7. Quantum Simulation

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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

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

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

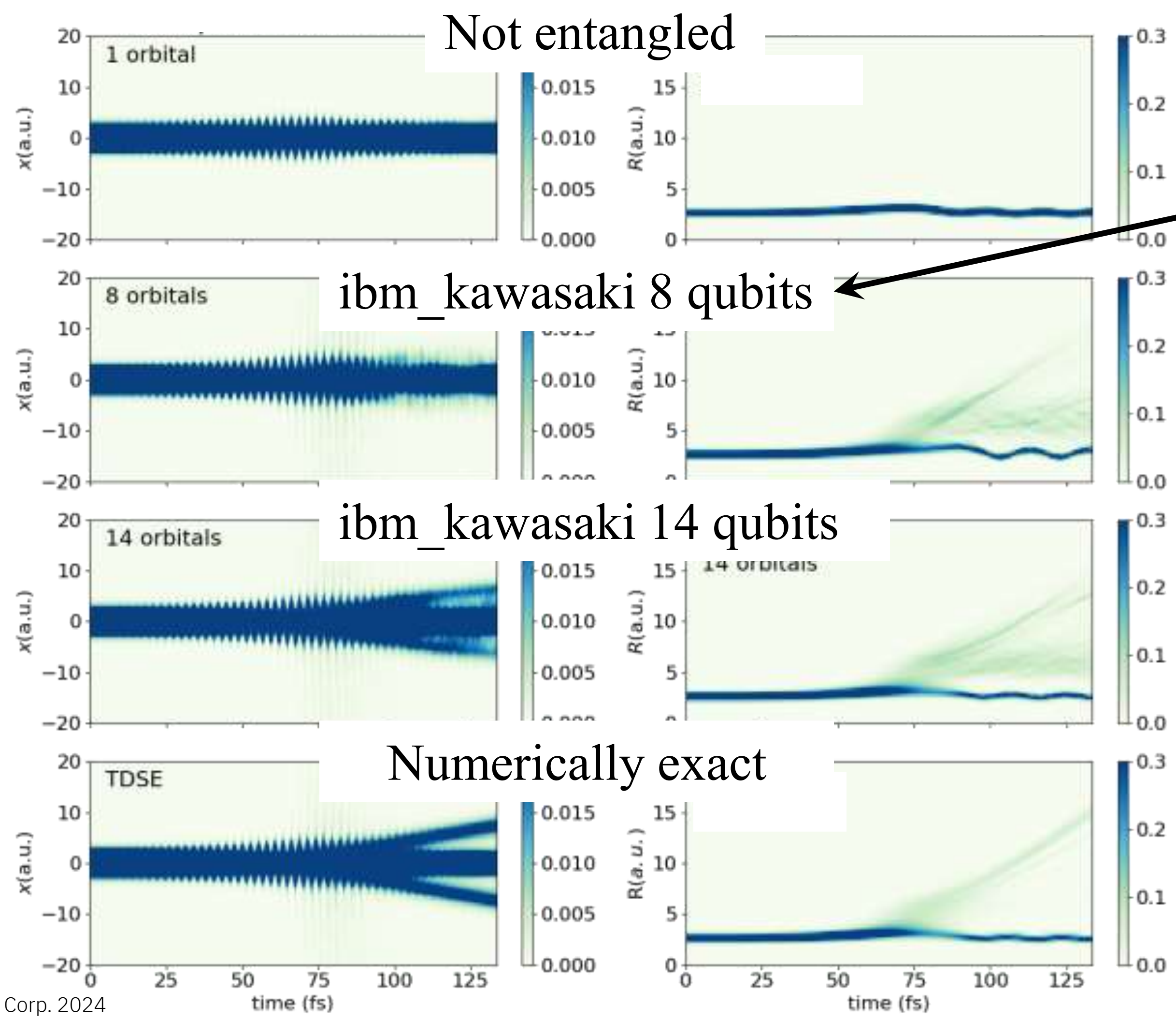
Very small time slice

Taylor series as an example

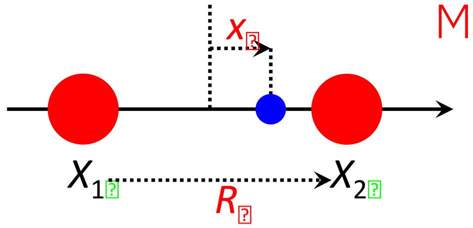
What can we do with quantum simulation: Electron and nuclear dynamics

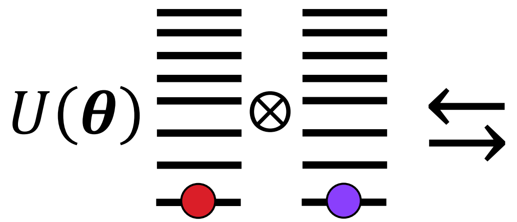
Univ of Tokyo, Professor Sato

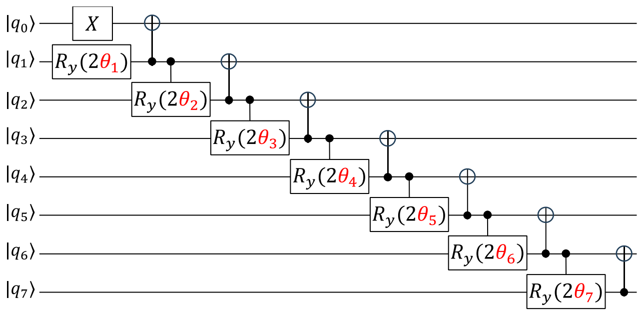
Electron density $\rho_e(x)$ Nuclear density $\rho_n(R)$

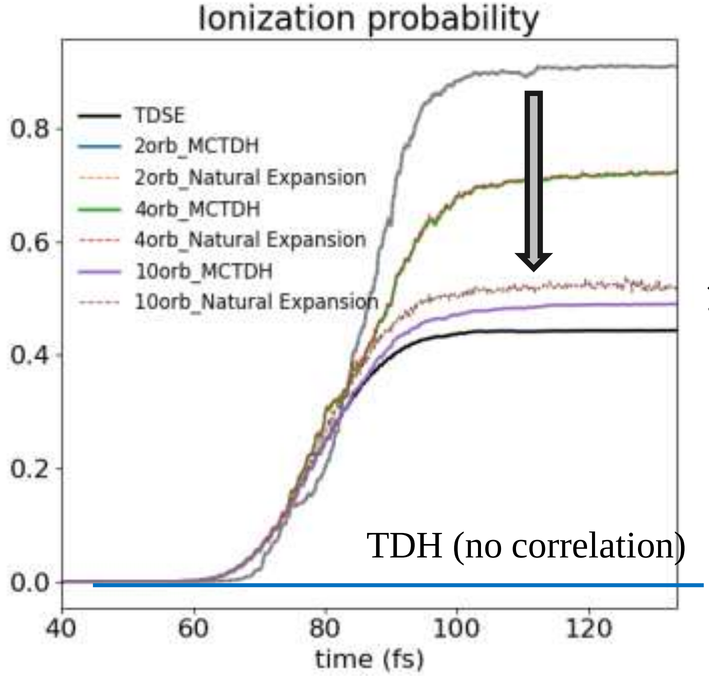


Molecule in a strong laser field









2 qubits

4 qubits

10 qubits

More accurate with more qubits

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

Quantum Simulation (Hamiltonian Simulation)

Solve the time-dependent Schrödinger equation

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Wavefunction

Hamiltonian

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Very small time slice

Taylor series as an example

Hamiltonian

Hamiltonian in general

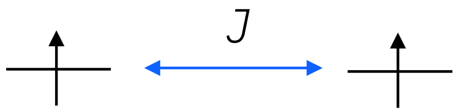
- Hamiltonian of a quantum system is an operator representing the total energy of the system
  - Kinetic energy and potential energy $\hat{H} = \hat{T} + \hat{V}$
- Time-dependent Hamiltonian & time-independent Hamiltonian
  - We will consider only time-independent Hamiltonian today
- Important in many fields
  - Quantum chemistry (material science)
  - Condensed matter physics
  - High-energy physics

Hamiltonian (Spin Hamiltonian)

Lattice models for spin systems to study magnetic systems

- *n*-vector models
  - Ising model (n=1)

$$H = -\overbrace{\sum_{\langle i,j \rangle} J \sigma_{Z_i} \sigma_{Z_j}}^{\text{Spin interaction}} - \overbrace{\sum_i h_i \sigma_{X_i}}^{\text{External field}}$$



  - 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)

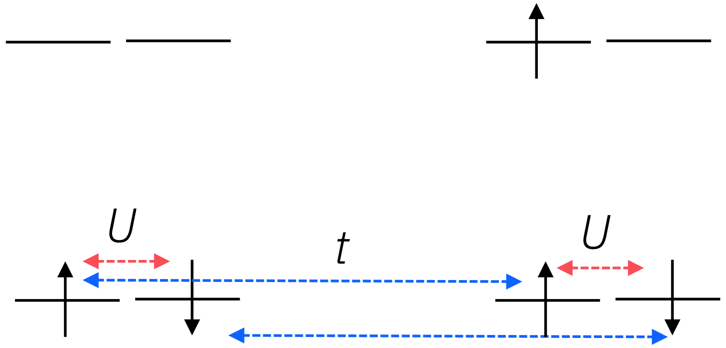
$$H = -\sum_{\langle i,j \rangle} \left(J_X \sigma_{X_i} \sigma_{X_j} + J_Y \sigma_{Y_i} \sigma_{Y_j} + J_Z \sigma_{Z_i} \sigma_{Z_j} \right) - \sum_i h_i \sigma_{Z_i}$$

Complexity & Computational resources

Hamiltonian (Fermionic Hamiltonian)

- Hubbard model

Describe conducting and insulating systems



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

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

Creation operator

Annhilation operator

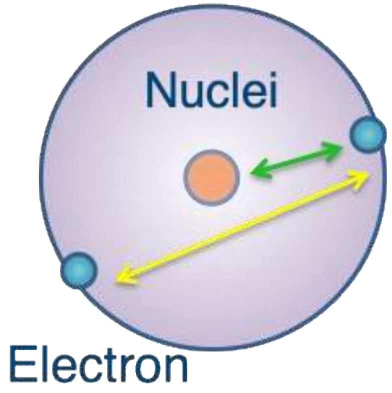
- Quantum Chemistry Hamiltonian

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

Kinetic energy of electrons

Electron-nucleus attraction

Electron-electron repulsion



Complexity & Computational resources

Mapping the Hamiltonian

Map the second-quantized Hamiltonian to qubits:

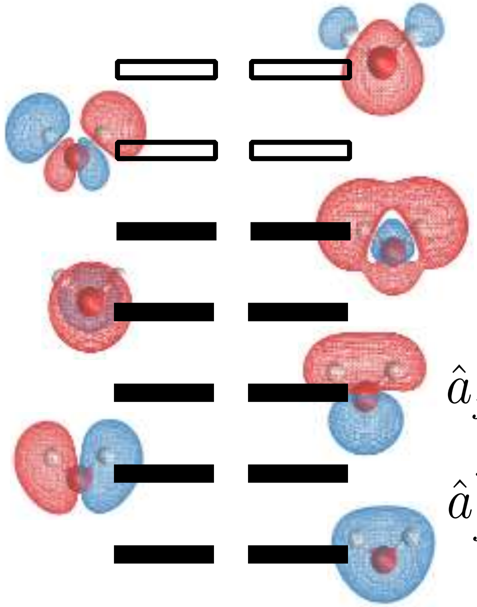
$$H = -t \sum_{i,\sigma} \left(\hat{c}^\dagger_{i,\sigma} \hat{c}_{i+1,\sigma} + \hat{c}^\dagger_{i+1,\sigma} \hat{c}_{i,\sigma} \right) + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}$$

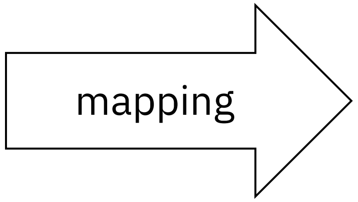
$$\hat{n}_{i,\sigma} = \hat{c}^\dagger_{i,\sigma} \hat{c}_{i,\sigma}$$

Hubbard, Quantum chemistry

Fermions

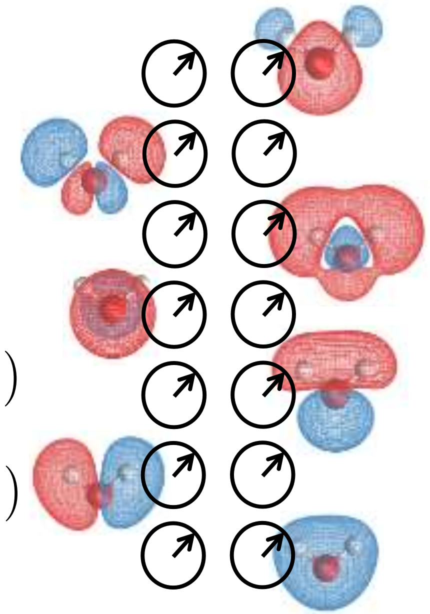
$$\{a_i, a_i\} = 0,\ \{a_i^\dagger, a_i^\dagger\} = 0, \{a_i, a_i^\dagger\} = \delta_{i,j}$$





Spins

$$[\sigma_i, \sigma_i] = 0,\ [\sigma_i^\dagger, \sigma_i^\dagger] = 0, [\sigma_i, \sigma_j^\dagger] = \delta_{i,j}$$



Jordan-Wigner

$$\hat{a}_j = \bigotimes_{i=1}^{j-1} \hat{\sigma}_i^z \otimes (\hat{\sigma}_j^x + i\hat{\sigma}_j^y)$$

$$\hat{a}_j^\dagger = \bigotimes_{i=1}^{j-1} \hat{\sigma}_i^z \otimes (\hat{\sigma}_j^x - i\hat{\sigma}_j^y)$$

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

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

Note that operators a and c are the same

Jordan–Wigner Mapping

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

Jordan–Wigner mapping

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

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

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

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

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

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

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

How will this be mapped?

Try mapping a one-body term

Use these relations $\sigma_X^2 = \sigma_Y^2 = \sigma_Z^2$

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

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

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

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

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

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

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

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

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

$$= \frac{1}{16}\Big[-X_3Y_2X_1Y_0 - iX_3Y_2Y_1Y_0 - iY_3Y_2X_1Y_0 + Y_3Y_2Y_1Y_0 - iX_3X_2X_1Y_0 + X_3X_2Y_1Y_0 + Y_3X_2X_1Y_0 + iY_3X_2Y_1Y_0$$
$$- iX_3Y_2X_1X_0 + X_3Y_2Y_1X_0 + Y_3Y_2X_1X_0 + iY_3Y_2Y_1X_0 + X_3X_2X_1X_0 + iX_3X_2Y_1X_0 + iY_3X_2X_1X_0 - Y_3X_2Y_1X_0\Big]$$

The equations are tedious, but the idea is simple

Mapping the Hamiltonian

General equation

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

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

Fermionic Hamiltonian

$$H_f = -1.26a_0^\dagger a_0 - 0.47a_1^\dagger a_1 - 1.26a_2^\dagger a_2 - 0.47a_3^\dagger a_3$$
$$+0.34a_0^\dagger a_0^\dagger a_0 a_0 + 0.33a_0^\dagger a_1^\dagger a_1 a_0 + 0.34a_0^\dagger a_2^\dagger a_2 a_0 + 0.33a_0^\dagger a_3^\dagger a_3 a_0 + \cdots$$
$$+0.09a_0^\dagger a_2^\dagger a_3 a_1 + \cdots$$

$$\downarrow$$

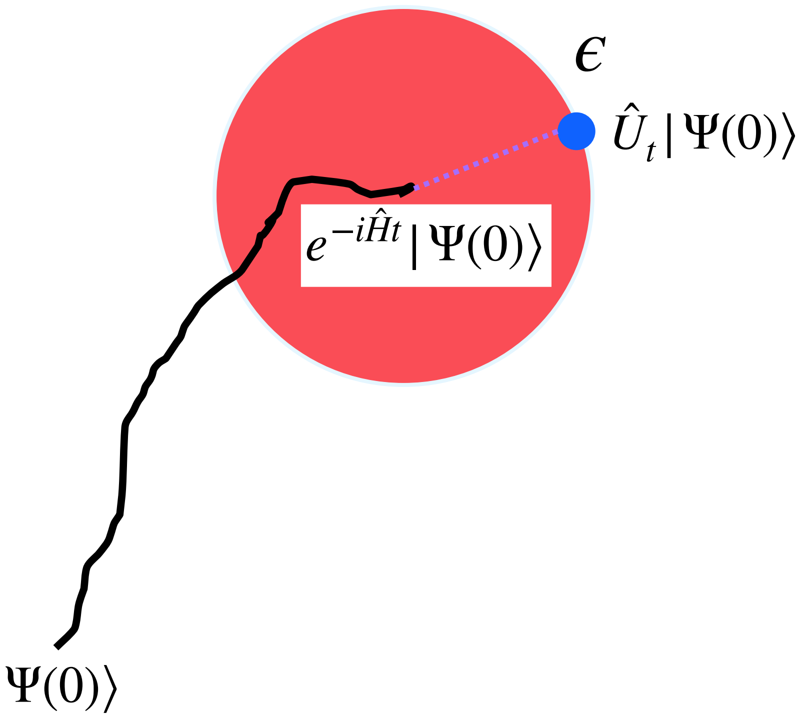
$$H_q = -0.81 + 0.17(Z_0 + Z_2) - 0.23(Z_1 + Z_3) + 0.12(Z_1Z_0 + Z_3Z_2) + 0.17Z_0Z_2 + 0.17Z_1Z_3$$
$$+ 0.17Z_1Z_2 + 0.17Z_0Z_3 + 0.05(Y_3Y_2Y_1Y_0 + X_3X_2X_1X_0 + Y_3Y_2X_1X_0 + X_3X_2Y_1Y_0)$$

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

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



- 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 $\hat{A} = 0$
    - $\|a\hat{A}\| = |a|\|\hat{A}\|$
    - $\|\hat{A} + \hat{B}\| \leq \|\hat{A}\| + \|\hat{B}\|$

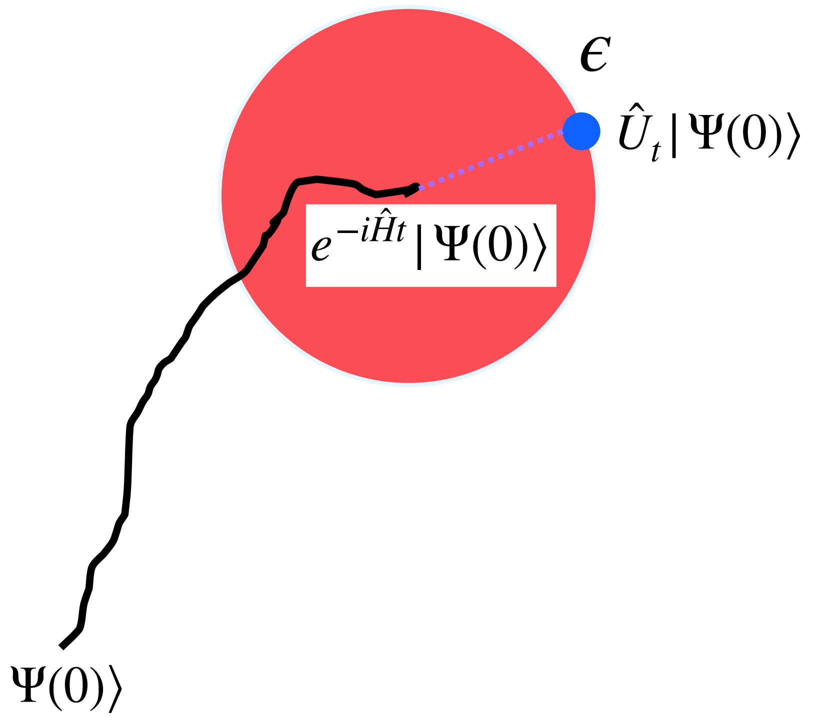
Algorithms for quantum simulations

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

- 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)

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



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)

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

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

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

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

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

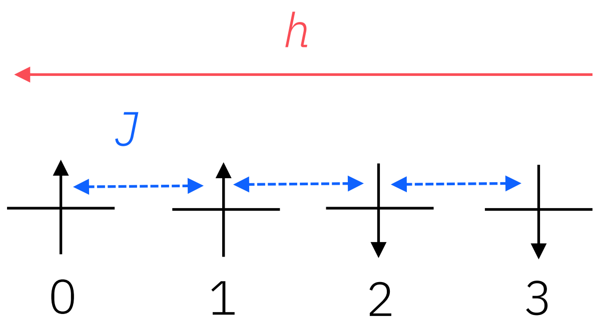
$$\|\hat{U}_{\text{exact}_2} - \hat{U}_{\text{trotter}_2}\| = \left\|\frac{(-i\Delta t)^2}{2}(\hat{H}_2\hat{H}_1 - \hat{H}_1\hat{H}_2) + O(\Delta t^3)\right\|$$

$$\leq \frac{1}{2}\|[\hat{H}_2, \hat{H}_1]\|\Delta t^2 + \|O(\Delta t^3)\|$$

(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

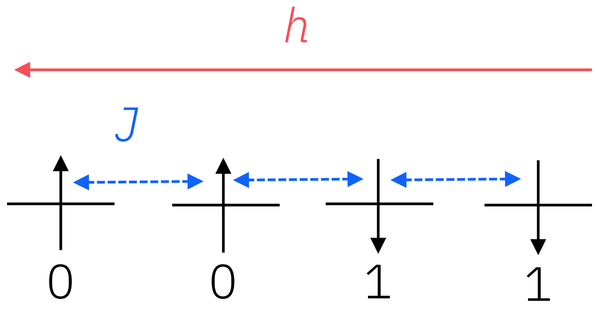
$$e^{-i\hat{H}\Delta t} = e^{-i\Delta t(-\sum_{i,j}^{N} J\sigma_{Z_i}\sigma_{Z_j} - \sum_{i}^{N} h_i\sigma_{X_i})} \approx \underbrace{e^{-i\Delta t(-\sum_{i,j}^{N} J\sigma_{Z_i}\sigma_{Z_j})}}_{R_{ZZ}(-2J\Delta t)} \underbrace{e^{-i\Delta t(-\sum_{i}^{N} h_i\sigma_{X_i})}}_{R_X(-2h\Delta t)}$$

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

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

Example: Trotterization (first-order)
Transverse Ising model

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



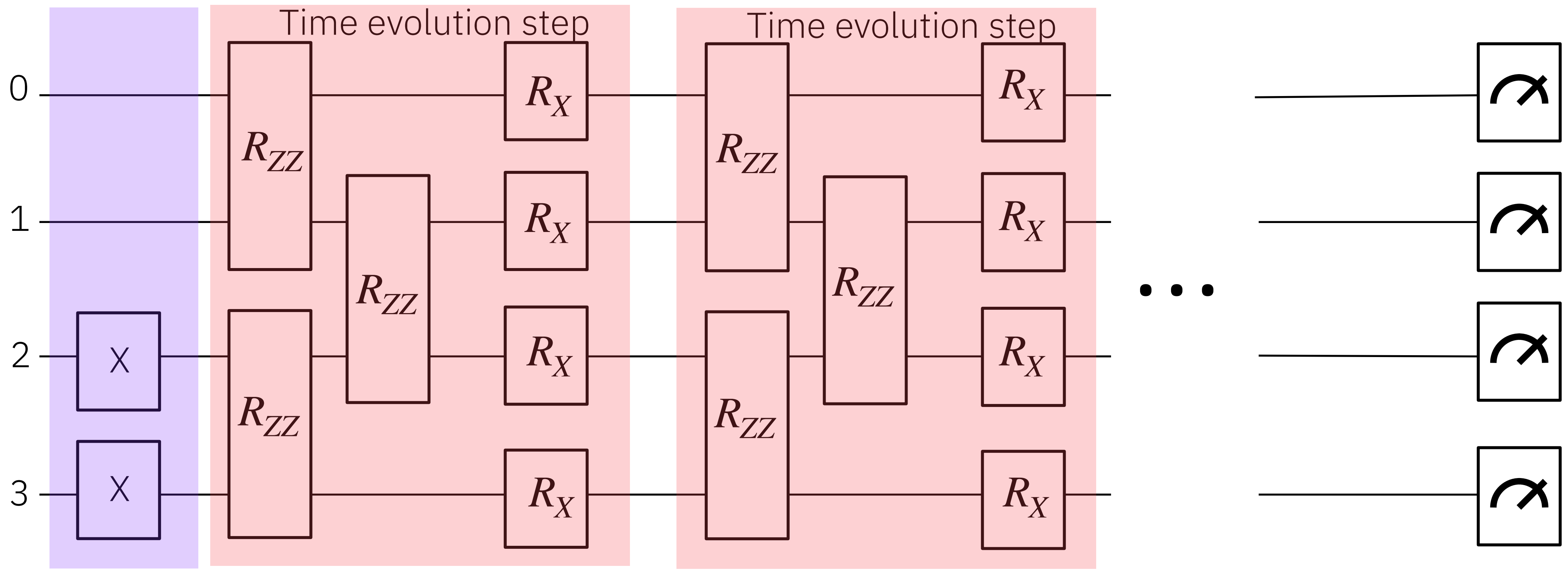
0: up spin

1: down spin

Bit strings

$|0011\rangle$

$|1100\rangle$



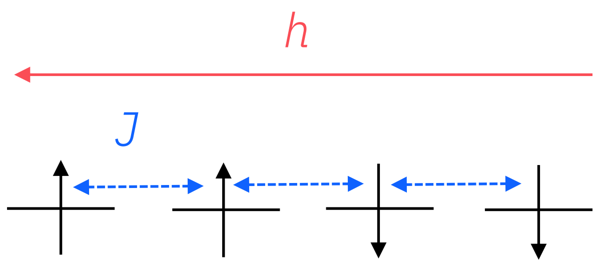
State preparation

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

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

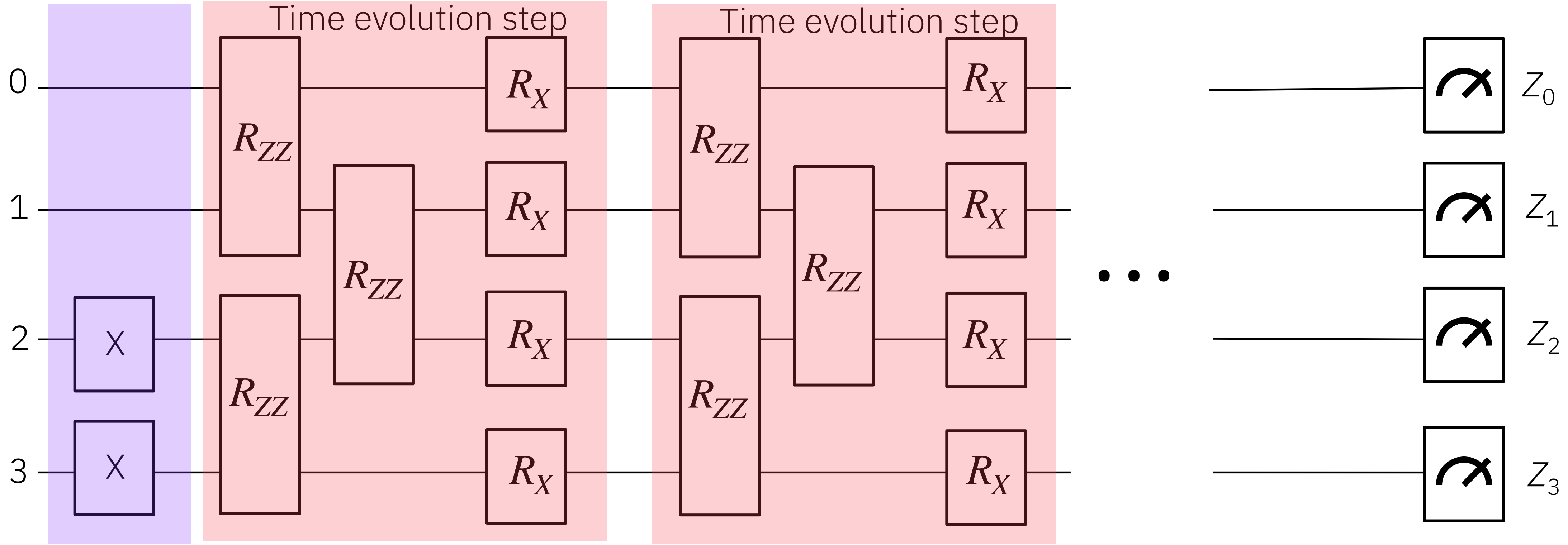
Example: Trotterization Transverse Ising model

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



Magnetization

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



State preparation

Measure expectation values of observables

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

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

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

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

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

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

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

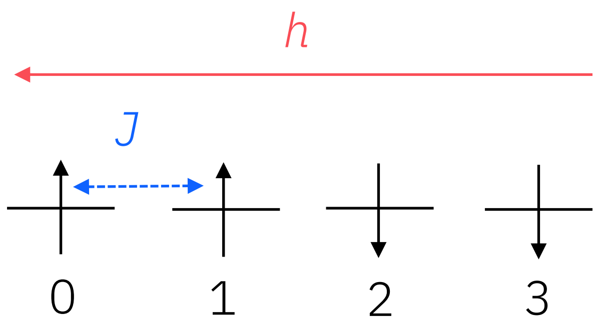
$$\hat{U}_{\text{ST2}_3} \approx \mathbb{I} + (-i\Delta t/2)(\hat{H}_1+\hat{H}_2) + \frac{(-i\Delta t/2)^2}{2}\left(\hat{H}_1+\hat{H}_2\right)^2$$

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

Error of the second-order Suzuki-Trotter

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

Example: Trotterization (second-order) Transverse Ising model



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

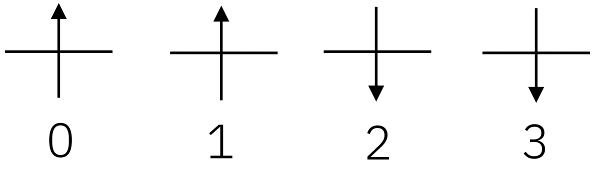
$$e^{-i\hat{H}\Delta t} = e^{-i\Delta t(-\sum_{i,j}^{N} J\sigma_{Z_i}\sigma_{Z_j} - \sum_{i}^{N} h_i\sigma_{X_i})}$$

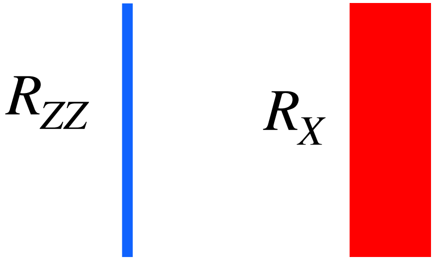
$$\approx e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_0}\sigma_{Z_1})} e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_1}\sigma_{Z_2})} e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_2}\sigma_{Z_3})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_0})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_1})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_2})}$$

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

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

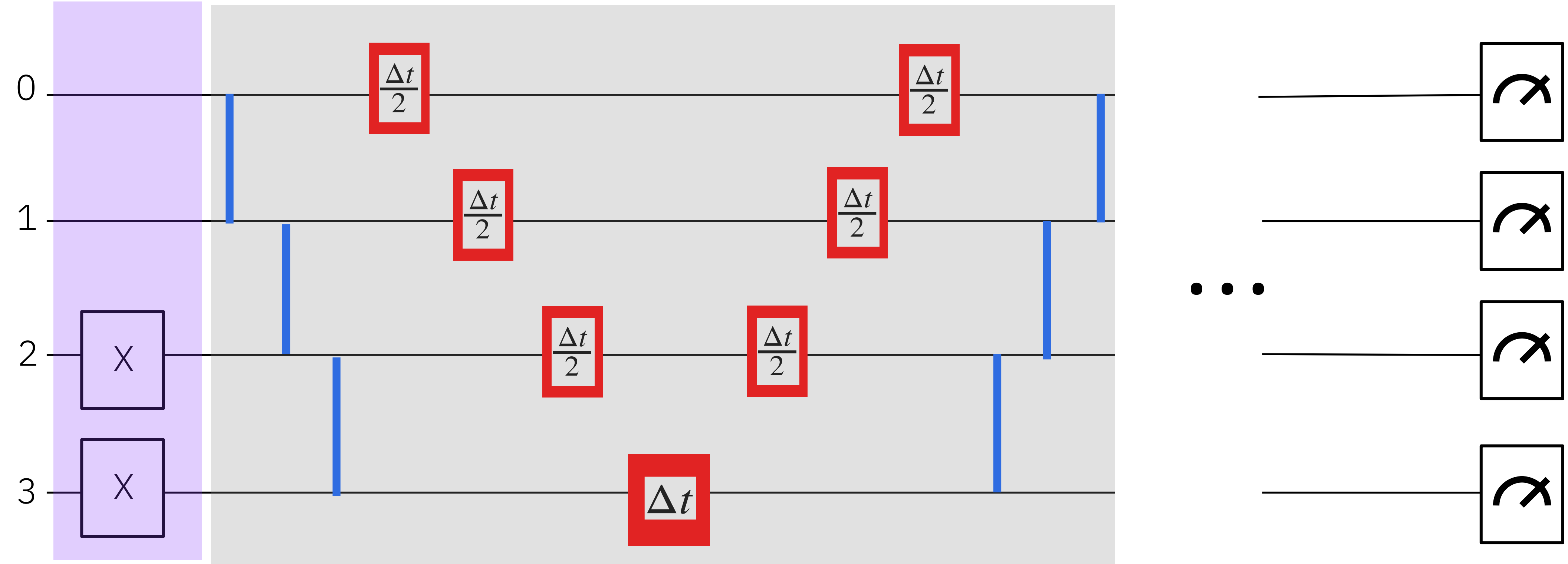
Example: Trotterization (second-order) Transverse Ising model





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

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

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

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

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

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

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

Connection with other lectures

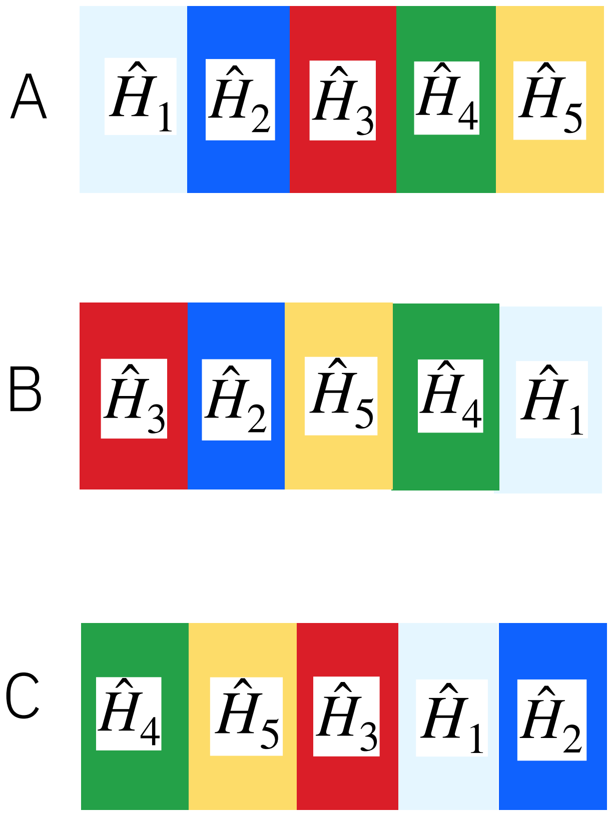
- Lecture 5: Quantum Phase Estimation
  - Quantum simulation can be a subroutine
  - The energy will emerge as the shift in the phase
  - Using the quantum chemistry Hamiltonian, we can get an accurate energy value of a molecule
- Lecture 6: Variational Quantum Eigensolver
  - We can use the quantum-classical 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

Hands-on session

- Quantum simulation with an ideal simulator
  - Monitoring time evolution of an observable
  - “Estimator” in Qiskit
- Quantum simulation with a quantum hardware
  - Time evolution of the wavefunction
  - “Sampler” in Qiskit

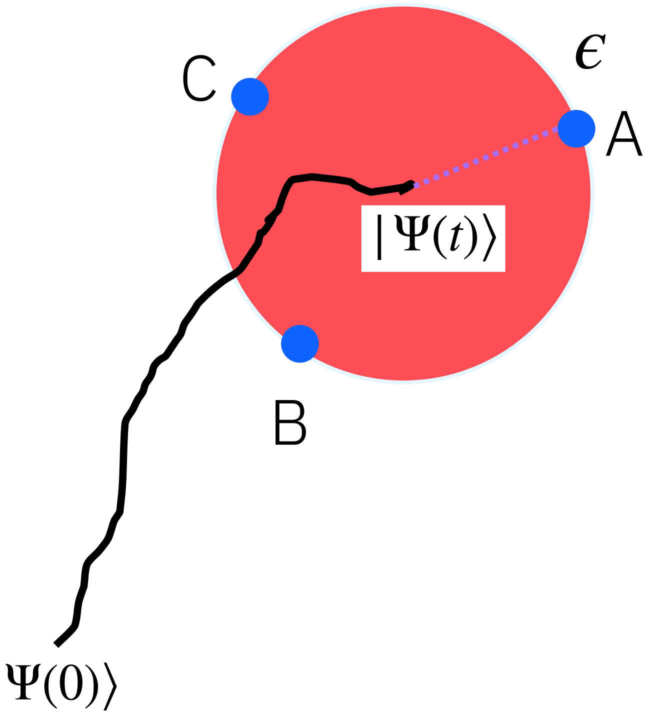
Randomization

Childs, Ostrander, Su, arXiv: 1805.08385



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

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



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

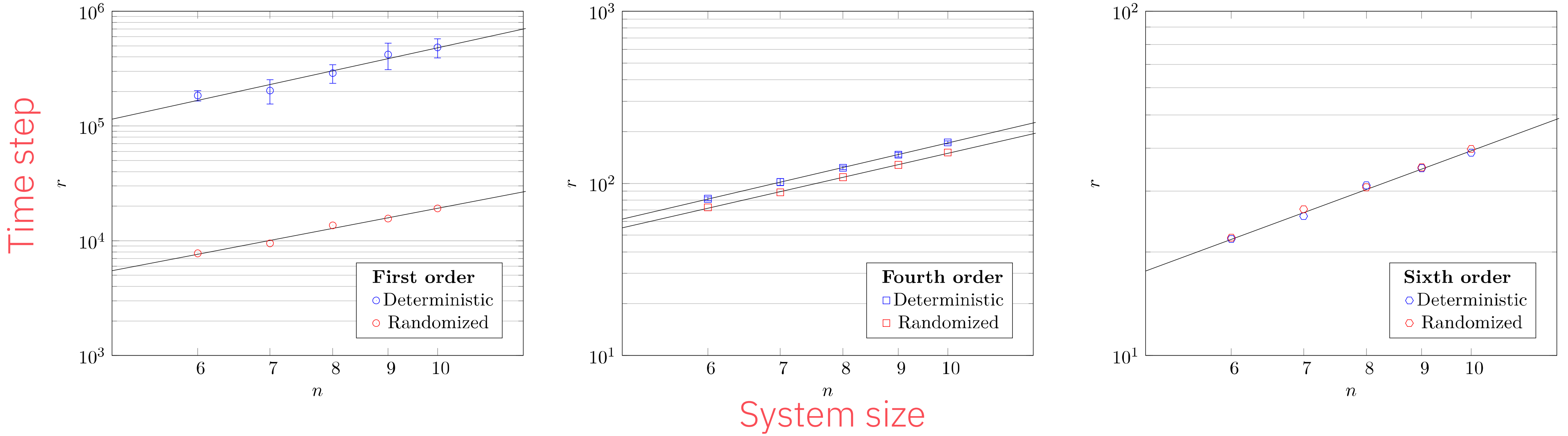


Figure 1: Comparison of the values of r between deterministic and randomized product formulas. Error bars are omitted when they are negligibly small on the plot. Straight lines show power-law fits to the data.

Calculation using a Heisenberg model

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

QDrift

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)

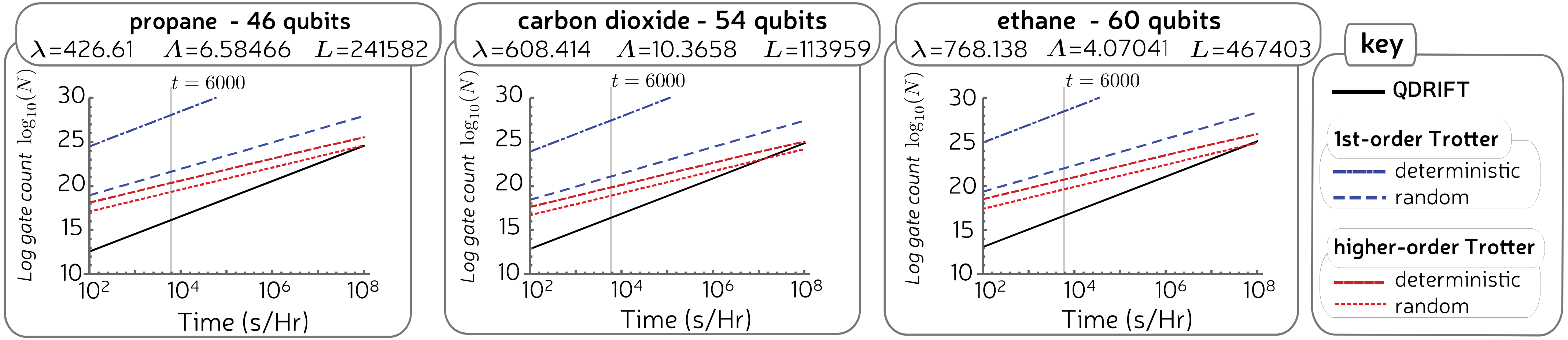


FIG. 2. The number of gates used to implement $U = \exp(iHt)$ for various t and $\epsilon = 10^{-3}$ and three different Hamiltonians (energies in Hartree) corresponding to the electronic structure Hamiltonians of propane (in STO-3G basis), carbon dioxide (in 6-31g basis), and ethane (in 6-31g basis).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

Randomization

- Scaling does not depend on the number of terms (QDrift)
- Advantageous for Hamiltonians with large number of terms (quantum chemistry)

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)

Thank you