The University of Tokyo
Special Lectures in Information Science Ⅱ
Introduction to Near-Term Quantum Computing

Lesson 13. Quantum Utility Ⅱ (Utility paper implementation)

1. Opening

Here, you will learn about the positioning of this lecture and we will provide an outline of its content.

13. Utility-Scale Experiment II

2024/07/12

Yukio Kawashima
IBM Research – Tokyo
Yukio.Kawashima@ibm.com

Lecturer
Yukio Kawashima

東京大学
THE UNIVERSITY OF TOKYO

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.

Course Schedule 2024 (subject to change)

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 / Tamiya Onodera
4/26	LOCC (Quantum teleportation/superdense coding/Remote CNOT)	Kifumi Numata	6/21	Quantum circuit optimization (transpilation)	Toshinari Itoko
5/10	Quantum Algorithms: Grover's algorithm	Atsushi Matsuo	6/28	Quantum noise and quantum error mitigation	Toshinari Itoko
5/15 (Wed)	Quantum Algorithms: Phase estimation	Kento Ueda	7/5	Utility Scale Experiment I	Tamiya Onodera
5/24	Quantum Algorithms: Variational Quantum Algorithms (VQA)	Takashi Imamichi	7/12	Utility Scale Experiment II	Yukio Kawashima
5/30 (Thu)	Quantum simulation (Ising model, Heisenberg, XY model), Time evolution (Suzuki Trotter, QDrift)	Yukio Kawashima	7/19	Utility Scale Experiment III	Kifumi Numata / Tamiya Onodera

Overview

1. Recap of Quantum simulation (Hamiltonian simulation, quantum dynamics)
   1. Hamiltonian (Model)
   2. Trotterization
2. About the experiment for the hands-on session and assignments
3. Break
4. Hands-on Session and assignments
   1. 20-qubit problem (state-vector and matrix product state simulator)
   2. 70-qubit problem (matrix product state simulator and quantum hardware)
   3. Assignments

2. Algorithm for Quantum Simulation

The time-dependent Schrödinger equation that needs to be solved for quantum simulation is very complex. Therefore, strategies that enable efficient computation with smaller errors and shallower circuit depths are used. In this section, we will provide an overview of quantum simulation and introduce some strategies employed for 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

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

Very small time slice

Taylor series as an example

Hamiltonian in general

- Hamiltonian of a quantum system is an operator representing the total energy of the system
  - Kinetic energy and potential energy $\hat{H} = \hat{T} + \hat{V}$
- 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

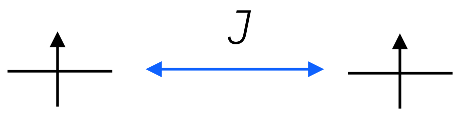
Spin interaction

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

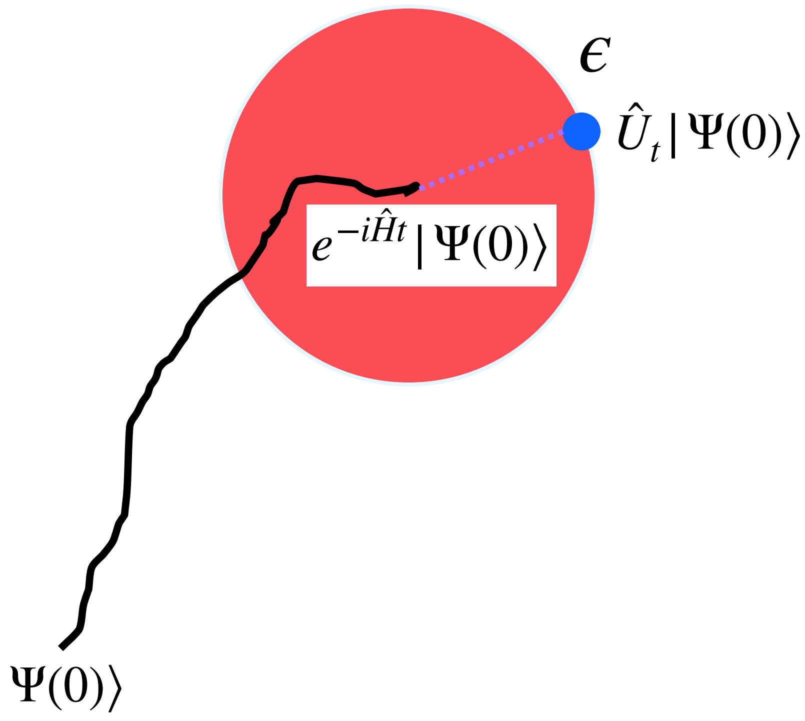
Algorithms for quantum simulations

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

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 $\| \hat{U}|\Psi\rangle - e^{-i\hat{H}t}|\Psi\rangle \| \leq \epsilon$

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

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



3. Trotterization

To perform quantum simulation, strategies like those introduced in the previous section are employed. In this section, we will learn about Trotterization. We will also examine an example of first-order Trotterization and study the complexity of its quantum circuit.

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

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

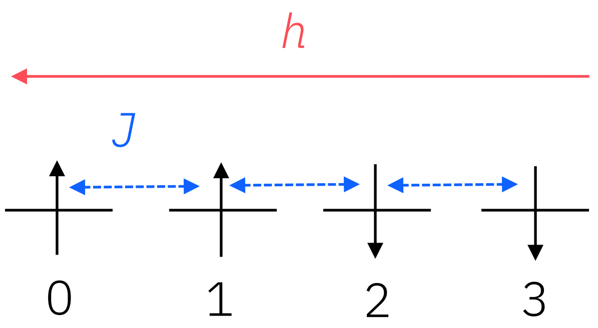
We will take “*n*” to be finite

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

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

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

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

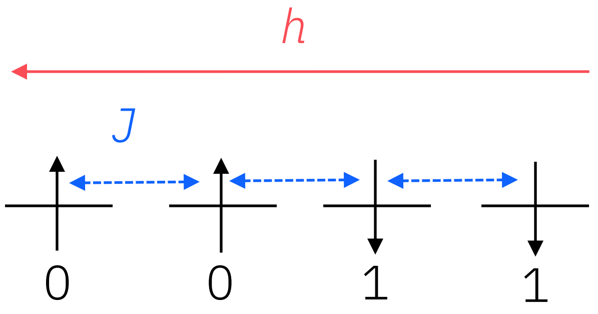
$R_{ZZ}(-2J\Delta t)$ $\qquad$ $R_X(-2h\Delta t)$

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

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

Example: Trotterization (first-order)
Transverse Ising model

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



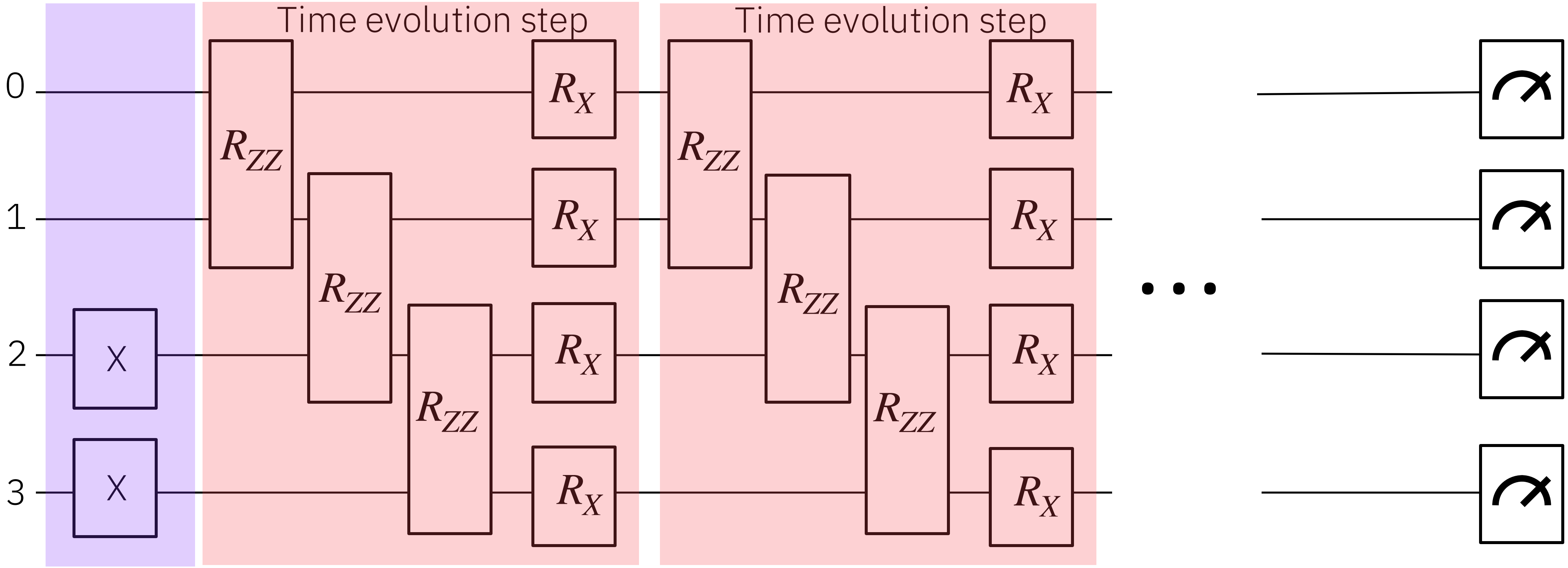
0: up spin

1: down spin

Bit strings

$|0011\rangle$

$|1100\rangle$



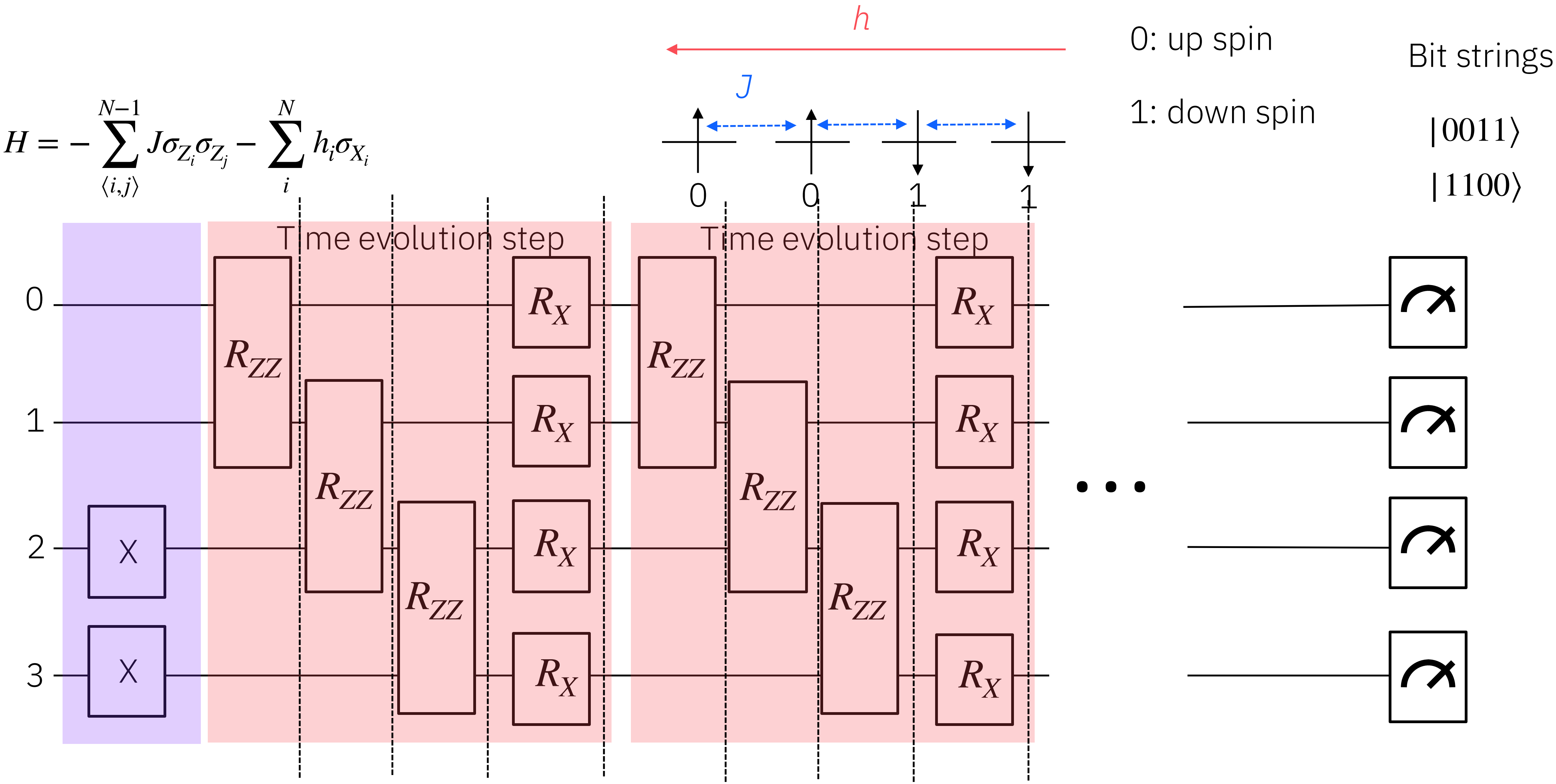
State preparation

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

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

The complexity of the circuit

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



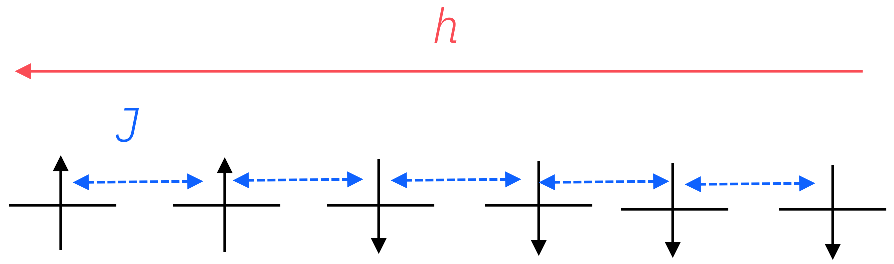
Number of (two-qubit) gates, depth of the circuit (reduction of them is important to improve the accuracy)

4. Magnetization

To handle the Transverse Ising Model on a quantum computer, it is necessary to monitor the time evolution of magnetization. In this section, we will learn about the theoretical background needed for implementation in the upcoming hands-on session.

Magnetization

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



Magnetization

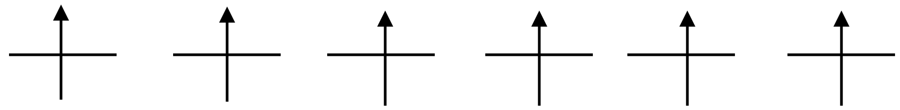
$$\sum_{i}^{N} Z_i/N$$

Expectation value

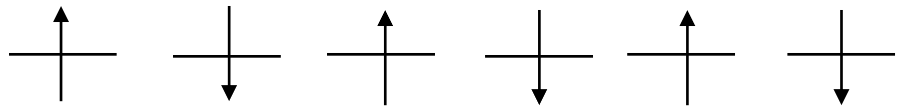
$Z|0\rangle = |0\rangle$ +1 $|0\rangle = |\uparrow\rangle$

$Z|1\rangle = -|1\rangle$ −1 $|1\rangle = |\downarrow\rangle$

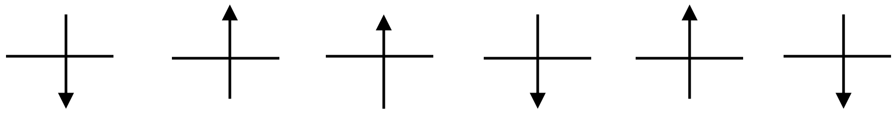
- Ferromagnetic
  - Aligned as same spin with the neighbor
  - Magnet at room temperature (iron)



- Antiferromagnetic
  - Aligned as opposite spin with the neighbor
  - Insulator (MnO)



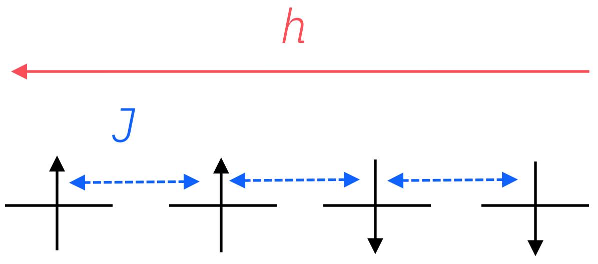
- Paramagnetic
  - Show no magnetization without external field



Metric for describing the magnetic state

Ground state of the 1D transverse-field 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

$$\sum_{i}^{N} Z_i / N$$

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

– Interaction energy

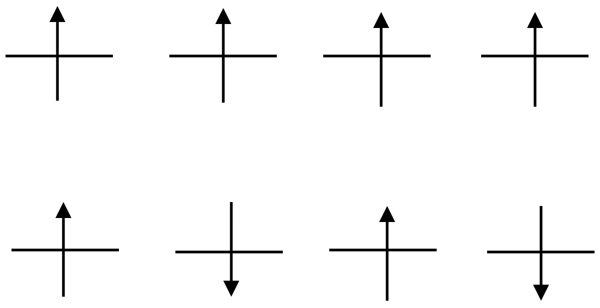
$$Z_k Z_{k+1} = 1 \qquad (1,1), (-1,-1)$$

$$Z_k Z_{k+1} = -1 \qquad (1,-1), (-1,1)$$

Ground state (ignoring h)

$-J < 0$

$-J > 0$

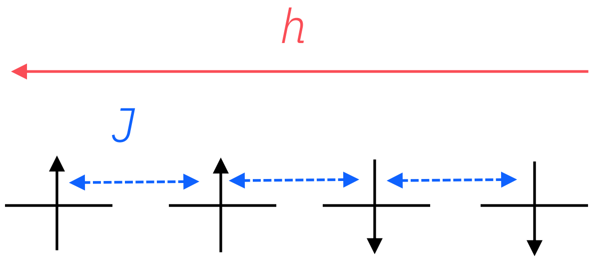


With large h: the configuration becomes disordered

The ground state (lowest energy) differs based on the parameters

Dynamical quantum phase transition

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

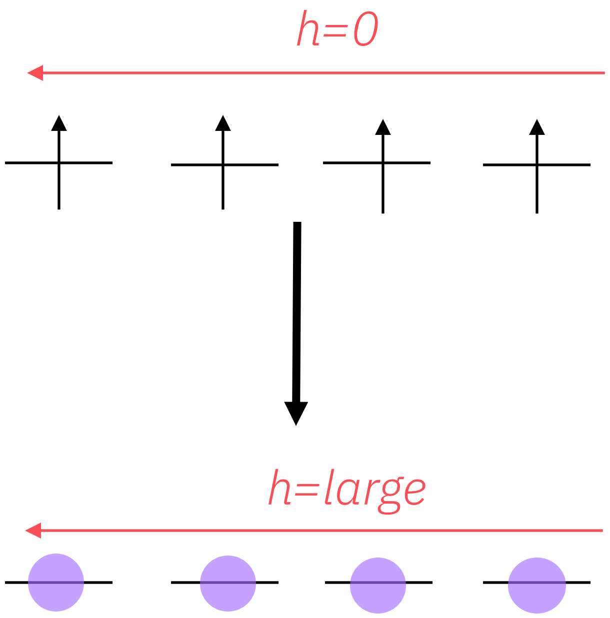


- A phase transition due to a nonequilibrium process
  - How about magnetic phase after a sudden quench (magnetic field)?

Magnetization

$$\sum_{i}^{N} Z_i / N$$

Ferromagnetic (–J < 0)



?

Monitor time evolution of the magnetization

5. Hands-on Part 1: Overview and Preparation

Here, we will learn about the overview of the hands-on session. We will also develop an understanding of the theoretical background and prepare for conducting simulations using Qiskit.

Hands-on session

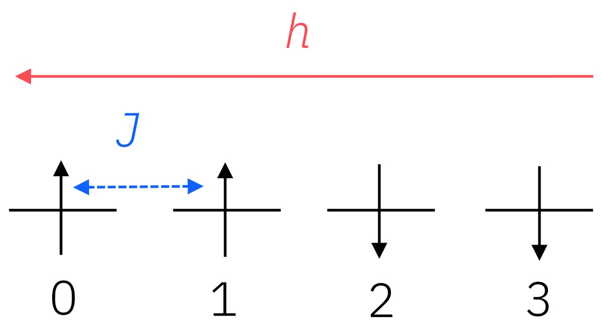
- Time evolution of magnetization and monitor the magnetic phase after change in magnetic field
  - Quantum simulation with an ideal simulator
    - 20 qubit-problem with state-vector and matrix product state simulator
  - Quantum simulation with a quantum hardware
    - 70 qubit-problem
      - matrix product state simulator
      - hardware

10. Innovations in Quantum Simulation

While increasing the order of Trotterization can reduce errors, it also increases the depth of the quantum circuit. To address this, methods such as QDrift are employed. In this section, we will learn about the theoretical background, characteristics, and performance of such methods.

Example: Trotterization (second-order)
Transverse Ising model

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



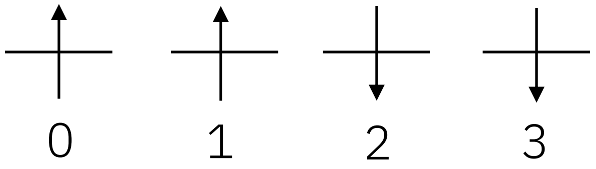
$$e^{-i\hat{H}\Delta t} = e^{-i\Delta t(-\sum_{i,j}^{N} J\sigma_{Z_i}\sigma_{Z_j} - \sum_{i}^{N} h_i\sigma_{X_i})}$$

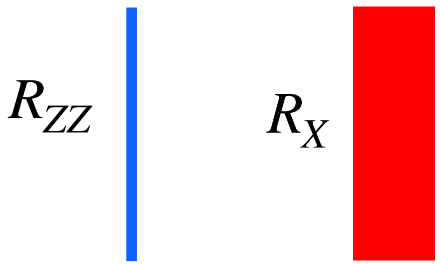
$$\approx e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_0}\sigma_{Z_1})} e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_1}\sigma_{Z_2})} e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_2}\sigma_{Z_3})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_0})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_1})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_2})}$$

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

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

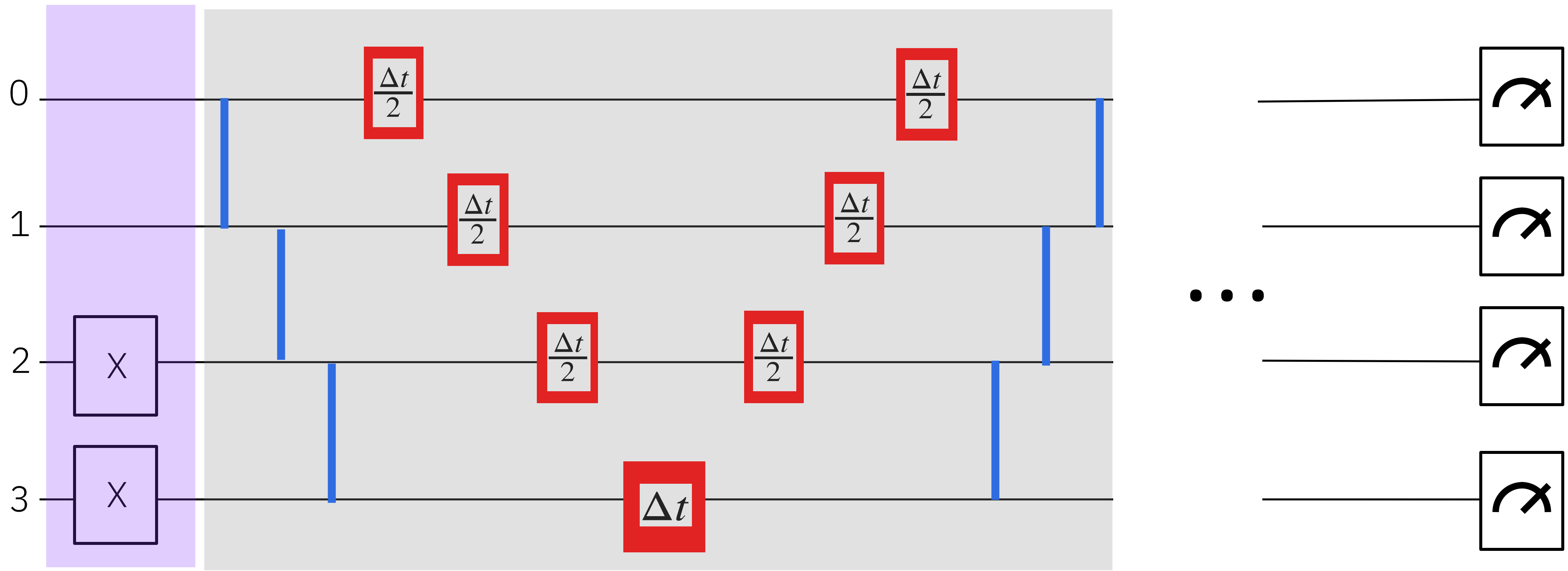
Example: Trotterization (second-order) Transverse Ising model





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

Time evolution step



State preparation

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

QDrift

Campbell, Phys Rev Lett 123, 070503 (2019)

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)

Campbell, Phys Rev Lett 123, 070503 (2019)

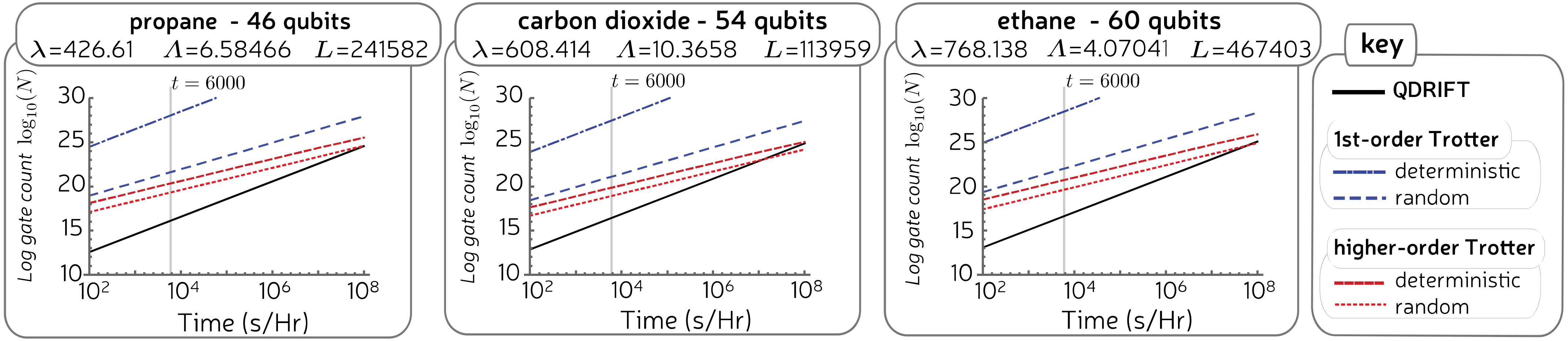


FIG. 2. The number of gates used to implement $U = \exp(iHt)$ for various t and $\epsilon = 10^{-3}$ and three different Hamiltonians (energies in Hartree) corresponding to the electronic structure Hamiltonians of propane (in STO-3G basis), carbon dioxide (in 6-31g basis), and ethane (in 6-31g basis). 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

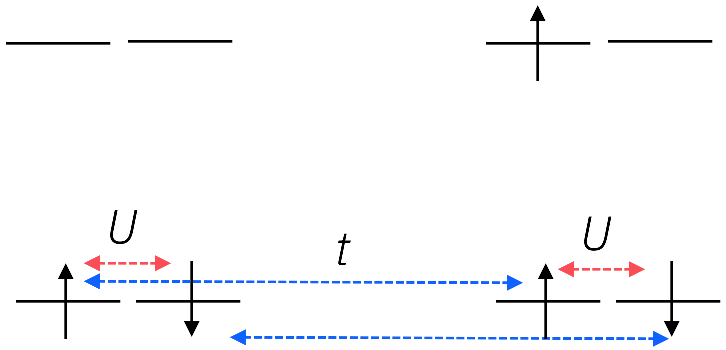
$$N_{\text{gates}} = O\left(\frac{2\lambda^2 t^2}{\epsilon}\right)$$

Powerful for Hamiltonians with large number of terms

Hamiltonian (Fermionic Hamiltonian)

– Hubbard model

Describe conducting and insulating systems



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

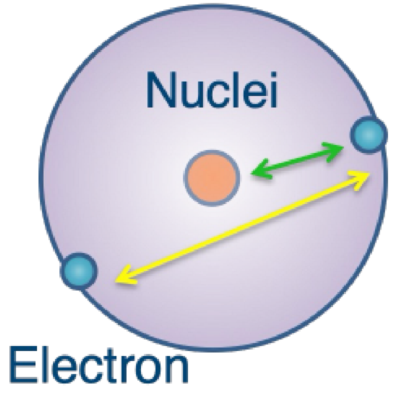
$$\hat{n}_{i,\sigma} = \hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i,\sigma}$$

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



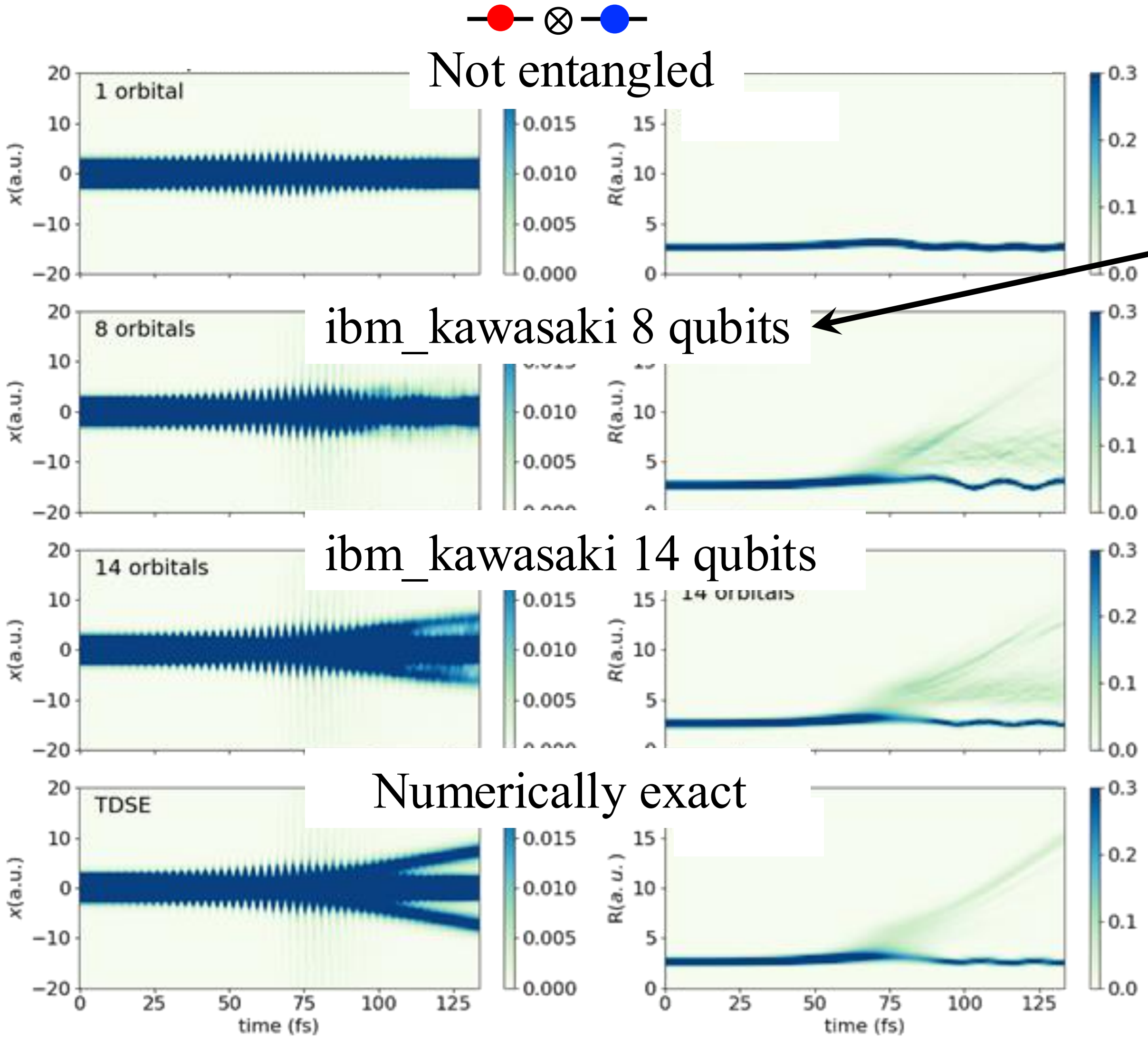
Complexity & Computational resources

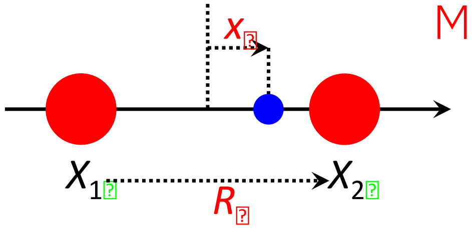
What can we do with quantum simulation: Electron and nuclear dynamics

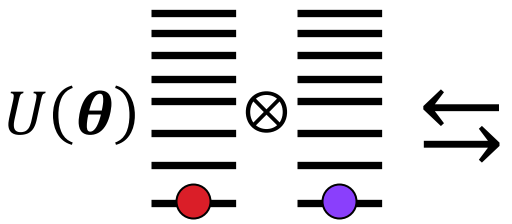
Univ of Tokyo, Professor Sato

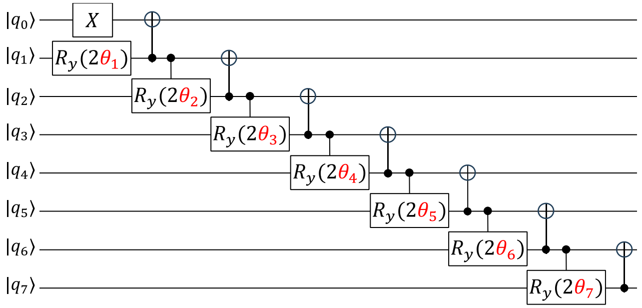
Molecule in a strong laser field

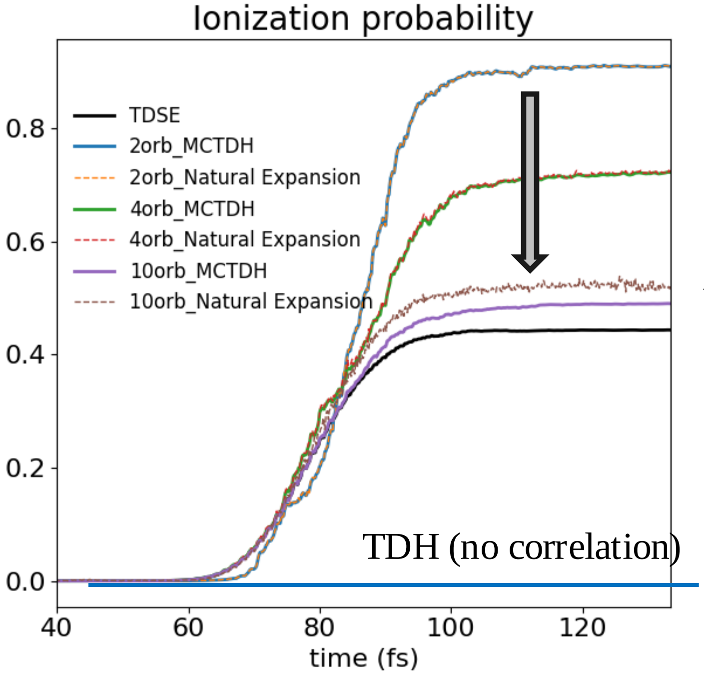
Electron density $\rho_e(x)$ Nuclear density $\rho_n(R)$











2 qubits

4 qubits

10 qubits

More accurate with more qubits

Reference

- Campbell, Phys. Rev. Lett., 123, 070503 (2019) (Slide 20)
- Slide shared from Professor Sato at the University of Tokyo (Slide 22)