Lesson 7. Quantum Simulation

1. Opening

Outline and Introduction of this Lecture. You will learn the role of this lecture in this course.

7. Quantum Simulation

2024/05/30

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Yukio Kawashima

Quantum Application Research Team

Doctor of Engineering at U. Tokyo (Applied chemistry)

Skills in quantum chemistry, and chemistry application in quantum computing.

Research on scaling up quantum chemistry calculations for both classical and quantum computers

Work experience at academic institutes and universities in Japan, and at a start-up in Canada. Client engagements with chemical industry.

The University of Tokyo
Special Lectures in Information Science II
Introduction to Near-Term Quantum Computing
情報科学科特別講義Ⅱ/量子計算論入門
2024年度の計画

Path to the Utility era in Quantum Computing
The goal of this course is to learn how to implement utility-scale applications on a quantum computer. To achieve the goal, the course covers from the basics of quantum information to recent advances of quantum algorithms for noisy quantum devices as well as circuit optimization and error mitigation techniques. The course also introduces how to implement quantum algorithms using open-source framework of quantum computing and real quantum device with more than 100 qubits. The course is intended to help students understand the potential and limitations of currently available quantum devices.

Schedule: Every Friday from 16:50 to 18:20 (except May 15 (Wed), May 30(Thu))

Notes: All lectures will be held in person. Recording also will be available for reviewing.

Course Schedule 2024

Date	Lecture Title	Lecturer	Date	Lecture Title	Lecturer
4/5	Invitation to the Utility era	Tamiya Onodera	6/7	Classical simulation (Clifford circuit, tensor network)	Yoshiaki Kawase
4/19	Quantum Gates, Circuits, and Measurements	Kifumi Numata	6/14	Quantum Hardware	Masao Tokunari
4/26	LOCC (Quantum teleportation/superdense coding/Remote CNOT)	Kifumi Numata/ Atsushi Matsuo	6/21	Quantum Circuit Optimization (transpiler)	Toshinari Itoko
5/10	Quantum Algorithms: Grover's algorithm	Atsushi Matsuo	6/28	Pauli twirling and Noise model (Pauli Transfer Matrix) Error mitigation (PEC, ZNE (PEA))	Toshinari Itoko
5/15 (Wed)	Quantum Algorithms: Phase estimation	Kento Ueda	7/5	Quantum Utility I (127Qubit GHZ)	Kifumi Numata
5/24	Quantum Algorithms: Variational Quantum Algorithms (VQA)	Takashi Imamichi	7/12	Quantum Utility II (Utility paper implementation)	Tamiya Onodera
5/30 (Thu)	Quantum simulation (Ising model, Heisenberg, XY model), Time evolution (Suzuki Trotter, QDrift)	Yukio Kawashima	7/19	Quantum Utility III (Krylov subspace expansion)	Yukio Kawashima

Overview

1. Quantum simulation (Hamiltonian simulation, quantum dynamics)
2. Hamiltonian (Model)
3. Algorithms for Quantum Simulation
   1. Trotterization
4. Hands-on Session
5. Algorithms for Quantum Simulation (if we have time...)
   1. Randomization

Lesson 7. Quantum Simulation

2. Introduction of Quantum Simulation

Quantum simulation is a critical application for quantum computers, addressing problems too large for classical methods, such as modeling quantum dynamics and solving complex optimization tasks. You will learn the overview of the quantum simulation and benefit of doing them on Quantum Computer .

Quantum Simulation?

Quantum Simulation (Hamiltonian Simulation)

Solve the time-dependent Schrödinger equation

$$i\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

Wavefunction

Hamiltonian

To compute this is the goal!

$$|\Psi(t)\rangle = e^{-i\hat{H}t}|\Psi(0)\rangle$$

Solve the problem numerically as accurate and efficient as possible

$$|\Psi(t+\Delta t)\rangle = e^{-i\hat{H}\Delta t}|\Psi(t)\rangle \approx \left(1 - iH\Delta t - \frac{\hat{H}^2\Delta t^2}{2} + \ldots\right)|\Psi(t)\rangle$$
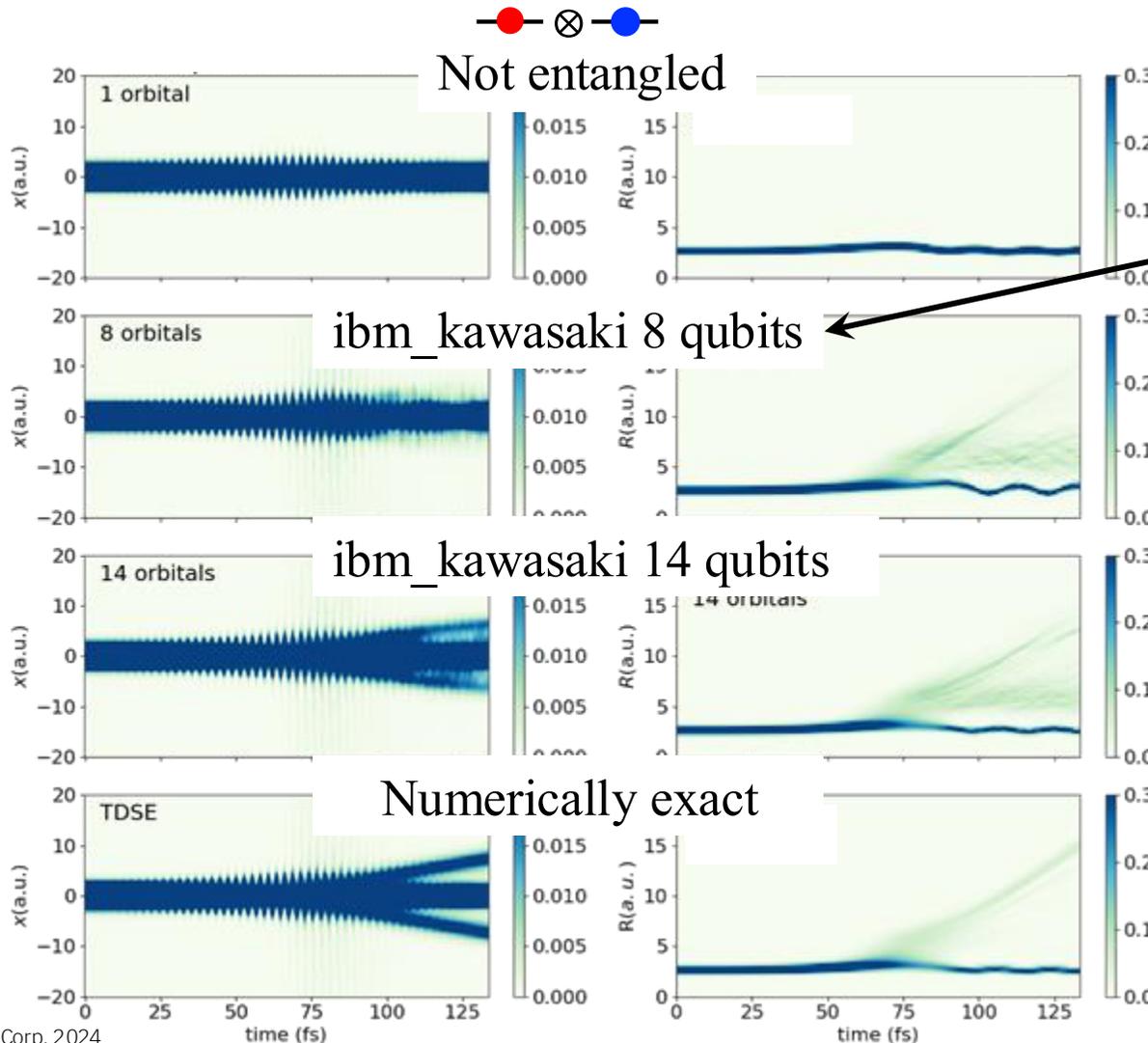
Very small time slice

Taylor series as an example

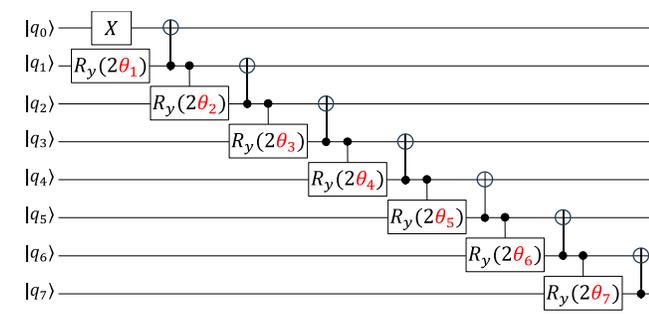# What can we do with quantum simulation: Electron and nuclear dynamics

Univ of Tokyo, Professor Sato

Molecule in a strong laser field

Electron density $\rho_e(x)$

Nuclear density $\rho_n(R)$
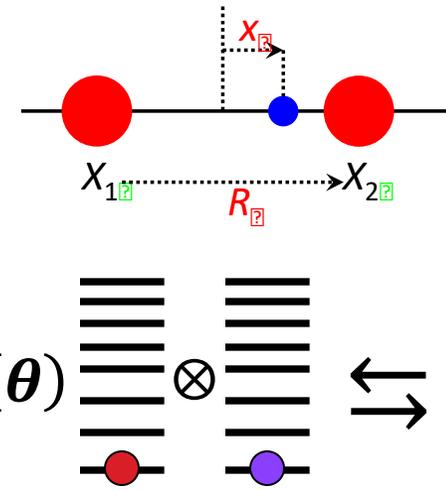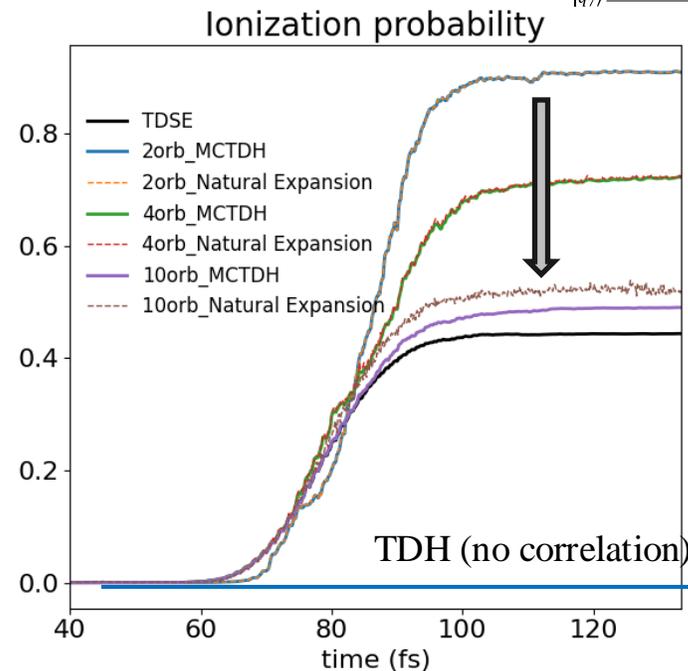
Why quantum simulation on quantum computers?

Storing the information of the wavefunction $\Psi(0)\rangle$ $|\Psi(t)\rangle$

– Requires extremely large memory on the classical computer

– Quantum computational resources (qubits) required to store them scale linear against the system size

One of the most important application on quantum computers

– Quantum chemistry (material science)

– High-energy physics

Lesson 7. Quantum Simulation

3. Hamiltonian

There are various types of Hamiltonians, and in this case, the quantum simulation involves the Fermionic Hamiltonian. Here, you will learn about the overview of Hamiltonians, including Spin Hamiltonians and Fermionic Hamiltonians.

Quantum Simulation (Hamiltonian Simulation)

Solve the time-dependent Schrödinger equation

$$i\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

Wavefunction

Hamiltonian

To compute this is the goal!

$$|\Psi(t)\rangle = e^{-i\hat{H}t}|\Psi(0)\rangle$$

Solve the problem numerically as accurate and efficient as possible

$$|\Psi(t+\Delta t)\rangle = e^{-i\hat{H}\Delta t}|\Psi(t)\rangle \approx \left(1 - iH\Delta t - \frac{\hat{H}^2\Delta t^2}{2} + \dots\right)|\Psi(t)\rangle$$

Very small time slice

Taylor series as an example

Hamiltonian

Hamiltonian in general

- Hamiltonian of a quantum system is an operator representing the total energy of the system

  - Kinetic energy and potential energy $\quad \hat{H} = \hat{T} + \hat{V}$

- Time-dependent Hamiltonian & time-independent Hamiltonian

  - We will consider only time-independent Hamiltonian today

- Important in many fields

  - Quantum chemistry (material science)

  - Condensed matter physics

  - High-energy physics

Hamiltonian (Spin Hamiltonian)

Lattice models for spin systems to study magnetic systems

Spin interaction   External field

- n-vector models

  - Ising model (n=1)

  $$H = -\sum_{\langle i,j \rangle} J\sigma_{Z_i}\sigma_{Z_j} - \sum_i h_i\sigma_{X_i}$$

  - XY model (n=2)

  $$H = -\sum_{\langle i,j \rangle} J\left(\sigma_{X_i}\sigma_{X_j} + \sigma_{Y_i}\sigma_{Y_j}\right) - \sum_i h_i\sigma_{Z_i}$$

  - Heisenberg model (n=3)

  $$H = -\sum_{\langle i,j \rangle} \left(J_X\sigma_{X_i}\sigma_{X_j} + J_Y\sigma_{Y_i}\sigma_{Y_j} + J_Z\sigma_{Z_i}\sigma_{Z_j}\right) - \sum_i h_i\sigma_{Z_i}$$

Complexity & Computational resources

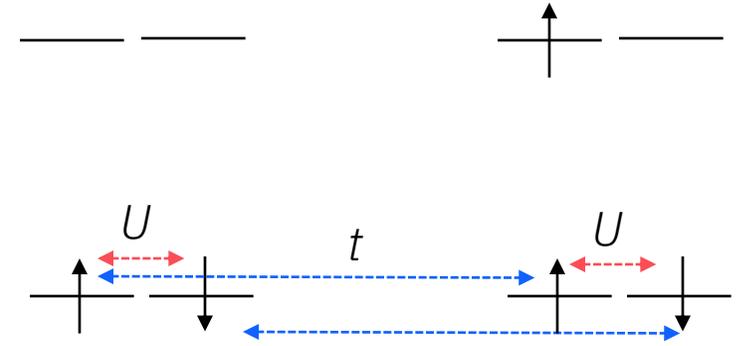# Hamiltonian (Fermionic Hamiltonian)

— Hubbard model   Describe conducting and insulating systems

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

$$\hat{n}_{i,\sigma} = \hat{c}_{i,\sigma}^{\dagger} \hat{c}_{i,\sigma}$$
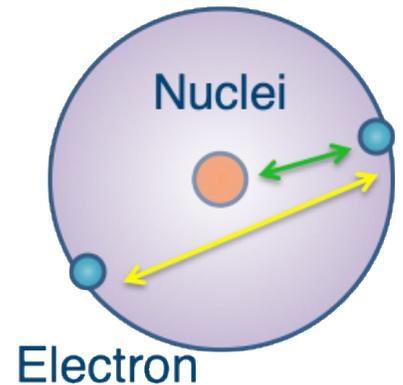
Creation operator   Annhilation operator

— Quantum Chemistry Hamiltonian

$$\hat{H}_{ele}(\mathbf{r}; \mathbf{R}) = -\sum_i^{N_{ele}} \frac{1}{2} \nabla_i^2 - \sum_A^{N_{nuc}} \sum_i^{N_{ele}} \frac{Z_A}{r_{iA}} + \sum_{i>j}^{N_{ele}} \frac{1}{r_{ij}}$$

Kinetic energy of electrons | Electron-nucleus attraction | Electron-electron repulsion

Complexity & Computational resources

Lesson 7. Quantum Simulation

4. Mapping of the Hamiltonian

When performing quantum simulation (Hamiltonian simulation) on a quantum computer, it is necessary to map the second-quantized Hamiltonian. This process converts a fermionic problem into a spin problem. Here, you will learn about the mapping process, including the Jordan–Wigner Mapping as one of its methods.

Mapping the Hamiltonian

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

Map the second-quantized Hamiltonian to qubits:

$$\hat{n}_{i,\sigma} = \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{i,\sigma}$$
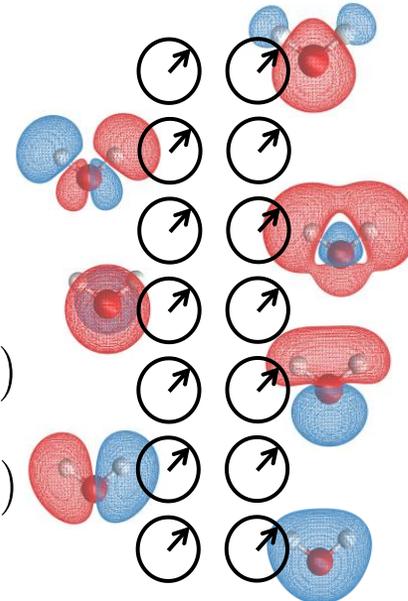
Hubbard, Quantum chemistry

Fermions

$$\{a_i, a_i\} = 0, \; \{a^{\dagger}_i, a^{\dagger}_i\} = 0, \; \{a_i, a^{\dagger}_i\} = \delta_{i,j}$$
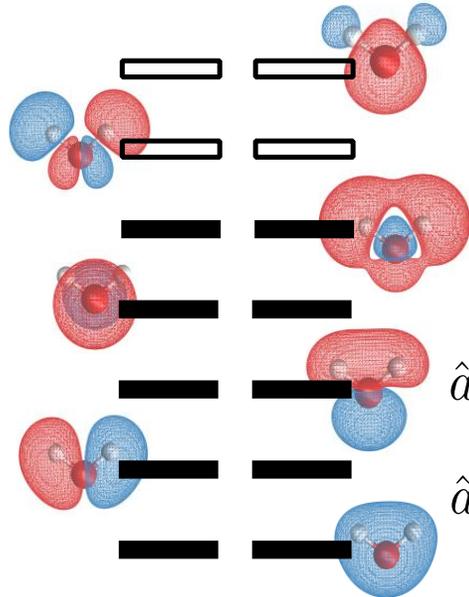
Spins

$$[\sigma_i, \sigma_i] = 0, \; [\sigma^{\dagger}_i, \sigma^{\dagger}_i] = 0, \; [\sigma_i, \sigma^{\dagger}_j] = \delta_{i,j}$$

mapping

Jordan-Wigner

$$\hat{a}_j = \bigotimes_{i=1}^{j-1} \hat{\sigma}^z_i \otimes \left(\hat{\sigma}^x_j + i\hat{\sigma}^y_j \right)$$

$$\hat{a}^{\dagger}_j = \bigotimes_{i=1}^{j-1} \hat{\sigma}^z_i \otimes \left(\hat{\sigma}^x_j - i\hat{\sigma}^y_j \right)$$

$$\hat{H}_{elec} = \sum_{pq} h_{pq} \hat{a}^{\dagger}_p \hat{a}_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} \hat{a}^{\dagger}_p \hat{a}^{\dagger}_q \hat{a}_r \hat{a}_s$$

$$\hat{H}_{elec} = \sum_{i} c_i \hat{P}_i$$

Note that operators a and c are the same

Jordan–Wigner Mapping

Fermionic Hamiltonian

$$\hat{H}_M = \sum_{pq} h_{pq} a_p^\dagger a_q + \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

Creation operator

$$a_p^\dagger = \frac{1}{2}\left(X_p - iY_p\right) \otimes Z_{p-1} \otimes \cdots \otimes Z_1$$

$$\sigma_{X_i}, \sigma_{Y_i}, \sigma_{Z_i} = X_i, Y_i, Z_i$$

Jordan–Wigner mapping

Annhilation operator

$$a_q = \frac{1}{2}\left(X_q + iY_q\right) \otimes Z_{q-1} \otimes \cdots \otimes Z_1$$

Hydrogen molecule (bond length=0.735 Angstrom, STO-3G basis set. 4 spin orbitals and 36 terms)

$$H_f = -1.26 a_0^\dagger a_0 - 0.47 a_1^\dagger a_1 - 1.26 a_2^\dagger a_2 - 0.47 a_3^\dagger a_3$$

$$+0.34 a_0^\dagger a_0^\dagger a_0 a_0 + 0.33 a_0^\dagger a_1^\dagger a_1 a_0 + 0.34 a_0^\dagger a_2^\dagger a_2 a_0 + 0.33 a_0^\dagger a_3^\dagger a_3 a_0 + \cdots$$

$$+0.09 a_0^\dagger a_2^\dagger a_3 a_1 + \cdots$$

How will this be mapped?

Try mapping a one-body term

$$\sigma_X \sigma_Y = -\sigma_Y \sigma_X = i\sigma_Z$$

Use these relations $\qquad \sigma_X^2 = \sigma_Y^2 = \sigma_Z^2 \qquad\qquad \sigma_Y \sigma_Z = -\sigma_Z \sigma_Y = i\sigma_X$

$$\sigma_{X_i}, \sigma_{Y_i}, \sigma_{Z_i} = X_i, Y_i, Z_i \qquad\qquad \sigma_Z \sigma_X = -\sigma_X \sigma_Z = i\sigma_Y$$

Let us try a one-body term as an example

$$a_3^\dagger a_3 = \frac{1}{2}\left(X_3 - iY_3\right) \otimes Z_2 Z_1 Z_0 \times \frac{1}{2}\left(X_3 + iY_3\right) \otimes Z_2 Z_1 Z_0$$

$$= \frac{1}{4}\left(X_3 Z_2 Z_1 Z_0 - iY_3 Z_2 Z_1 Z_0\right) \times \left(X_3 Z_2 Z_1 Z_0 + iY_3 Z_2 Z_1 Z_0\right) = \frac{1}{4}\left(I + I + iX_3 Y_3 - iY_3 X_3\right)$$

$$= \frac{1}{4}\left(I + I + iX_3 Y_3 - iY_3 X_3\right) = \frac{1}{2}\left(I + iX_3 Y_3\right) = \frac{1}{2}\left(I - Z_3\right)$$

How about a two-body term?

Use these relations

$$\sigma_X^2 = \sigma_Y^2 = \sigma_Z^2$$

$$\sigma_X \sigma_Y = -\sigma_Y \sigma_X = i\sigma_Z$$

$$\sigma_Y \sigma_Z = -\sigma_Z \sigma_Y = i\sigma_X$$

$$\sigma_Z \sigma_X = -\sigma_X \sigma_Z = i\sigma_Y$$

$$a_0^\dagger a_2^\dagger a_3 a_1 = \frac{1}{2}\left(X_0 - iY_0\right) \times \frac{1}{2}\left(X_2 - iY_2\right) \otimes Z_1 Z_0 \times \frac{1}{2}\left(X_3 + iY_3\right) \otimes Z_2 Z_1 Z_0 \times \frac{1}{2}\left(X_1 + iY_1\right) \otimes Z_0$$

$$= \frac{1}{16}\left[-X_3 Y_2 X_1 Y_0 - iX_3 Y_2 Y_1 Y_0 - iY_3 Y_2 X_1 Y_0 + Y_3 Y_2 Y_1 Y_0 - iX_3 X_2 X_1 Y_0 + X_3 X_2 Y_1 Y_0 + Y_3 X_2 X_1 Y_0 + iY_3 X_2 Y_1 Y_0 \right.$$

$$\left. - iX_3 Y_2 X_1 X_0 + X_3 Y_2 Y_1 X_0 + Y_3 Y_2 X_1 X_0 + iY_3 Y_2 Y_1 X_0 + X_3 X_2 X_1 X_0 + iX_3 X_2 Y_1 X_0 + iY_3 X_2 X_1 X_0 - Y_3 X_2 Y_1 X_0\right]$$

The equations are tedious, but the idea is simple

Mapping the Hamiltonian

General equation

$$h_{pq}a_p^\dagger a_q = \frac{1}{4}h_{pq}\left(X_p - iY_p\right)\otimes Z_{p-1}\otimes\cdots\otimes Z_{q+1}\otimes\left(X_q + iY_q\right)$$

$$h_{pqrs}a_p^\dagger a_q^\dagger a_r a_s = \frac{1}{16}h_{pqrs}\left(X_p - iY_p\right)\otimes Z_{p-1}\otimes\cdots\otimes Z_{q+1}\otimes\left(X_q - iY_q\right)$$
$$\left(X_r + iY_r\right)\otimes Z_{r-1}\otimes\cdots\otimes Z_{s+1}\otimes\left(X_s - iY_s\right)$$

$$H_f = -1.26a_0^\dagger a_0 - 0.47a_1^\dagger a_1 - 1.26a_2^\dagger a_2 - 0.47a_3^\dagger a_3$$

Fermionic Hamiltonian

$$+0.34a_0^\dagger a_0^\dagger a_0 a_0 + 0.33a_0^\dagger a_1^\dagger a_1 a_0 + 0.34a_0^\dagger a_2^\dagger a_2 a_0 + 0.33a_0^\dagger a_3^\dagger a_3 a_0 + \cdots$$

$$+0.09a_0^\dagger a_2^\dagger a_3 a_1 + \cdots$$

$$H_q = -0.81 + 0.17(Z_0 + Z_2) - 0.23(Z_1 + Z_3) + 0.12(Z_1 Z_0 + Z_3 Z_2) + 0.17Z_0 Z_2 + 0.17Z_1 Z_3$$

$$+ 0.17Z_1 Z_2 + 0.17Z_0 Z_3 + 0.05(Y_3 Y_2 Y_1 Y_0 + X_3 X_2 X_1 X_0 + Y_3 Y_2 X_1 X_0 + X_3 X_2 Y_1 Y_0)$$

Lesson 7. Quantum Simulation

5. Algorithm for quantum simulation

In quantum simulation, instead of calculating the Hamiltonian exactly, several methods have been proposed to achieve minimal error and shallow circuit depth during computation. Here, you will learn about the overview of algorithms for quantum simulation and their theoretical background.

Algorithms for Quantum Simulation

Algorithms for quantum simulations

The Hamiltonian is known, but how to compute $e^{-i\hat{H}t}$ is not trivial

It is extremely difficult to compute this exactly

We try to implement U such that $\qquad \|\hat{U}|\Psi\rangle - e^{-i\hat{H}t}|\Psi\rangle\| \leq \epsilon$

- Operator norm $\hat{A} : V \to W$

  - A linear operator $\hat{A}$ is bounded if there exists a real number $c > 0$ such that for any v

    $$\|\hat{A}v\| \leq c\||v\|$$

  - The smallest M (size) that satisfies this requirement is the norm of the operator

    $$\|\hat{A}\| := \min\{c \geq 0 : \|\hat{A}v\| \leq c\|v\| \text{ for all } v \in V\}$$
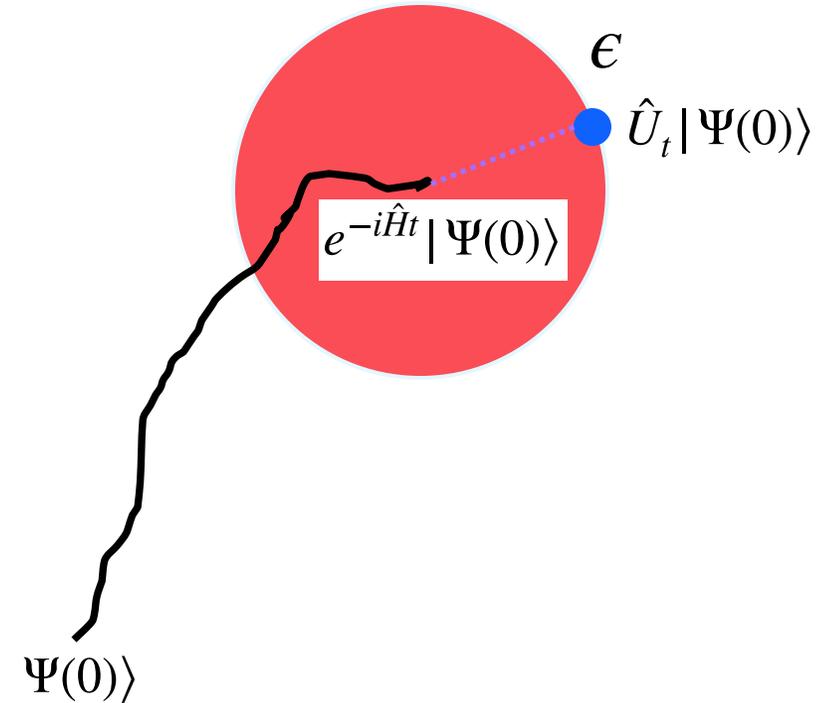
  - Properties:

    - $\|\hat{A}\| \geq 0$ and $\|\hat{A}\| = 0$ if and only if $\hat{A} = 0$

    - $\|a\hat{A}\| = |a|\|\hat{A}\|$

    - $\|\hat{A} + \hat{B}\| \leq \|\hat{A}\| + \|\hat{B}\|$

$$|\Psi(t)\rangle = e^{-i\hat{H}t}|\Psi(0)\rangle$$

ϵ

$\hat{U}_t|\Psi(0)\rangle$

$e^{-i\hat{H}t}|\Psi(0)\rangle$

$\Psi(0)\rangle$

Algorithms for quantum simulations

The Hamiltonian is known, but how to compute $e^{-i\hat{H}t}$ is not trivial
It is extremely difficult to compute this exactly
We try to implement U such that $\quad \|\hat{U}|\Psi\rangle - e^{-i\hat{H}t}|\Psi\rangle\| \leq \epsilon$

- There are several strategies to compute it efficiently
  - Small error
  - Shallow circuit depth

- Methods
  - Trotter formula
  - Randomization (QDrift)
  - "Post Trotter"
    - Linear combination of unitaries
    - Qubitization (quantum signal processing)

$$|\Psi(t)\rangle = e^{-i\hat{H}t}|\Psi(0)\rangle$$

ϵ

$\hat{U}_t|\Psi(0)\rangle$

$e^{-i\hat{H}t}|\Psi(0)\rangle$

$\Psi(0)\rangle$

Lesson 7. Quantum Simulation
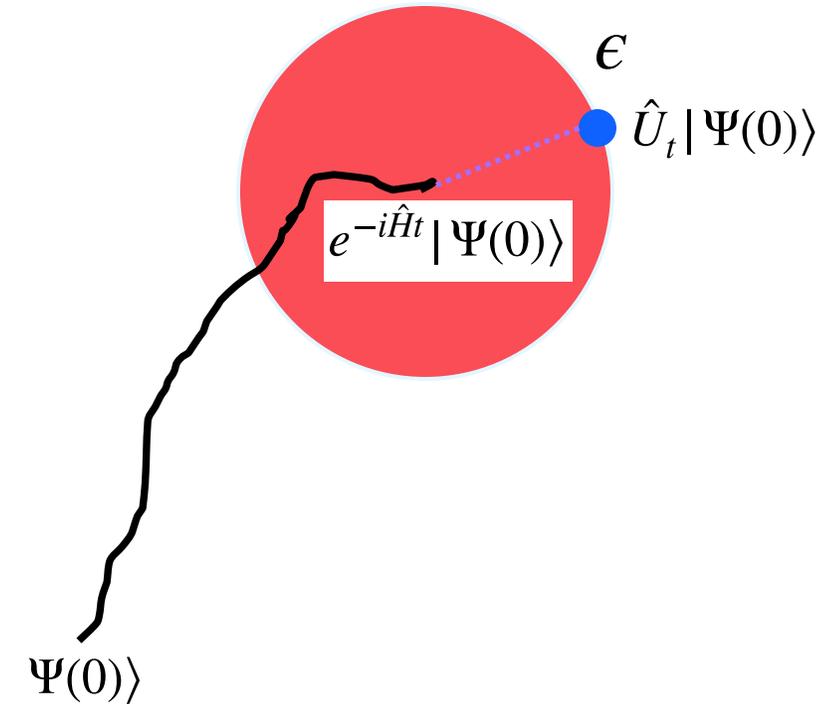
6. Trotterization

The Hamiltonian is transformed into a form suitable for quantum computation using Trotterization. Here, you will learn how this transformation is performed, as well as the errors that arise from first-order Trotterization. The Transverse Ising model is provided as an example.

Trotterization

We here assume that the Hamiltonian is k-local (P are Pauli strings that act on at most "k" qubits)

$$\hat{H} = \sum_{i=1}^{L} a_i P_i$$

Let us focus on a simple Hamiltonian

$$\hat{H} = \hat{H}_1 + \hat{H}_2$$

Lie Product Formula

$$e^{-it(H_1+H_2)} = \lim_{n \to \infty} \left(e^{-iH_1\frac{t}{n}} e^{-iH_2\frac{t}{n}} \right)^n$$

We will take "n" to be finite

$$e^{-i(\hat{H}_1+\hat{H}_2)\Delta t} = e^{-i\hat{H}_1\Delta t} e^{-i\hat{H}_2\Delta t}$$

This only holds when H_1 and H_2 commute, but this is often not the case

Error in Trotterization (First order)

$$\hat{U}_{\text{exact}} = e^{-i(\hat{H}_1 + \hat{H}_2)\Delta t}$$

$$\hat{U}_{\text{trotter}} = e^{-i\hat{H}_1 \Delta t} e^{-i\hat{H}_2 \Delta t}$$

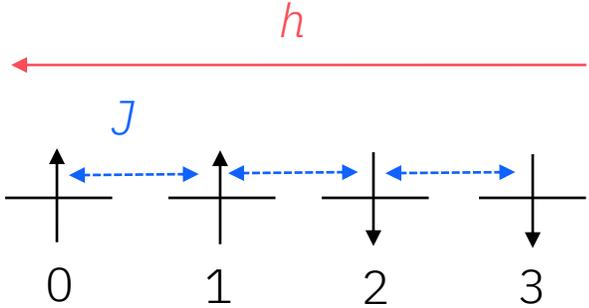$$\hat{U}_{\text{exact}_2} = \mathbb{I} + (-i\Delta t)(\hat{H}_1 + \hat{H}_2) + \frac{(-i\Delta t)^2}{2}\left(\hat{H}_1^2 + \hat{H}_2^2 + \hat{H}_1\hat{H}_2 + \hat{H}_2\hat{H}_1\right)$$

$$\hat{U}_{\text{trotter}_2} = \left[\mathbb{I} + (-i\Delta t)\hat{H}_1 + \frac{(-i\Delta t)^2}{2}\left(\hat{H}_1^2\right)\right]\left[\mathbb{I} + (-i\Delta t)\hat{H}_2 + \frac{(-i\Delta t)^2}{2}\left(\hat{H}_2^2\right)\right]$$

$$\approx \mathbb{I} + (-i\Delta t)(\hat{H}_1 + \hat{H}_2) + \frac{(-i\Delta t)^2}{2}\left(\hat{H}_1^2 + \hat{H}_2^2 + 2\hat{H}_1\hat{H}_2\right)$$

$$\|\hat{U}_{\text{exact}_2} - \hat{U}_{\text{trotter}_2}\| = \|\frac{(-i\Delta t)^2}{2}(\hat{H}_2\hat{H}_1 - \hat{H}_1\hat{H}_2) + O(\Delta t^3)\|$$

$$\leq \frac{1}{2}\|[\hat{H}_2, \hat{H}_1]\|\Delta t^2 + \|O(\Delta t^3)\| \qquad \text{(Triangle inequality of the operator norm)}$$

Example: Trotterization (first-order)
Transverse Ising model

$$H = -\sum_{\langle i,j \rangle}^{N-1} J\sigma_{Z_i}\sigma_{Z_j} - \sum_i^N h_i\sigma_{X_i}$$

N: Number of qubits

$$e^{-i\hat{H}\Delta t} = e^{-i\Delta t(-\sum_{i,j}^N J\sigma_{Z_i}\sigma_{Z_j} - \sum_i^N h_i\sigma_{X_i})} \approx e^{-i\Delta t(-\sum_{i,j}^N J\sigma_{Z_i}\sigma_{Z_j})} e^{-i\Delta t(-\sum_i^N h_i\sigma_{X_i})}$$
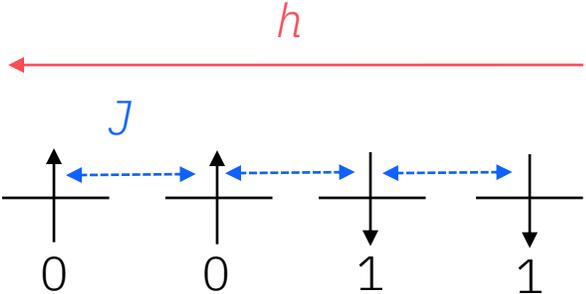
$$R_{ZZ}(-2J\Delta t) \qquad\qquad R_X(-2h\Delta t)$$

$$R_{ZZ}(\theta) = e^{-i\frac{\theta}{2}\sigma_Z\sigma_Z} = \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 & 0 & 0 \\ 0 & e^{i\frac{\theta}{2}} & 0 & 0 \\ 0 & 0 & e^{i\frac{\theta}{2}} & 0 \\ 0 & 0 & 0 & e^{-i\frac{\theta}{2}} \end{pmatrix}$$

$$R_X(\theta) = e^{-i\frac{\theta}{2}\sigma_X} = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -i\sin\left(\frac{\theta}{2}\right) \\ -i\sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix}$$

Example: Trotterization (first-order)
Transverse Ising model

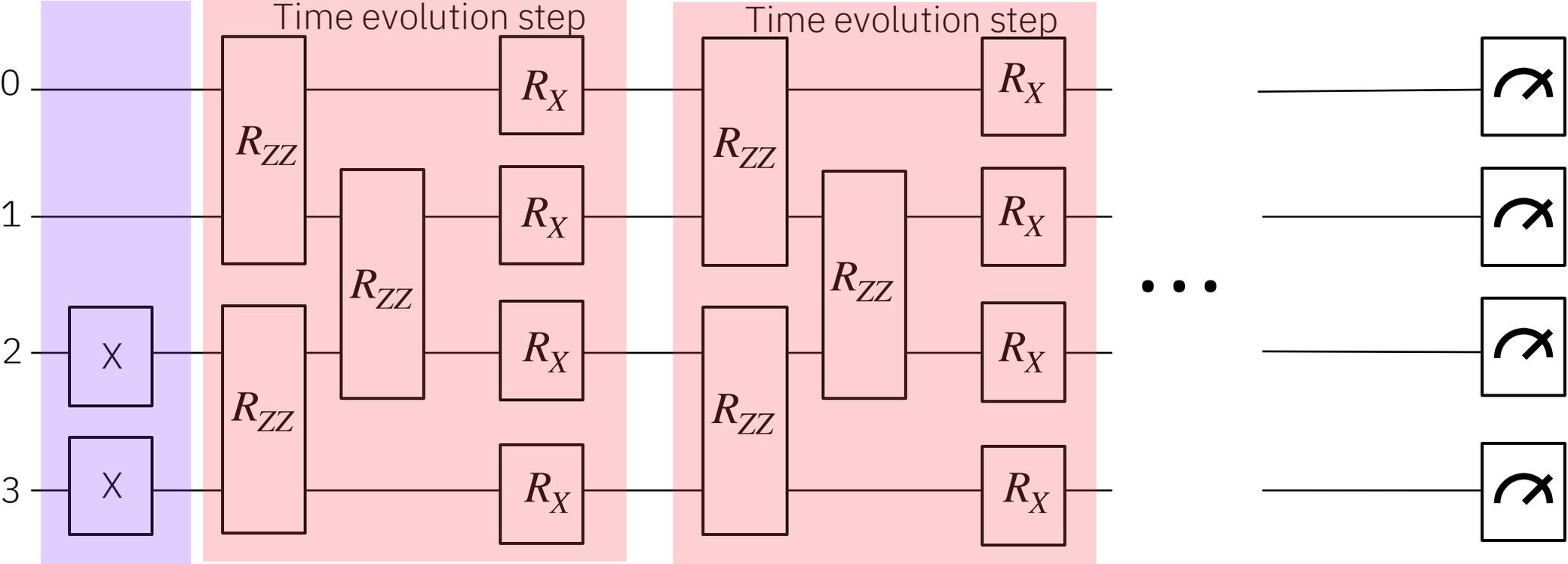$$H = -\sum_{\langle i,j \rangle}^{N-1} J\sigma_{Z_i}\sigma_{Z_j} - \sum_i^N h_i\sigma_{X_i}$$

0: up spin

1: down spin

Bit strings

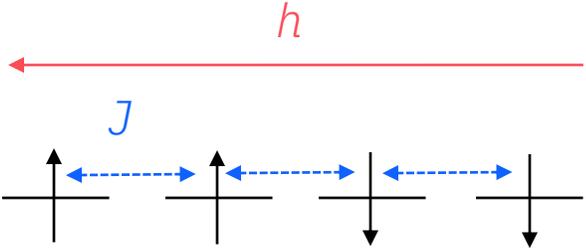$|0011\rangle$

$|1100\rangle$

State preparation

By repeating this, we can get the wavefunction of time t
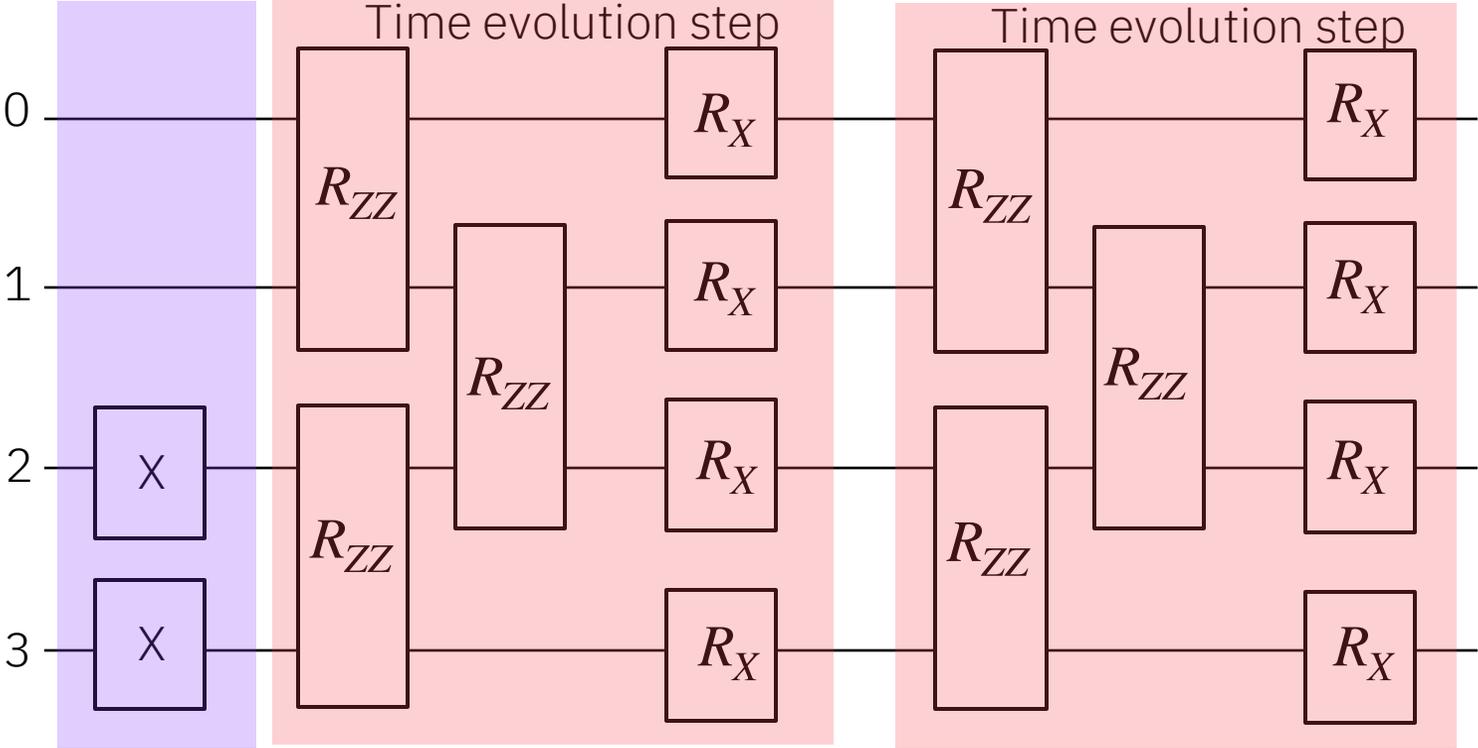
$$|\Psi(t)\rangle = e^{-i\hat{H}t}|\Psi(0)\rangle$$

Example: Trotterization Transverse Ising model

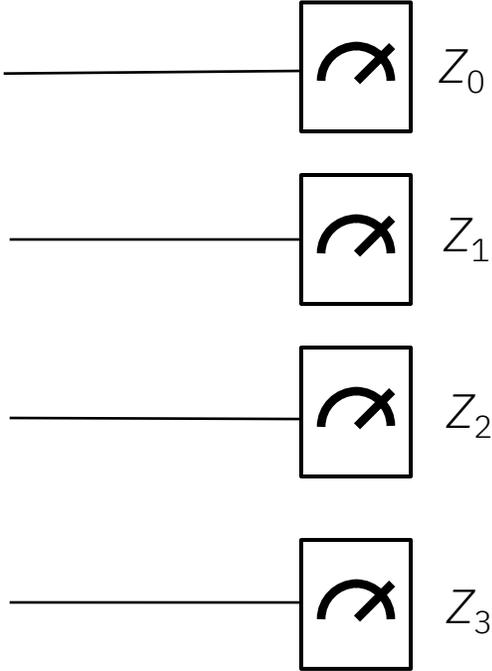$$H = -\sum_{\langle i,j \rangle}^{N-1} J\sigma_{Z_i}\sigma_{Z_j} - \sum_i^N h_i \sigma_{X_i}$$

Magnetization

$$\sum_i^N Z_i / N$$

Lesson 7. Quantum Simulation

7. Suzuki-Trotter Formula (Second order)

Here, the second-order Suzuki–Trotter formula is used for Trotterization.
You will learn about the transformation of the Hamiltonian using the Suzuki–Trotter formula and the associated errors. Additionally, higher-order Suzuki–Trotter formulas for more complex cases will also be discussed.

Suzuki-Trotter Formula
(2nd order)

Hamiltonian (general form)

$$\hat{H} = \sum_{i=1}^{L} a_i P_i$$

Second-order Suzuki–Trotter formula

$$U_{ST2} = \prod_{j=1}^{L} e^{-ia_j P_j \frac{t}{2}} \prod_{j'=L}^{1} e^{-ia_{j'} P_{j'} \frac{t}{2}}$$

Again, let us focus on a simple Hamiltonian

$$\hat{H} = \hat{H}_1 + \hat{H}_2$$

$$\hat{U}_{ST2} = e^{-i\hat{H}_1 \frac{\Delta t}{2}} e^{-i\hat{H}_2 \Delta t} e^{-i\hat{H}_1 \frac{\Delta t}{2}}$$

Error in Suzuki-Trotter Formula (2nd order)

$$\hat{U}_{\text{exact}} = e^{-i(\hat{H}_1 + \hat{H}_2)\Delta t}$$

$$\hat{U}_{\text{ST2}} = e^{-i\hat{H}_1\frac{\Delta t}{2}} e^{-i\hat{H}_2\Delta t} e^{-i\hat{H}_1\frac{\Delta t}{2}}$$

The exact Taylor expansion truncated at the 3rd order

$$\hat{U}_{\text{exact}_3} = \mathbb{I} + (-i\Delta t)(\hat{H}_1 + \hat{H}_2) + \frac{(-i\Delta t)^2}{2}\left(\hat{H}_1 + \hat{H}_2\right)^2 + \frac{(-i\Delta t)^3}{6}\left(\hat{H}_1 + \hat{H}_2\right)^3$$

The Taylor expansion for each term (3rd order)

in the 2nd order Suzuki-Trotter Formula

$$\hat{U}_{\text{ST2}_3} = \left[\mathbb{I} + (-i\Delta t/2)\hat{H}_1 + \frac{(-i\Delta t/2)^2}{2}\left(\hat{H}_1^2\right) + \frac{(-i\Delta t/2)^3}{6}\left(\hat{H}_1^3\right)\right]$$

$$\left[\mathbb{I} + (-i\Delta t)\hat{H}_2 + \frac{(-i\Delta t)^2}{2}\left(\hat{H}_2^2\right) + \frac{(-i\Delta t)^3}{6}\left(\hat{H}_2^3\right)\right]$$

$$\left[\mathbb{I} + (-i\Delta t/2)\hat{H}_1 + \frac{(-i\Delta t/2)^2}{2}\left(\hat{H}_1^2\right) + \frac{(-i\Delta t/2)^3}{6}\left(\hat{H}_1^3\right)\right]$$
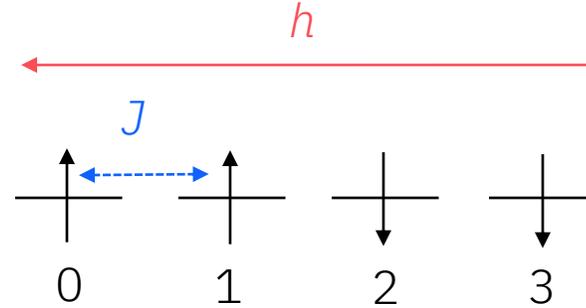
$$\hat{U}_{\text{ST2}_3} \approx \mathbb{I} + (-i\Delta t/2)(\hat{H}_1 + \hat{H}_2) + \frac{(-i\Delta t/2)^2}{2}\left(\hat{H}_1 + \hat{H}_2\right)^2$$

$$+ \frac{(-i\Delta t/2)^3}{6}\left[\hat{H}_1^3 + \frac{3}{2}(\hat{H}_1\hat{H}_2^2 + \hat{H}_2^2\hat{H}_1 + \hat{H}_1\hat{H}_2\hat{H}_1) + \frac{3}{2}(\hat{H}_2\hat{H}_1^2 + \hat{H}_1^2\hat{H}_2 + \hat{H}_2^3)\right]$$

Error of the second-order Suzuki-Trotter

$$\|\hat{U}_{\text{exact}_3} - \hat{U}_{\text{ST2}_3}\| \le \frac{1}{24}\|\hat{H}_2^2\hat{H}_1 + \hat{H}_1\hat{H}_2^2 + \hat{H}_1\hat{H}_2\hat{H}_1 + \hat{H}_2\hat{H}_1\hat{H}_2\|\Delta t^3$$

Example: Trotterization (second-order)
Transverse Ising model

$$H = - \sum_{\langle i,j \rangle}^{N-1} J\sigma_{Z_i}\sigma_{Z_j} - \sum_i^N h_i \sigma_{X_i}$$

h

J

$$0 \quad 1 \quad 2 \quad 3$$

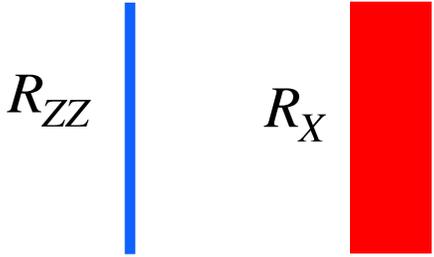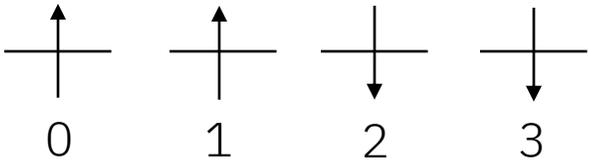$$e^{-i\hat{H}\Delta t} = e^{-i\Delta t(-\sum_{i,j}^N J\sigma_{Z_i}\sigma_{Z_j} - \sum_i^N h_i \sigma_{X_i})}$$

$$\approx e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_0}\sigma_{Z_1})} e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_1}\sigma_{Z_2})} e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_2}\sigma_{Z_3})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_0})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_1})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_2})}$$

$$e^{-i\Delta t(-h\sigma_{X_3})}$$

$$e^{-i\frac{\Delta t}{2}(-h\sigma_{X_2})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_1})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_0})} e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_2}\sigma_{Z_3})} e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_1}\sigma_{Z_2})} e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_0}\sigma_{Z_1})}$$
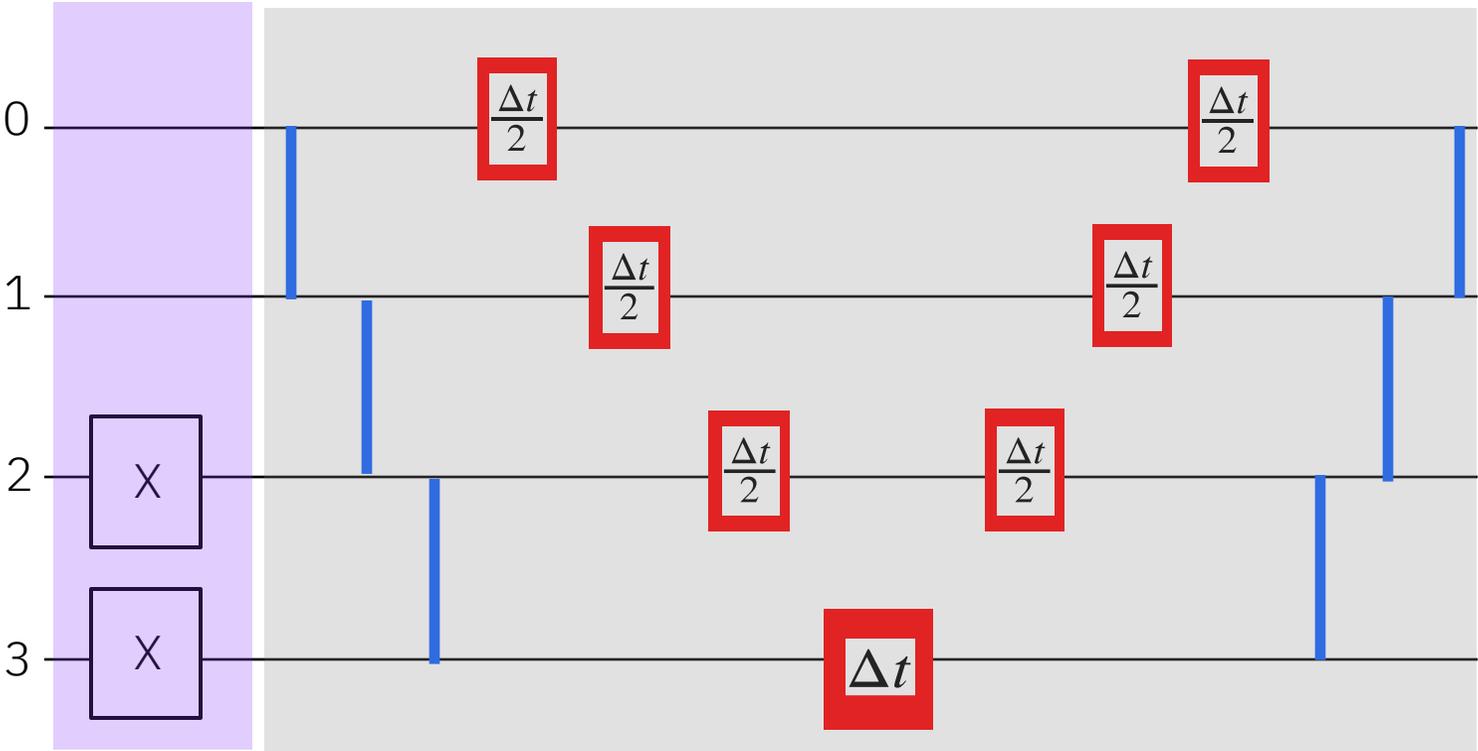
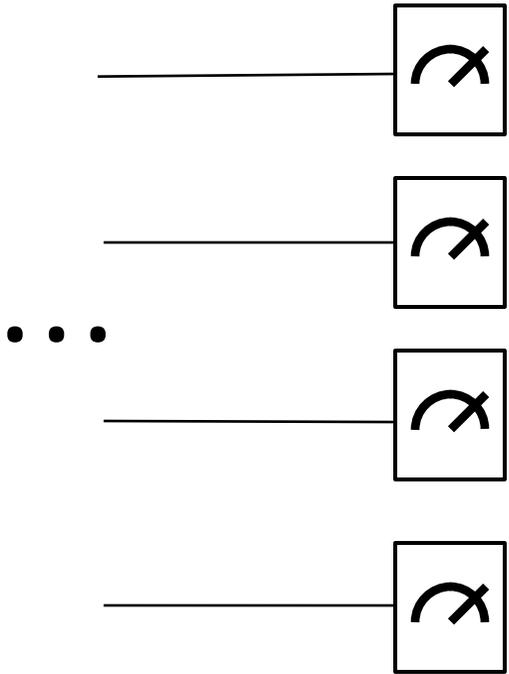# Example: Trotterization (second-order) Transverse Ising model

$$H = -\sum_{\langle i,j \rangle}^{N-1} J\sigma_{Z_i}\sigma_{Z_j} - \sum_{i}^{N} h_i\sigma_{X_i}$$

Time evolution step

State preparation

By repeating this, we can get the wavefunction of time t

Suzuki-Trotter recursion formula for higher order

Second-order Suzuki–Trotter formula

$$e^{-itH} \approx \hat{U}_{ST2}(t) = \prod_{j=1}^{L} e^{-ia_j P_j \frac{t}{2}} \prod_{j'=L}^{1} e^{-ia_j P_{j'} \frac{t}{2}}$$

Recursion relation

$$U_{ST(2k)}(t) = \left[U_{ST(2k-2)}(p_k t) \right]^2 U_{ST(2k-2)} \left((1-4p_k)t \right) \left[U_{ST(2k-2)}(p_k t) \right]^2$$

$$p_k = 1/\left(4 - 4^{\frac{1}{2k-1}} \right)$$

Fourth order Suzuki–Trotter

$$\hat{U}_{ST4}(t) = \left[\hat{U}_{ST2}(p_2 t) \right]^2 \hat{U}_{ST2} \left((1-4p_2)t \right) \left[\hat{U}_{ST2}(p_2 t) \right]^2$$

$$p_2 = 1/\left(4 - 4^{\frac{1}{2*2-1}} \right) = 1/\left(4 - 4^{\frac{1}{3}} \right) \approx 0.4145$$

$$\hat{U}_{ST4}(\Delta t) = \hat{U}_{ST2}(0.4145\Delta t) \, \hat{U}_{ST2}(0.4145\Delta t) \, \hat{U}_{ST2}(-0.6579\Delta t) \, \hat{U}_{ST2}(0.4145\Delta t) \, \hat{U}_{ST2}(0.4145\Delta t)$$

Trotterization

- The method is intuitive and easy to implement

- Number of qubits required is minimal (no ancilla required)

- The scaling of the gate depth against the error is not optimal

  - First-order Trotterization scaling: $O\left(t^2/\epsilon\right)$

  - Second-order Suzuki-Trotter scaling: $O\left(t^{1.5}/\epsilon^{0.5}\right)$

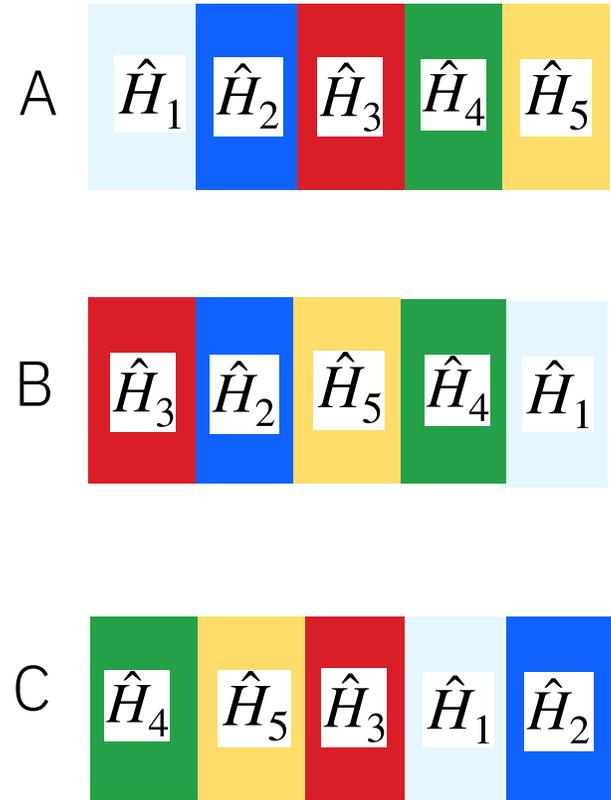   L: Number of terms in the Hamiltonian

    t: time

Lesson 7. Quantum Simulation

11. Randomization

Trotterization has been used for quantum simulation, but methods like Randomization and QDrift have been proposed as effective approaches to average out errors caused by the same error bounds. Here, you will learn about these methods, their overviews, and their performance .
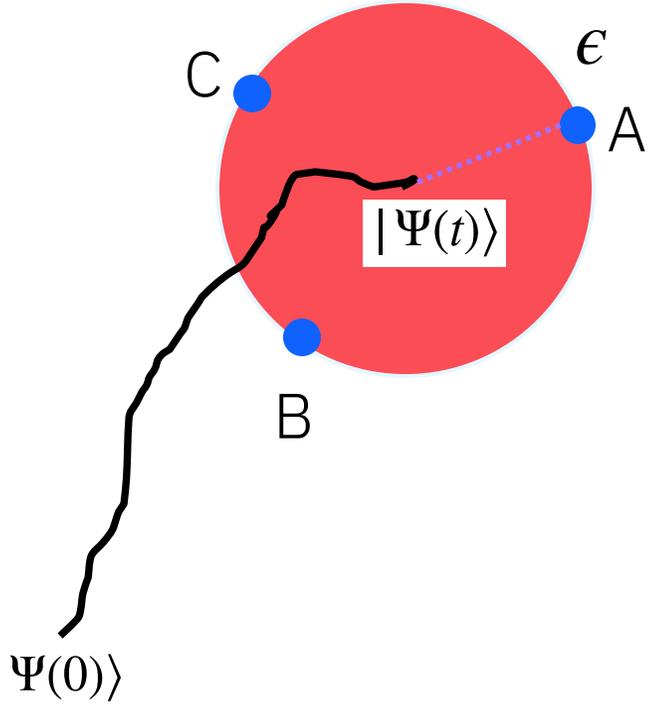
Randomization

A $\hat{H}_1$ $\hat{H}_2$ $\hat{H}_3$ $\hat{H}_4$ $\hat{H}_5$

$$\hat{H} = \sum a_j \hat{H}_j \qquad \|\hat{H}_j\| = 1$$
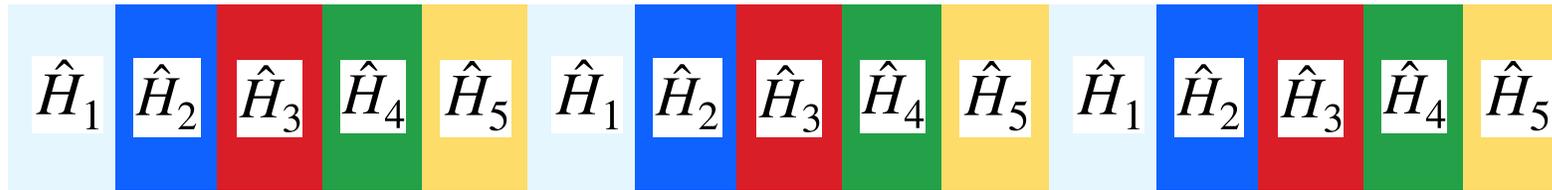
B $\hat{H}_3$ $\hat{H}_2$ $\hat{H}_5$ $\hat{H}_4$ $\hat{H}_1$

$$e^{-i\hat{H}_1 \Delta t} e^{-i\hat{H}_2 \Delta t} e^{-i\hat{H}_3 \Delta t} e^{-i\hat{H}_4 \Delta t} e^{-i\hat{H}_5 \Delta t}$$

C $\hat{H}_4$ $\hat{H}_5$ $\hat{H}_3$ $\hat{H}_1$ $\hat{H}_2$

These sequences have the same error bound

Trotterization vs Randomization

Conventional Trotterization (first order)

$\hat{H}_1$ $\hat{H}_2$ $\hat{H}_3$ $\hat{H}_4$ $\hat{H}_5$ $\hat{H}_1$ $\hat{H}_2$ $\hat{H}_3$ $\hat{H}_4$ $\hat{H}_5$ $\hat{H}_1$ $\hat{H}_2$ $\hat{H}_3$ $\hat{H}_4$ $\hat{H}_5$

$$N_{\text{gates}} = O\left(\frac{L^4 t^2}{\epsilon}\right)$$

Randomization

$\hat{H}_1$ $\hat{H}_2$ $\hat{H}_3$ $\hat{H}_4$ $\hat{H}_5$ $\hat{H}_3$ $\hat{H}_2$ $\hat{H}_5$ $\hat{H}_4$ $\hat{H}_1$ $\hat{H}_4$ $\hat{H}_5$ $\hat{H}_3$ $\hat{H}_1$ $\hat{H}_2$
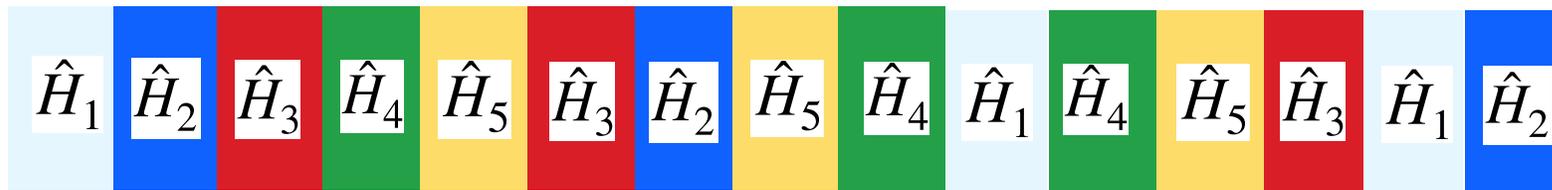
$$N_{\text{gates}} = O\left(\frac{L^{2.5} t^{1.5}}{\epsilon^{0.5}}\right)$$

Can we average out the errors by randomly selecting the ordering?

Performance of randomization
(time steps required to achieve a given accuracy)
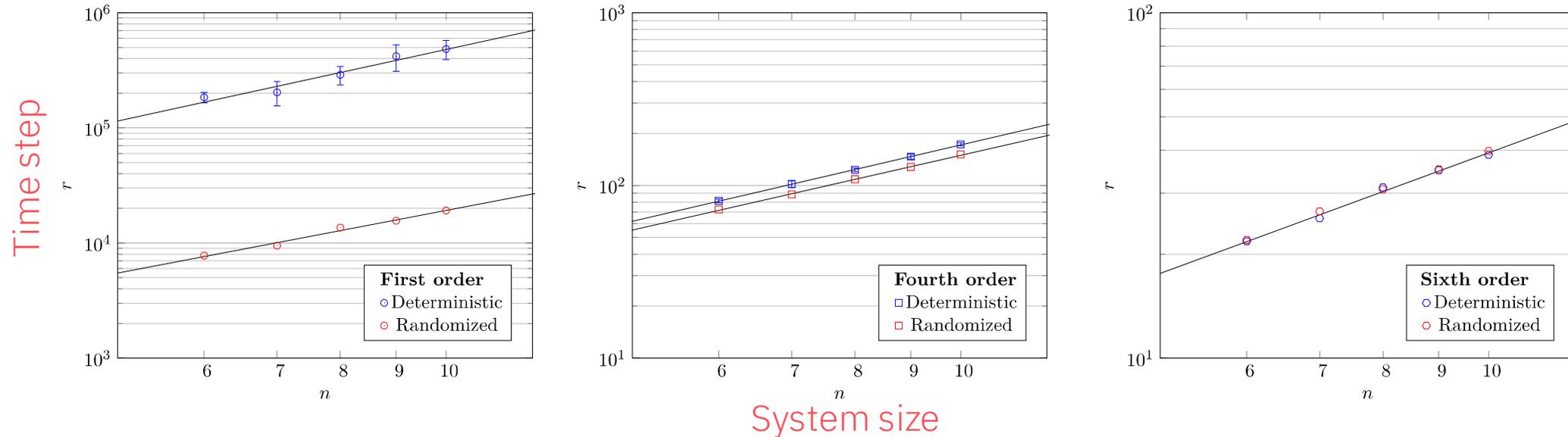
Childs, Ostrander, Su, arXiv: 1805.08385

Figure 1: Comparison of the values of r between deterministic and randomized product formulas. Error bars are omitted when they are negligibly small on the plot. Straight lines show power-law fits to the data.

Calculation using a Heisenberg model

Randomization is effective for Trotterization of low order (good for near term)
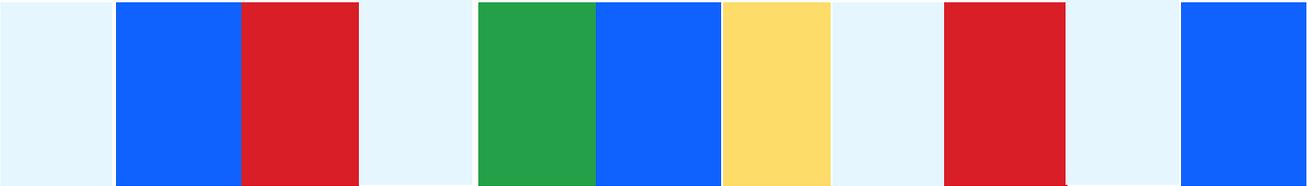
QDrift

Randomization

$$\hat{H} = \sum a_j \hat{H}_j \qquad a_j \geq 0 \qquad \|\hat{H}_j\| = 1$$

Let us try to average out the error further

Can we make it applicable to systems with large number of terms?

Sample $e^{-i\lambda \hat{H}_j \Delta t}$ with weights $p_j = a_j / \lambda$ $\qquad \lambda = \sum_j a_j$

Performance of Qdrift
(gate counts required to achieve a given accuracy)

propane - 46 qubits
λ=426.61 Λ=6.58466 L=241582

carbon dioxide - 54 qubits
λ=608.414 Λ=10.3658 L=113959

ethane - 60 qubits
λ=768.138 Λ=4.07041 L=467403

key

QDRIFT

1st-order Trotter
— deterministic
— random

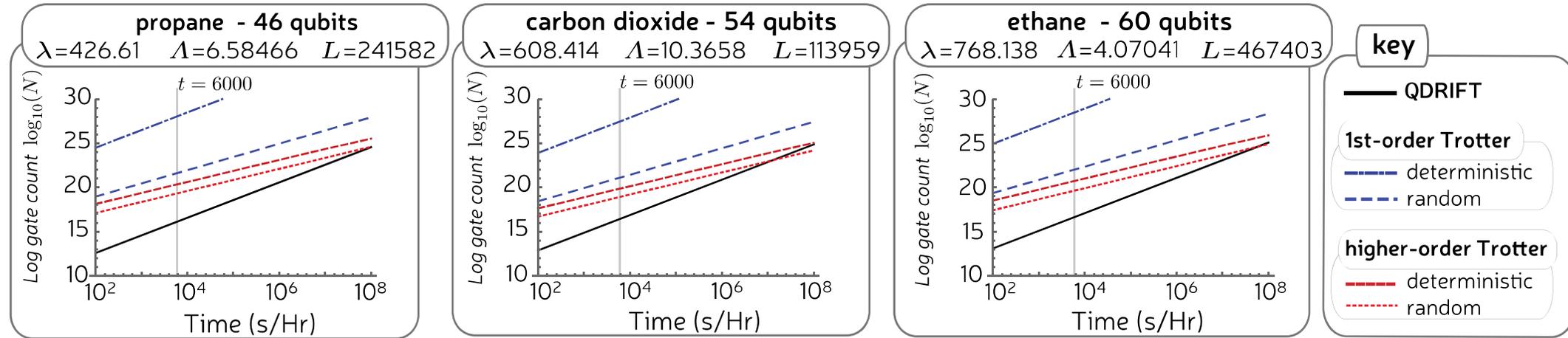**higher-order Trotter**
— deterministic
— random

FIG. 2.   The number of gates used to implement $U = \exp(iHt)$ for various t and $\epsilon = 10^{-3}$ and three different Hamiltonians (energies in Hartree) corresponding to the electronic structure Hamiltonians of propane (in STO-3G basis), carbon dioxide (in 6-31g basis), and ethane (in 6-31g basis). Since the Hamiltonian contains some very small terms, one can argue that conventional Trotter-Suzuki methods would fare better if they truncate the Hamiltonian by eliminating negligible terms. For this reason, whenever simulating to precision ϵ we also remove from the Hamiltonian the smallest terms with weight summing to ϵ. This makes a fairer comparison, though in practice we found it made no significant difference to performance. For the Suzuki decompositions we choose the best from the first four orders, which is sufficient to find the optimal.

Performance is better than randomization only

$$N_{\text{gates}} = O\left(\frac{2\lambda^2 t^2}{\epsilon}\right)$$

Powerful for Hamiltonians with large number of terms

Randomization

- Scaling does not depend on the number of terms (QDrift)

- Advantageous for Hamiltonians with large number of terms (quantum chemistry)

Lesson 7. Quantum Simulation

12. Summary

The Quantum Simulation techniques covered in this lecture are related to areas such as Quantum Phase Estimation and Variational Quantum Algorithms. Here, you will learn not only the summary of this lecture but also its connections to other lectures .

Connection with other lectures

- Lecture 5: Quantum Phase Estimation

  - Quantum simulation can be a subroutine

  - The energy will emerge as the shift in the phase

  - Using the quantum chemistry Hamiltonian, we can get an accurate energy value of a molecule

- Lecture 6: Variational Quantum Eigensolver

  - We can use the quantum-classical hybrid algorithm to get energies and other physical properties

  - QAOA circuits are extremely similar with the time-evolution circuits

- For utility experiments

  - Time-evolution circuits play an important role

Further Reading

1. "Quantum Computation and Quantum Information", Michael A. Nielsen and Isaac L. Chuang, Cambridge University Press.
2. "Quantum Information Science", Riccardo Manenti and Mario Motta, Oxford University Press.

Overview

1. Quantum simulation (Hamiltonian simulation, quantum dynamics)
2. Hamiltonian (Model)
3. Algorithms for Quantum Simulation
   1. Trotterization
4. Hands-on Session
5. Algorithms for Quantum Simulation (if we have time...)
   1. Randomization

Reference

- Slide shared from Professor Sato at the University of Tokyo (Slide 8)
- Childs et al., Quantum 3, 182 (2019) (Slide 38)
- Campbell, Phys. Rev. Lett., 123, 070503 (2019) (Slide 40)