Hamiltonian Simulation

An overview

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FRIB-TA Summer School 2022

Recap

- Basics of quantum computing (morning)
- Afternoon: Quantum dynamics
  - Hamiltonian simulation
  - Phase estimation (phase ➞ eigenvalue)
  - Adiabatic evolution (state preparation, ground state determination)

- Next hour: a deeper dive into Hamiltonian simulation (HS)

By the end of this talk…

You should be able to

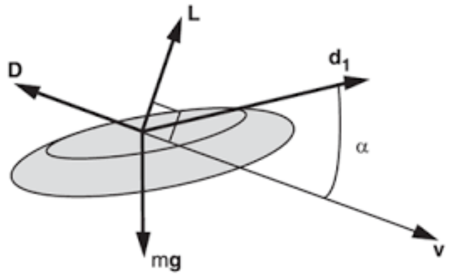
- Define Hamiltonian simulation (in the context of quantum computing)
- Recognize the scope and limitations of quantum simulations
- Understand the phrase "k-local Hamitonian simulation is BQP-complete"

Suppose you had a quantum computer today, with 10^9 perfect logical qubits to use for quantum dynamical simulations.

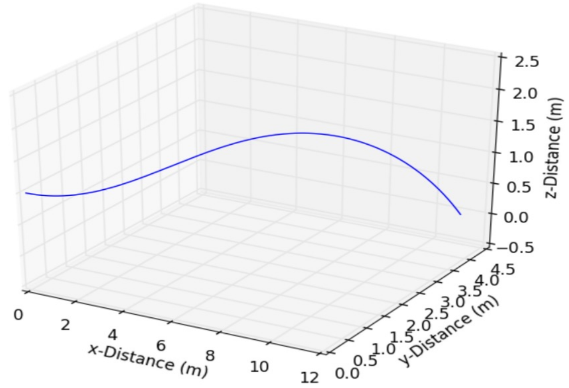
What would you do first?

Why care about dynamical sims?

- Gets to the basic goals of physics and science!
- Concrete predictions + Empirical verification = Confidence in theory
- Leads to *new* phenomena not obvious from basic theory. (e.g. phase transitions)



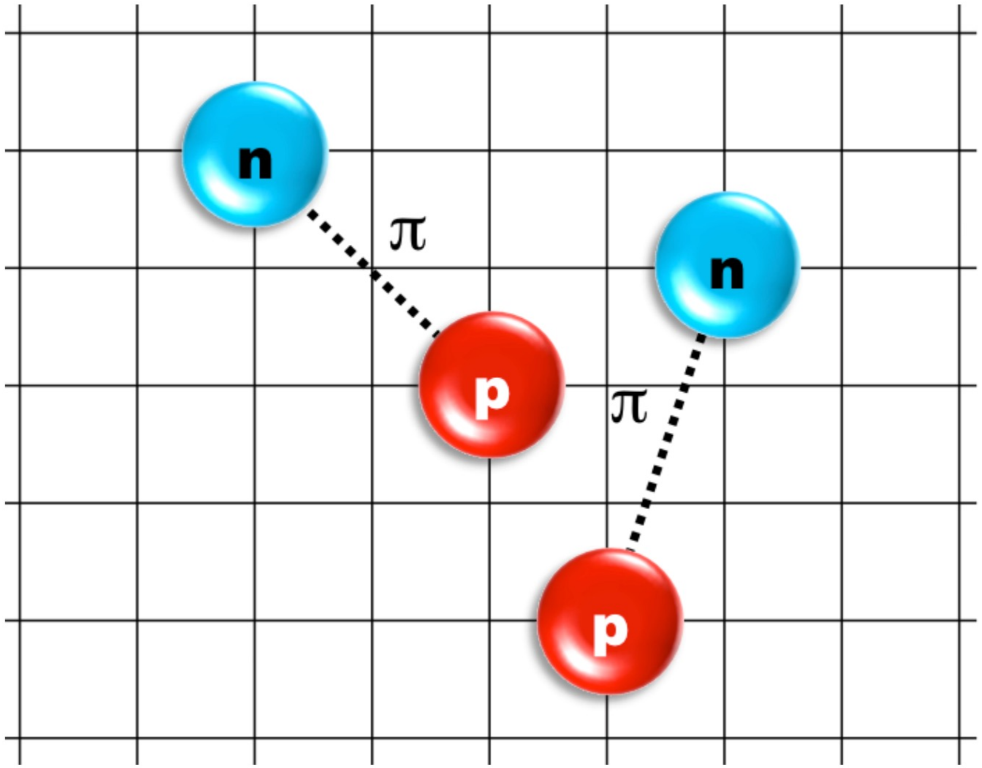
Hubbard & Hummel, 2000.



Hannah, 2017.

Why care about Hamiltonian simulation (HS)?

1. A significant fraction of computing power is currently dedicated to simulating quantum systems (many of you know this well!)
2. HS algs are promising first (useful) app of quantum computers



Lattice EFT principle, courtesy of Dean Lee

Quantum dynamics

The time evolution of a (closed, isolated) quantum system is described by a unitary operator U_t

$$\rho_t = U_t \, \rho_0 \, U_t^\dagger \qquad \text{(Schrödinger picture)}$$

$$O_t = U_t^\dagger O_0 U_t \qquad \text{(Heisenberg picture)}$$

From Unitaries to Hamiltonians

(to the white board)

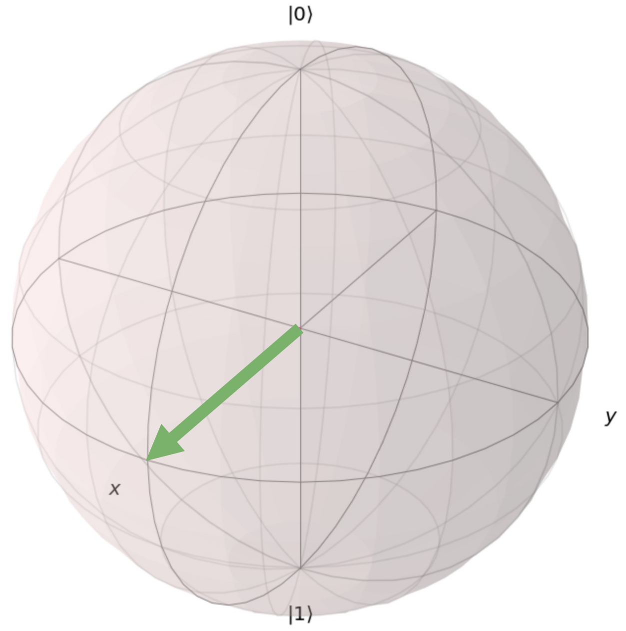
Can you think of reasons why you might *prefer* a classical simulation over a quantum one?

Representing quantum objects

$$\vec{p} = \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix}$$

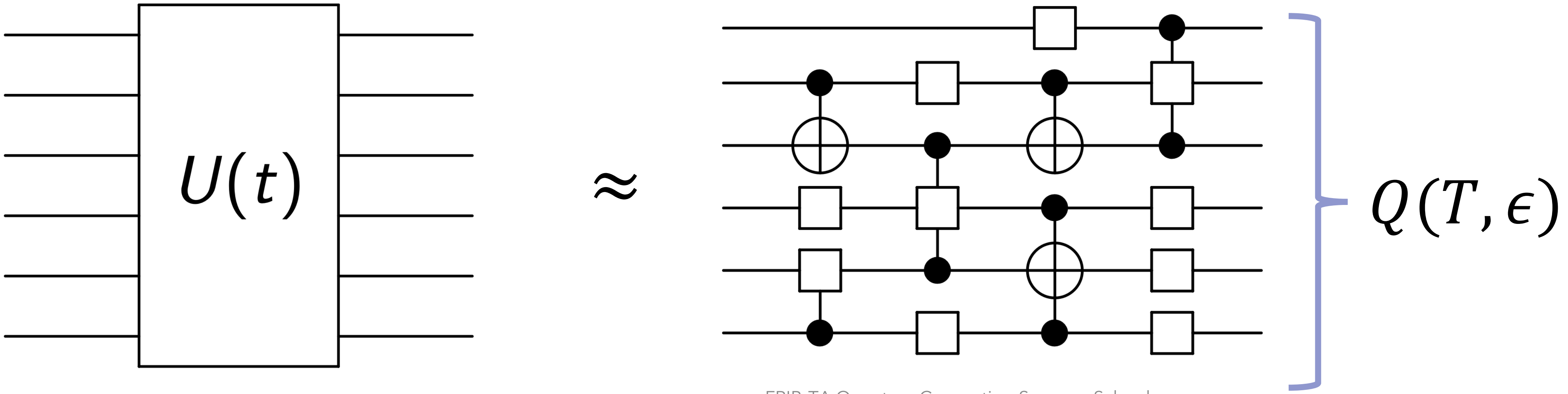
Representing quantum objects

$$|\psi\rangle = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$



Towards a formal definition.

Given a Hamiltonian H, simulation time T, construct a quantum circuit Q which approximates U to accuracy ϵ.

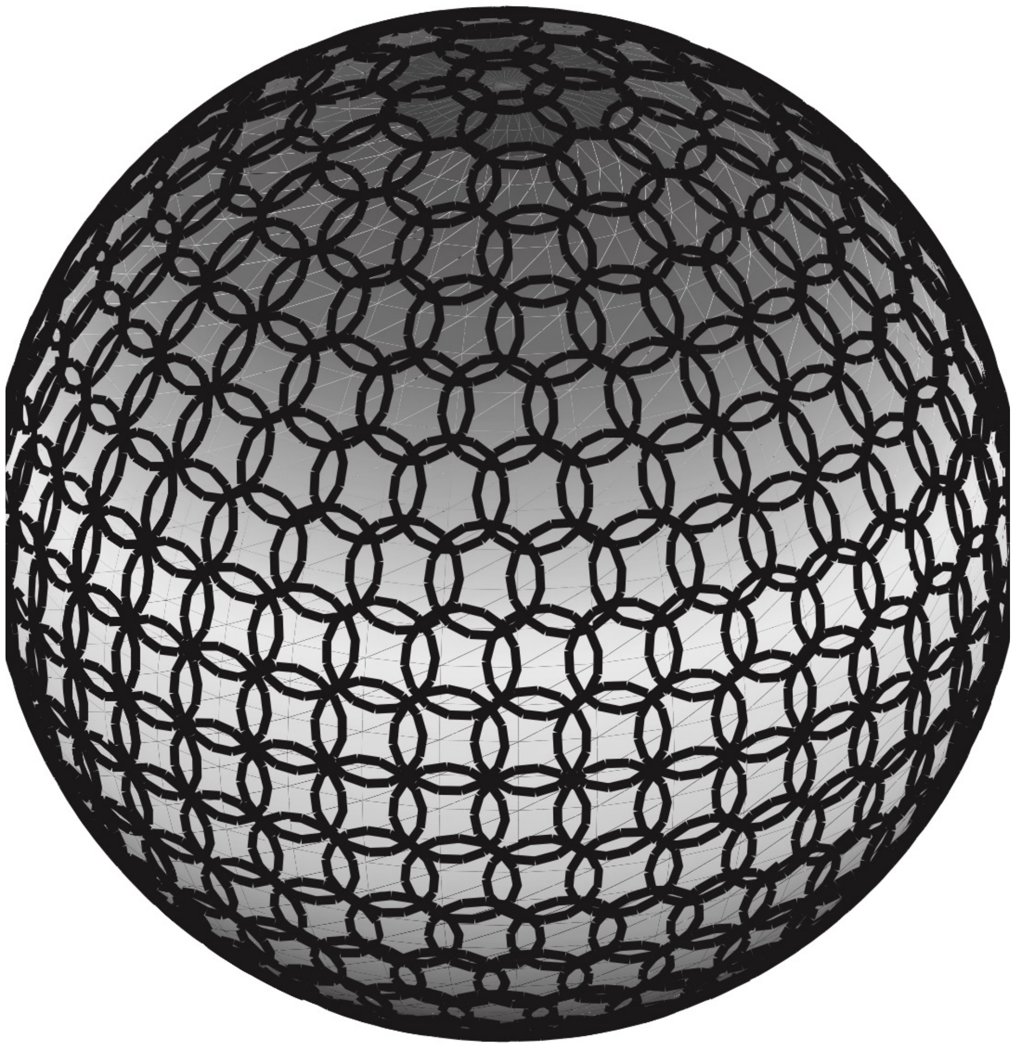


How hard is simulating U? Really hard.

Fact: *every* unitary is generated by *some* Hamiltonian

$U = e^{i\,H}$ for some H

Some U are very difficult

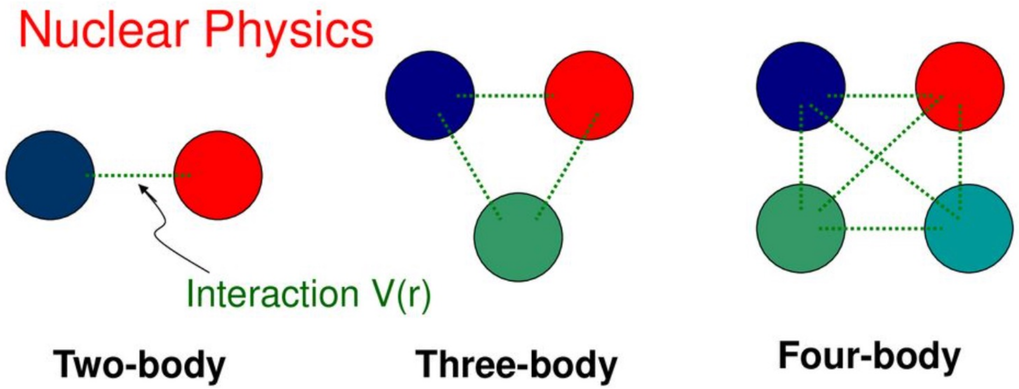


Counting argument for inefficiency of arbitrary *U*
Nielsen and Chuang, Ch. 4.5.4

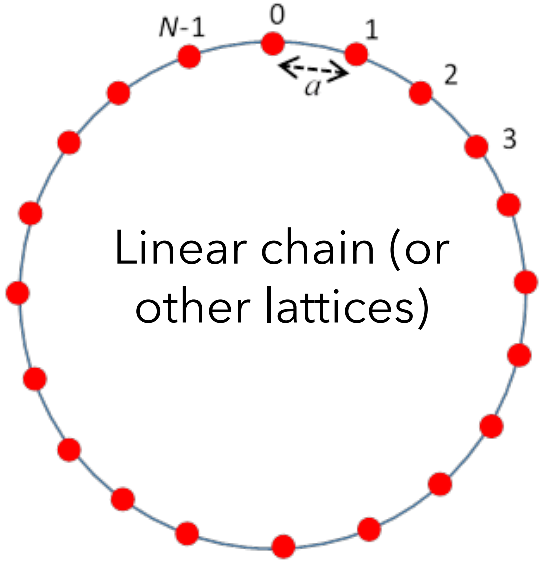
Are physical Hamiltonians arbitrary?

1-body   2-body

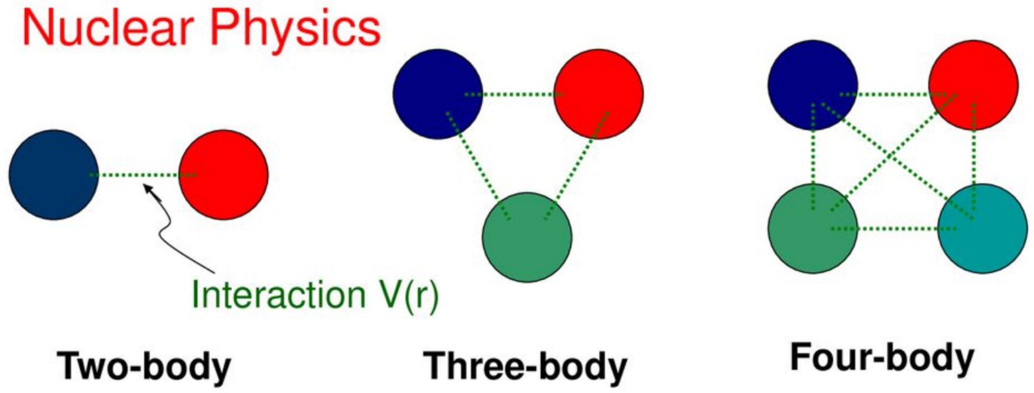
$$\hat{H} = -\frac{\hbar^2}{2}\sum_{j=1}^{N}\frac{1}{m_j}\nabla_j^2 + \frac{1}{8\pi\varepsilon_0}\sum_{j=1}^{N}\sum_{i\neq j}\frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j|}$$



E. Hiyama, RIKEN,
https://slideplayer.com/slide/12920762/



Lesson: “Divide and conquer”



Physical Hamiltonians are often *k-local*

$$H = \sum_n H_n$$

where k is a fixed integer. Each H_n acts on only k subsystems.

People also generalize to *sparse Hamiltonians* (at most $\log N$ nonzero entries per row).

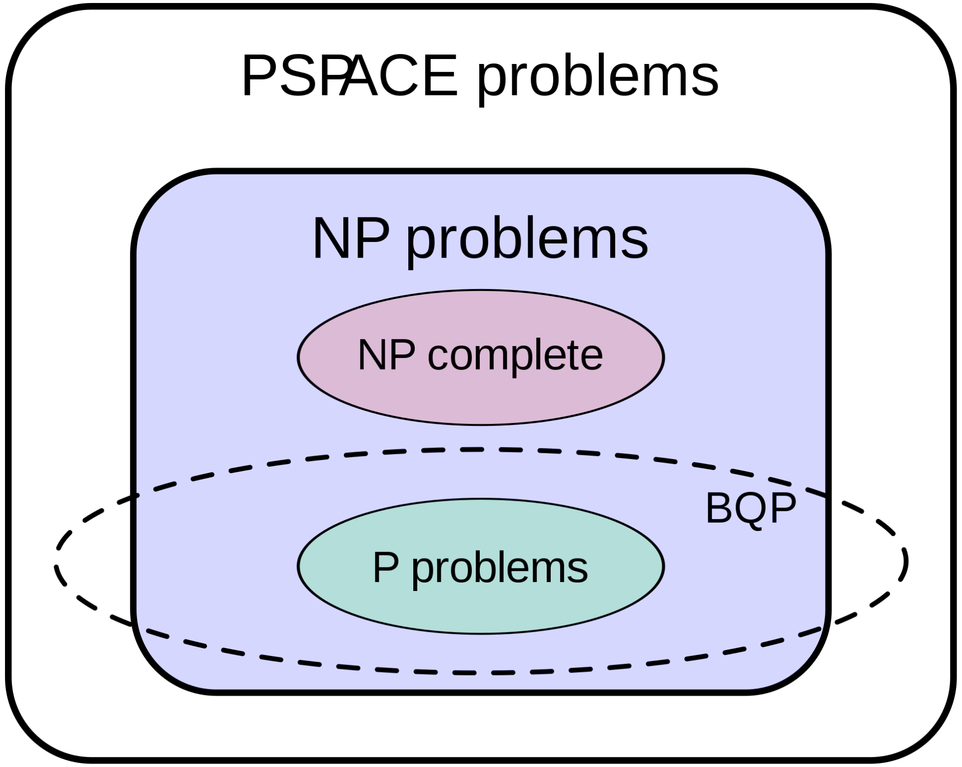
An improved definition of Ham sim

Given a k-local (or sparse) Hamiltonian H and simulation time T, construct a polynomially-sized quantum circuit Q approximating $U(T)$ to accuracy ϵ.

How hard is k-local Hamiltonian simulation?

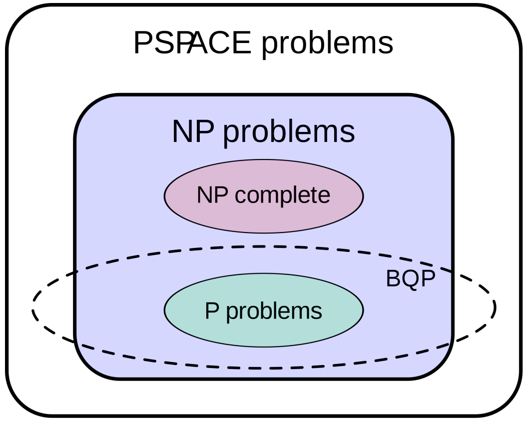
We need a little complexity theory.

- **P** - problems which are efficiently solvable with deterministic computers (adding two numbers, linear programming, primality testing)
- **BPP** - problems efficiently solvable with Monte Carlo methods
- **BQP** – problems solvable with polynomially sized quantum circuit. (factoring, discrete log, Ham sim)



By Mike1024, Wikipedia, BQP

More on BQP



- **BQP** – problems solvable with polynomially sized quantum circuit.
- A problem is **BQP-hard** if it is at least as hard as any problem in BQP.

  (More formally, any problem in BQP can be reduced to the hard problem in polynomial time)
- A problem is **BQP-complete** if it is both in BQP and BQP-hard

  (These are the "hardest problems" in BQP. Solving these essentially solves them all)

Hamiltonian simulation is BQP-complete

HS is BQP-Hard: For any quantum circuit, there is a k-local Hamiltonian which simulates that circuit

HS is in BQP: Trotterization (aka product formulas) allow for any Hamiltonian to be efficiently simulated.

In summary

- Hamiltonian simulation is an important scientific goal. Quantum computers may be able to help.
- “Physical Hamiltonians” admit efficient simulation algorithms on quantum computers.
- Hamiltonian simulation and quantum circuits are equivalent. This can be helpful for constructing algorithms.