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OUTLINE OF PART II: QUANTUM SIMULATION AND QUANTUM-COMPUTING BASICS

i) Quantum-simulation steps: A brief introduction

ii) Various modes of quantum simulation: Digital, analog, hybrid

iii) Digital-quantum-simulations basics:

- qubits and gates
- Encoding fermions and bosons onto qubits
- State-preparation strategies
- Time evolution (via product formulas)
- Measurement strategies and observables

Presenter:
Zhengrong Qian

Reference: ZD, TASI/CERN/KITP Lecture Notes on "Toward Quantum Computing Gauge Theories of Nature", arXiv:2507.15840 [hep-lat].

- These slides are based on materials prepared by Prof. Zohreh Davoudi, with minor modifications.

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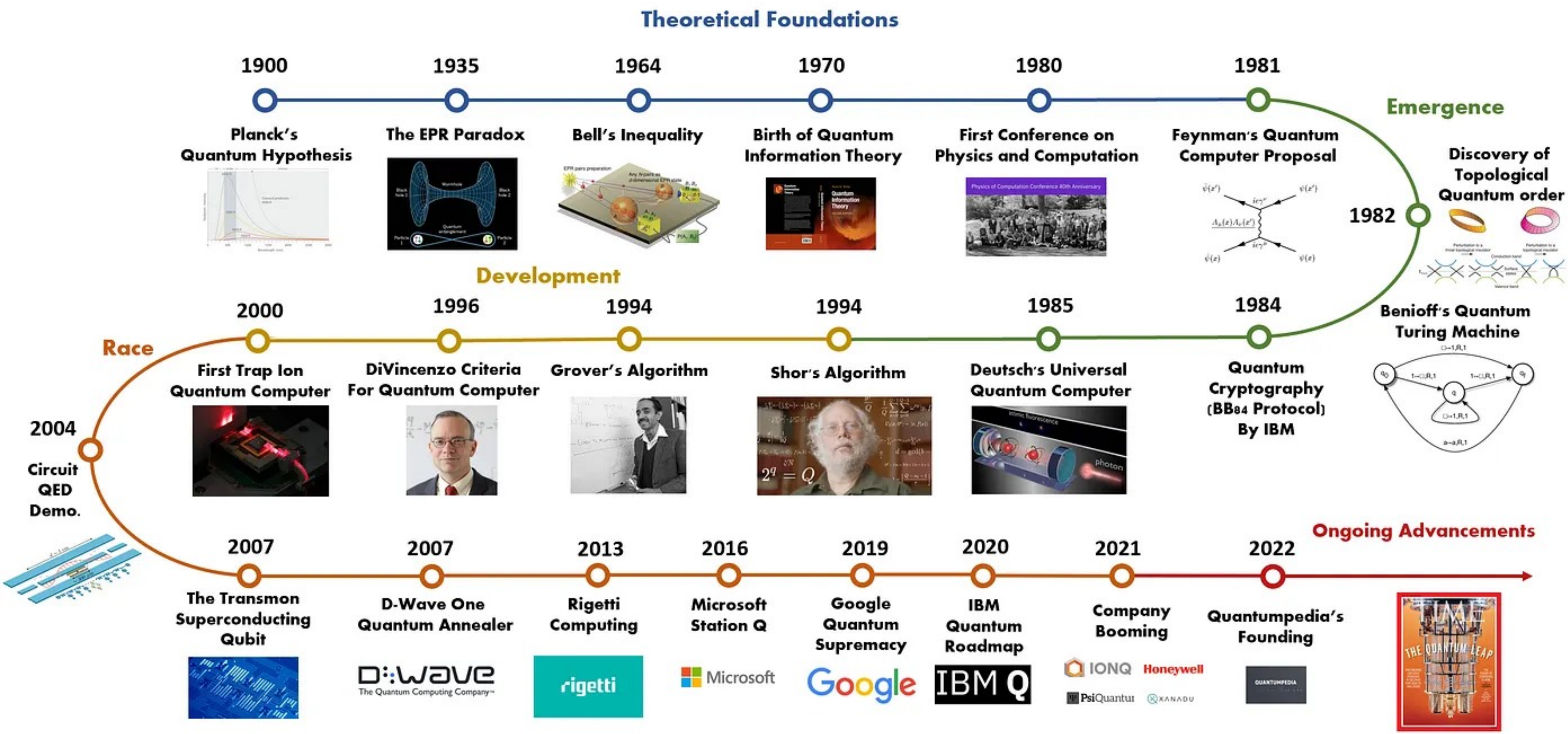
A MICRO-TIMELINE FOR QUANTUM COMPUTING & SIMULATION

- 1982 Feynman – simulators idea
- 1993–96 Trotter/Lloyd – digital QS
- 2002+ Optical lattices – analog Hubbard
- 2010s Trapped-ion Ising – analog/digital
- 2016+ Rydberg arrays – gauge analogs
- 2019–25 NISQ scaling – IBM/Google/Quantinuum/IonQ/QuEra/Pasqal



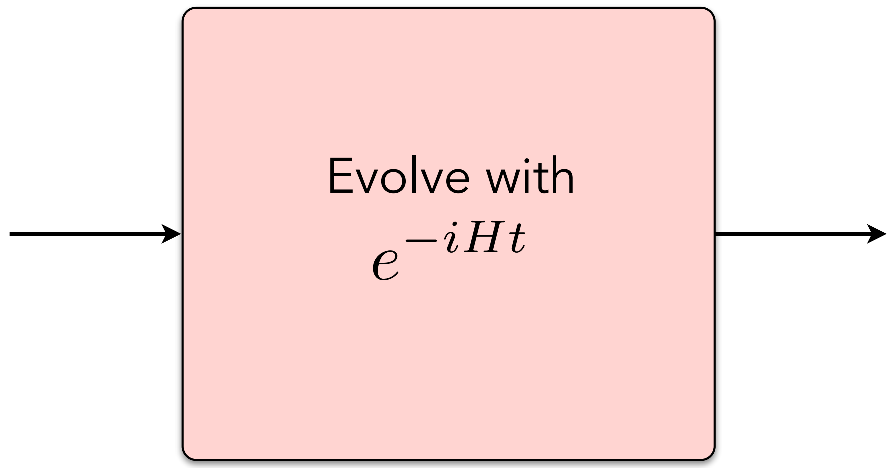
- Source: quantumpedia.uk

ON A QUANTUM COMPUTING MACHINE, WE CAN IN PRINCIPLE:

Prepare the initial state →

- Nontrivial specially in strongly-interacting theories like quantum chromodynamics (QCD).
- Thermal states possible.

ON A QUANTUM COMPUTING MACHINE, WE CAN IN PRINCIPLE:



- Depends on the mode of the simulator.
- The choice of formulation and basis states impacts the implementation.

ON A QUANTUM COMPUTING MACHINE, WE CAN IN PRINCIPLE:

Measure observables

- May require non-trivial circuits given the observable
- Exponentially large number of amplitudes to be measured. Efficient but approximate protocols are being developed.

CAN WE COMBINE THIS WITH CLASSICAL COMPUTING?

QUANTUM SUBPROCESS

Prepare the initial state

Evolve with e^{-iHt}

Measure observables

?

Conventional lattice QCD

?

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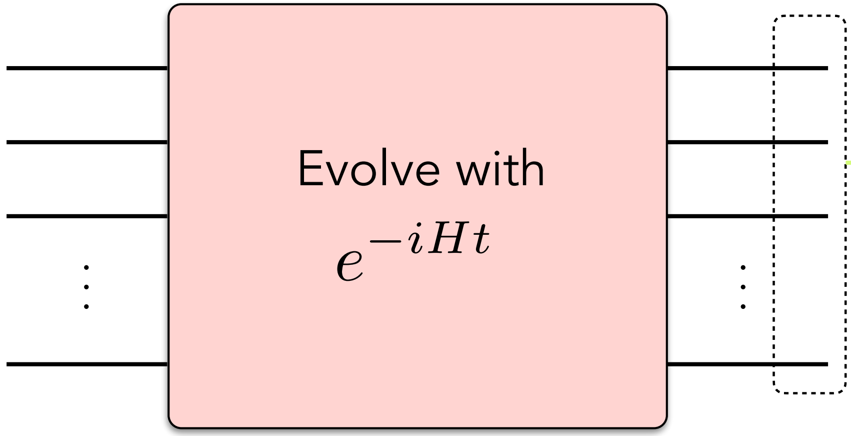
THIS LECTURE CONCERNS PRIMARILY TIME EVOLUTION.

Evolve with

$$e^{-iHt}$$

DIFFERENT APPROACHES TO QUANTUM SIMULATION

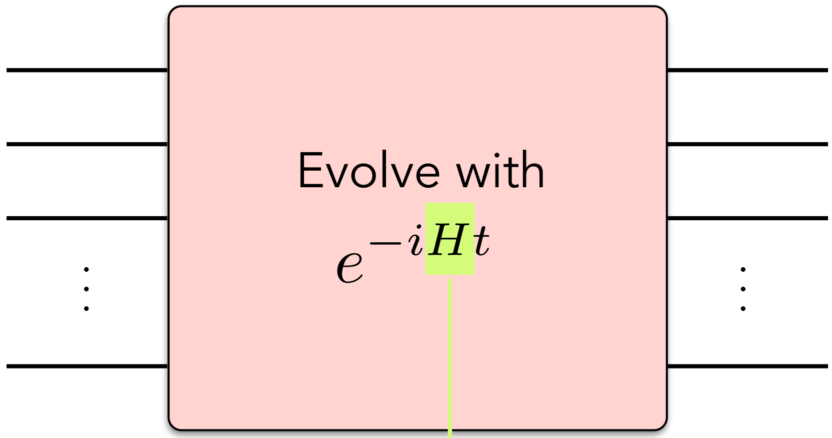
Analog



Degrees of freedom in the simulator: fermions, bosons, spins (of various dimensions), etc.

DIFFERENT APPROACHES TO QUANTUM SIMULATION

Analog



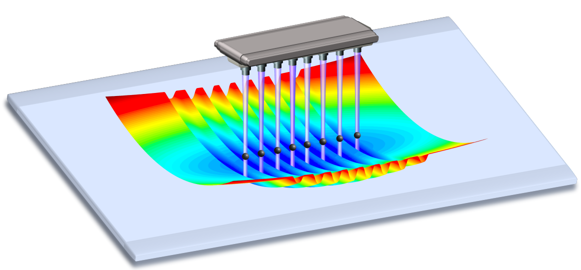
- Optical-lattice potential (1D slice) $V_{lat}(x) = V_0 \sin^2(kx)$

- Bose-Hubbard (lowest band)

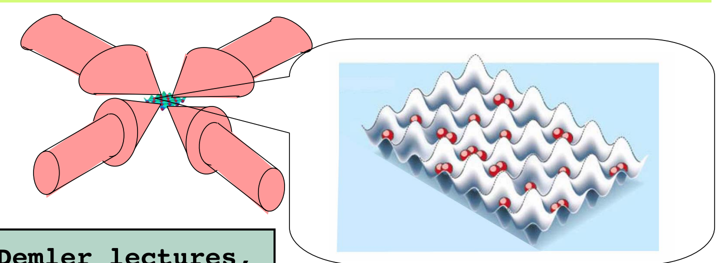
$$H_{BH} = -J \sum_{\langle i,j \rangle} b_i^{\dagger} b_j + \frac{U}{2} \sum_i n_i (n_i - 1) + \sum_i \mu_i n_i$$

The engineered simulator Hamiltonian that mimics the Hamiltonian of target system.

Some of the leading analog simulators are: cold-atoms in optical lattices, Rydberg atoms with optical tweezers, trapped ions, superconducting circuits (including when coupled to photonics systems), etc.



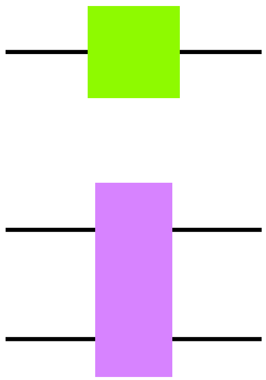
CREDIT: ANDREW SHAW, UNIVERSITY OF MARYLAND



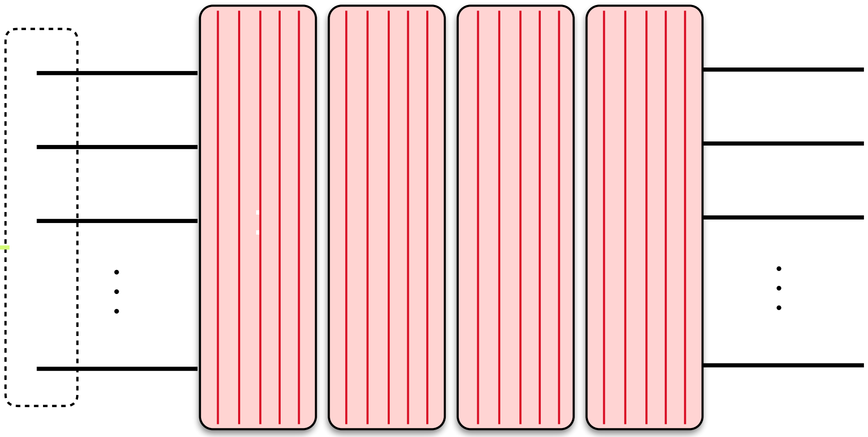
Eugene Demler lectures, Harvard University.

DIFFERENT APPROACHES TO QUANTUM SIMULATION

Digital



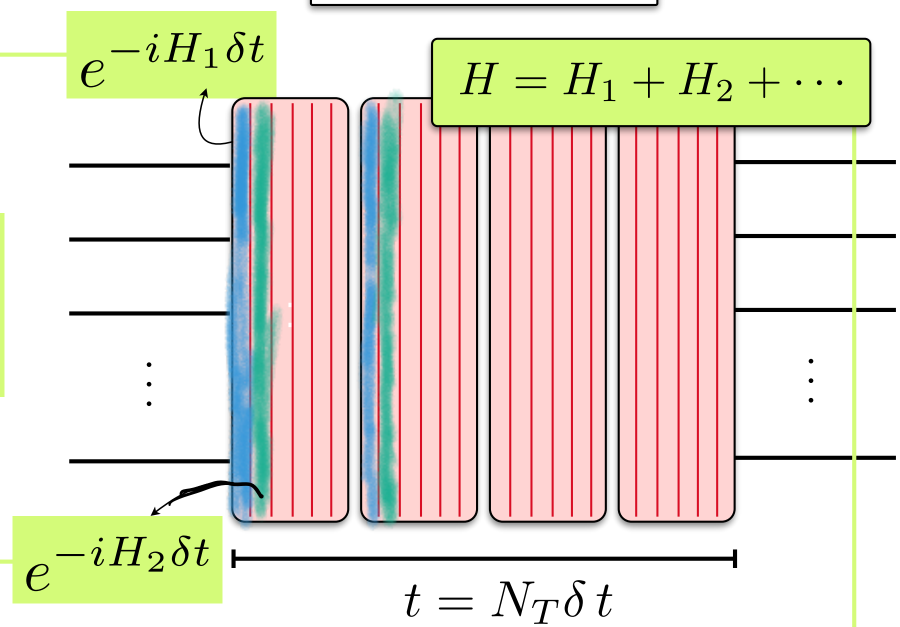
Only qubits as DOF. Only universal single- and two-qubit operations allowed.



DIFFERENT APPROACHES TO QUANTUM SIMULATION

Example of a digital scheme:

Digital



Each of these can now potentially be decomposed to a universal set of single and two-qubit gates.

Trotter-Suzuki expansion:

$$e^{-i(H_1+H_2+\cdots)t} = \left[e^{-iH_1\delta t} e^{-iH_2\delta t} \cdots\right]^{t/\delta t} + \mathcal{O}((\delta t)^2)$$

Other digitalization schemes also exist.

…other methods exist too.

Andrew Childs lectures on Quantum Simulation, University of Maryland.

Some classical algorithms approximate exponential of a matrix using a Taylor expansion. Would a Taylor expansion of unitary time-evolution operator be straightforward to perform on a digital quantum computer?

Extra workspace

Not Directly!

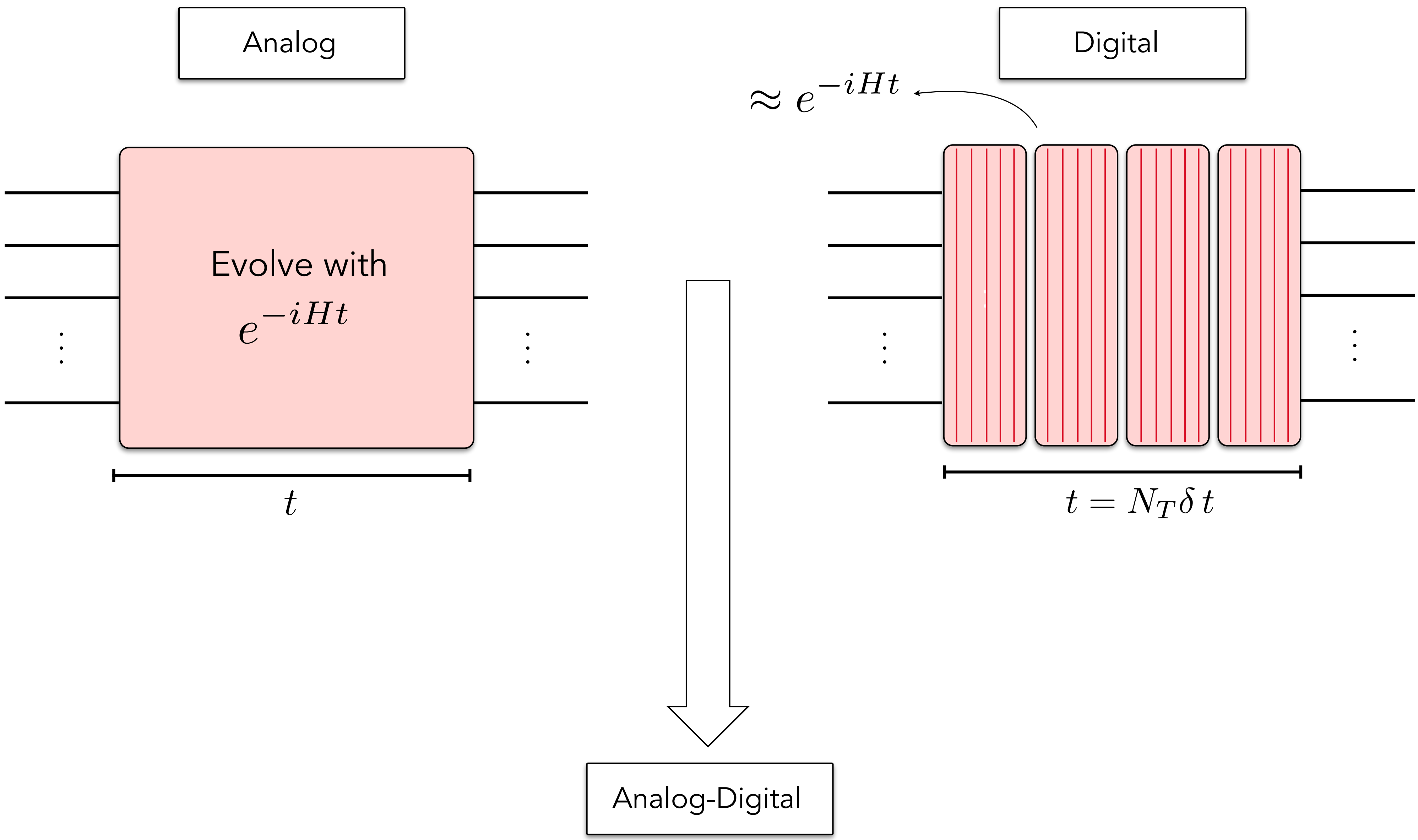
Taylor expansion : $e^{-iHt} \sim \sum_{k=0}^{K} \frac{(-iHt)^k}{k!}$

linear sum, not a unitary.

need LCU / Qubitization to turn that in sum into a unitary procedure

(if one insists)

DIFFERENT APPROACHES TO QUANTUM SIMULATION



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A textbook of extreme popularity: Nielson and Chuang, Quantum Computation and Quantum Information. But some of the newer notions not there.

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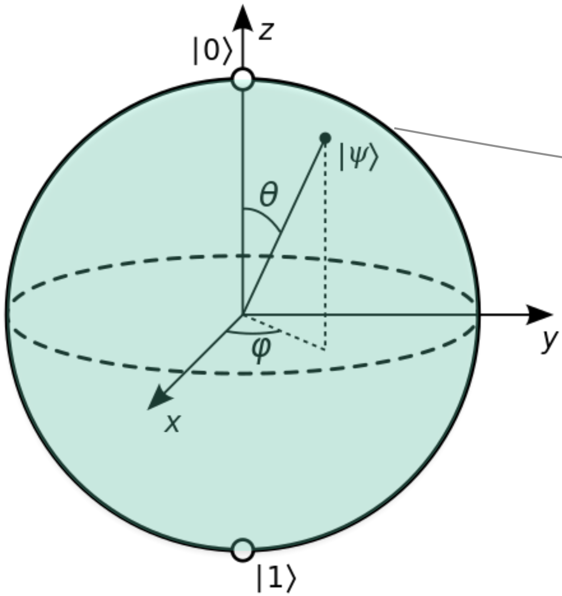


State of a single qubit: $|\psi\rangle = a|0\rangle + b|1\rangle \equiv a\begin{pmatrix}1\\0\end{pmatrix} + b\begin{pmatrix}0\\1\end{pmatrix}$

$$\equiv \cos(\theta/2)|0\rangle + ie^{i\phi}\sin(\theta/2)|1\rangle$$

State of two qubits: $|\psi\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$

$$\equiv a\begin{pmatrix}1\\0\\0\\0\end{pmatrix} + b\begin{pmatrix}0\\1\\0\\0\end{pmatrix} + c\begin{pmatrix}0\\0\\1\\0\end{pmatrix} + d\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

(Examples of) quantum logic gates

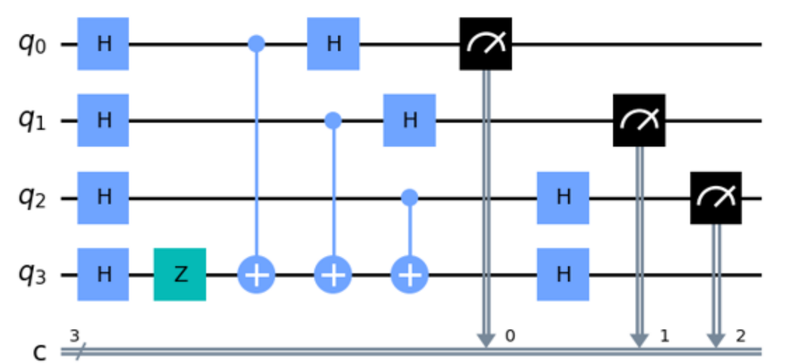
Operator	Gate(s)	Matrix
Pauli-X (X)	X	$\begin{bmatrix}0&1\\1&0\end{bmatrix}$
Pauli-Y (Y)	Y	$\begin{bmatrix}0&-i\\i&0\end{bmatrix}$
Pauli-Z (Z)	Z	$\begin{bmatrix}1&0\\0&-1\end{bmatrix}$
Hadamard (H)	H	$\frac{1}{\sqrt{2}}\begin{bmatrix}1&1\\1&-1\end{bmatrix}$
Phase (S, P)	S	$\begin{bmatrix}1&0\\0&i\end{bmatrix}$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

Any unitary on a finite number of qubits can be approximated *efficiently* by a finite sequence of a universal gate set. `Solovay (1995) and Kitaev (1997).`

Two common choices for these gate sets are:

- $R^x(\theta) = e^{-i\theta\sigma^x/2}$, $R^y(\theta) = e^{-i\theta\sigma^y/2}$, $R^z(\theta) = e^{-i\theta\sigma^z/2}$, $P_\phi = \begin{pmatrix}1&0\\0&e^{i\phi}\end{pmatrix}$, CNOT
- H, S, CNOT, T (S not strictly needed but more economical.)

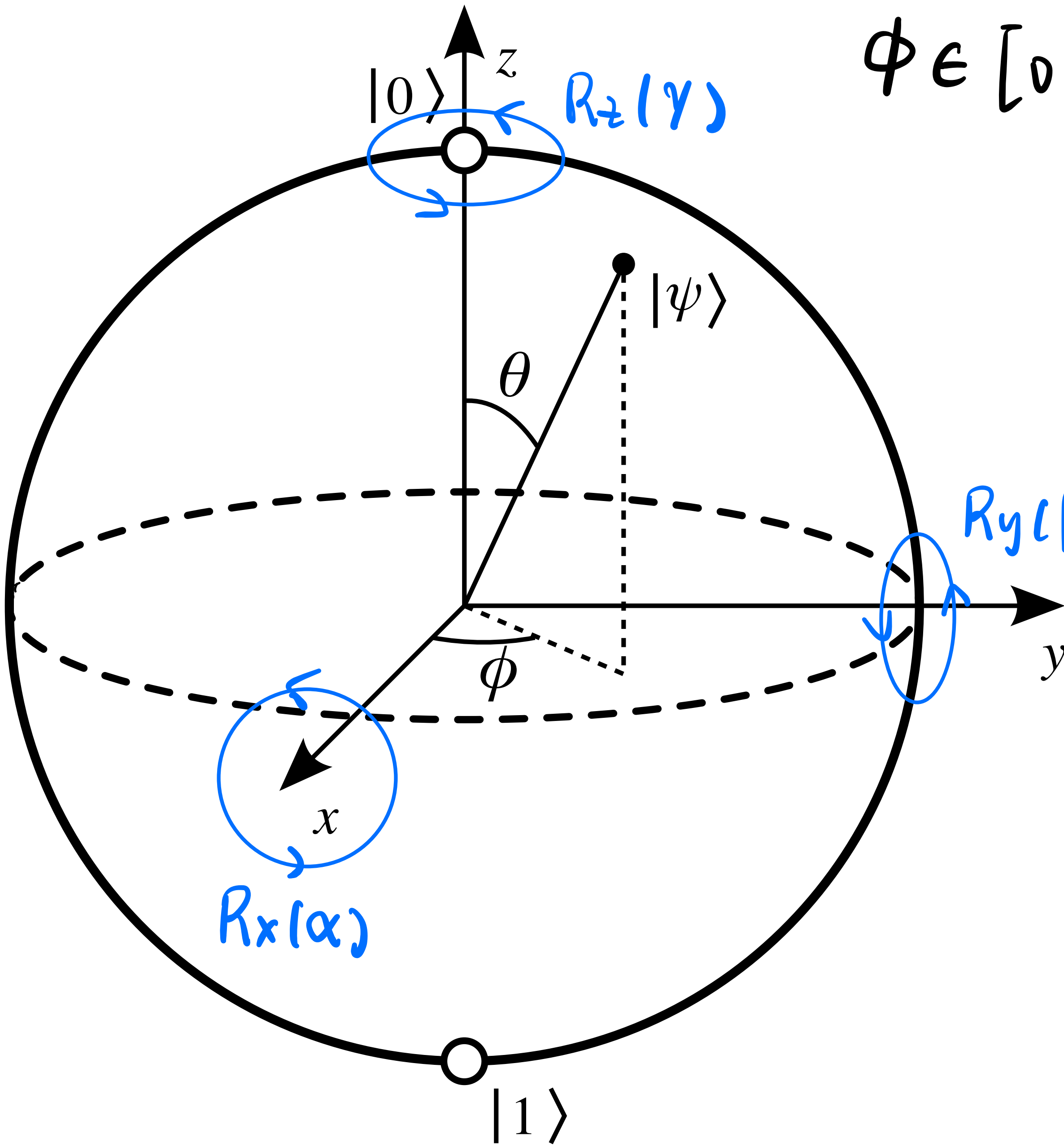
Example of) a quantum circuit:



THE BLOCH SPHERE

$\theta \in [0, \pi]$

$\phi \in [0, 2\pi)$



SINGLE & TWO-QUBIT GATE IDENTITIES

Single-qubit identities $\{\sigma_i, \sigma_j\} = 2\delta_{ij} I$, $[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k$

$\sigma_i^\dagger = \sigma_i$, $\sigma_i^2 = I$, $\sigma_i \in \{X, Y, Z\}$

'Pauli Sandwich'

> if $P, Q \in \{X, Y, Z\}$, w/ $\{P, Q\} = 0$, $P^2 = I$

$$XZX = -Z, \quad XYX = -Y, \quad ZXZ = -X$$

$$R_a(\theta) = e^{-i\theta\sigma_a/2}, \quad U e^A U^\dagger = e^{UAU^\dagger}$$

$$X R_z(\theta) X = R_z(-\theta) \qquad Z R_x(\theta) Z = R_x(-\theta) \quad \ldots$$

Extra workspace

'Conjugation by rotations'

$$R_a(\theta)\,\sigma_b\,R_a(-\theta) = \sigma_b \cos\theta + \sum_c \varepsilon_{abc}\,\sigma_c \sin\theta$$

$$R_x(\theta)\,Z\,R_x(-\theta) = Z\cos\theta + Y\sin\theta\,, \quad R_x\left(\tfrac{\pi}{2}\right) Z\, R_x\left(-\tfrac{\pi}{2}\right) = Y$$

$$R_y(\theta)\,Z\,R_y(-\theta) = Z\cos\theta + X\sin\theta\,, \quad R_y\left(\tfrac{\pi}{2}\right) Z\, R_y\left(-\tfrac{\pi}{2}\right) = X$$

'Basis Change identities'

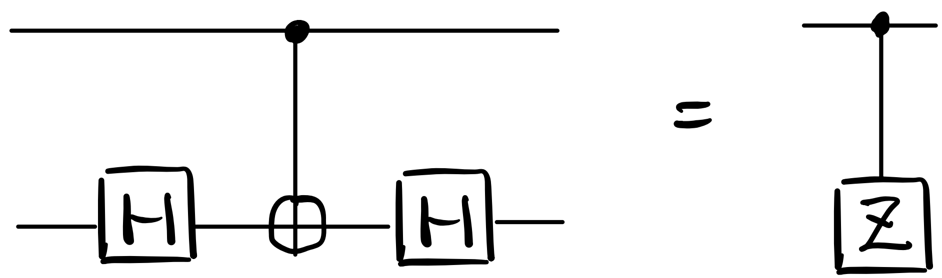
$$HXH = Z\,, \quad HZH = X\,, \quad HYH = -Y$$

SINGLE & TWO-QUBIT GATE IDENTITIES

Two-qubit identities

①. Basis Change = Rename the controlled Pauli.

$$(I \otimes H)\, CNOT\, (I \otimes H) = CZ$$



$$(I \otimes S)\, CNOT\, (I \otimes S^{\dagger}) = CY \qquad (S X S^{\dagger}) = Y$$

$$(H \otimes H)\, CNOT_{a \to b}\, (H \otimes H) = CNOT_{b \to a}$$

Extra workspace

② Propagation Rules = how Paulis move through CNOT

Exercise 4.31: (More circuit identities) Let subscripts denote which qubit an operator acts on, and let C be a CNOT with qubit 1 the control qubit and qubit 2 the target qubit. Prove the following identities:

$$CX_1C = X_1X_2 \tag{4.32}$$

$$CY_1C = Y_1X_2 \tag{4.33}$$

$$CZ_1C = Z_1 \tag{4.34}$$

$$CX_2C = X_2 \tag{4.35}$$

$$CY_2C = Z_1Y_2 \tag{4.36}$$

$$CZ_2C = Z_1Z_2 \tag{4.37}$$

$$R_{z,1}(\theta)C = CR_{z,1}(\theta) \tag{4.38}$$

$$R_{x,2}(\theta)C = CR_{x,2}(\theta). \tag{4.39}$$

③ Decomposition = build other 2-qubit ops from CNOTs (+1 qubit)

e.g. $\text{SWAP} = \text{CNOT}_{c\to t}\,\text{CNOT}_{t\to c}\,\text{CNOT}_{c\to t}$

UNIVERSAL QUANTUM GATES

$\forall n \geq 1$

n : # of qubits.

Approximately Universal

$$\overline{\langle \mathcal{G} \rangle_n} = PU(2^n)$$

$\varepsilon > 0$: Arbitrary accuracy.

finite gate library

{H, S, CNOT}

Clifford + T

Exactly Universal

$$\langle \mathcal{G} \rangle_n = PU(2^n)$$

$\varepsilon = 0$.

continuous family of gates

All single qubit unitaries

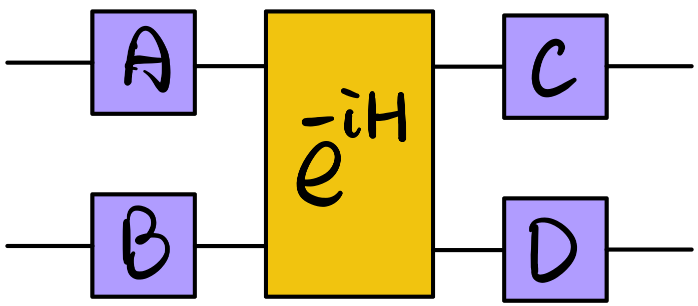
Single qubit + CNOT

AN OPTIMAL DECOMPOSITION OF TWO-QUBIT UNITARIES

2- qubit

$n=2$

Implementing CNOT gates is expensive!!



local : $SU(2)\otimes SU(2)$

non local : $SU(4)\setminus SU(2)\otimes SU(2)$

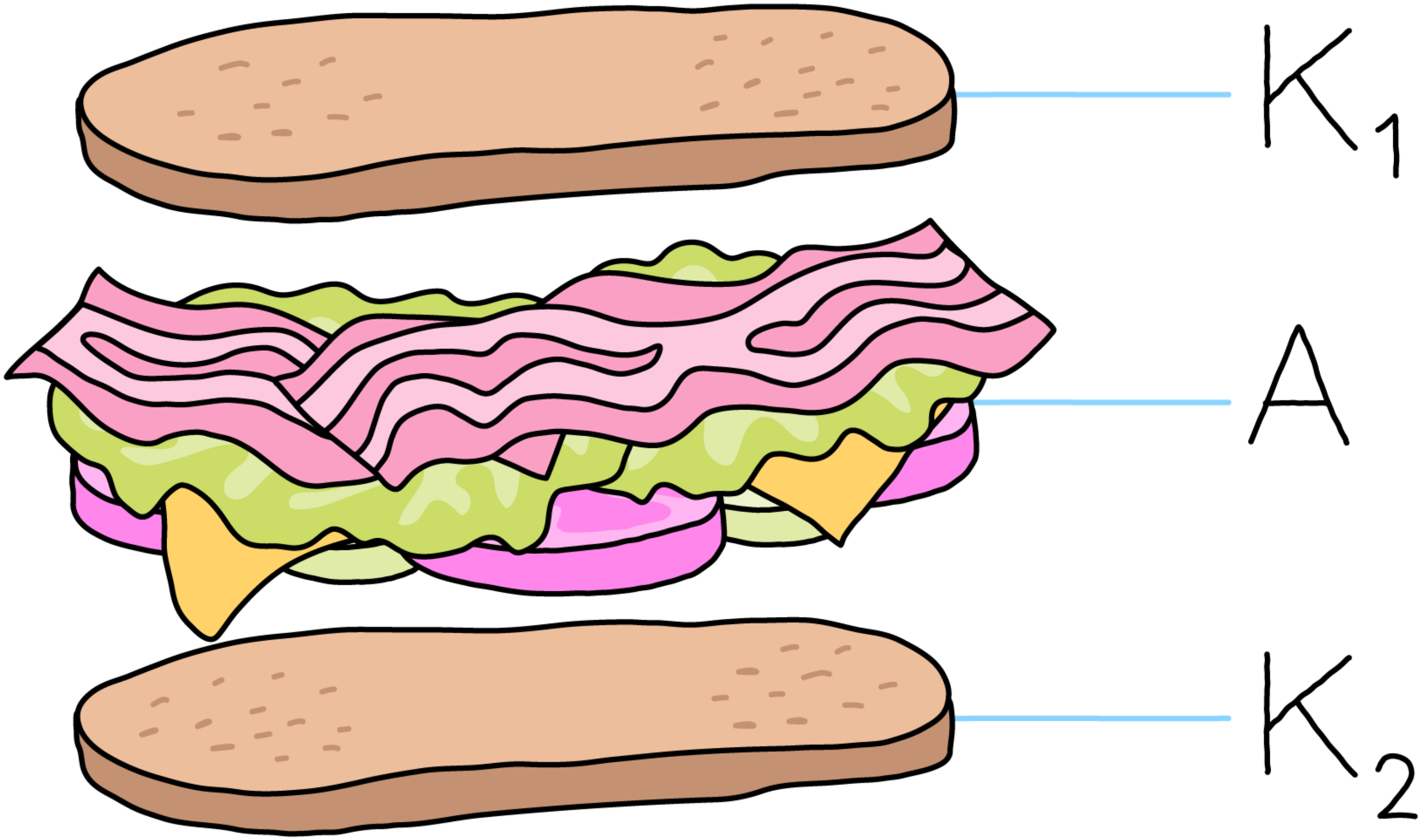
$$\mathcal{U} = (A\otimes B)\exp\left\{-i\left(c_1XX+c_2YY+c_3ZZ\right)\right\}(C\otimes D)$$

$$0\leq c_3\leq c_2\leq c_1\leq \frac{\pi}{4}$$

ref:

1. $(c_1,c_2,c_3)=(0,0,0)\rightarrow$ 0 CNOTs
2. $(c_1,c_2,c_3)=(\frac{\pi}{4},0,0)\rightarrow$ 1 CNOT
3. $c_3=0$ (excluding 1. & 2.) $\rightarrow$ 2 CNOTs
4. $c_3>0$ (generic) $\rightarrow$ 3 CNOTs

Extra workspace

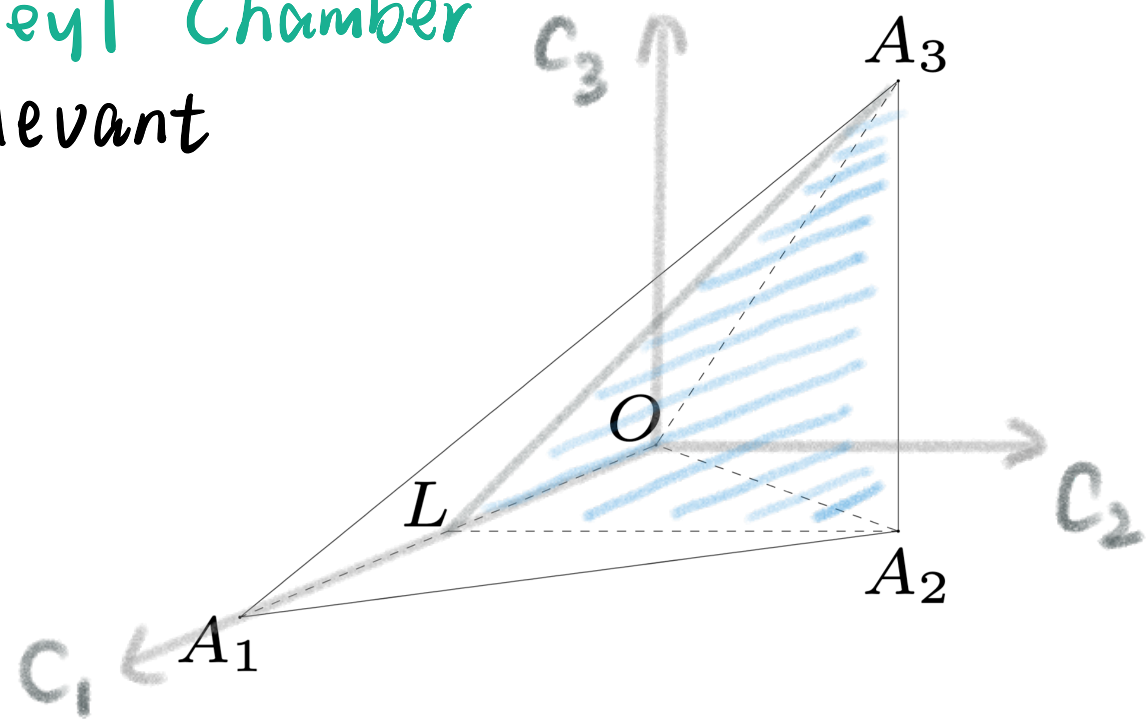


ref: Pennylane.ai

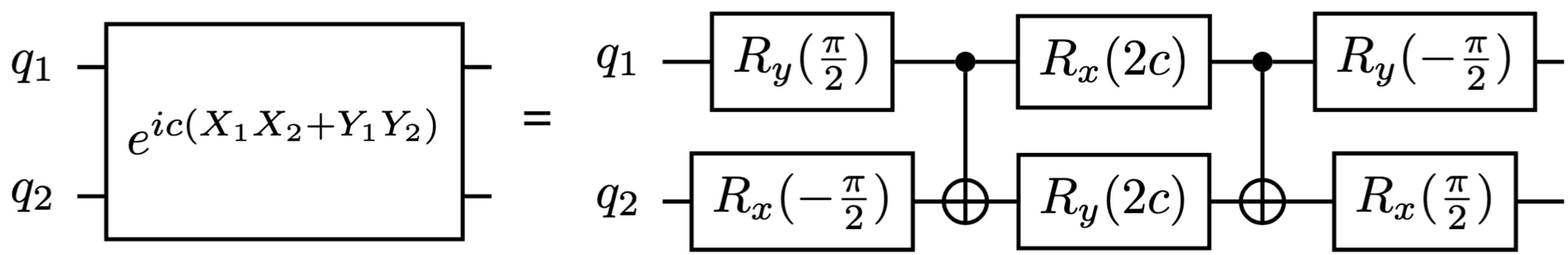
Extra workspace

'Weyl Chamber'

How is this relevant to Hamiltonian Simulation ?



example:



ref. arXiv: 2208.13557

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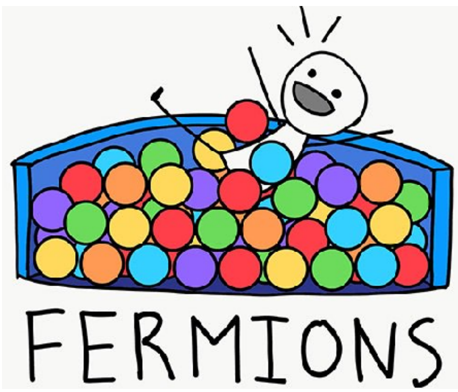
Fermions are **finite-dimensional** locally but obey **Fermi statistics**. Mapping a fermionic Hamiltonian into a qubit Hamiltonian can be done:

- using one qubit per fermion but at the cost of non-local qubit interactions using Jordan-Wigner transformation:

$$\psi_i = \Big(\prod_{j<i} \sigma_j^z\Big)\sigma_i^+, \quad \psi_i^\dagger = \Big(\prod_{j<i} \sigma_j^z\Big)\sigma_i^-$$

- using more than one qubit per fermion to assist retaining any existing locality in the original fermionic Hamiltonian (e.g. Verstrate-Cirac, compact, superfast encodings).



$|0\rangle$: empty

$|1\rangle$: occupied

$$a_j^\dagger = \Big(\prod_{k<j} Z_k\Big)\sigma_j^- . \quad a_j = \Big(\prod_{k<j} Z_k\Big)\sigma_j^+ . \quad \sigma^\pm = \tfrac{1}{2}(X \pm iY)$$

$$a_1 a_2 = \sigma_1^+ (Z_1 \sigma_2^+) = -\sigma_1^+ \sigma_2^+$$

$$a_2 a_1 = Z_1 \sigma_2^+ \sigma_1^+ = \sigma_1^+ \sigma_2^+$$

$$\Rightarrow \{a_1, a_2\} = 0$$

Similarly: $\{a_1, a_2^\dagger\} = 0$

$$Z\sigma^- = -\sigma^-, \quad \sigma^- Z = +\sigma^-, \quad Z\sigma^+ = \sigma^+, \quad \sigma^+ Z = -\sigma^+$$

Extra workspace

$$H \supset -\mu n_j \xrightarrow{JW} -\frac{\mu}{2}(1-Z_j)$$

chemical potential

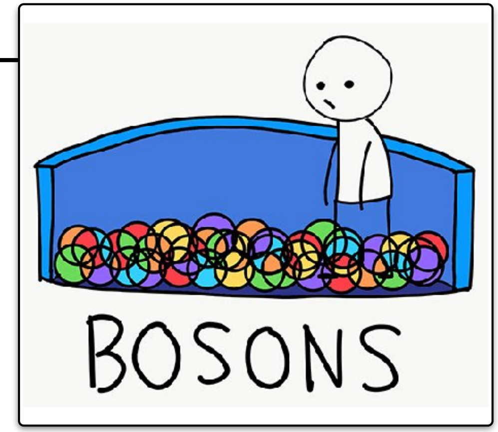
$$H \supset -t(a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) \xrightarrow{JW} -\frac{t}{2}(X_j X_{j+1} + Y_j Y_{j+1})$$

tight-binding 'hop'

$$H \supset \Delta(a_j a_{j+1} + a_{j+1}^\dagger a_j^\dagger) \xrightarrow{JW} \frac{\Delta}{2}(Y_j Y_{j+1} - X_j X_{j+1})$$

nearest-neighbor pairing

Bosons are **infinite-dimensional** locally but obey **Bose statistics**. Mapping a bosonic Hamiltonian into a qubit Hamiltonian can be done, e.g.,



- using binary encoding, requiring $\eta = \log(\Lambda + 1)$ qubits per boson, where Λ is the cutoff on boson occupation per site:

$$\hat{N}_p |p\rangle = p|p\rangle \text{ where } |p\rangle = \otimes_{j=0}^{\eta-1} |p_j\rangle \text{ with } p = \sum_{j=0}^{\eta-1} 2^j p_j$$

- using unary encoding, requiring Λ qubits per boson.

e.g. $\Lambda = 3$. $\eta = 2$ qubits.

L.S.B.

P	(q_1, q_0)
0	$\|00\rangle$
1	$\|01\rangle$
2	$\|10\rangle$
3	$\|11\rangle$

q z

$0 \to 1$

$1 \to -1$

$$\hat{n} = \sum_{j=0}^{\eta-1} 2^j \hat{P}_j \quad . \qquad \hat{P}_j = \frac{1 - z_j}{2}$$

$$= \frac{1-z_0}{2} + 2\,\frac{1-z_1}{2} = \frac{1}{2}(3 - z_0 - 2z_1)$$

Extra workspace

$$a^\dagger = \sum_{p=0}^{n-1} \sqrt{p+1}\, |p+1\rangle\langle p|$$

$$a^\dagger|p\rangle = \begin{cases} \sqrt{p+1}\,|p+1\rangle, & p < n \\ 0, & p = n \end{cases} \qquad a = (a^\dagger)^\dagger$$

$$a^\dagger = |01\rangle\langle 00| + \sqrt{2}\,|10\rangle\langle 01| + \sqrt{3}\,|11\rangle\langle 10|$$

$$a = |00\rangle\langle 01| + \sqrt{2}\,|01\rangle\langle 10| + \sqrt{3}\,|10\rangle\langle 11|$$

$$\hat{x} = \frac{1}{\sqrt{2}}(a + a^\dagger), \qquad \hat{H} = \omega\hat{n} + \frac{\lambda}{\sqrt{2}}(a + a^\dagger)$$

$\rightarrow$ Trotterize.

Extra workspace

Rewrite single-qubit outer products in Paulis:

$$|0\rangle\langle 0| = \frac{1+Z}{2}, \quad |1\rangle\langle 1| = \frac{1-Z}{2}$$

$$|0\rangle\langle 1| = \frac{X+iY}{2}, \quad |1\rangle\langle 0| = \frac{X-iY}{2}$$

e.g. $$a+a^\dagger = \frac{1+\sqrt{3}}{2} I\otimes X + \frac{1}{\sqrt{2}}(X\otimes X + Y\otimes Y)$$

$$+ \frac{1-\sqrt{3}}{2} Z\otimes X$$

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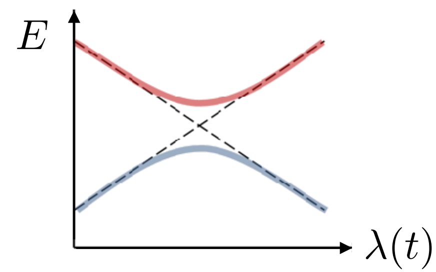
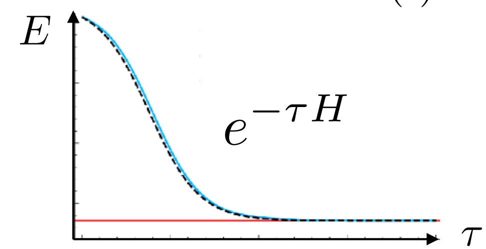
EXAMPLES OF (GROUND-)STATE PREPARATION METHODS

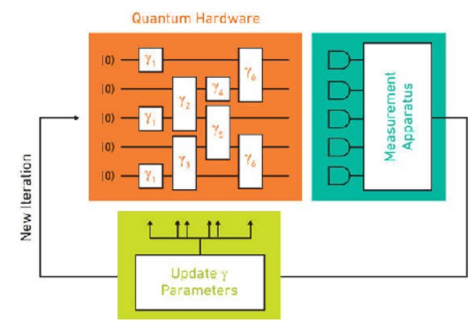
- **Adiabatic state preparation:** Prepare the ground state of a simple Hamiltonian, then adiabatically turn the Hamiltonian to that of the target Hamiltonian. Requires a non-closing energy gap.



- **Imaginary time evolution:** Start with an easily prepared state and evolve with imaginary time operator to settle in the ground state. Require implementing non-unitary operator which can be costly.



- **Variational quantum eigensolver (VQE):** Use the variational principle of quantum mechanic and classical pre-processing to minimize the energy of a non-trivial ansatz wavefunction generated by a quantum circuit. The optimized circuit corresponding to the minimum energy generates an approximation to ground-state wavefunction. Can fail if stuck in local minima manifolds or manifolds with exponentially small gradients in qubit number.



- **Classically computed states:** Use classical computing such as Monte Carlo or Tensor Networks to learn the state or features of the state when possible, for a direct implementation of the state as a quantum circuit, or as close enough state to the ground state as a starting point of the above algorithms so to achieve more efficient implementations.

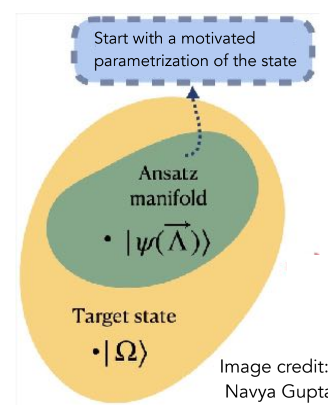


Image credit: Navya Gupta (UMD)

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(IMPROVED) THEORY OF PRODUCT FORMULAS

Consider the Hamiltonian
$$H = \sum_{i=1}^{\Gamma} H_i$$

First-order product formula

$$\boxed{V_1(t)} = e^{-itH_1} e^{-itH_2} \cdots e^{-itH_\Gamma}$$

is bounded by:

$$\|\boxed{V_1(t)} - e^{-itH}\| \le \frac{t^2}{2} \sum_{i=1}^{\Gamma} \left\| \left[\sum_{j=i+1}^{\Gamma} H_j, H_i \right] \right\|$$

Second-order formula

$$\boxed{V_2(t)} = (e^{-itH_\Gamma/2} \cdots e^{-itH_2/2} e^{-itH_1/2})(e^{-itH_1/2} e^{-itH_2/2} \cdots e^{-itH_\Gamma/2})$$

is bounded by:

$$\|\boxed{V_2(t)} - e^{-itH}\| \le \frac{t^3}{12} \sum_{i=1}^{\Gamma} \left\| \left[\sum_{k=i+1}^{\Gamma} H_k, \left[\sum_{j=i+1}^{\Gamma} H_j, H_i \right] \right] \right\| + \frac{t^3}{24} \sum_{i=1}^{\Gamma} \left\| \left[H_i, \left[H_i, \sum_{j=i+1}^{\Gamma} H_j \right] \right] \right\|$$

tighter, locality-aware bounds.

A general bound also exist, see: **Childs, Su, Tran, Wiebe, Zhu, Phys. Rev. X 11, 011020 (2021).**

Extra workspace

OUTLINE OF PART II: QUANTUM SIMULATION AND QUANTUM-COMPUTING BASICS

i) Quantum-simulation steps: A brief introduction
ii) Various modes of quantum simulation: Digital, analog, hybrid
iii) Digital-quantum-simulations basics:

- qubits and gates
- Encoding fermions and bosons onto qubits
- State-preparation strategies
- Time evolution (via product formulas)
- Measurement strategies and observables

EXAMPLES OF ACCESSIBLE OBSERVABLES

One can measure the following quantities to learn properties of the outcome state. Some of these can be measured directly in the computational basis, but others need a change of basis or other dedicated quantum circuits to access them.

- Energy and momentum, particle and charge (both locally and globally)
- Various correlation functions (both static and dynamical)
- Asymptotic S-matrix elements (assuming asymptotic final states are reached and overlap with a specified final state is desired)
- Entanglement measures such as entanglement spectrum (which can signal thermalization or lack of) using efficient ansatze.

Fidelities and full state tomography are hard as they demand exponentially large number of measurements.

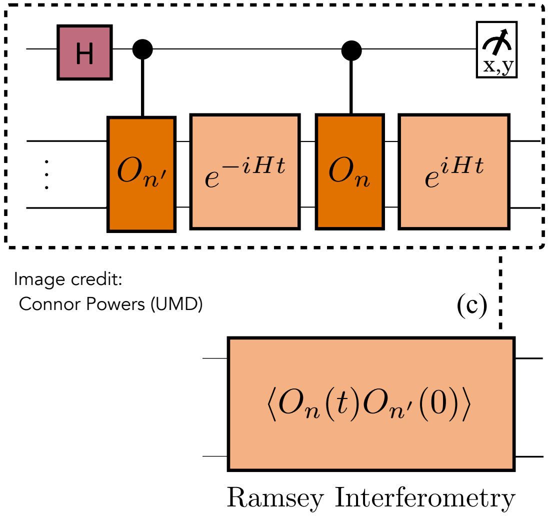
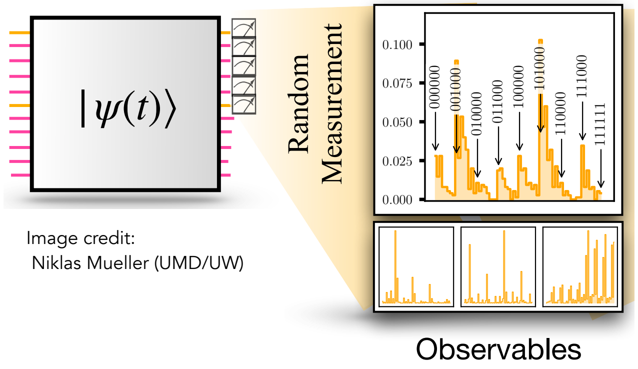


Image credit:
Connor Powers (UMD)



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Niklas Mueller (UMD/UW)

TO BE CONTINUED…
QUESTIONS?