Lecture 4

Quantum algorithms beyond the circuit model

Quantum optimization - **Quantum simulation**

Quantum Simulators

A quantum machine that could imitate any quantum system, including the physical world

Richard Feynman

Quantum Simulation: Simulation of real quantum systems by implementing the relevant Hamiltonian

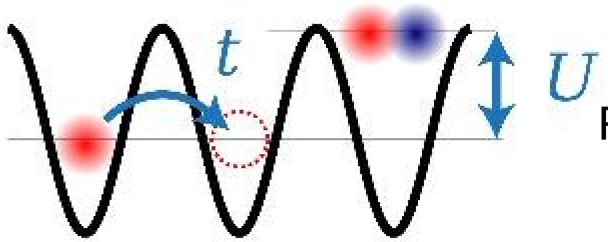
Applications: High-Tc superconductivity, High-energy Physics, Frustrated magnetism, Topological materials, quantum chemistry, etc

Outline

- 1. What kind of model Hamiltonians?
- 2. What kind of systems/machines?
- 3. What kind of algorithms?

Quantum Simulators

Example 1: Hubbard Model



R. Hulet's lab

$$\hat{H} = -t\sum_{i,\sigma}\left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i+1,\sigma} + \hat{c}^{\dagger}_{i+1,\sigma}\hat{c}_{i,\sigma}\right) + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow},$$

$$\{\hat{c}_{\mathbf{j}\sigma}, \hat{c}^{\dagger}_{\mathbf{l}\sigma'}\} = \delta_{\mathbf{j},\mathbf{l}}\,\delta_{\sigma,\sigma'} \qquad \{\hat{c}^{\dagger}_{\mathbf{j}\sigma}, \hat{c}^{\dagger}_{\mathbf{l}\sigma'}\} = 0 \qquad \{\hat{c}_{\mathbf{j}\sigma}, \hat{c}_{\mathbf{l}\sigma'}\} = 0$$

- Model dynamics of valence electrons in solids

- Cannot be solved numerically in many cases

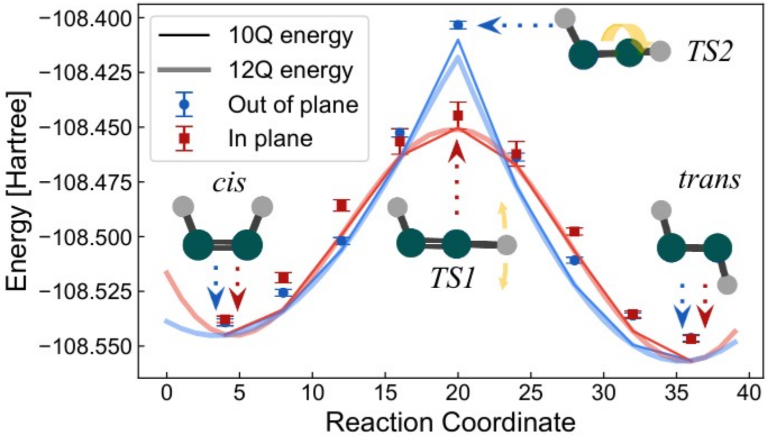
- Candidate to explain high-Tc superconductivity

Quantum Simulators

Example 2: Quantum Chemistry

$$\mathcal{H}(R) = \sum_{pq} h_{pq}(R)\hat{a}_p^\dagger \hat{a}_q + \sum_{pqrs} h_{pqrs}(R)\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

electronic orbital



$$h_{pq} = \int dr\ \chi_p(r)^* \left(-\frac{1}{2}\nabla^2 - \sum_\alpha \frac{Z_\alpha}{|r_\alpha - r|}\right)\chi_q(r) \quad (2)$$

Single-electron orbital wavefunction

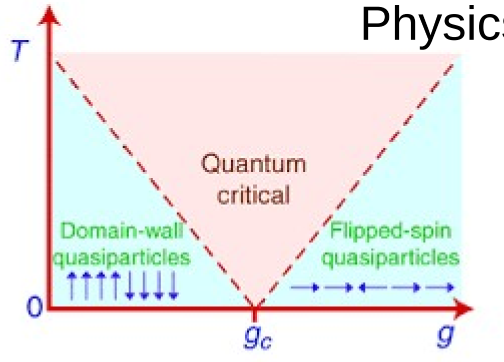
$$h_{pqrs} = \int dr_1\ dr_2\ \frac{\chi_p(r_1)^*\chi_q(r_2)^*\chi_r(r_1)\chi_s(r_2)}{|r_1 - r_2|} \quad (3)$$

Electron-Electron-term

(Google AI)

Quantum Simulators

Physics.harvard.edu



Example 3: quantum Ising Models

$$H = h \sum_i X_i + J \sum_i Z_i Z_{i+1}$$

- Fundamental in condensed matter:
quantum magnetism, frustration, quantum Phase transitions

- Easily implementable in many platforms, including quantum computers

Other topics for quantum simulation:

- Quantum electrodynamics (Schwinger's model)
- Topological phases (Hofstadter model)
- Analog black holes (SYK model) and many more

Systems for quantum simulation

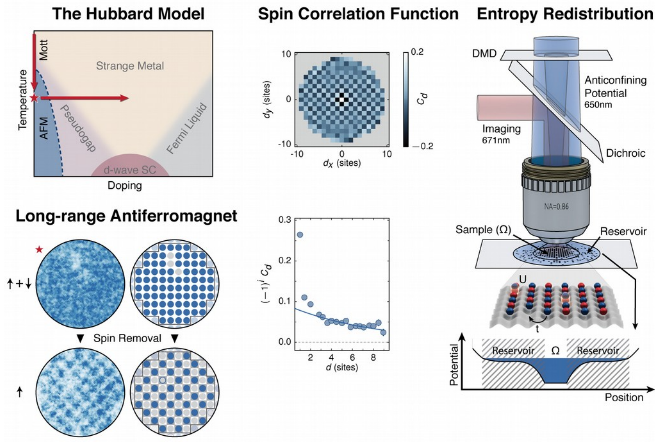
Quantum machines to implement fermions

$$H = -t \sum_{\langle i,j \rangle,\sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

1) We need fermionic particles', i.e

→ Ultra-cold atoms in optical lattices.

→ Quantum dots in silicons



M. Greiner's lab

Quantum Simulators

What kind of quantum machine to simulate Fermions

2) We can also use a quantum computer and map fermions to qubits

Jordan-Wigner Transformation (TD4)

$$\hat{a}_j \to I^{\otimes j-1} \otimes \sigma_+ \otimes \sigma_z^{\otimes N-j}$$
$$\hat{a}_j^\dagger \to I^{\otimes j-1} \otimes \sigma_- \otimes \sigma_z^{\otimes N-j}$$

Advantage: Any model can be implemented (universal quantum computing)

Drawback: Overhead ($\rightarrow$ errors) due to the mapping to qubits

Quantum Simulators

Three ways to study a model via Quantum Simulation

$$\hat{H} = -t\sum_{i,\sigma}\left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i+1,\sigma} + \hat{c}^{\dagger}_{i+1,\sigma}\hat{c}_{i,\sigma}\right) + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow},$$

1) Ground-state Cooling
(prepare ground state
by cooling the sample)

$$|\psi\rangle_0$$

2) Quantum Dynamics

$$|\psi(t)\rangle = e^{-iHt}\,|\psi(t=0)\rangle$$

3) Adiabatic/Variational preparation
via quantum dynamics
(Lecture 5)

$$|\psi\rangle_0$$

Quantum dynamics

$$|\psi(t)\rangle = e^{-iHt}\,|\psi(t=0)\rangle$$

Option 1: One can realize physically the model Hamiltonian H
(eg Fermi-Hubbard with fermions)

→ Just let the system evolve with the Schrodinger equation!

Option 2: One has a quantum computer, I.e we can create any state
but we need an efficient quantum algorithm..

Digital Quantum Simulation (Lloyd 1996)

Step 1: Mapping to a qubit Hamiltonian H
(ex: Fermi-Hubbard → Spin via Jordan-Wigner transformation)

Step 2: Decompose H in sums of terms which can associated with a quantum circuit

Example with the quantum Ising model:

$$H = \underbrace{h \sum_i X_i}_{H_1} + \underbrace{J \sum_i Z_i Z_{i+1}}_{H_2}$$

Quantum Simulators via Quantum Computers: Digital Quantum Simulation

Step 2: Decompose H in sums of terms which can be associated with a quantum circuit

$$H = h\underbrace{\sum_i X_i} + J\underbrace{\sum_i Z_i Z_{i+1}}$$

$$e^{-iH_1 t} = \prod_i e^{-ihX_i t} = R_{X,1}(2ht)\ldots R_{X,n}(2ht)$$

I can do that because…?

$$e^{-iH_2 t} = \prod_i e^{-ihZ_i Z_{i+1} t} = R_{ZZ,12}(2ht)\ldots R_{ZZ,n-1\,n}(2ht)$$

Quantum Simulators via Quantum Computers: Digital Quantum Simulation

Step 3: Suzuki-Trotter expansion

$$\psi(t) = e^{-iHt}\psi(0) \quad H = H_1 + H_2$$

$$\psi(t) \approx \left(e^{-iH_1(t/n)}e^{-iH_2(t/n)}\right)^n \psi(0)$$

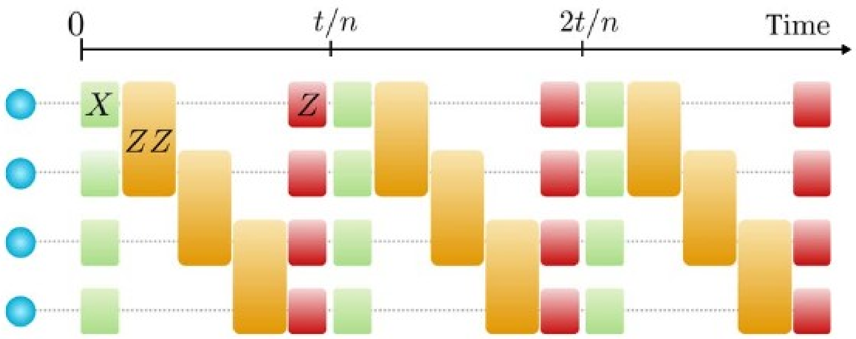
Error for a finite n $\mathcal{E} \sim \frac{t^2}{n}||[H_1, H_2]||$

→ For a given accuracy, and local Hamiltonians, the algorithm requires polynomial time

Quantum computers offer an exponential speedup for quantum dynamics
(but this is not a surprise..)

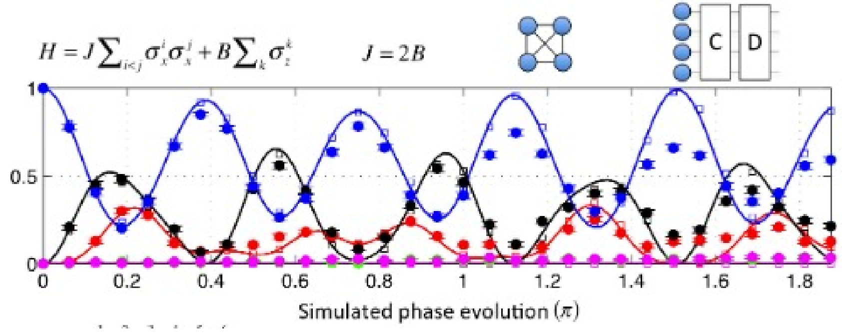
Quantum Simulators via Quantum Computers: Digital Quantum Simulation

$$\underbrace{H = h\sum_i \sigma_i^x}_{H_1} + \underbrace{J\sum_i \sigma_i^z\sigma_{i+1}^z}_{H_2} \longrightarrow \psi(t) \approx \left(e^{-iH_1(t/n)}e^{-iH_2(t/n)}\right)^n \psi(0)$$



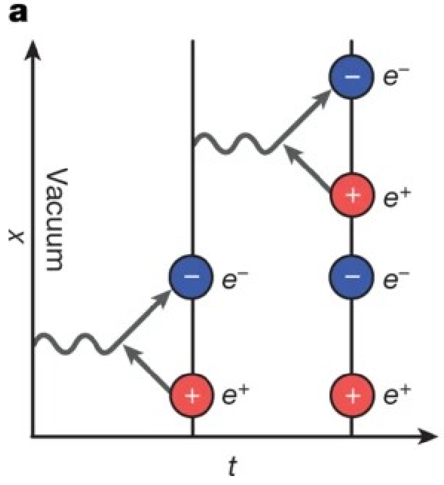
Sci. Adv.2019;5

Experimental demonstration with trapped ions (Lanyon 2011)



Quantum Simulation of high-energy physics phenomena

Illustration: Nature volume 534, pages516–519(2016)

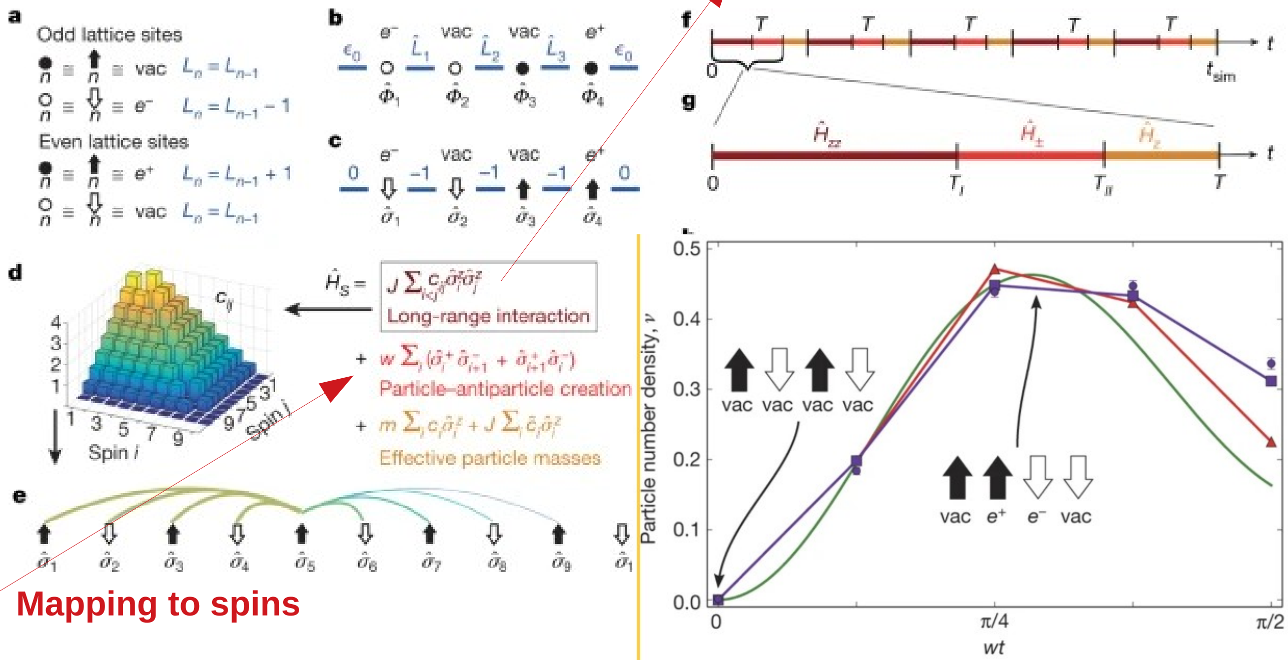


Swinger Model
(1 dimensional quantum-electro dynamics)

$$\hat{H}_{\text{lat}} = -iw\sum_{n=1}^{N-1}[\hat{\Phi}_n^{\dagger}e^{i\hat{\theta}_n}\hat{\Phi}_{n+1} - \text{h.c.}] + J\sum_{n=1}^{N-1}\hat{L}_n^2 + m\sum_{n=1}^{N}(-1)^n\hat{\Phi}_n^{\dagger}\hat{\Phi}_n$$

Kogut–Susskind fermions

Digital quantum simulation



Mapping to spins