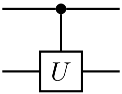

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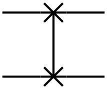

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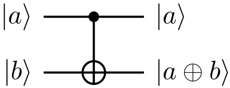

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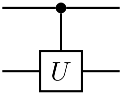

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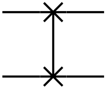
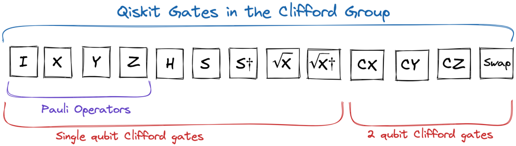


Clifford gates: elements of Clifford group
$\mathbf{C}_n = \{V \in U_{2^n} \mid V\mathbf{P}_n V^\dagger = \mathbf{P}_n\}$. Here P_n is the n-qubit Pauli group.
Generators: $\{$H, S, CNOT$\}$.



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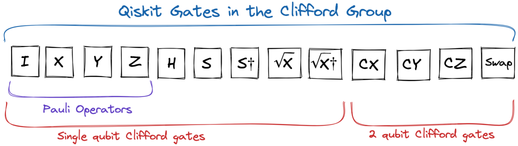

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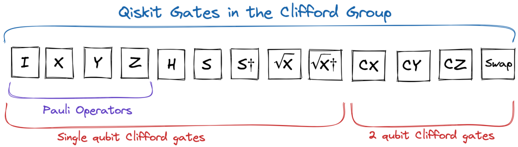

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Upshot: Universality!

A set of quantum gates is called universal, if composing gates from it can approximate any quantum gate to any desired precision.
Some examples of universal gate sets are:

- {CNOT, all single-qubit gates}
- {CNOT, H, T}
- {Toffoli, H}

Basic QC Glossary – Measurements

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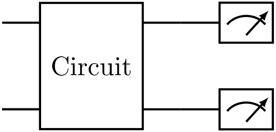
  2-qubit example $|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$



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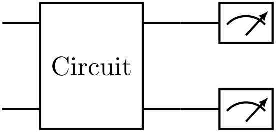

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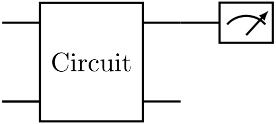

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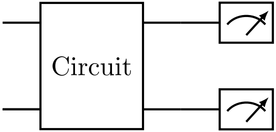

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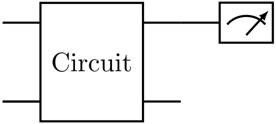

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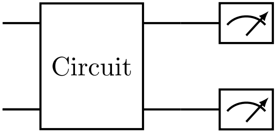

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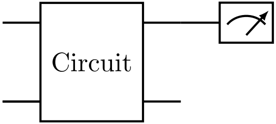

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If we observe 0, the joint state after the measurement becomes

$$\frac{\alpha_{00}|00\rangle + \alpha_{01}|01\rangle}{\sqrt{|\alpha_{00}|^2 + |\alpha_{01}|^2}} = |0\rangle \otimes \frac{\alpha_{00}|0\rangle + \alpha_{01}|1\rangle}{\sqrt{|\alpha_{00}|^2 + |\alpha_{01}|^2}}.$$ "Unentangled"

Wave function collapse after measurement

Basic QC Glossary – quantum circuits

Quantum algorithms (QA) are represented by quantum circuits.

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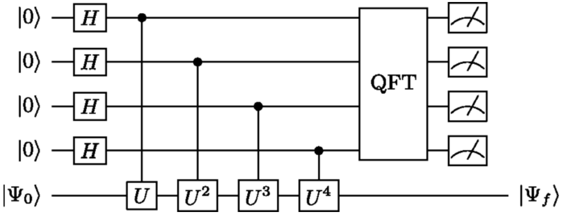

Complexity of a QA: Gate complexity, Query complexity (oracle)

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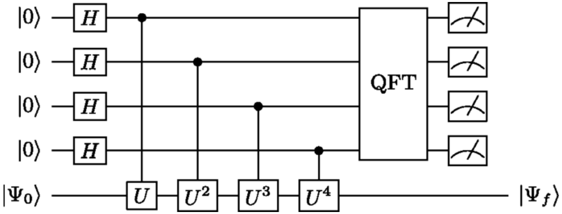

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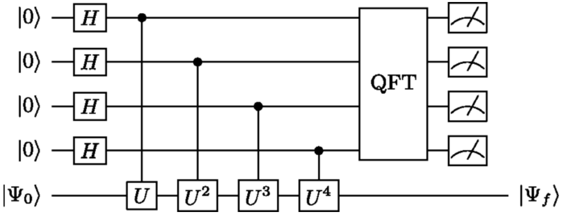

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- Is QC at least as powerful as classical computing?
- Is there always an exponential (superpolynomial) quantum advantage?

Basic QC Glossary – QC vs CC

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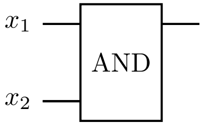

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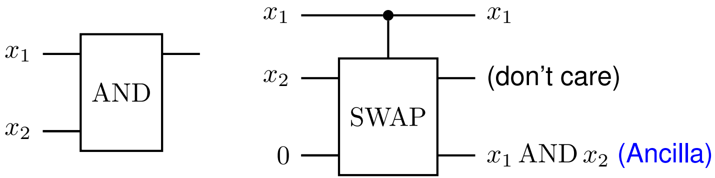

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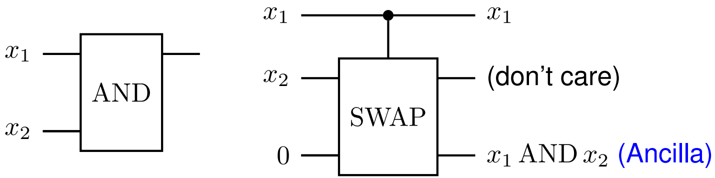

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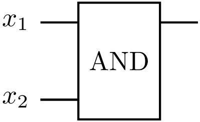

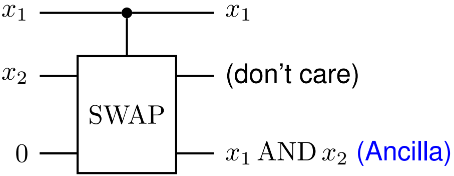

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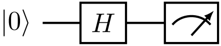

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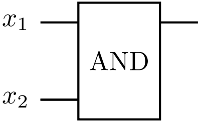

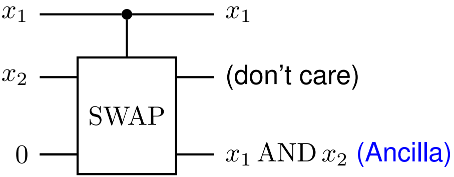

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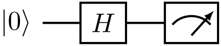
$\boxed{\text{CoinFlip}}$



Question 2: Always exponential quantum speedup (b/c $2^n = N$)?
No!! Restrictions:

- Unitary + Measurement (Needs structure of tasks!)
- No cloning theorem

Basic QC Glossary: No-cloning Theorem

There is no quantum circuit that clones an arbitrary quantum state!

Basic QC Glossary: No-cloning Theorem

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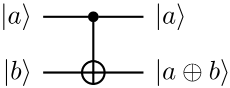

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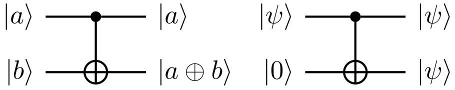

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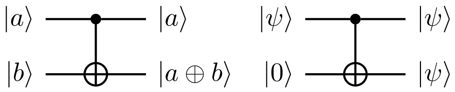

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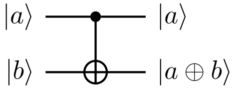

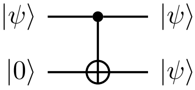

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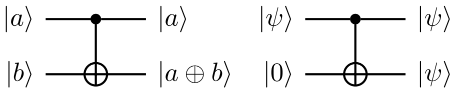

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$$(I \otimes U)\,|\psi\rangle\,|s\rangle = |\psi\rangle\,|\psi\rangle\,.$$

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Exponential Quantum Advantage (EQA) (often this is also used to refer superpolynomial speedup)

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Examples of Tasks with EQA:

- Factoring $\Rightarrow$ Shor's Algorithm (A)
- Invert a large sparse linear system $\Rightarrow$ HHL Algorithm (A)(B)
- Hamiltonian Simulation (B)

Summary of Part 1

- Motivation: first principle, potential EQA
- Quantum State
- Quantum Gates / Circuits
- Measurement
- QA v.s. CA; no-cloning; EQA

Part 2: Block-encoding and Hamiltonian Simulation

Hamiltonian Simulation

Hamiltonian Simulation Problem: Given a description of the Hamiltonian $H(t)$, an evolution time t and an initial state $|\psi(0)\rangle$, to produce the final state $|\psi(t)\rangle$ within in some error tolerance ϵ.

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No-fast-forwarding Theorem *(informal)*: Simulating Hamiltonian dynamics for time t requires complexity $\Omega(t)$.

Hamiltonian Simulation Algorithms

- Trotterization (= Product Formulae = Time/Operator Splitting)
  1st-order Trotter formula (Lie-Trotter) for $H = H_1 + H_2$

$$e^{-\mathrm{i}Ht} \approx \left(e^{-\mathrm{i}H_2 t/L} e^{-\mathrm{i}H_1 t/L}\right)^L$$

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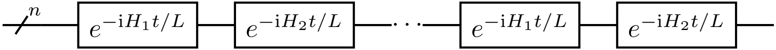

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$$e^{-\mathrm{i}Ht} \approx \sum_{k=0}^{K} \frac{(-\mathrm{i}Ht)^k}{k!} = \sum_{k=0}^{K} \sum_{\ell_1,\cdots,\ell_k} \frac{(-\mathrm{i}t)^k}{k!} H_{\ell_1} H_{\ell_2} \cdots H_{\ell_k}.$$

Upshot: $\Rightarrow \mathcal{O}(t \log(1/\epsilon))$

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Upshot: $\Rightarrow \mathcal{O}(t \log(1/\epsilon))$ $\Rightarrow$ Even better, say, $\mathcal{O}(t + \log(1/\epsilon))$?

Block-Encoding – Definition

Let A be a general $2^n \times 2^n$ matrix.

Idea:

$$U_A = \begin{pmatrix} A & * \\ * & * \end{pmatrix} \quad \rightarrow \text{ancilla qubits}$$

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U_A is an (α, m, ϵ)-block-encoding of A, if

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for some $\alpha \geq \|A\|$, $m > 0$ and $\epsilon > 0$. Here α is called the *subnormalization* factor and m is the number of ancilla qubits, and n is the number of system qubits. When $\epsilon = 0$, it is also called an (α, m)-block-encoding.

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Understanding: $U_A : 2^{m+n} \times 2^{m+n}$.

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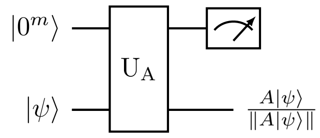
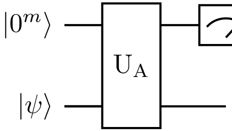


(upon getting 0 in measurement)

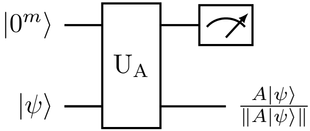
Block-Encoding – Definition cont'd



$\frac{A|\psi\rangle}{\|A|\psi\rangle\|}$ (upon getting 0 in measurement)

$$|0,\psi\rangle = |0\rangle \otimes |\psi\rangle = \begin{pmatrix} |\psi\rangle \\ 0 \end{pmatrix}, \quad U_A\,|0,\psi\rangle = \begin{pmatrix} \frac{\tilde{A}}{\alpha} & * \\ * & * \end{pmatrix} \begin{pmatrix} |\psi\rangle \\ 0 \end{pmatrix} = \begin{pmatrix} \tilde{A}\,|\psi\rangle \\ * \end{pmatrix}.$$

Block-Encoding – Definition cont'd



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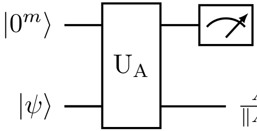
Block-Encoding – Definition cont'd



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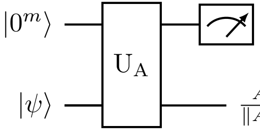

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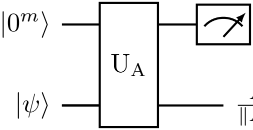

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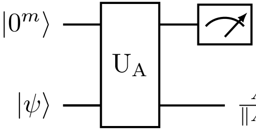

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$$U_A := \begin{pmatrix} W & 0 \\ 0 & I_n \end{pmatrix} \begin{pmatrix} \Sigma & \sqrt{I_n - \Sigma^2} \\ \sqrt{I_n - \Sigma^2} & -\Sigma \end{pmatrix} \begin{pmatrix} V^\dagger & 0 \\ 0 & I_n \end{pmatrix}$$
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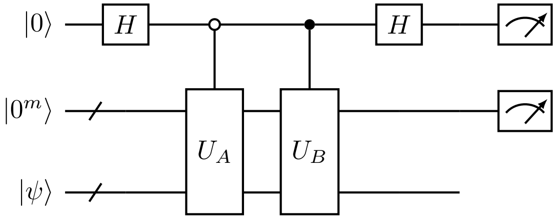
   The following circuit constructs a $(2, m, \delta + \epsilon)$-BE of $A + B$.



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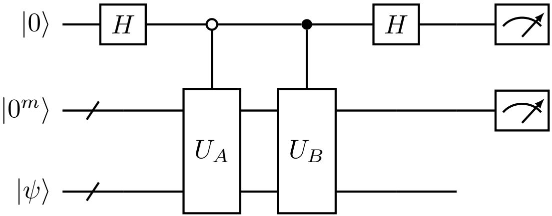

More generally, linear combination of block-encodings can be constructed via Linear Combination of Unitaries (LCU) Lemma.

LCU Lemma

LCU Lemma: $T = \sum_{j \in [L]} c_j U_j$ for unitaries U_j. $\|c\|_1 = \sum_{j \in [L]} |c_j|$.

LCU [Berry-Childs-Kothari 2015], General LCBE [Gilyen-Su-Low-Wiebe 2018]

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- $\mathrm{SEL} := \sum_{j\in[L]} |j\rangle\langle j| \otimes U_j$
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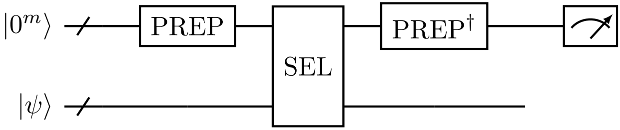

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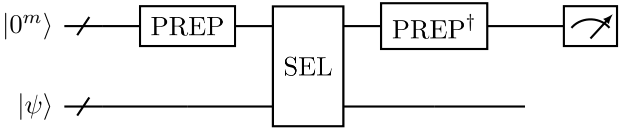

General LCBE: $\max_j m_j + \lceil \log_2 L \rceil$ ancillas

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Quantum Singular Value Transformation (QSVT) / Quantum Signal Processing (QSP)

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Theorem (QSVT with odd real polynomial)

Let U_A be a $(1, m)$-block-encoding of $A \in \mathbb{C}^{2^n \times 2^n}$. Given an odd polynomial $P_\Re(x) \in \mathbb{R}[x]$ of odd degree d satisfying

$$|P_\Re(x)| \leqslant 1, \forall x \in [-1, 1].$$

We can find a sequence of phase factors $\Phi \in \mathbb{R}^{d+1}$ and construct a $(1, m+1)$-block-encoding of $P_\Re^\diamond(A)$ that uses $U_A, U_A^\dagger$, m-qubit controlled NOT, and single qubit rotation gates for $\mathcal{O}(d)$ times.

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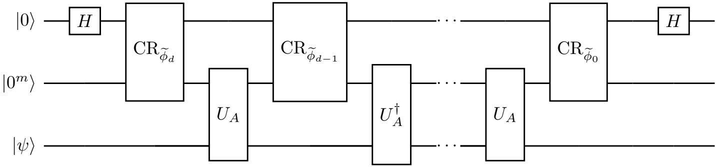

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Given U_H: an $(\alpha, m, 0)$-block-encoding of H.
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- Jacobi-Anger expansion on $[-1, 1]$:

$$\cos(tx) = J_0(t) + 2\sum_{k=1}^{\infty}(-1)^k J_{2k}(t)T_{2k}(x),$$

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$J_\nu(t)$ denotes Bessel functions of the first kind.

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- This series converges rapidly. Truncating it with

$$r = \Theta\left(t + \frac{\log(1/\epsilon)}{\log(e + \log(1/\epsilon)/t)}\right)$$

terms gives a polynomial approximation (with precision ϵ and degree $2r+1$) of $\cos(tx) + i\sin(tx) = e^{itx}$.

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Query Complexity: ($\alpha \geq \|H\|$.)

$$\mathcal{O}\left(\alpha t + \frac{\log(1/\epsilon)}{\log(e + \log(1/\epsilon)/t)}\right).$$

Success Probability

e^{-iHt} is unitary. Success probability upon measurement is ok. [1]

[1] In fact, it is an issue even for Hamiltonian simulation that leads to exponential cost in time. But for unitary dynamics, OAA (can be viewed as a form of QSVT) can solve the issue.

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$$|\psi\rangle = \sqrt{p}\,|\psi_{\text{good}}\rangle + \sqrt{1-p}\,|\psi_{\text{bad}}\rangle\,.$$

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Amplitude Amplification (AA): The success probability can be boosted from p to $\Omega(1)$ via AA that accesses $\mathcal{O}(1/\sqrt{p})$ times of the circuit U.

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Summary of Part 2

- Hamiltonian simulation and Trotterization
- Block-encoding: Definition and Properties
- LCU and QSVT
- Optimal Hamiltonian Simulation via QSVT
- Success Probability

Other advanced topics

- General Linear Differential Equation *(optional)*
- Hamiltonian Simulation – time dependent case? with unboundeded operator? *(workshop talk)*

References on Quantum Algorithms

- M. Nielsen and I. Chuang. Quantum Computation and Quantum Information, Cambridge University Press *(classics)*
- Lecture Notes on Quantum Computation by Umesh Vazirani (UC Berkeley) *(entry level)*
- Lecture Notes on Quantum Computation by John Preskill (Caltech) *(entry level)*
- Lecture Notes on Quantum Computation by Ryan O'Donnell (CMU) *(entry level)*
- Lecture notes on Quantum Algorithms for Scientific Computations by Lin Lin (UC Berkeley) [arXiv:2201.08309] *(advanced topics)*
- Lecture notes on Quantum Algorithms by Andrew Childs (U Maryland) *(advanced topics)*
- Qiskit Textbook by IBM (https://qiskit.org/learn) *(Algorithm Demos)*

Thank you for your attention!