Utility-Scale Experiment II

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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

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)

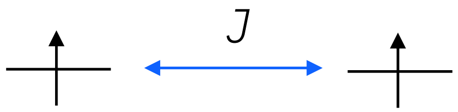
Lattice models for spin systems to study magnetic systems

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

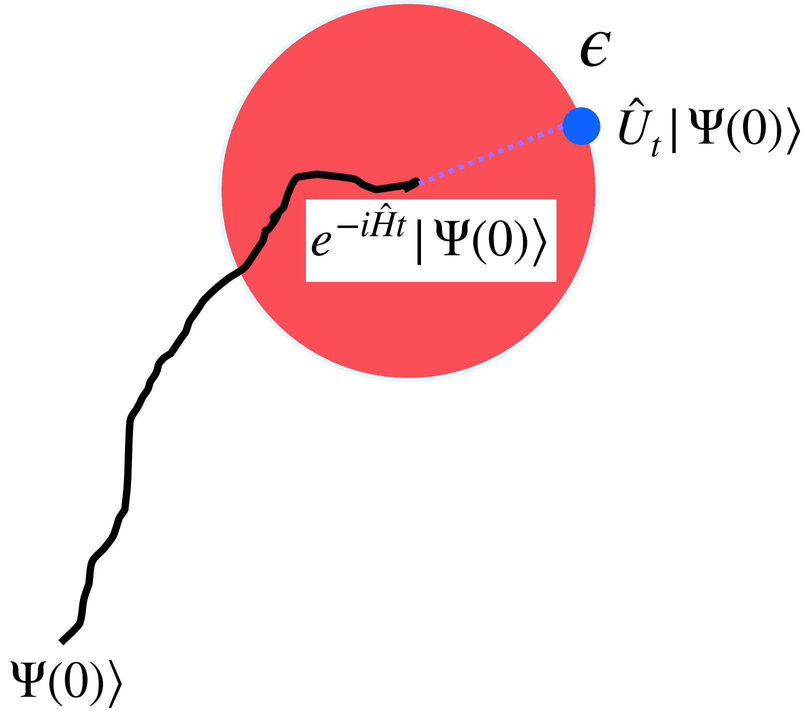
Algorithms for quantum simulations

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

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)



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

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

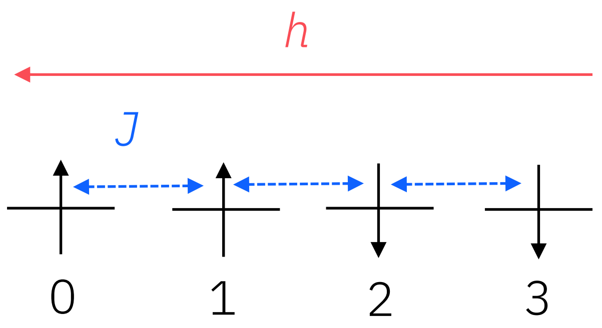
We will take "*n*" to be finite

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

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

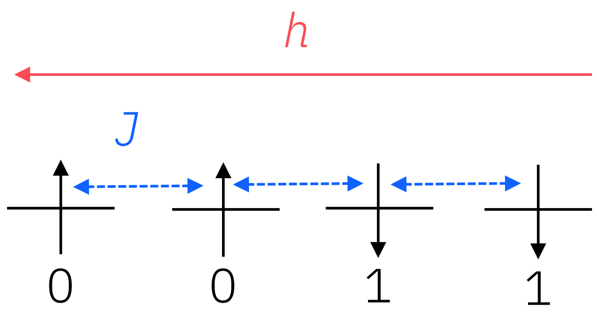
$$e^{-i\hat{H}\Delta t} = e^{-i\Delta t(-\sum_{i,j}^N J\sigma_{Z_i}\sigma_{Z_j} - \sum_i^N h_i\sigma_{X_i})} \approx \underbrace{e^{-i\Delta t(-\sum_{i,j}^N J\sigma_{Z_i}\sigma_{Z_j})}}_{R_{ZZ}(-2J\Delta t)} \underbrace{e^{-i\Delta t(-\sum_i^N h_i\sigma_{X_i})}}_{R_X(-2h\Delta t)}$$

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

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

Example: Trotterization (first-order)
Transverse Ising model

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



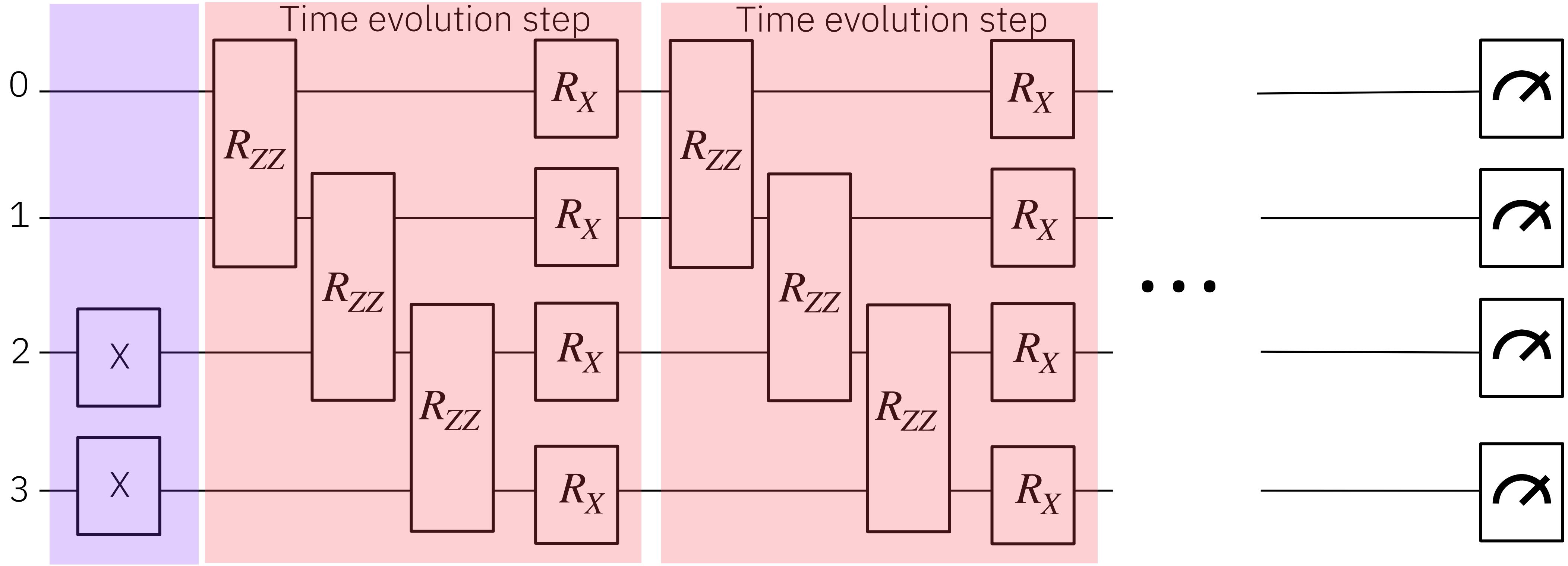
0: up spin

1: down spin

Bit strings

$|0011\rangle$

$|1100\rangle$



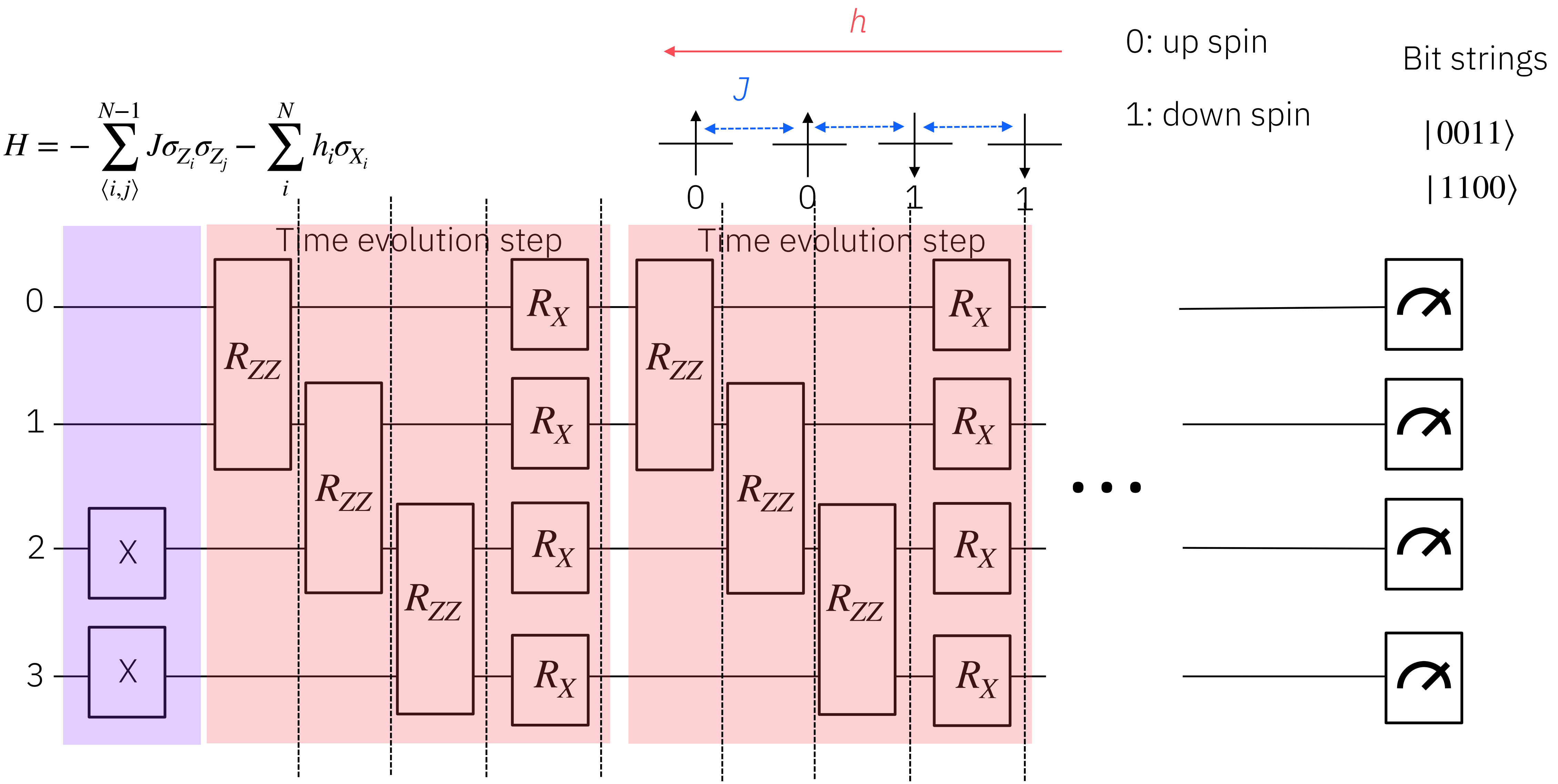
State preparation

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

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

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)

Magnetization

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

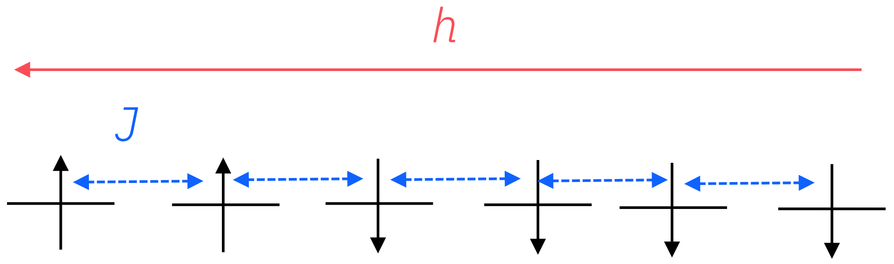
Expectation value

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

$Z|1\rangle = -|1\rangle$ −1

$|0\rangle = |\uparrow\rangle$

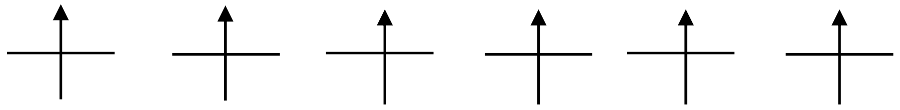
$|1\rangle = |\downarrow\rangle$



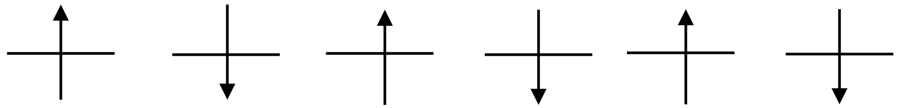
Magnetization

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

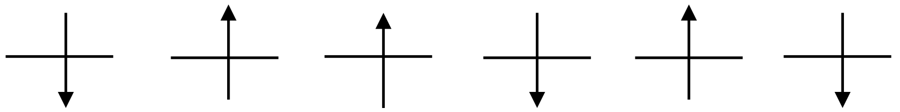
- Ferromagnetic
  - Aligned as same spin with the neighbor
  - Magnet at room temperature (iron)



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



- Paramagnetic
  - Show no magnetization without external field



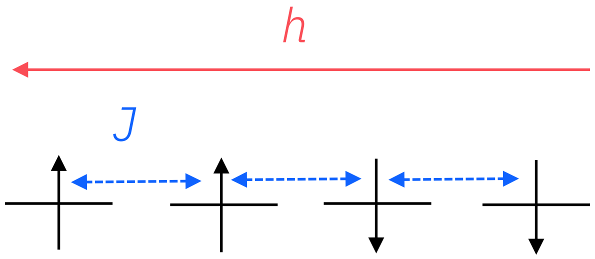
Metric for describing the magnetic state

Ground state of the 1D transverse-field Ising model

Magnetization

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

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



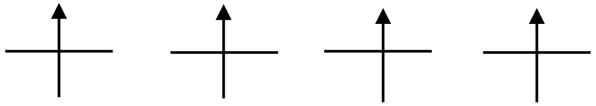
$$\sigma_{X_i}, \sigma_{Y_i}, \sigma_{Z_i} = X_i, Y_i, Z_i$$

– Interaction energy

Ground state (ignoring h)

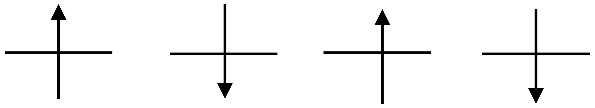
$Z_k Z_{k+1} = 1 \quad (1,1), (-1,-1)$

$-J < 0$



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

$-J > 0$

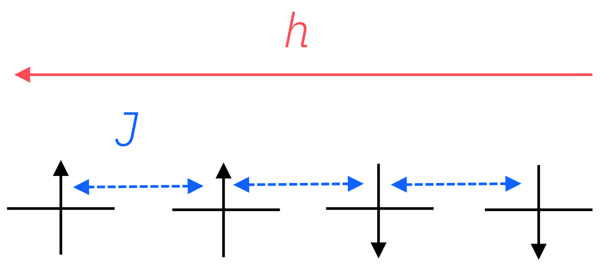


With large h: the configuration becomes disordered

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

Dynamical quantum phase transition

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



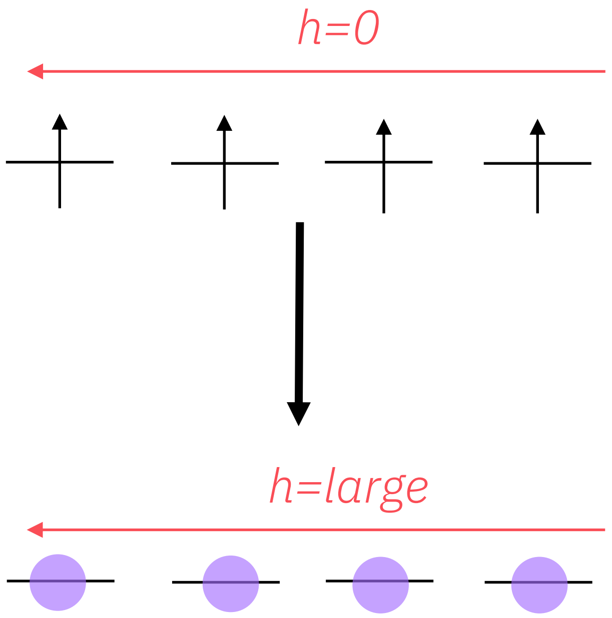
Magnetization

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

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

Ferromagnetic (–J < 0)

?



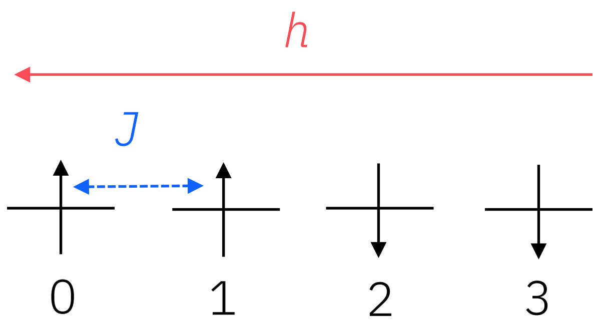
Monitor time evolution of the magnetization

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

Example: Trotterization (second-order)
Transverse Ising model

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



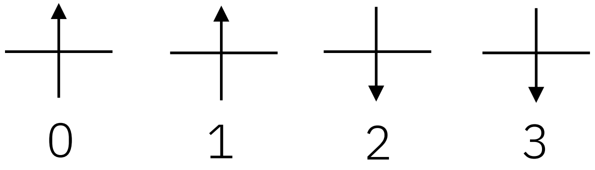
$$e^{-i\hat{H}\Delta t} = e^{-i\Delta t(-\sum_{i,j}^{N} J\sigma_{Z_i}\sigma_{Z_j} - \sum_{i}^{N} h_i\sigma_{X_i})}$$

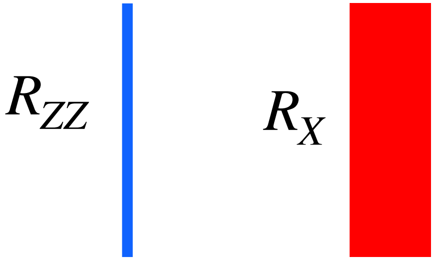
$$\approx e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_0}\sigma_{Z_1})} e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_1}\sigma_{Z_2})} e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_2}\sigma_{Z_3})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_0})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_1})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_2})}$$

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

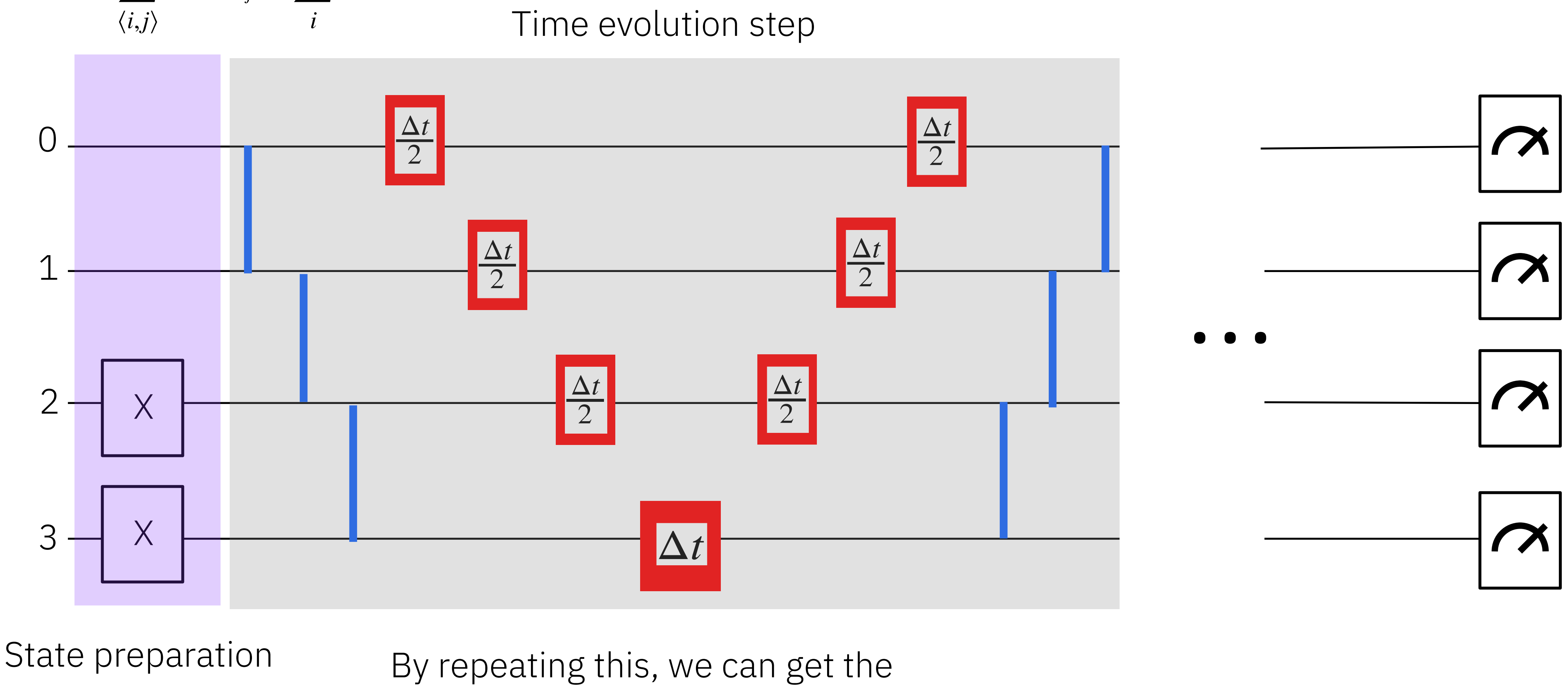
$$e^{-i\frac{\Delta t}{2}(-h\sigma_{X_2})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_1})} e^{-i\frac{\Delta t}{2}(-h\sigma_{X_0})} e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_2}\sigma_{Z_3})} e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_1}\sigma_{Z_2})} e^{-i\frac{\Delta t}{2}(-J\sigma_{Z_0}\sigma_{Z_1})}$$

Example: Trotterization (second-order)
Transverse Ising model





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



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)

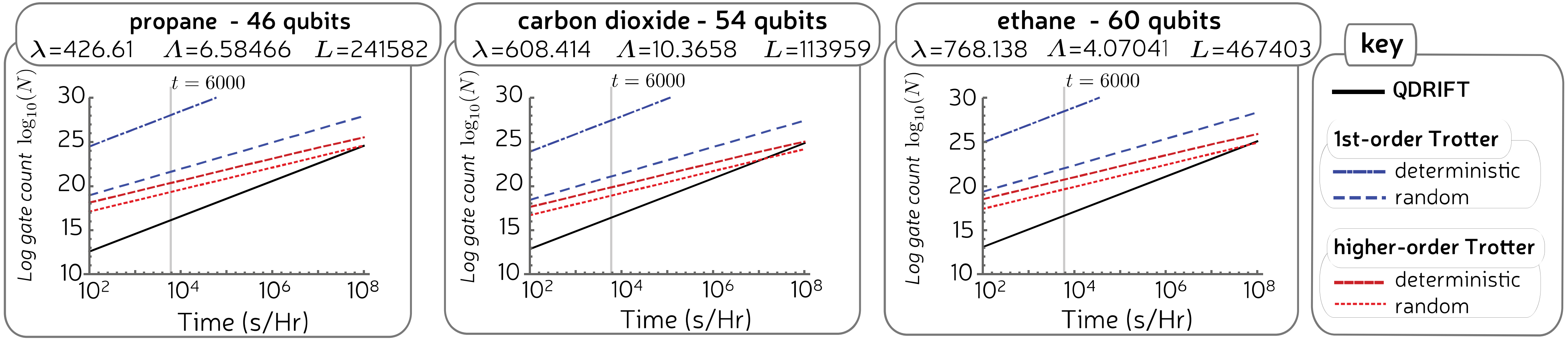


FIG. 2. The number of gates used to implement $U = \exp(iHt)$ for various t and $\epsilon = 10^{-3}$ and three different Hamiltonians (energies in Hartree) corresponding to the electronic structure Hamiltonians of propane (in STO-3G basis), carbon dioxide (in 6-31g basis), and ethane (in 6-31g basis).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

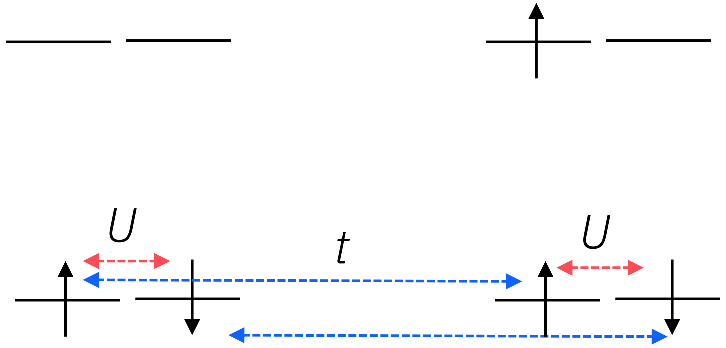
$$N_{\text{gates}} = O\left(\frac{2\lambda^2 t^2}{\epsilon}\right)$$

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

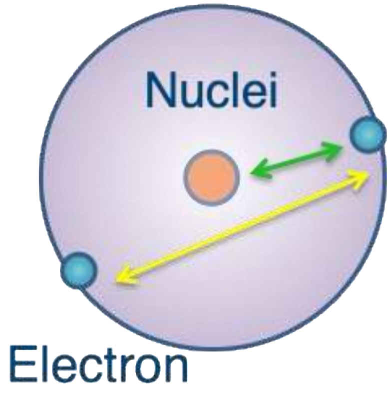
– Quantum Chemistry Hamiltonian

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

Kinetic energy of electrons

Electron-nucleus attraction

Electron-electron repulsion



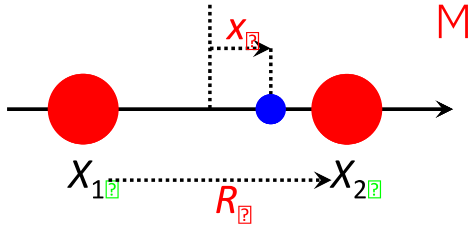
Complexity & Computational resources

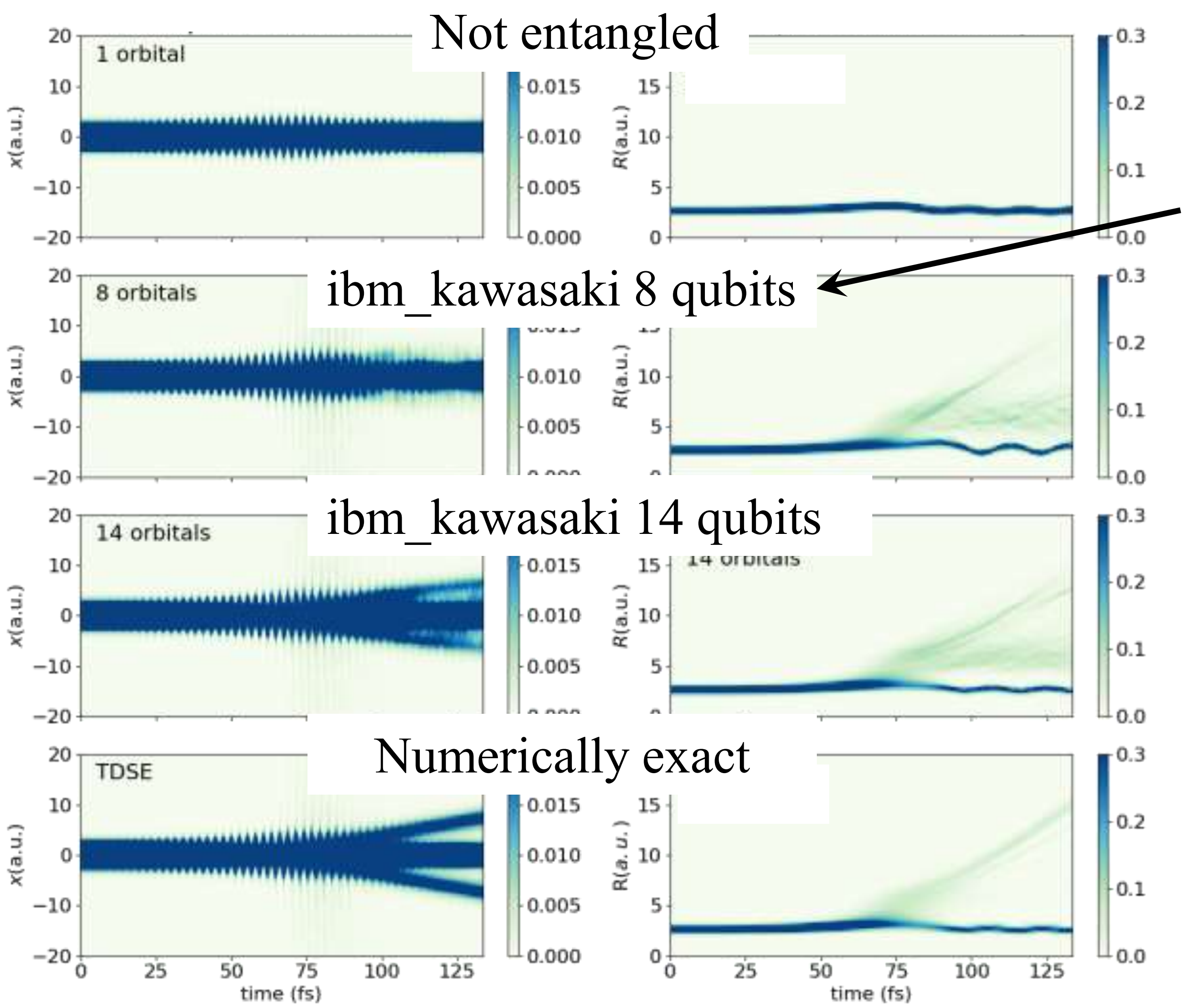
What can we do with quantum simulation: Electron and nuclear dynamics

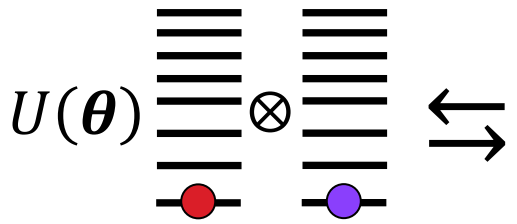
Univ of Tokyo, Professor Sato

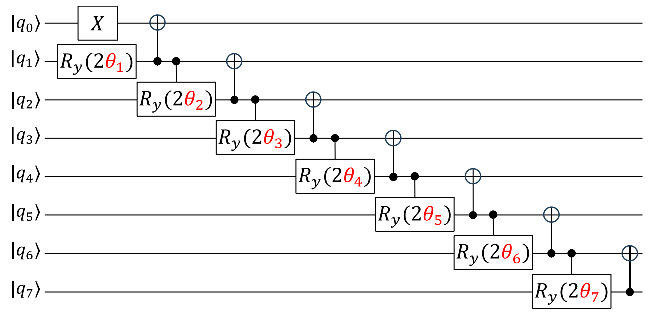
Electron density $\rho_e(x)$ Nuclear density $\rho_n(R)$

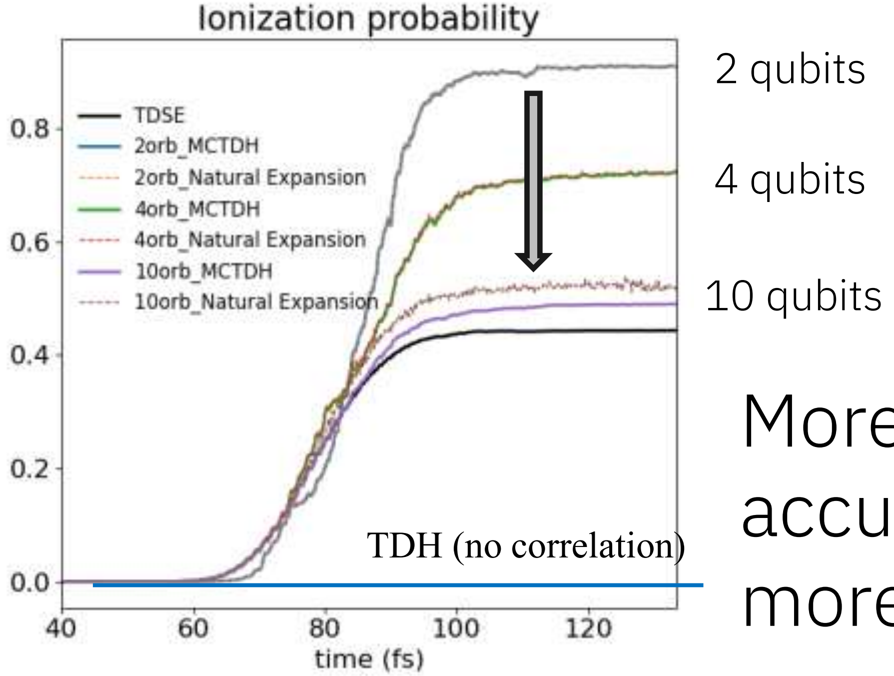
Molecule in a strong laser field











More accurate with more qubits

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Reference

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

Thank you