Introduction to Adiabatic Evolution and Variational Quantum Eigensolver

application to simulate 1D Heisenberg model and its Qiskit realization

Jerry TianShen He

M.S. in Physics – Quantum Computing

WQCC: Advanced Topics in Quantum Computing Study Session I
October 2022

Table of Contents

WQCC
Wisconsin Quantum Computing Club

Table of Contents

|WQCC⟩ Wisconsin Quantum Computing Club

Significance of ground state simulation

- electronic structures of matter
- molecular formations
- magnetization
- quantum phase transitions

One of the key tasks in condensed matter physics

WQCC
Wisconsin Quantum Computing Club

Introduction

Classical approaches:
Impossible, due to the exponential growth of the Hilbert space with respect to the system size.

Semiclassical approaches:

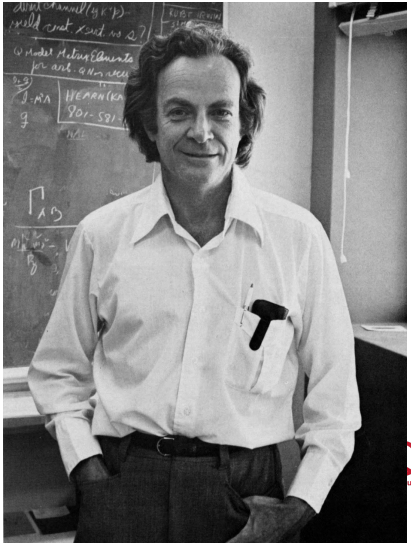
- Density functional theory
- Quantum Monte Carlo
- Density matrix renormalization group
- Machine learning

It's difficult to unravel quantum features with classical simulations.

WQCC Wisconsin Quantum Computing Club

Introduction

"Nature isn't classical, and if you want to make a simulation of Nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem because it doesn't look so easy."
– Richard Phillips Feynman



Introduction

On quantum simulators:

- Imaginary time evolution
- Adiabatic evolution (AE)
- Variational Quantum Eigensolver (VQE)

VQE fits the current Noisy Intermediate Scale Quantum (NISQ) simulators.

Table of Contents

WQCC
Wisconsin Quantum Computing Club

Adiabatic evolution

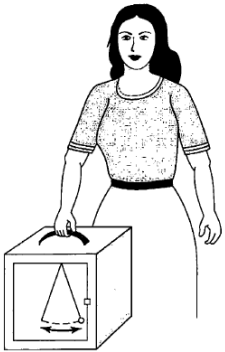
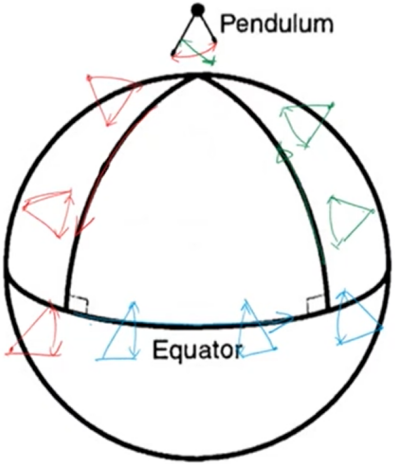


Figure 12.1: Adiabatic motion: If the case is transported gradually, the pendulum inside keeps swinging with the same amplitude, in a plane parallel to the original one.



[1]Images: Lecture Notes on Quantum Mechanics, Jiang Xiao

Adiabatic evolution

Adiabatic theorem

- Suppose through time H_i changes into H_f
- The n^{th} eigenstate of H_i evolves into the n^{th} eigenstate of H_f if
  - 1. The change is slow
  - 2. The energy gap is finite
- with an additional geometric phase (Berry phase)

We can prepare the ground state of a complex Hamiltonian starting from a simpler one.

Complex = Many-body
Simple = Two-body

|WQCC⟩ Wisconsin Quantum Computing Club

Proof of adiabatic condition

$$H(t)|n(t)\rangle = E_n(t)|n(t)\rangle, |\psi(t)\rangle = \Sigma_n c_n(t)|n(t)\rangle, i\hbar|\dot{\psi}(t)\rangle = H(t)|\psi(t)\rangle$$

$$i\hbar\dot{c}_m(t) + i\hbar\Sigma_n c_n(t)\langle m(t) \mid \dot{n}(t)\rangle = c_m(t)E_m(t)$$

$$\dot{H}(t)|n(t)\rangle + H(t)|\dot{n}(t)\rangle = \dot{E}_n(t)|n(t)\rangle + E_n(t)|\dot{n}(t)\rangle$$

$$\langle m(t) \mid \dot{n}(t)\rangle = -\frac{\langle m(t)|\dot{H}(t)|n(t)\rangle}{E_m(t) - E_n(t)} \quad (m \neq n)$$

$$\dot{c}_m(t) + \left(\frac{i}{\hbar}E_m(t) + \langle m(t) \mid \dot{m}(t)\rangle\right) c_m(t) = \sum_{n\neq m} \frac{\langle m(t)|\dot{H}|n(t)\rangle}{E_m(t) - E_n(t)} c_n(t)$$

$$c_m(t) = c_m(0)e^{i\theta_m(t)}e^{i\gamma_m(t)}, \theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n\left(t'\right)dt'$$

$$0 = \frac{d}{dt}(\langle m(t) \mid m(t)\rangle) = \langle \dot{m}(t) \mid m(t)\rangle + \langle m(t))|\dot{m}(t)\rangle$$

$$= \langle m(t))|\dot{m}(t)\rangle^* + \langle m(t))|\dot{m}(t)\rangle = 2\,\mathrm{Re}(\langle m(t))|\dot{m}(t)\rangle)$$

Example: 1D antiferromagnetic Heisenberg chain

$$H = J\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 = J(X_1X_2 + Y_1Y_2 + Z_1Z_2)$$

$$|\mathrm{GS}\rangle = |\psi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$$

Example: 1D antiferromagnetic Heisenberg chain

$$H = J \sum_{i=1}^{N-1} \boldsymbol{\sigma}^i \cdot \boldsymbol{\sigma}^{i+1}$$

$|\mathrm{GS}\rangle = ???$

Adiabatic path

$$H = J\sum_{i=1}^{N-1} \boldsymbol{\sigma}^i \cdot \boldsymbol{\sigma}^{i+1}$$

$$H_{\text{ad}}(t) = H_{\text{odd}} + \frac{t}{T_{\text{max}}} H_{\text{even}}$$
$$0 \le t \le T_{\text{max}}, H_{\text{odd}} = J\sum_{\text{odd } i} \boldsymbol{\sigma}^i \cdot \boldsymbol{\sigma}^{i+1}, H_{\text{even}} = J\sum_{\text{even } i} \boldsymbol{\sigma}^i \cdot \boldsymbol{\sigma}^{i+1}$$

$t = 0, H_{\text{ad}} = H_{\text{odd}}$

still a two-body Hamiltonian

$|\text{GS}\rangle = |\psi^-\rangle \otimes \cdots \otimes |\psi^-\rangle$

$|\psi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$

$t = 0.5\,T_{\text{max}}$

gradually turn up the even couplings

Adiabatic evolution

$$H = J\sum_{i=1}^{N-1} \boldsymbol{\sigma}^i \cdot \boldsymbol{\sigma}^{i+1}$$

$$H_{\text{ad}}(t) = H_{\text{odd}} + \frac{t}{T_{\text{max}}} H_{\text{even}}$$
$$0 \leq t \leq T_{\text{max}}, H_{\text{odd}} = J\sum_{\text{odd } i} \boldsymbol{\sigma}^i \cdot \boldsymbol{\sigma}^{i+1}, H_{\text{even}} = J\sum_{\text{even } i} \boldsymbol{\sigma}^i \cdot \boldsymbol{\sigma}^{i+1}$$

$t = 0, H_{\text{ad}} = H_{\text{odd}}$

basically a two-body Hamiltonian

$|\text{GS}\rangle = |\psi^-\rangle \otimes \cdots \otimes |\psi^-\rangle$

$|\psi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$

$t = T_{\text{max}}, H_{\text{ad}} = H$

For large $T_{\text{max}}(T_{\text{max}} \sim N^2)$, system remains in the ground state.

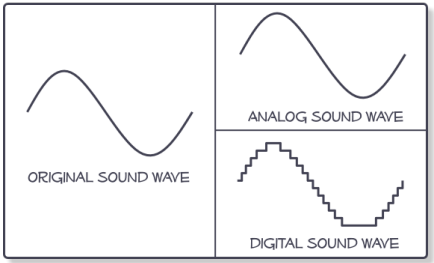
Digital quantum simulation

Digital = Using quantum gates (single-qubit / two-qubit)

$$H_{\text{ad}}(t) = H_{\text{odd}} + \frac{t}{T_{\text{max}}} H_{\text{even}}$$

Quantum Dynamics

Goal: simulate $U = e^{iH_{\text{ad}}(t)t}$



- First Step:

Discretize the time evolution into M steps, each with a fixed Hamiltonian $U_k = e^{-iH_{ad}(k\Delta t)\Delta t}, \Delta t = T_{\text{max}}/M$

Suzuki-Trotter expansion

$$H_{\text{ad}}(t) = H_{\text{odd}} + \frac{t}{T_{\text{max}}} H_{\text{even}}$$

Goal: In the k^{th} step, simulate $U = e^{-iH_{ad}(k\Delta t)\Delta t}$

$H_{ad}(k\Delta t)$ is still a many-body Hamiltonian, so generally we don't know how to decompose U into quantum gates.

- Second step:

Exploit the Suzuki-Trotter expansion in each step

To separate a many-body Hamiltonian into the sum of several two-body Hamiltonians

Suzuki-Trotter expansion

$$H_{\text{ad}}(t) = H_{\text{odd}} + \frac{t}{T_{\text{max}}} H_{\text{even}}$$

Goal: In the k^{th} step, simulate $U = e^{-iH_{ad}(k\Delta t)\Delta t}$

Suzuki-Trotter expansion[HS05]

First order: $e^{\delta(A+B)} = e^{\delta A} e^{\delta B} + O\left(\delta^2\right)$

Second order: $e^{\delta(A+B)} = e^{\delta B/2} e^{\delta A} e^{\delta B/2} + O\left(\delta^3\right)$

Suzuki-Trotter expansion of U_k

$$U_k^{\text{ST1}} = e^{-iH_{\text{even}} \frac{k\Delta t^2}{T_{\text{max}}}} e^{-iH_{\text{odd}}\, \Delta t}$$

$$U_k^{\text{ST2}} = e^{-iH_{\text{odd}} \frac{\Delta t}{2}} e^{-iH_{\text{even}} \frac{k\Delta t^2}{T_{\text{max}}}} e^{-iH_{\text{odd}} \frac{\Delta t}{2}}$$

We know the optimal decomposition of any two-qubit unitary[VW04]

WQCC Wisconsin Quantum Computing Club

Towards higher order ST expansion[HS05]

$$S_2(x) \equiv \mathrm{e}^{\frac{x}{2}A}\mathrm{e}^{xB}\mathrm{e}^{\frac{x}{2}A} = \mathrm{e}^{x(A+B)+x^3R_3+x^5R_5+\cdots}$$

$$S_2(x)S_2(-x) = \mathrm{e}^{\frac{x}{2}A}\mathrm{e}^{xB}\mathrm{e}^{\frac{x}{2}A}\mathrm{e}^{-\frac{x}{2}A}\mathrm{e}^{-xB}\mathrm{e}^{-\frac{x}{2}A} = I$$

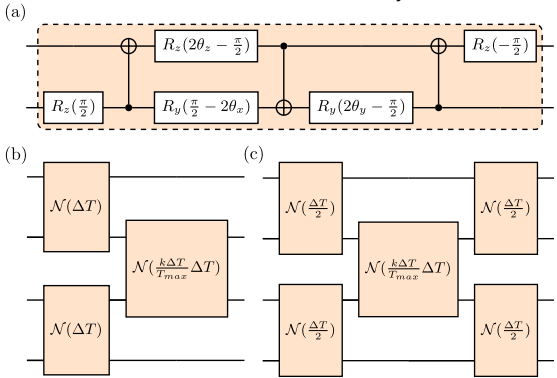
$$\begin{aligned} S(x) &= S_2(sx)S_2((1-2s)x)S_2(sx) \\ &= \mathrm{e}^{sx(A+B)+s^3x^3R_3+\mathrm{O}\left(x^5\right)}\mathrm{e}^{(1-2s)x(A+B)+(1-2s)^3x^3R_3+\mathrm{O}\left(x^5\right)}\mathrm{e}^{sx(A+B)+s^3x^3R_3+\mathrm{O}\left(x^5\right)} \\ &= \mathrm{e}^{x(A+B)+\left[2s^3+(1-2s)^3\right]R_3+\mathrm{O}\left(x^5\right)}. \end{aligned}$$

$$\begin{aligned} S_4(x) &\equiv S_2\left(s_2x\right)^2 S_2\left(\left(1-4s_2\right)x\right) S_2\left(s_2x\right)^2 \\ &= \mathrm{e}^{\frac{s_2}{2}xA}\mathrm{e}^{s_2xB}\mathrm{e}^{s_2xA}\mathrm{e}^{s_2xB}\mathrm{e}^{\frac{1-3s_2}{2}xA}\mathrm{e}^{(1-4s_2)xB}\mathrm{e}^{\frac{1-3s_2}{2}xA}\mathrm{e}^{s_2xB}\mathrm{e}^{s_2xA}\mathrm{e}^{s_2xB}\mathrm{e}^{\frac{s_2}{2}xA} \end{aligned}$$

Circuit realization

$$\mathcal{N}(\theta_x, \theta_y, \theta_z) = e^{i(\theta_x \sigma_x \otimes \sigma_x + \theta_y \sigma_y \otimes \sigma_y + \theta_z \sigma_z \otimes \sigma_z)}$$

For Heisenberg model, $\theta_x = \theta_y = \theta_z = \theta$.



[1]Figure: [LMB20]

Summary of AE on a Digital Quantum Simulator

Steps to prepare the ground state of a many-body hamiltonian

- Come up with an adiabatic path
- Prepare the easy ground state
- Discretize the time evolution
- Adopt Suzuki-Trotter expansion
- Run the circuit

Disadvantage of AE

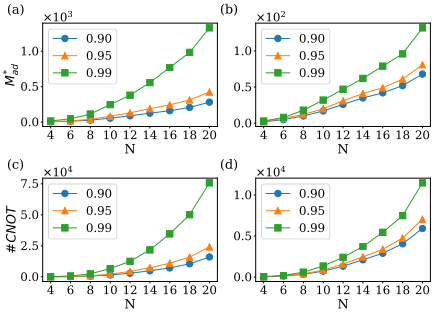


Figure 2: The minimum circuit depth M^*_{ad} as a function of N for various threshold fidelities using: (a) first order Suzuki-Trotter approximation; and (b) Second order Suzuki-Trotter procedure. The number of CNOT gates required for the adiabatic evolution as a function of length N for required for various threshold fidelities using: (c) first order Suzuki-Trotter approximation; and (d) Second order Suzuki-Trotter procedure.

[1]Figure: [LMB20]

Fidelity $= \langle \psi_{\text{exact}} | \psi \rangle$

- Second order is better
- Too deep a circuit for NISQ

Table of Contents

|WQCC⟩ Wisconsin Quantum Computing Club

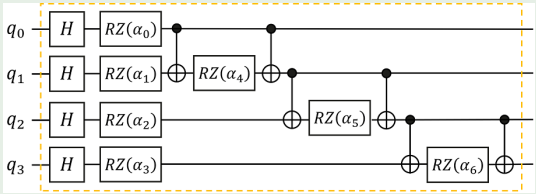
Variational Quantum Eigensolver

The variational principle

$$\langle H \rangle = \langle \psi(\vec{\theta}) | H | \psi(\vec{\theta}) \rangle \geq E_{\text{GS}}, \vec{\theta} = (\theta_1, \theta_2, \cdots, \theta_L)$$

Examples

This circuit generates an ansatz $\psi(\vec{\alpha})$.



Gradient: Parameter Shift Rule

$$\frac{\partial \langle H \rangle}{\partial \theta_i} = \frac{\langle H \rangle|_{\theta_i + \pi/2} - \langle H \rangle|_{\theta_i - \pi/2}}{2}$$

WQCC Wisconsin Quantum Computing Club

Parameter Shift Rule[MNKF18][SBG+19][MBK21]

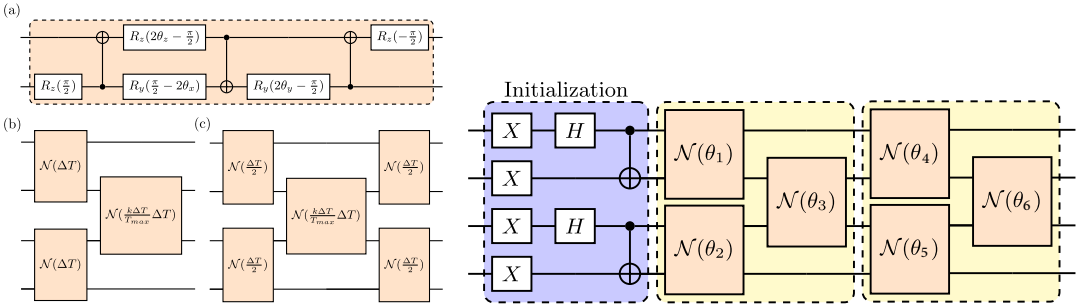
Suppose $|\psi\rangle = U(\vec{\theta})|0\rangle = U_N(\theta_N)\, U_{N-1}(\theta_{N-1}) \cdots U_i(\theta_i) \cdots U_1(\theta_1)\,|0\rangle$

$$\frac{\partial \langle\psi|H|\psi\rangle}{\partial \theta_i} = \frac{d}{d\theta_i}\left\langle \psi_{i-1} \left| U^\dagger(\theta_i)\, MU(\theta_i) \right| \psi_{i-1} \right\rangle$$

where $|\psi_{i-1}\rangle = U_{i-1}(\theta_{i-1}) \cdots U_1(\theta_1)\,|0\rangle$ and $M = U^\dagger(\theta_{i+1}) \cdots U^\dagger(\theta_N) H U(\theta_N) \cdots U(\theta_{i+1})$.
Originally stated as $U(\theta_i) = e^{-iG\theta_i}$, and G is a Hermitian Operator with only two unique eigenvectors $\pm r$, $U\left(\frac{\pi}{4r}\right) = \frac{1}{\sqrt{2}}\left(1 - ir^{-1}G\right)$.

But actually $\frac{\partial}{\partial \theta_j}\hat{K}(\theta_j) = \frac{\hat{K}\left(\theta_j+s\right) - \hat{K}\left(\theta_j - s\right)}{2\sin(s)}$

PQC design



[1]Figure: Adapted from [LXYB23]

Resource comparison

	ST 1st $order$		ST 2nd $order$		VQE	
N	M^*_{ad}	$\#CNOT$	M^*_{ad}	$\#CNOT$	M^*_{VQE}	$\#CNOT$
4	15	135	3	45	2	18
8	113	2373	18	594	3	63
10	247	6669	32	1344	3	81
16	770	34650	79	5451	5	225
20	1330	75810	132	11484	6	342

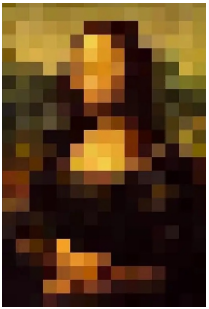
Table 1: A comparison for the circuit depth M^* between the adiabatic approach (with both first and second order Suzuki-Trotter approximation) and the VQE algorithm for various system sizes when the threshold fidelity is chosen to be $F = 0.99$.

[1]Table: [LMB20]

PQC design: generalization

The adiabatic circuit can be considered as a special case of VQE.

Adiabatic evolution



Shallow layers

VQE

One can always adapt the adiabatic circuit and add local rotations to all the qubits of each layer[LMB20].

Symmetry considerations

1d Heisenberg model

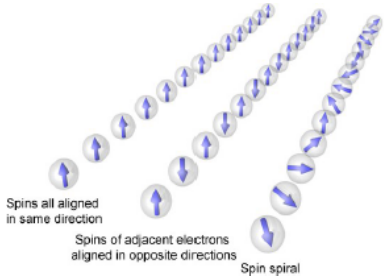
$H = J\sum_{i=1}^{N-1} \boldsymbol{\sigma}^i \cdot \boldsymbol{\sigma}^{i+1}, J > 0$

Open boundaries

Spin Conservation

$[H, S_\alpha] = 0, S_\alpha = \sum_i \sigma_\alpha^i, \alpha = x, y, z$
$[H, S_{tot}^2] = 0, S_{tot}^2 = S_x^2 + S_y^2 + S_z^2$

N gate conserves total spin[LXYB23].



Summary of VQE

Procedure of VQE

- Design a parameterized quantum circuit
- Measure the energy expectation
- "Measure" the gradient via parameter shift rule
- Gradient descent optimization on a classical computer
- Go back and repeat until convergence

Table of Contents

|WQCC⟩
Wisconsin Quantum Computing Club

Qiskit AE & VQE

- qiskit.quantum_info.SparsePauliOp
- qiskit.synthesis.SuzukiTrotter
- qiskit.algorithms.TimeEvolutionProblem
- qiskit.circuit.Parameter
- qiskit_algorithms.optimizers
- qiskit_algorithms.minimum_eigensolvers.VQE

Other related topics

- Quantum Chemistry

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

- Quantum Machine Learning

$$K_{ij} = |\langle \phi(\vec{x}_i) \mid \phi(\vec{x}_j) \rangle|^2$$

|WQCC⟩ Wisconsin Quantum Computing Club

Reference

- N. Hatano and M. Suzuki, *Finding exponential product formulas of higher orders*, Quantum Annealing and Other Optimization Methods (2005), 37–68.
- C. Lyu, V. Montenegro, and A. Bayat, *Accelerated variational algorithms for digital quantum simulation of many-body ground states*, Quantum **4** (2020), 324.
- C. Lyu, X. Xu, M. Yung, and A. Bayat, *Symmetry enhanced variational quantum spin eigensolver*, Quantum **7** (2023), 899.
- Andrea Mari, Thomas R. Bromley, and Nathan Killoran, *Estimating the gradient and higher-order derivatives on quantum hardware*, Phys. Rev. A **103** (2021), 012405.
- K. Mitarai, M. Negoro, M. Kitagawa, and K. Fujii, *Quantum circuit learning*, Phys. Rev. A **98** (2018), 032309.
- Maria Schuld, Ville Bergholm, Christian Gogolin, Josh Izaac, and Nathan Killoran, *Evaluating analytic gradients on quantum hardware*, Phys. Rev. A **99** (2019), 032331.
- Farrokh Vatan and Colin Williams, *Optimal quantum circuits for general two-qubit gates*, Phys. Rev. A **69** (2004), 032315.