Road to Quantum Utility Workshop 2025

Quantum Chemistry

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Overview

1. Why Quantum Chemistry?
2. The goal of Hamiltonian simulation
3. A real experiment example
4. Hamiltonian
5. Approximation Methods for Hamiltonian Simulations
6. Qiskit Coding Session
7. Summary

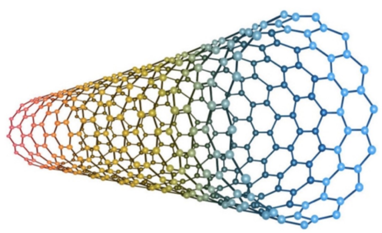
Why Quantum Simulation?

Certain tasks like simulating nature is not tractable with classical computation

Quantum computations are viable candidates to handle such simulations

Also frequently referred to as Hamiltonian Simulation

Materials Science and Chemistry



Drug Discovery and Development

Energy Optimization and Renewable Energy

...and more!

The Goal: Obtain the wave function

Time-dependent Schrödinger equation

$$\hat{H}\Psi(t) = i\hbar\frac{\partial}{\partial t}\Psi(t)$$

$\hat{H}$ **Hamiltonian**
corresponds to the total energy of the system

The goal is to compute the **wave function** that satisfies the above

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

The wave function contains vital information about a particle system

$\hat{E}$	$\hat{x}$	$\hat{p}$	$\hat{L}$
energy	position	momentum	orbital angular momentum ~ Spin

Hamiltonian

Hamiltonian in general

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

$$\hat{H} = \underbrace{\hat{T}}_{\text{Kinetic Energy}} + \underbrace{\hat{V}}_{\text{Potential Energy}}$$

Important in many fields

- Quantum chemistry (material science)
- Condensed matter physics
- High-energy physics

Spin Hamiltonian

In Quantum Simulations, these energies can come from spin 1/2 interactions and external magnetic fields

$$\hat{H} = \underbrace{\hat{T}}_{\text{KE: spin interactions}} + \underbrace{\hat{V}}_{\text{PE: external magnetic field}}$$

Spin Hamiltonian in different lattice models

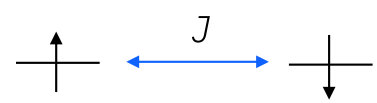
Lattice models for spin systems to study magnetic systems

Spin interaction

External field

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

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

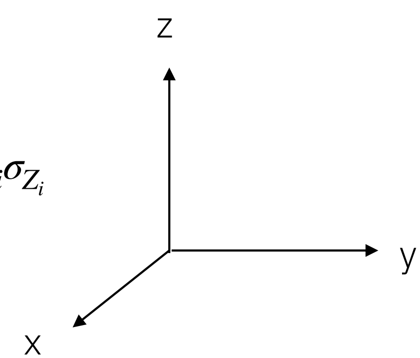


  - XY model (*n*=2)

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

  - 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

Pauli matrices

- Pauli matrices play a critical role in describing spin ½. (Usually written as $\boldsymbol{\sigma_x}, \boldsymbol{\sigma_y}, \boldsymbol{\sigma_z},$)
- Linear algebraic characteristics: Hermitian, traceless, and unitary
- They represent operators which gives us a projection of spin of electrons along the x, y, z, axis
- And the good news is that they **can be implemented as quantum gates** on a quantum computer!

Pauli Operators

Pauli x $$\sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Pauli y $$\sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Pauli z $$\sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Rotational gates

$$\boldsymbol{R_x(\theta) = e^{-i\frac{\theta}{2}\sigma_x} = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -i\sin\left(\frac{\theta}{2}\right) \\ -I\,sin\left(\frac{\theta}{2}\right) & cos\left(\frac{\theta}{2}\right) \end{pmatrix}}$$

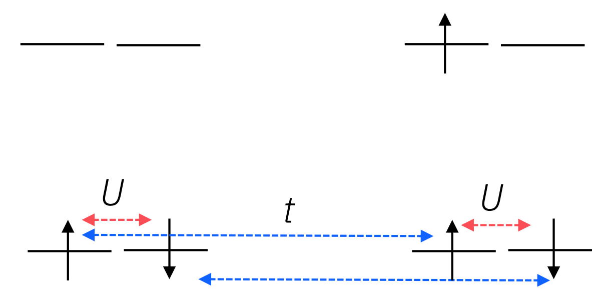
$$\boldsymbol{R_y(\theta) = e^{-i\frac{\theta}{2}\sigma_y} = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right) \\ sin\left(\frac{\theta}{2}\right) & cos\left(\frac{\theta}{2}\right) \end{pmatrix}}$$

$$\boldsymbol{R_z(\theta) = e^{-i\frac{\theta}{2}\sigma_z} = \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix}}$$

Second quantization

– Hubbard model

Describe conducting and insulating systems



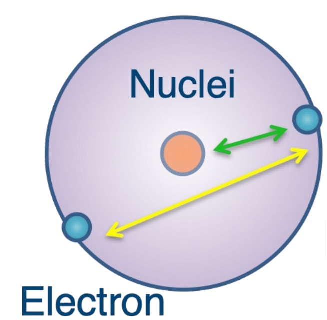
$$H = -t \sum_{i,\sigma} \left(\hat{a}^{\dagger}_{i,\sigma} \hat{a}_{i+1,\sigma} + \hat{a}^{\dagger}_{i+1,\sigma} \hat{a}_{i,\sigma} \right) + U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}$$

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

Creation operator   Annihilation operator

– Quantum Chemistry Hamiltonian

The Born-Oppenheimer approximation neglects the motion of the atomic nuclei



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

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

Complexity & Computational resources

Mapping the Hamiltonian

Map the second-quantized Hamiltonian to qubits:

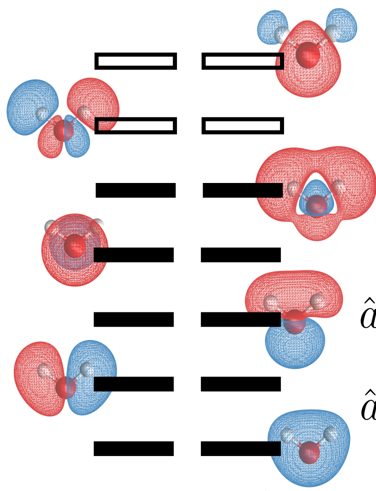
$$H = -t \sum_{i,\sigma} \left(\hat{a}^\dagger_{i,\sigma} \hat{a}_{i+1,\sigma} + \hat{a}^\dagger_{i+1,\sigma} \hat{a}_{i,\sigma} \right) + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}$$

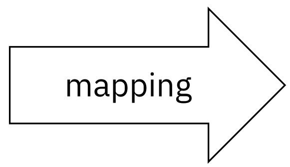
Hubbard, Quantum chemistry

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

Fermions

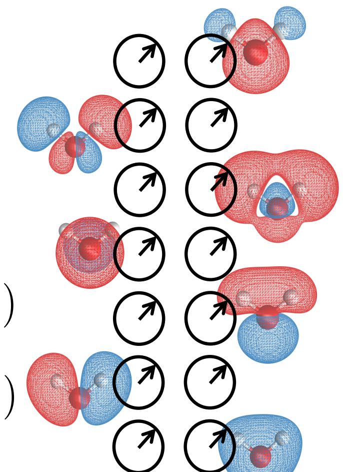
$$\{a_i, a_i\} = 0,\ \{a_i^\dagger, a_i^\dagger\} = 0, \{a_i, a_i^\dagger\} = \delta_{i,j}$$





Spins

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



Jordan-Wigner

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

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

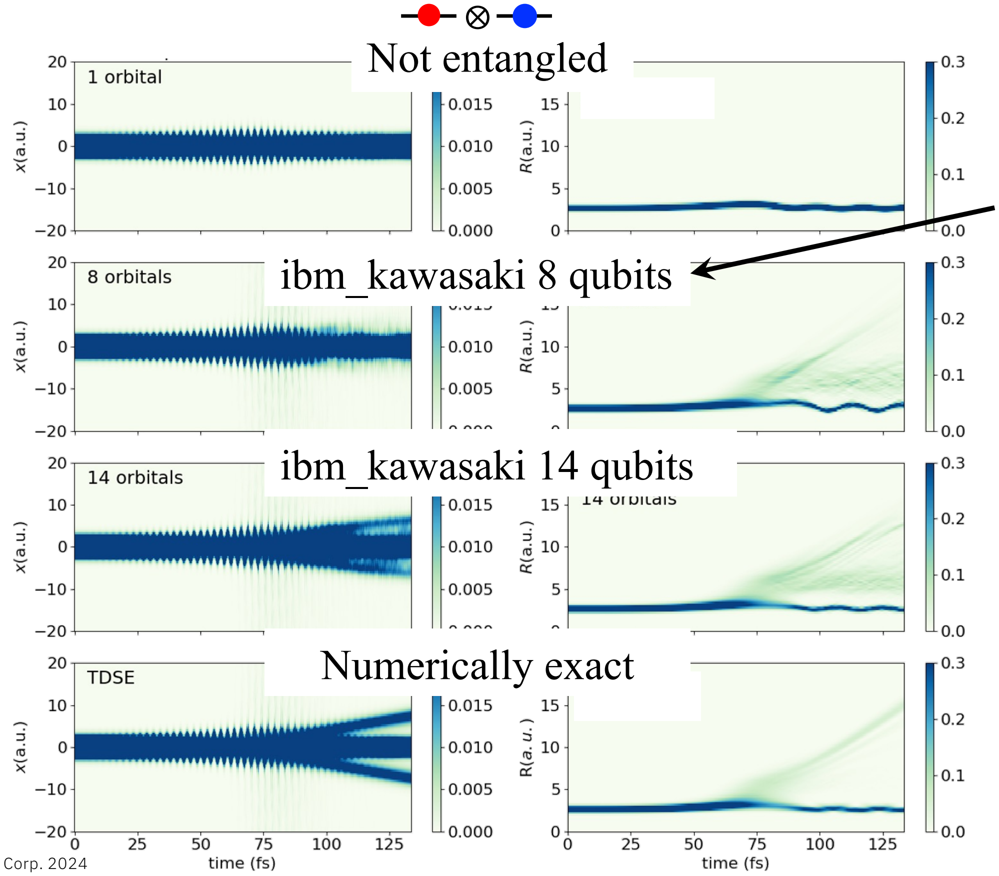
$$\hat{H}_{elec} = \sum_{pq} h_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

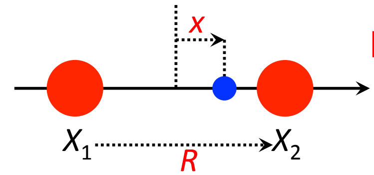
$$\hat{H}_{elec} = \sum_i c_i \hat{P}_i$$

Simulation example: H^+_2

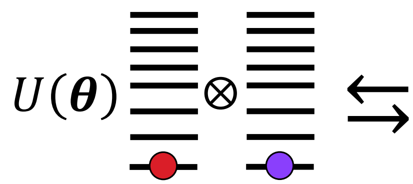
Experimental results provided by Prof. Sato at the University of Tokyo

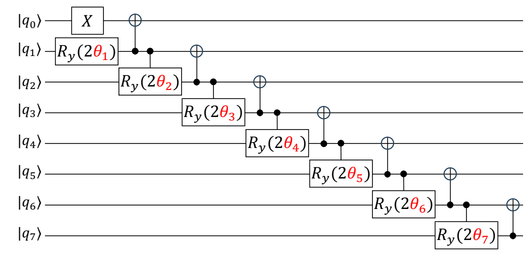
Electron density $\rho_e(x)$ Nuclear density $\rho_n(R)$

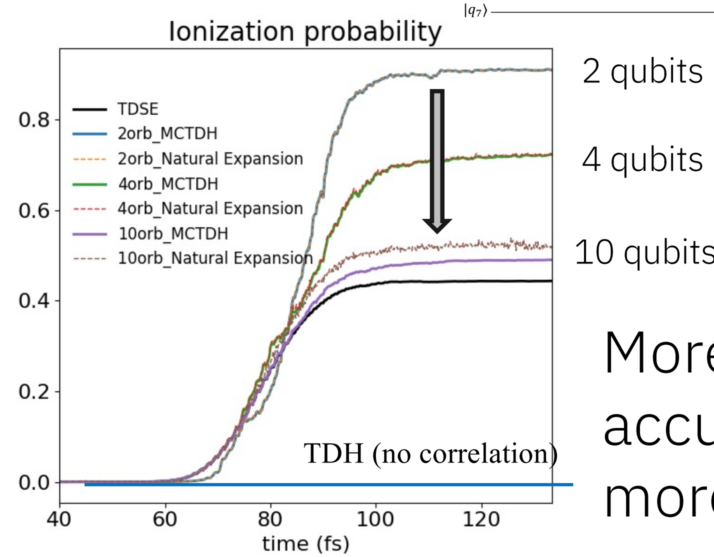




Molecule in a strong laser field





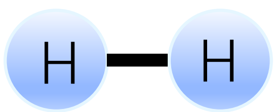


More accurate with more qubits

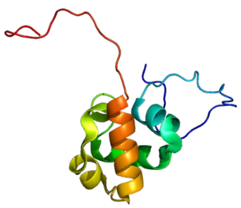
Motivation

$$\hat{H}\Psi = E\Psi$$

Computing and storing information of the wave function is very challenging



Ψ is $\sim 10^{12}$



Ψ is $\sim 10^{100,000}$

Simulating larger molecules requires extremely large memory on the classical computer

One of the most important application on quantum computers

- Quantum chemistry (material science)
- High-energy physics

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Subatomic particles

	Spin	Elementary particle examples
Bosons	1	photons, gluons, mesons, W bosons, Z bosons
Fermions	1/2	electrons, protons, neutrons, neutrinos
Higgs-Boson	0	Higgs particle

Bosons have integer spins (e.g.,1, 2, 3, etc.)

Fermions have half-odd integer spins (e.g., $^1/_2$, $^3/_2$, etc.)

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

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

These our Pauli operators!

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

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

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

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

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

How will this be mapped?

Try mapping a one-body term

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

$$a_3^\dagger a_3 = \frac{1}{2}\left(X_3 - iY_3\right) \otimes Z_2Z_1Z_0 \times \frac{1}{2}\left(X_3 + iY_3\right) \otimes Z_2Z_1Z_0$$

$$= \frac{1}{4}\left(X_3Z_2Z_1Z_0 - iY_3Z_2Z_1Z_0\right) \times \left(X_3Z_2Z_1Z_0 + iY_3Z_2Z_1Z_0\right) = \frac{1}{4}\left(I + I + iX_3Y_3 - iY_3X_3\right)$$

$$= \frac{1}{4}\left(I + I + iX_3Y_3 - iY_3X_3\right) = \frac{1}{2}\left(I + iX_3Y_3\right) = \frac{1}{2}\left(I - Z_3\right)$$

How about a two-body term?

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

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

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

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

The equations are tedious, but the idea is simple

Mapping the Hamiltonian

General equation

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

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

Fermionic Hamiltonian

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

$$\downarrow$$

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

Procedure for Quantum Simulation

The Challenge

Computing this is not easy

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

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

Approximating the solution

Recall: The goal was to compute the wave function at time t.

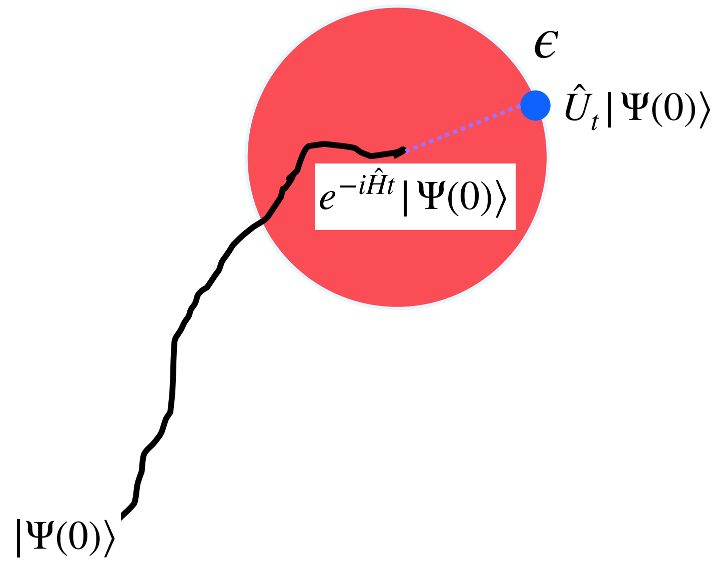
$$|\Psi(t)\rangle = e^{-i\hat{H}t}|\Psi(0)\rangle$$

Obtaining an exact solution is extremely difficult.
We approximate the solution within a small error range

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

- There are several strategies for keeping the error small
  - Small error -> Shallow circuit depth

- Methods
  - 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 (also known as the Trotter 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

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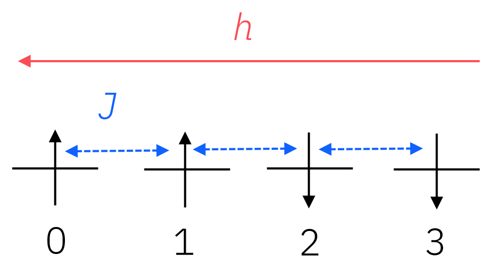
We will take “*n*” to be finite

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

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

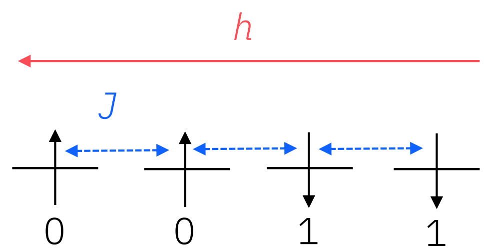
$$e^{-i\hat{H}\Delta t} = e^{-i\Delta t(-\sum_{i,j}^{N} J\sigma_{Z_i}\sigma_{Z_j} - \sum_{i}^{N} h_i\sigma_{X_i})} \approx \underbrace{e^{-i\Delta t(-\sum_{i,j}^{N} J\sigma_{Z_i}\sigma_{Z_j})}}_{R_{ZZ}(-2J\Delta t)} \underbrace{e^{-i\Delta t(-\sum_{i}^{N} h_i\sigma_{X_i})}}_{R_X(-2h\Delta t)}$$

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

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

Trotterization (1st order): Time evolution of the **wave function**
Transverse Ising Model

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



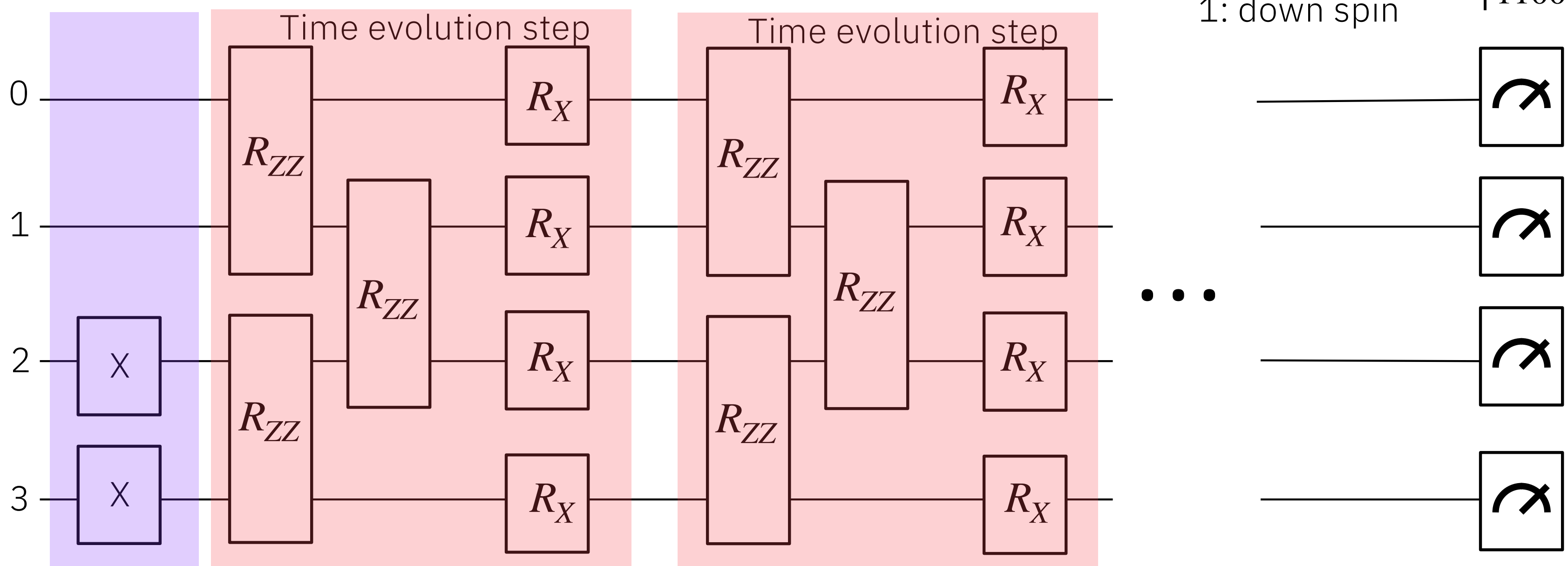
0: up spin

1: down spin

Bit strings

$|0011\rangle$

$|1100\rangle$

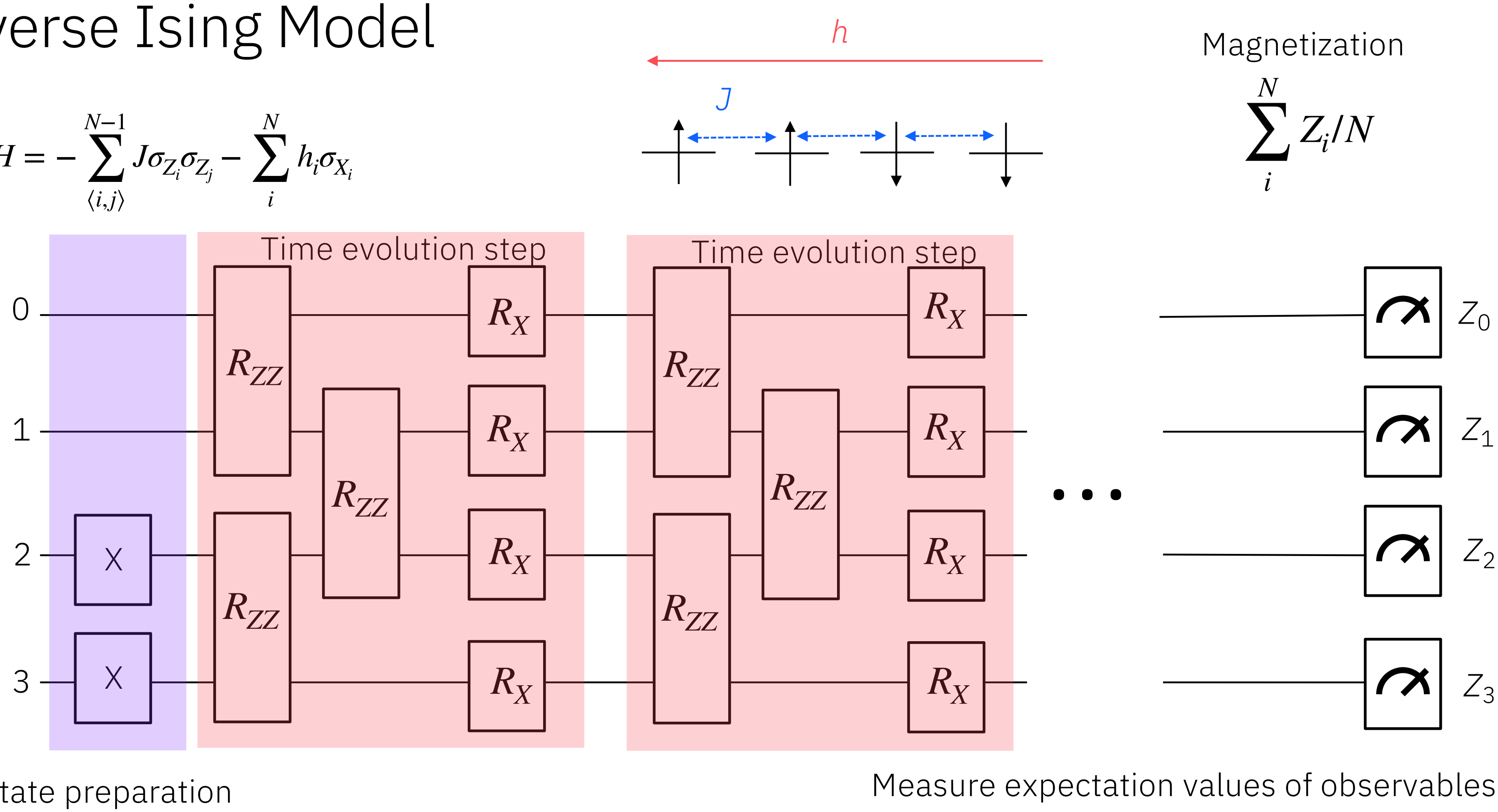


State preparation

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

Trotterization (1st order): Time evolution of an **observable**
Transverse Ising Model

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



Suzuki-Trotter Formula (2nd order)

Hamiltonian (general form)

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

Second-order Suzuki–Trotter formula

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

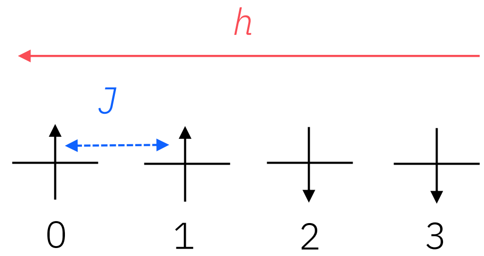
Again, let us focus on a simple Hamiltonian

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

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

Example: Trotterization (second-order)
Transverse Ising model

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



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

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

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

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

Error in Suzuki-Trotter Formula (2nd order)

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

The exact Taylor expansion truncated at the 3rd order

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

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

The Taylor expansion for each term (3rd order) in the 2nd order Suzuki-Trotter Formula

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

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

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

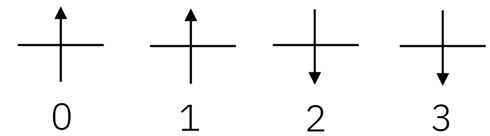
$$\hat{U}_{\text{ST2}_3} \approx \mathbb{I} + (-i\Delta t/2)(\hat{H}_1 + \hat{H}_2) + \frac{(-i\Delta t/2)^2}{2}\left(\hat{H}_1 + \hat{H}_2\right)^2$$

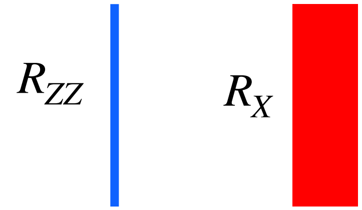
$$+\frac{(-i\Delta t/2)^3}{6}\left[\hat{H}_1^3 + \frac{3}{2}(\hat{H}_1\hat{H}_2^2 + \hat{H}_2^2\hat{H}_1 + \hat{H}_1\hat{H}_2\hat{H}_1) + \frac{3}{2}(\hat{H}_2\hat{H}_1^2 + \hat{H}_1^2\hat{H}_2 + \hat{H}_2^3)\right]$$

Error of the second-order Suzuki-Trotter

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

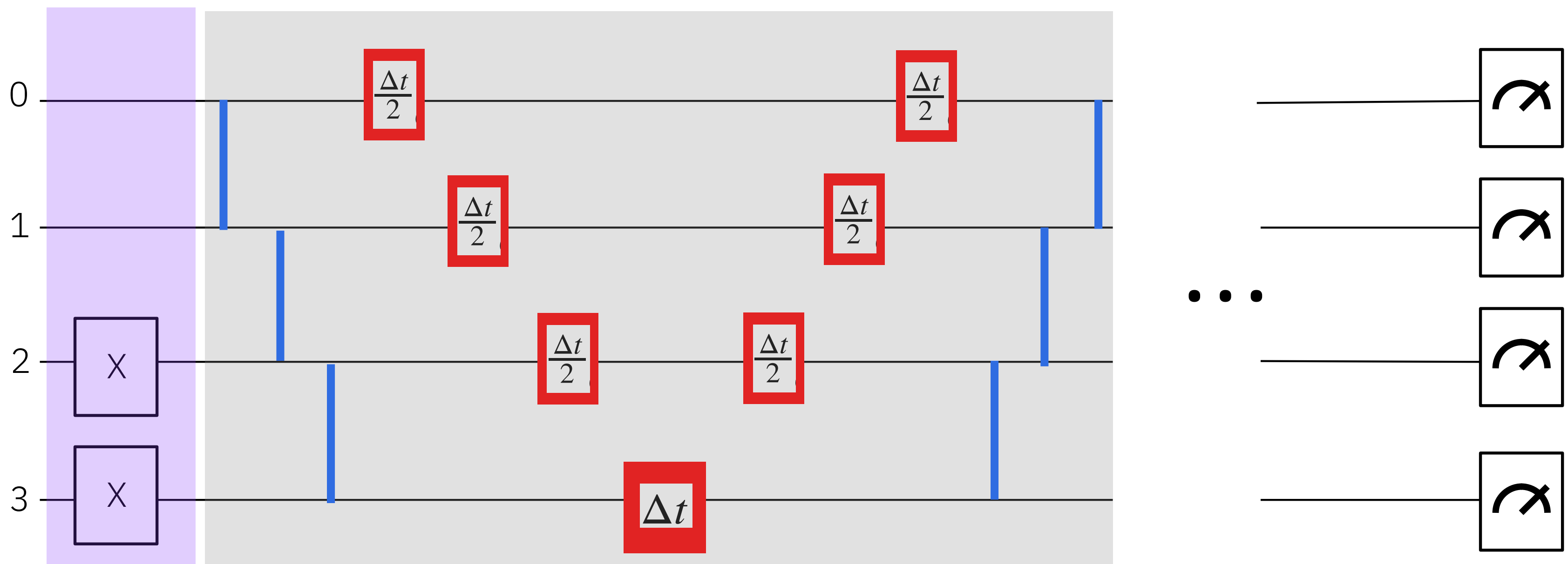
Example: Trotterization (second-order)
Transverse Ising model





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

Time evolution step



State preparation

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

Suzuki-Trotter recursion formula for higher ($\mathcal{P}^{\text{th}}$) order

Second-order Suzuki–Trotter formula $$e^{-itH} \approx \hat{U}_{ST2}(t) = \prod_{j=1}^{L} e^{-ia_j P_j \frac{t}{2}} \prod_{j'=L}^{1} e^{-ia_{j'} P_{j'} \frac{t}{2}}$$

$\mathcal{P} = 2k$

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

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

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

Reasons to study product formulas (trotterization)

- The method is intuitive and easy to implement
- Number of qubits required is minimal (no auxiliary qubits required)
- The scaling of the gate depth against the error is not optimal
  - First-order trotter error: $O\left(t^2/\epsilon\right)$
  - Second-order trotter error: $O\left(t^{1.5}/\epsilon^{0.5}\right)$

Qiskit Coding Session

Building utility-scale circuits

Evolution of the transverse Ising model

The `PauliEvolutionGate` implements $U(t) = e^{-itH}$

Ising model on spin-1/2 particles:

$$H = \underbrace{-J \sum_{jk} Z_j Z_k}_{H_{ZZ}} + \underbrace{h \sum_j X_j}_{H_X}$$

```python
from qiskit.circuit.library import PauliEvolutionGate
from qiskit.quantum_info import Statevector, SparsePauliOp

def get_hamiltonian(nqubits, J, h, alpha):

    # List of Hamiltonian terms as 3-tuples containing
    # (1) the Pauli string,
    # (2) the qubit indices corresponding to the Pauli string,
    # (3) the coefficient.
    Hzz = [("ZZ", [i, i + 1], -J) for i in range(0, nqubits - 1)]
    Hz = [("Z", [i], -h * np.sin(alpha)) for i in range(0, nqubits)]
    Hx = [("X", [i], -h * np.cos(alpha)) for i in range(0, nqubits)]

    # We create the Hamiltonian as a SparsePauliOp, via the method
    # `from_sparse_list`, and multiply by the interaction term.
    hamiltonian = SparsePauliOp.from_sparse_list([*Hzz, *Hz, *Hx], num_qubits=nqubits)
    return hamiltonian.simplify()
```


IBM quantum utility paper: https://www.nature.com/articles/s41586-023-06096-3
API docs: https://docs.quantum.ibm.com/api/qiskit/qiskit.circuit.library.PauliEvolutionGate

Qiskit Coding Session

Please have the Jupyter notebook downloaded and ready

What we will demonstrate in this coding session:

1. Quantum simulation with an ideal simulator
   - Time evolution of an observable
   - Estimator in Qiskit
2. Quantum simulation with a quantum hardware
   - Time evolution of the wavefunction
   - Sampler in Qiskit

Summary

Hamiltonian Simulations in the context of simulating nature (e.g., chemistry, condensed matter physics applications) are one of the most promising areas for quantum computing to show advantage.

Solving the wave function is key to simulation and obtaining physical observables of interest

However, calculating the wave function exactly is very challenging and algorithms that can approximate the solution effectively is an active area of research

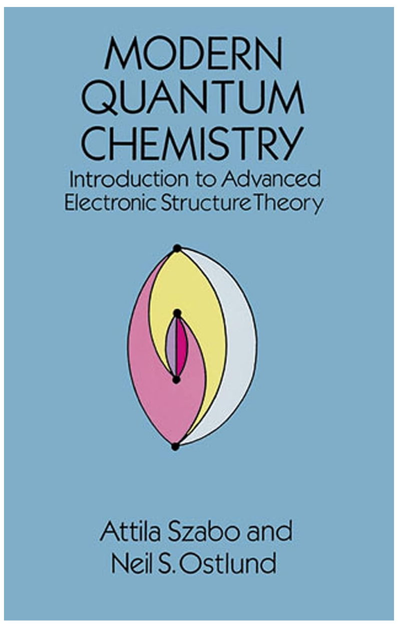
Trotterization is a widely used mathematical approach to simulate Hamiltonians on a quantum computer

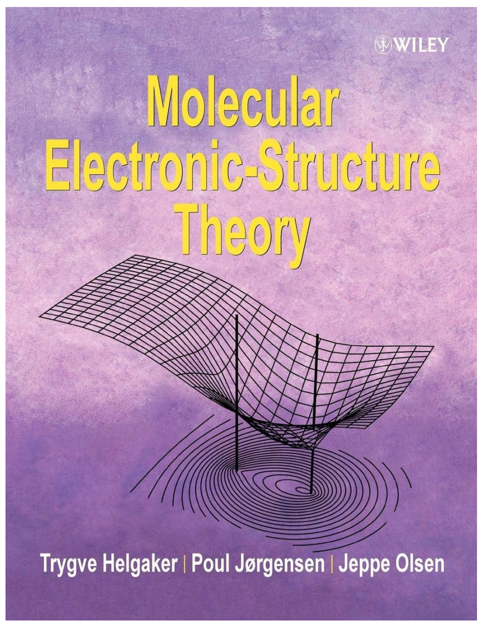
While higher order trotterization may provide better accuracy of results, it increases circuit depth and is something to consider when computing on near-term quantum computers.

Time evolution circuits we saw today play an important role in running utility-scale experiments.

Further Reading

1. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory by Attila Szabo, Neil S. Ostlund
2. Molecular Electronic-Structure Theory 1st Edition by Trygve Helgaker, Poul Jorgensen, Jeppe Olsen





Thank you!