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
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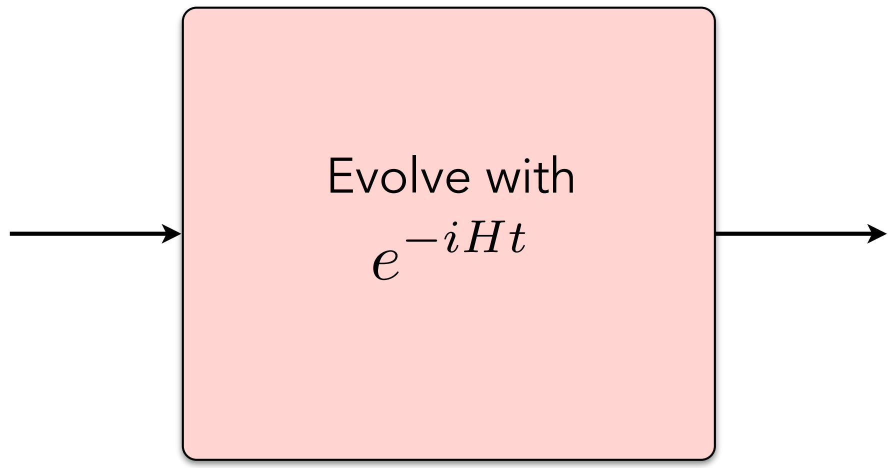
- Time evolution (via product formulas)
- Measurement strategies and observables

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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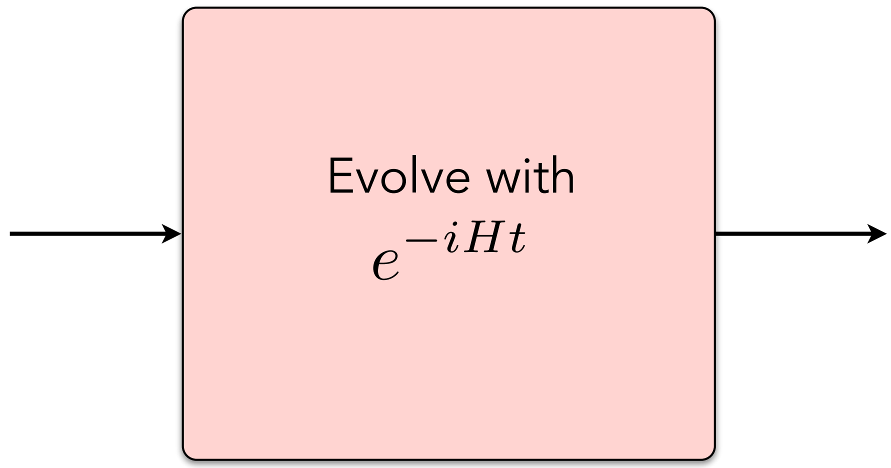
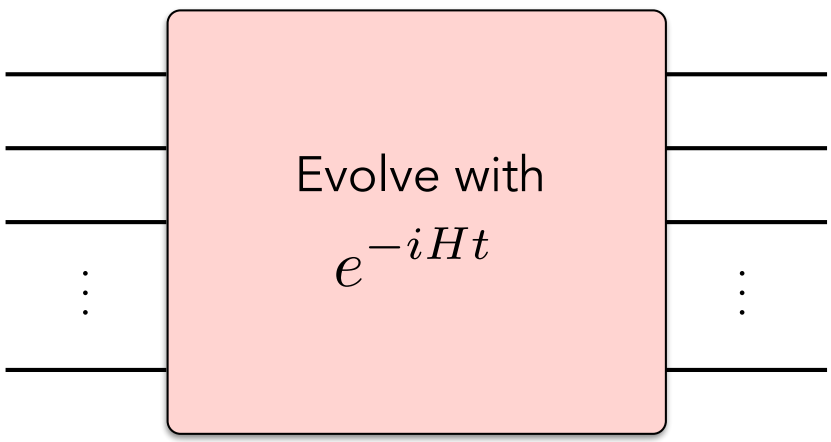
THIS LECTURE CONCERNS PRIMARILY TIME EVOLUTION.



DIFFERENT APPROACHES TO QUANTUM SIMULATION

Analog



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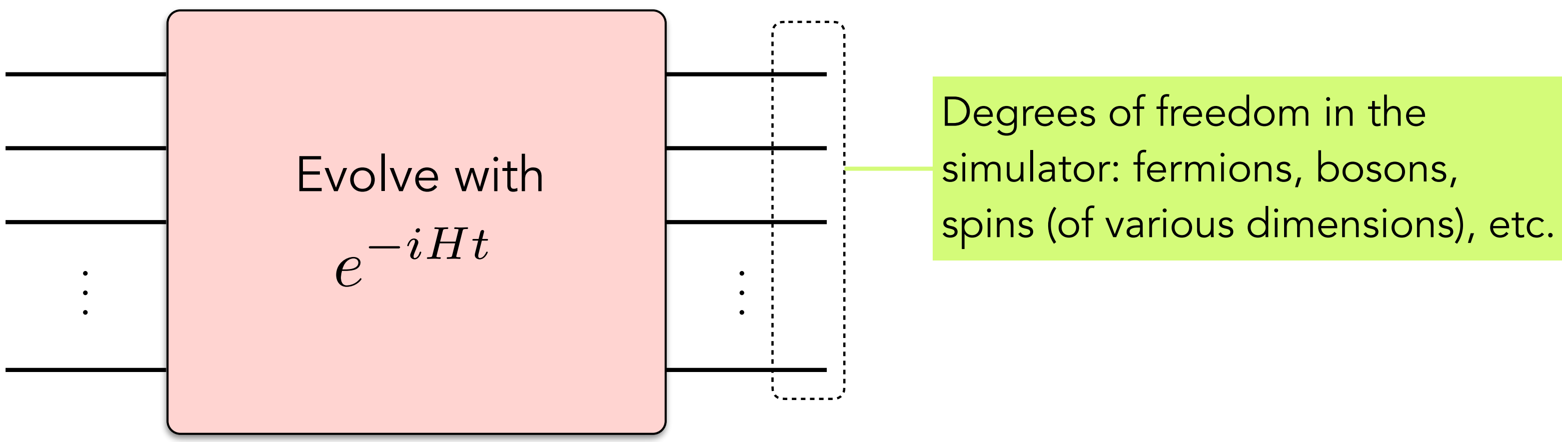
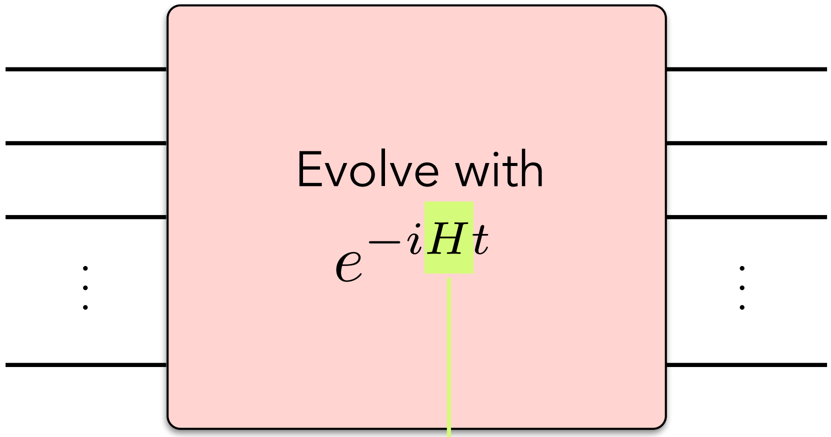


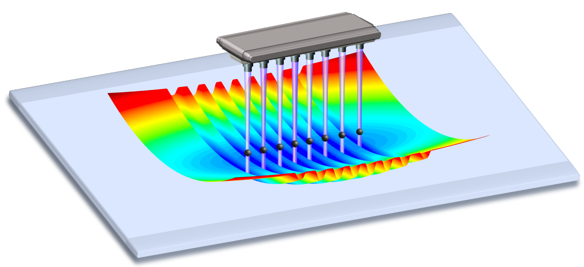
DIFFERENT APPROACHES TO QUANTUM SIMULATION

Analog

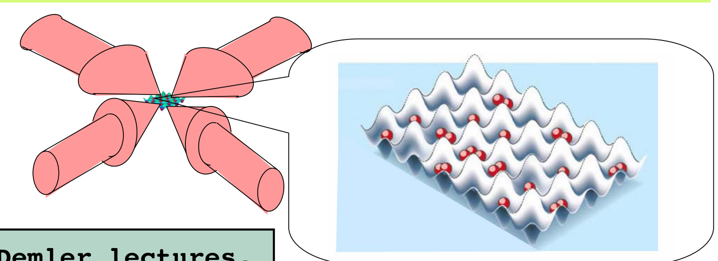


The engineered simulator Hamiltonian that mimics the Hamiltonian of target system.

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.



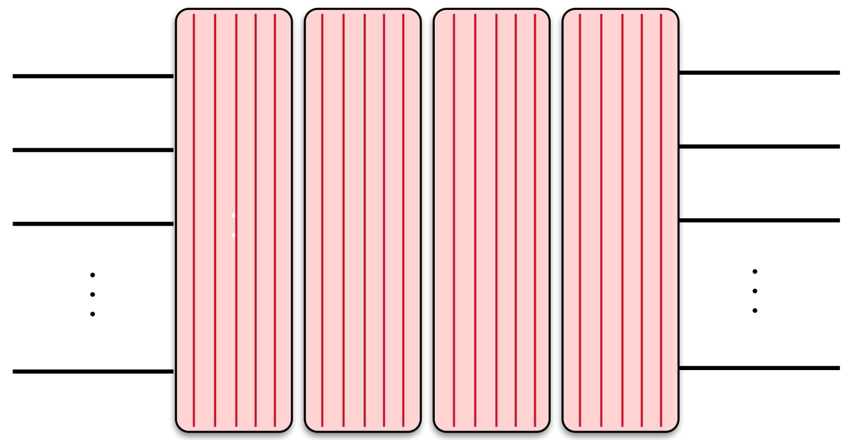
CREDIT: ANDREW SHAW, UNIVERSITY OF MARYLAND



Eugene Demler lectures, Harvard University.

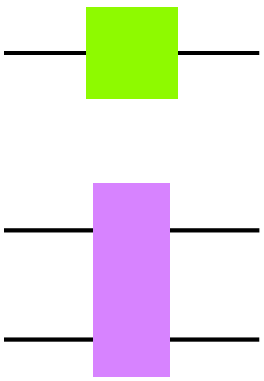
DIFFERENT APPROACHES TO QUANTUM SIMULATION

Digital

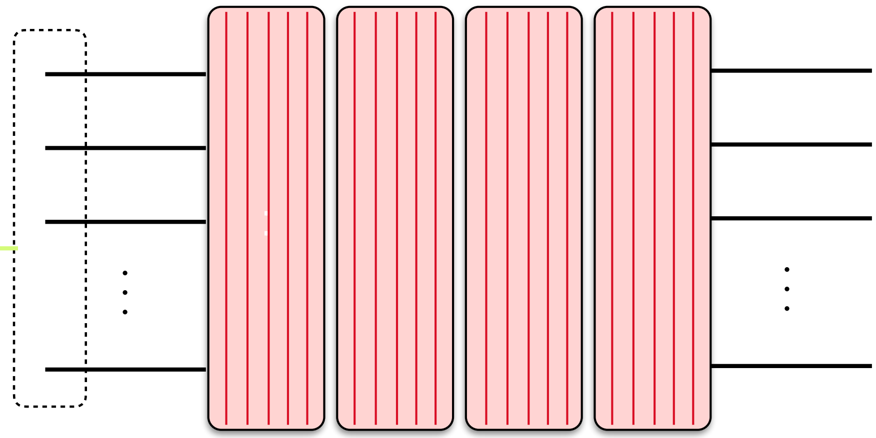


DIFFERENT APPROACHES TO QUANTUM SIMULATION

Digital



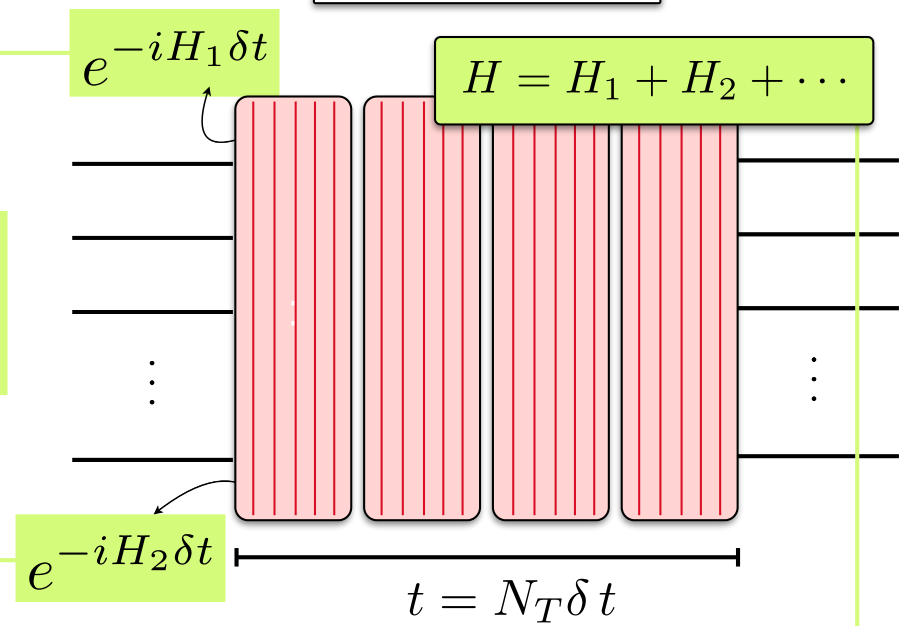
Only qubits as DOF. Only universal single- and two-qubit operations allowed.



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.

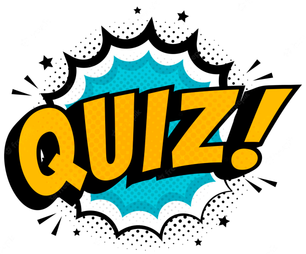
Trotter-Suzuki expansion:

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

Other digitalization schemes also exist.

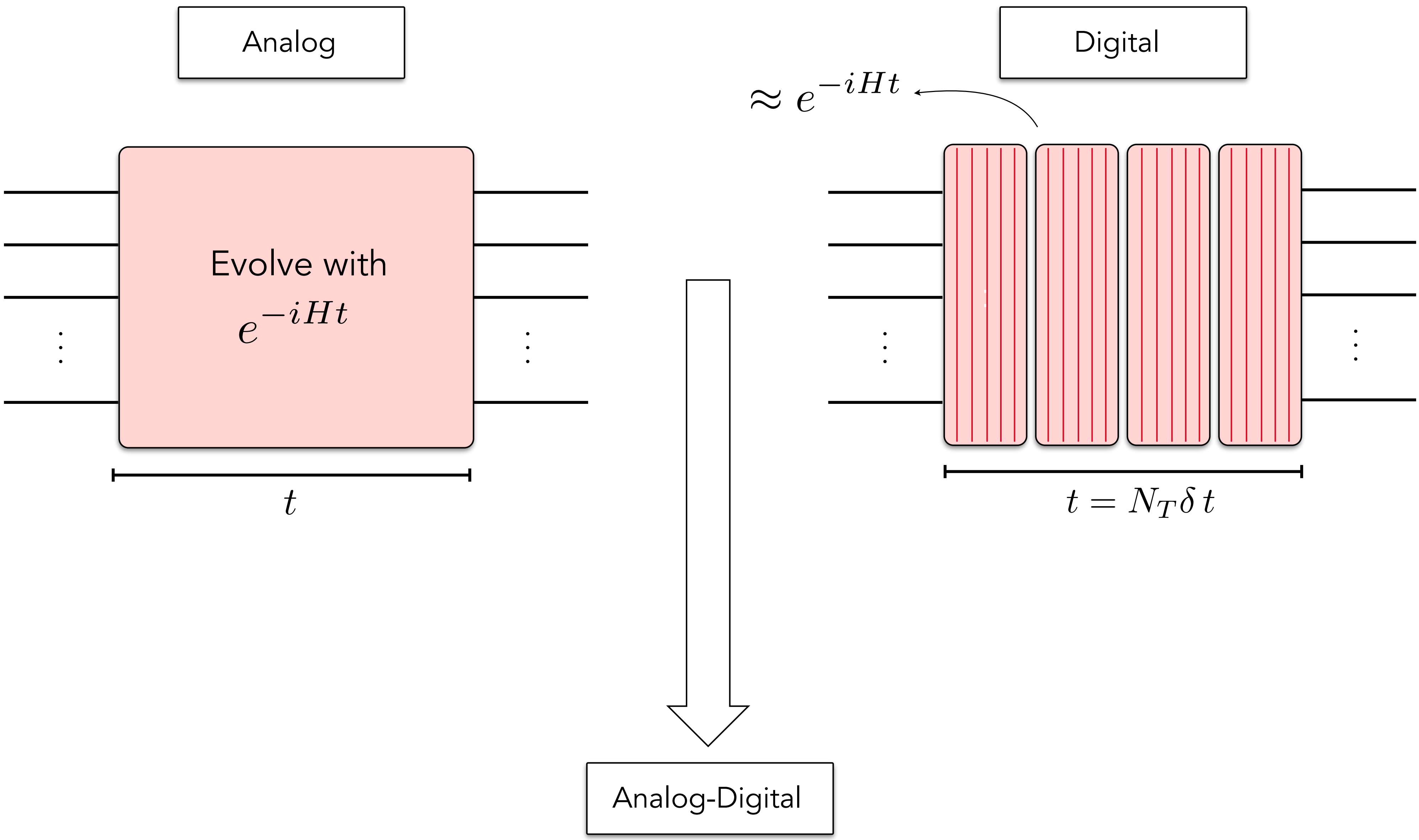
…other methods exist too.

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?

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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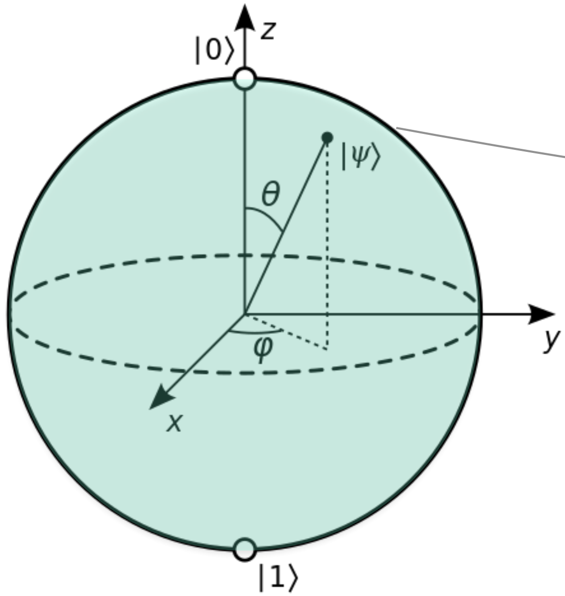


State of a single qubit: $|\psi\rangle = a|0\rangle + b|1\rangle \equiv a\begin{pmatrix}1\\0\end{pmatrix} + b\begin{pmatrix}0\\1\end{pmatrix}$

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

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

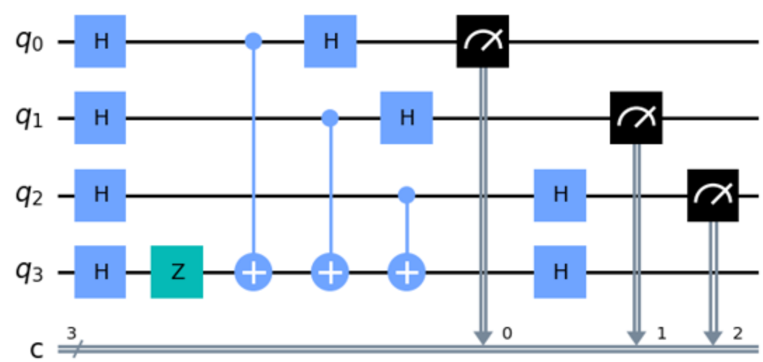
Operator	Gate(s)	Matrix
Pauli-X (X)	X	$\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$
Pauli-Y (Y)	Y	$\begin{bmatrix}0 & -i\\i & 0\end{bmatrix}$
Pauli-Z (Z)	Z	$\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$
Hadamard (H)	H	$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}$
Phase (S, P)	S	$\begin{bmatrix}1 & 0\\0 & i\end{bmatrix}$
$\pi/8$ (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, T, CNOT

Example of) a quantum circuit:



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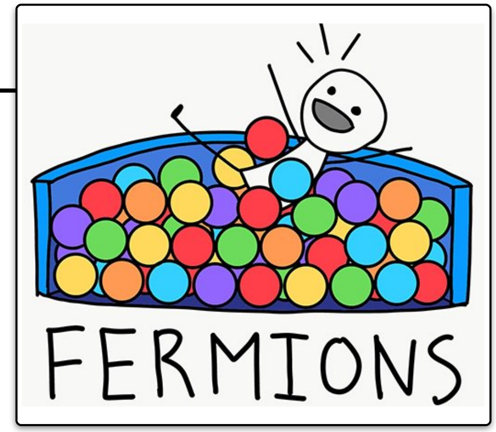
Fermions are **finite-dimensional** locally but obey **Fermi statistics**. Mapping a fermionic Hamiltonian into a qubit Hamiltonian can be done:

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

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

- 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).

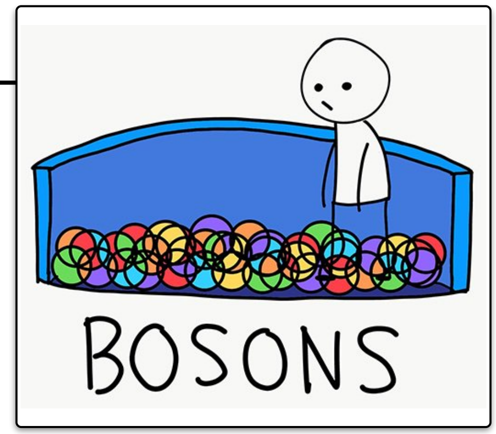


Bosons are **infinite-dimensional** locally but obey **Bose statistics**. Mapping a bosonic Hamiltonian into a qubit Hamiltonian can be done, e.g.,

- 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.



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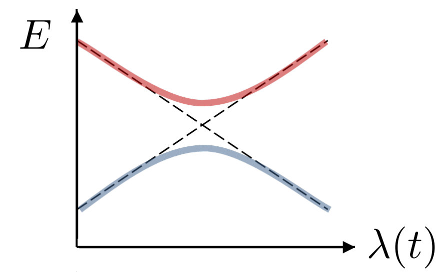
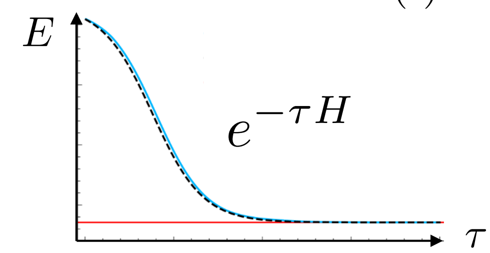
EXAMPLES OF (GROUND-)STATE PREPARATION METHODS

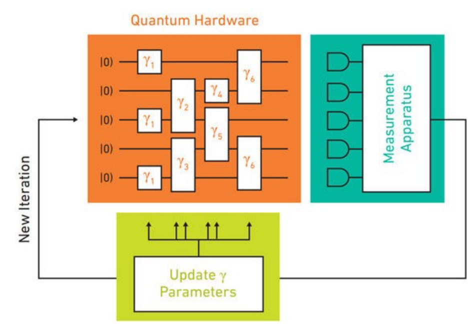
- **Adiabatic state preparation:** Prepare the ground state of a simple Hamiltonian, then adiabatically turn the Hamiltonian to that of the target Hamiltonian. Requires a non-closing energy gap.



- **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.

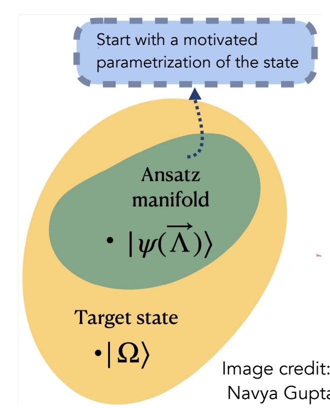


Image credit:
Navya Gupta (UMD)

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(IMPROVED) THEORY OF PRODUCT FORMULAS

Consider the Hamiltonian

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

First-order product formula

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

is bounded by:

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

Second-order formula

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

is bounded by:

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

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

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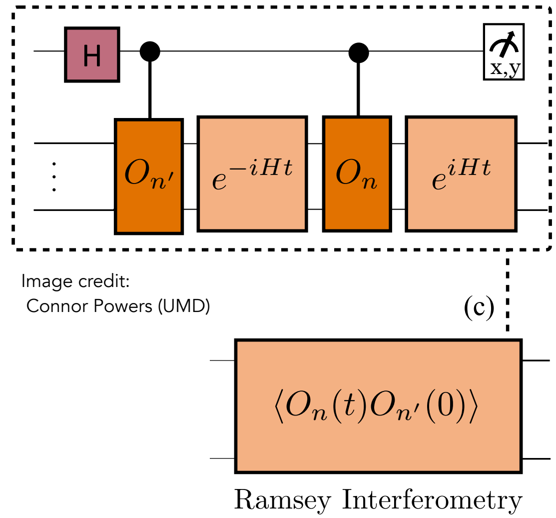
EXAMPLES OF ACCESSIBLE OBSERVABLES

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.



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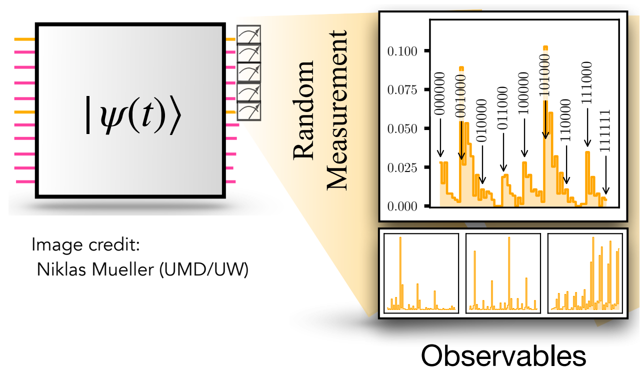

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TO BE CONTINUED…

QUESTIONS?