ICEPP The University of Tokyo

Hands-on session 2:
Representation of physical systems and dynamics simulation

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Re(-re-...-)visiting how it started

Simulating Physics with Computers

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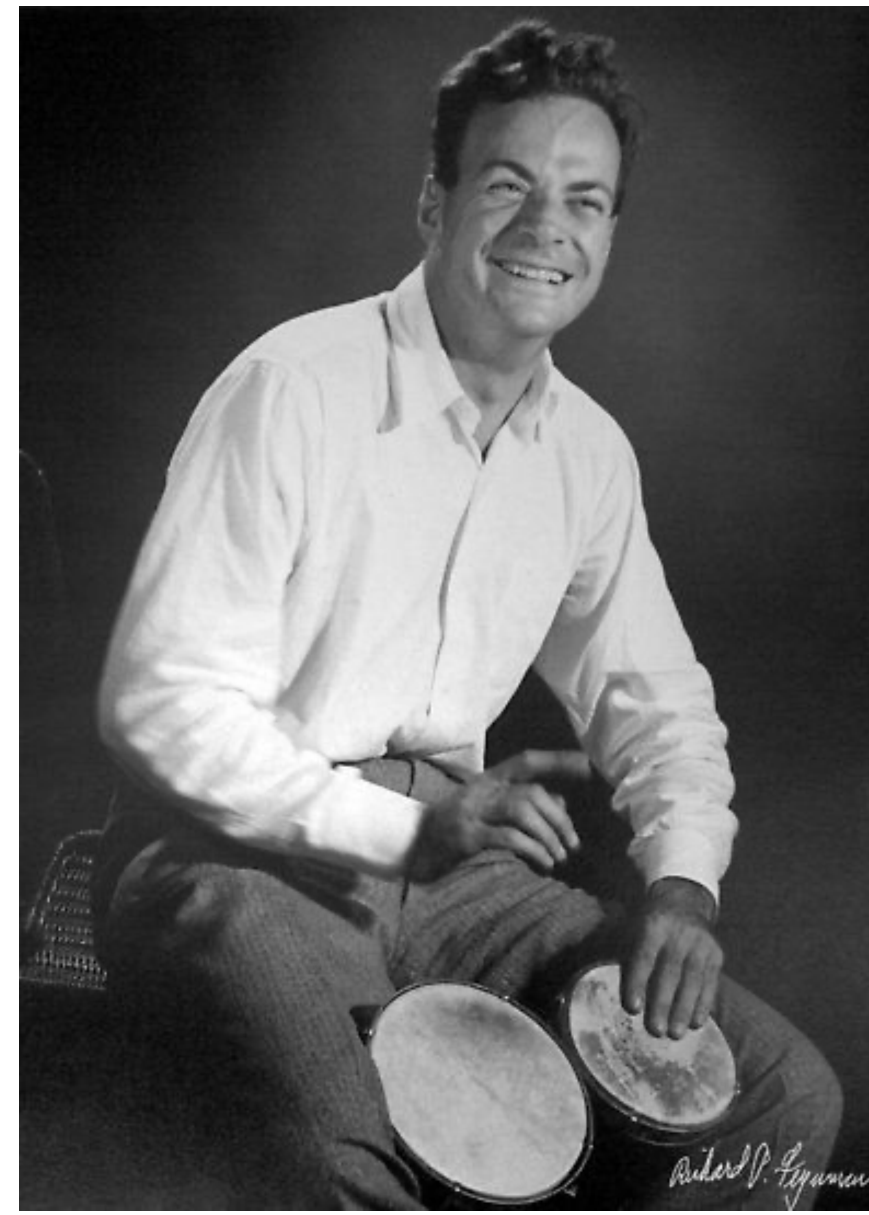
1. INTRODUCTION

On the program it says this is a keynote speech—and I don't know what a keynote speech is. I do not intend in any way to suggest what should be in this meeting as a keynote of the subjects or anything like that. I have my own things to say and to talk about and there's no implication that



... because nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, ...

Dynamics in the Hamiltonian formalism

Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$ (differential form)

$$|\psi(t)\rangle = T\left[\exp\left(-\frac{i}{\hbar}Ht\right)\right]|\psi(0)\rangle$$ (integral form)

$$= \lim_{\substack{\Delta t \to 0 \\ N\Delta t = t}} \prod_{k=0}^{N} e^{-\frac{i}{\hbar}H(k\Delta t)\Delta t}|\psi(0)\rangle$$

Form usable in numerical simulation

Calculation is conceptually easy

To compute $\prod_{k=0}^{N} e^{-\frac{i}{\hbar}H(k\Delta t)\Delta t}|\psi(0)\rangle$,

- At each k:
  - Find the eigenvalues $\hbar\omega_j$ and eigenvectors $|\phi_j\rangle$ of $H(k\Delta t)$:
    $H(k\Delta t) = \sum_{j=1}^{M} \hbar\omega_j|\phi_j\rangle\langle\phi_j|$
  - Decompose $|\psi(k\Delta t)\rangle$ into eigenvectors $|\phi_j\rangle$:
    $|\psi(k\Delta t)\rangle = \sum_{j=1}^{M} c_j|\phi_j\rangle$
  - Update the complex phase of the coefficients and take the sum:
    $|\psi((k+1)\Delta t)\rangle \simeq \sum_{j=1}^{M} e^{-i\omega_j\Delta t}c_j|\phi_j\rangle$
- Repeat

But practically impossible

- Hilbert space dimension is exponential with respect to the degrees of freedom n of the system:
  $M = O(\exp(Cn))$ $(C > 0)$
  - Computer will run out of memory to store M eigenvectors
  - Diagonalization of $M \times M$ Hamiltonian even more impractical
- Less significant but still formidable:
  How many time steps N do we need for a relevant simulation?

Using a quantum computer

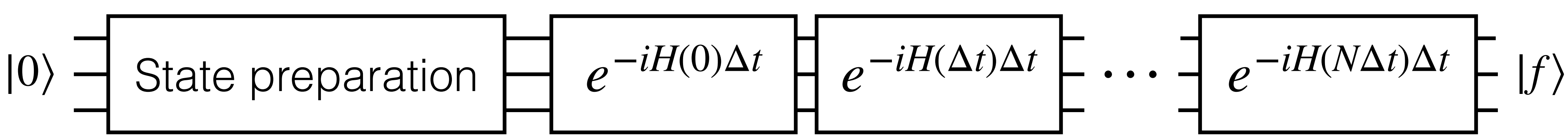
- Hilbert space of an n-qubit register has 2^n dimensions
- $e^{-iH\Delta t}$ is a unitary operator, just as quantum gates are

→ Quantum computer is useful for certain classes of systems

If we have:

- A mapping of system state to register state
- A decomposition of the Hamiltonian into implementable gates

then



$|f\rangle$ represents the qubit-mapped final state of the system

Mapping physical systems to qubits

Examples

- Spin-1/2 systems
  - Spin $\leftrightarrow$ qubit
  - $|\uparrow\rangle \leftrightarrow |0\rangle$, $|\downarrow\rangle \leftrightarrow |1\rangle$
  - Pauli $\sigma^{X,Y,Z} \leftrightarrow X, Y, Z$ gates
- Fermion systems (second quantization)
  - Orbital (site) $\leftrightarrow$ qubit
  - $|e\rangle \leftrightarrow |0\rangle$, $|o\rangle \leftrightarrow |1\rangle$
  - Creation / annihilation $\leftrightarrow X \mp iY$

Mapping physical systems to qubits

- Harmonic oscillators
  - Oscillator ↔ K-qubit register (truncated at 2^K modes)
  - $|n\rangle \leftrightarrow \bigotimes_{k=0}^{K-1} |n_k\rangle$ $(n = \sum_{k=0}^{K-1} 2^k n_k)$
  - Ladder operator ↔ Incrementer / decrementer circuit
- Fermion systems (first quantization)
  - Particle ↔ register
  - Single-particle eigenstates ↔ computational basis states

Mapping continuous and/or unbounded states requires ingenuity

Expressing the Hamiltonian with gates

Gates natively supported on a typical digital quantum computer:

- Single particle rotations (~arbitrary)
- One or two multi-qubit operations

There is no “gate for time evolution of system X”

→ Must find a decomposition $H = \sum_{l=1}^{L} H_l$ where each $e^{-iH_l\Delta t}$ is implementable with native gates

Two problems arise:

- $\prod e^{-iH_l\Delta t} \neq e^{-i\sum_l H_l\Delta t}$ (H_ls don't commute in general)
- What if $L = O(\exp(Cn))$?
  Example:
  Space of Hermitian ops of an n-spin system is spanned by $\{I, X, Y, Z\}^{\otimes n}$

Suzuki-Trotter decomposition

From Trotter formula

$$\lim_{n\to\infty}\left(e^{iAt/n}e^{iBt/n}\right)^n = e^{i(A+B)t}$$

product-of-exponentials is a valid first-order approximation:

$$\exp\left(-\frac{i\Delta t}{\hbar}H\right) = \prod_{k=1}^{L}\exp\left(-\frac{i\Delta t}{\hbar}H_k\right) + O((\Delta t)^2)$$

i.e. the approximation accuracy improves as $\Delta t \to 0$.

Most interesting Hamiltonians are local

Natural systems are governed by local interactions

Even in n-spin systems we usually consider 2- and 3-body interactions
→ In terms of Paulis, a typical Hamiltonian term looks like
$I \otimes \cdots \otimes I \otimes X \otimes Y \otimes I \otimes \cdots \otimes I$

System ↔ qubit mapping should consider Hamiltonian locality

Exercise 1: Driven spin 1/2

Let us simulate a single spin-1/2 system with a single qubit.

The spin is externally driven by an oscillating field:

$$H(t) = \omega |\uparrow\rangle\langle\uparrow| + \frac{A}{2}\cos\alpha t\left(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right) = H_Z + H_X(t)$$

Using the previously discussed mapping,

$$|\uparrow\rangle, |\downarrow\rangle \rightarrow |0\rangle, |1\rangle$$

$$\exp\left(-i\omega\Delta t|\uparrow\rangle\langle\uparrow|\right) \rightarrow$$
$$\exp\left(-\frac{i\omega\Delta t}{2}\left[(|0\rangle\langle 0| - |1\rangle\langle 1|) + (|0\rangle\langle 0| + |1\rangle\langle 1|)\right]\right) = e^{-i\omega\Delta t/2(Z+I)}$$

$$= e^{-i\omega\Delta t/2} R_Z(\omega\Delta t)$$

$$\exp\left(-i\frac{A}{2}\cos(\alpha t)\Delta t\left[|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right]\right) \rightarrow$$
$$e^{-iA\cos(\alpha t)\Delta t/2X} = R_X(A\cos(\alpha t)\Delta t)$$

Qiskit note: Sampler and Estimator

Sampler:

- User passes full circuits (including measurements)
- Returns occurrence frequencies of bit strings
- Optionally applies various error mitigation techniques

Estimator:

- User passes unmeasured circuits and observables (sums of Pauli products)
- Measures and returns expectation values of the observables
- Optionally applies various error mitigation techniques

Basis transformation

- Measurements are implemented only for $|0\rangle/|1\rangle$ (Z) basis
- Native multi-qubit gates have very specific forms

→ Basis transformation (π/2 rotations in Bloch sphere) is an important technique

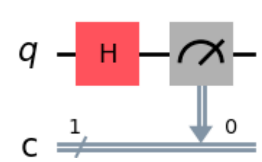
- Z basis ↔ X basis: $HZH = X \Leftrightarrow Z = HXH$

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

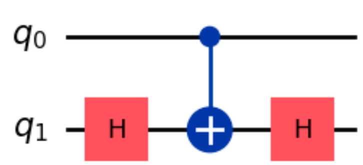
$$S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

Examples:

- Measurement of $\langle X \rangle$:



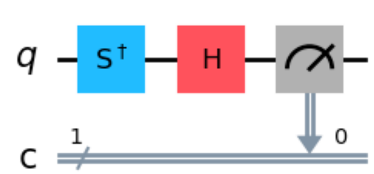
- Controlled-Z



- Z basis ↔ Y basis: $SHZHS^\dagger = Y \Leftrightarrow Z = S^\dagger HYHS$

Examples:

- Measurement of $\langle Y \rangle$:



Exercise 2: Heisenberg model

Next we look at a multi-body system with a static Hamiltonian.

$$H = -J\sum_{j=0}^{n-2}(\sigma_{j+1}^X\sigma_j^X + \sigma_{j+1}^Y\sigma_j^Y + \sigma_{j+1}^Z\sigma_j^Z) - h\sum_{j=0}^{n-1}\sigma_j^Z$$

With the usual mapping

$$U_{XX}(\Delta t) = \exp\left(iJ\Delta t\sum_{j=0}^{n-2}\sigma_{j+1}^X\sigma_j^X\right) = \prod_{j=0}^{n-2}\exp\left(iJ\Delta t\sigma_{j+1}^X\sigma_j^X\right) \to R_{XX}^{j,j+1}(-2J\Delta t)$$

$$U_{YY}(\Delta t) = \exp\left(iJ\Delta t\sum_{j=0}^{n-2}\sigma_{j+1}^Y\sigma_j^Y\right) = \prod_{j=0}^{n-2}\exp\left(iJ\Delta t\sigma_{j+1}^Y\sigma_j^Y\right) \to R_{YY}^{j,j+1}(-2J\Delta t)$$

$$U_{ZZ}(\Delta t) = \exp\left(iJ\Delta t\sum_{j=0}^{n-2}\sigma_{j+1}^Z\sigma_j^Z\right) = \prod_{j=0}^{n-2}\exp\left(iJ\Delta t\sigma_{j+1}^Z\sigma_j^Z\right) \to R_{ZZ}^{j,j+1}(-2J\Delta t)$$

$$U_{Z}(\Delta t) = \exp\left(ih\Delta t\sum_{j=0}^{n-1}\sigma_j^Z\right) = \prod_{j=0}^{n-1}\exp\left(ih\Delta t\sigma_j^Z\right) \to R_{Z}^{j}(-2h\Delta t)$$

Implementation of $R_{XX/YY/ZZ}$

Qiskit has built-in support of these gates.

But we implement them "by hand" using single-qubit gates + CX as an exercise.

Note that

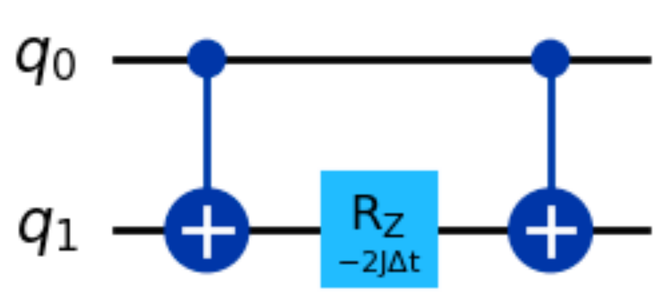
$$Z_j Z_{j+1}|00\rangle = |00\rangle \qquad e^{i\phi Z_j Z_{j+1}}|00\rangle = e^{i\phi}|00\rangle$$

$$Z_j Z_{j+1}|01\rangle = -|01\rangle \qquad e^{i\phi Z_j Z_{j+1}}|01\rangle = e^{-i\phi}|01\rangle$$

$$Z_j Z_{j+1}|10\rangle = -|10\rangle \qquad e^{i\phi Z_j Z_{j+1}}|10\rangle = e^{-i\phi}|10\rangle$$

$$Z_j Z_{j+1}|11\rangle = |11\rangle \qquad e^{i\phi Z_j Z_{j+1}}|11\rangle = e^{i\phi}|11\rangle$$

A gate sequence that performs this operation is



$$|00\rangle \to e^{iJ\Delta t}|00\rangle$$
$$|01\rangle \to e^{-iJ\Delta t}|01\rangle$$
$$|10\rangle \to e^{-iJ\Delta t}|10\rangle$$
$$|11\rangle \to e^{iJ\Delta t}|11\rangle$$

Implementation of $R_{XX/YY/ZZ}$

R_{XX} and R_{YY} are obtained from R_{ZZ} using basis transformations: