

Quantum simulation for correlated quantum many-body systems on noisy quantum devices

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- Introduction: Quantum simulation & quantum computer
 - Quantum simulation by quantum computer
 - Near-term noisy intermediate-scale quantum (NISQ) devices
- Variational quantum algorithm in NISQ era
 - Variational quantum eigensolver (VQE)
 - Issues and challenges in VQE
- Applications to correlated quantum many-body systems
 - To gapless fermion: <u>T. Shirakawa, K. Seki & S. Yunoki, PRResearch 3, 013004 (2021)</u>
 - To Heisenberg model: <u>K. Seki, T. Shirakawa & S. Yunoki, PRA 101, 052340 (2020)</u>
 - To topological order: <u>R.-Y. Sun, T. Shirakawa & S. Yunoki, PRB 107, L041109 (2023)</u>
- Summary







Introduction: Quantum simulation & quantum computer





"...Nature isn't classical, dammit, 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..."



Simulating a quantum system by using other quantum systems (i.e. controllable quantum devices)

Quantum simulation by quantum computer R-ccs

—— R. P. Feynman, Int. J. Theor. Phys. 21, 467 (1982)



R. P. Feynman







Quantum simulation by quantum computer R-ccs

Circuit-based quantum computer

- Quantum circuit model
 - Qubit
 - form a quantum state
 - Two-level quantum mechanical system: $|0\rangle$ and $|1\rangle$
 - Quantum logic gate
 - update the quantum state
 - basic quantum circuit operating on a small number of qubits

One-qubit gate / two-qubit gate / ...

- Measurement
 - information readout: classical bit strings







Google



Quantum simulation by quantum computer R-ccs

In principle: quantum adiabatic process

- Goal: find the ground state $|\Psi_f
 angle$ of Hamiltonian \hat{H}_f
- Start from \hat{H}_i
 - Simple Hamiltonian with the known ground state $|\Psi_i\rangle = \hat{U}_i |0\rangle$
- Construct the mixture Hamiltonian

•
$$\hat{H}(t) = s_i(t)\hat{H}_i + s_f(t)\hat{H}_f$$

Evolution operator:
$$\hat{U}(T) = \mathcal{T} \exp\{-i \int_0^T \hat{H}(t) dt\}$$

Perform adiabatic time evolution

•
$$|\Psi(T)\rangle = \hat{U}(T)|\Psi_i\rangle$$

- Quantum adiabatic theorem
 - For sufficiently long T, $|\Psi(T)\rangle = |\Psi_f\rangle$





Fault-tolerant quantum computer ~ solve quantum many-body problem

- How to design mixture hamiltonian?
- How to decompose the evolution operator on quantum device?
- **Fatal weakness:**

Long time evolution on current accessible quantum devices is impossible!









- Noisy intermediate-scale quantum (NISQ) era
 - A few $\mathcal{O}(10^1 \sim 10^2)$ qubits without error correction
 - A few $\mathcal{O}(10^0 \sim 10^1)$ depths circuit evolution
 - E.g. "Google's quantum supremacy" circuit: 53 qubits with 40 depths

In comparison: Construct $\hat{U}(\delta t) = e^{-i\delta t\hat{H}}$ use ~ 20 (40) depths in 1D (2D) case when δt is very small

Quantum adiabatic evolution is hopeless in NISQ era Special algorithms for NISQ devices are required Key point: Only shallow circuits are considered

Near-term noisy quantum devices

Quantum Computing in the NISQ era and beyond

John Preskill

Institute for Quantum Information and Matter and Walter Burke Institute for Theoretical Physics, California Institute of Technology, Pasadena CA 91125, USA 30 July 2018



Quantum 2, 79 (2018)



Near-term aim: achieve useful quantum advantage on NISQ devices

Useful example: understand correlated quantum many-body problems







Variational quantum algorithm in NISQ era





Quantum-classical loop

quantum computer



describe a quantum state & extract information



Quantum-classical hybrid paradigm in NISQ era R-ccs



pre/post processing less demanding tasks

 \bullet \bullet \bullet \bullet \bullet





- Objective function (OF)
 - With parameters related to quantum circuit
 - Goal: minimize the OF
 - Example: system energy
- Parametrized quantum circuit (PQC)
 - Take parameters in OF
 - Be performed on quantum computer
 - Example: wavefunction ansatz to describe ground state
- Classical optimization
 - Classical optimizer for updating parameters in PQC
 - Based on values of OF and functions related to OF (for instance, derivatives)
 - Be performed on classical computer
 - Example: gradient descent optimizer

Variational quantum algorithm (VQA)







A VQA for finding the ground state of quantum many-body system



- **Objective function**
 - Energy
- Parametrized quantum circuit (PQC)
 - Parametrized circuit ansatz state

variational quantum state: parametrized circuit ansatz

$$|\Psi(\{\theta_i\})\rangle = \hat{U}$$

 $|\Psi(\{\theta_i\})\rangle$: 2^N dimensional vector (variational state)

 $\{\theta_i\}$: poly(N) dimensional vector

(variational parameters)

N: number of qubits

A path to achieve useful quantum advantage (find the ground state of quantum many-body system) on NISQ devices



 $\hat{H}|\Psi(\{\theta_i\})\rangle = E(\{\theta_i\})|\Psi(\{\theta_i\})\rangle$



classical computer

optimization of variational parameters $\{\theta_i\}$

 $\theta_i \leftarrow \theta_i - \lambda \partial E(\{\theta_i\}) / \partial \theta_i$

Nat. Commun. 5, 4213 (2014)









- Parametrized circuit ansatz
 - Scalability on NISQ devices
 - Expressibility to the ground state
 - Optimizable or not
- **Classical optimization**
 - Capability to get the global minimal
 - Efficiency for NISQ device
- Suitable problem
 - Lower spacial dimension (1D and 2D)
 - Simple system (spins)



Issues & challenges

Scalable VQE (up to 500~1000 qubits) \sim Solve a small group of quantum many-body problems \sim Achieve useful quantum advantage in the near-term







Applications to correlated quantum many-body systems





Quantum simulation for gapless fermion

T. Shirakawa, K. Seki & S. Yunoki, Phys. Rev. Research 3, 013004 (2021)





Let us assume
$$\hat{H}_{\!f}=\hat{V}_1+\hat{V}_2$$
, where $[\hat{V}_1,\hat{V}_2]\neq 0$,

and
$$\hat{H}_i = \hat{V}_1$$

The time-evolution operator is

$$\hat{U}(T) = \lim_{M \to \infty} \hat{U}_d(\boldsymbol{\theta}_M) \hat{U}_d(\boldsymbol{\theta}_{M-1}) \cdots \hat{U}_d(\boldsymbol{\theta}_1)$$

where

$$\begin{split} \hat{U}_{d}(\boldsymbol{\theta}_{m}) &= \mathrm{e}^{-\mathrm{i}\boldsymbol{\theta}_{1}^{(m)}\hat{V}_{1}}\mathrm{e}^{-\mathrm{i}\boldsymbol{\theta}_{2}^{(m)}\hat{V}_{2}} \\ \theta_{1}^{(m)} &= [s_{i}(\tau_{m}) + s_{f}(\tau_{m})]\delta\tau \\ \theta_{2}^{(m)} &= s_{f}(\tau_{m})\delta\tau \end{split} \right\} \xrightarrow{\rightarrow} \mathrm{e.g., \ linear \ schedul} \\ s_{i}(\tau) &= 1 - \frac{\tau}{T} \\ \mathrm{with} \\ \delta\tau &= T/M \\ \tau_{m} &= m\delta\tau \end{split}$$

Set *M* to be finite and consider $\{\theta_1^{(m)}, \theta_2^{(m)}\}$ as variational parameters A parametrized circuit ansatz $\hat{U}_M(\theta_1, \theta_2, \dots, \theta_M) | \Psi_i \rangle$ with M depths **DQAP** ansatz or quantum approximate optimization ansatz (QAOA)

A quantum adiabatic evolution path itself is to be optimized

Discretized quantum adiabatic process (DQAP) ansatz









DQAP ansatz for 1D free fermions

1D free fermions (spinless) with L sites at half filling (gapless ground state)



T. Shirakawa, K. Seki & S. Yunoki, Phys. Rev. Research 3, 013004 (2021)

$$\begin{aligned} \hat{c}(\hat{c}_{1}^{\dagger}\hat{c}_{L}+\hat{c}_{L}^{\dagger}\hat{c}_{1}) &= \hat{\mathcal{V}}_{1}+\hat{\mathcal{V}}_{2} \\ \hat{c}_{2x-1}^{\dagger}\hat{c}_{2x}) \\ \gamma &= \begin{cases} 1 & \text{periodic} \\ -1 & \text{antiperiodic} \end{cases} \end{aligned}$$

$$\hat{c}_{2x}^{\dagger}\hat{c}_{2x+1}) - \gamma t(\hat{c}_1^{\dagger}\hat{c}_L + \hat{c}_L^{\dagger}\hat{c}_1)$$

$$| \psi_{M}(\boldsymbol{\theta}) \rangle = \hat{\mathcal{U}}_{M}(\boldsymbol{\theta}) | \psi_{i} \rangle$$

$$\hat{\mathcal{U}}_{M}(\boldsymbol{\theta}) = \hat{\mathcal{U}}_{d}(\boldsymbol{\theta}_{M}) \hat{\mathcal{U}}_{d}(\boldsymbol{\theta}_{M-1}) \cdots \hat{\mathcal{U}}_{d}(\boldsymbol{\theta}_{1})$$

$$\hat{\mathcal{U}}_{d}(\boldsymbol{\theta}_{m}) = e^{-i\theta_{1}^{(m)}\hat{\mathcal{V}}_{1}} e^{-i\theta_{2}^{(m)}\hat{\mathcal{V}}_{2}}$$

$$\boldsymbol{\theta} = \{\boldsymbol{\theta}_{m}\}_{m=1}^{M} \quad \boldsymbol{\theta}_{m} = \{\theta_{1}^{(m)}, \theta_{2}^{(m)}\}$$

$$\rightarrow \text{ variational parameters}$$

$$\# \text{ of parameters: } 2M$$

Natural gradient decent method in classical computer



Ground state energy





T. Shirakawa, K. Seki & S. Yunoki, Phys. Rev. Research 3, 013004 (2021)

$$\Delta E = E(\theta) - E_{exact}(L)$$

$$E(\theta) = \langle \psi_{M}(\theta) | \hat{\mathscr{X}} | \psi_{M}(\theta) \rangle$$

$$E_{exact}(L): \text{ exact ground state energy for system size } L$$
exact ground state at $M=L/4$

$$= E(\theta)/L - \lim_{L \to \infty} E_{exact}(L)/L$$

$$= E(\theta)/L - \lim_{L \to \infty} E_{exact}(L)/L$$
states $| \psi_{M}(\theta) \rangle$ with $M < L/4$ are independent of system size L

$$= U(h)/L - \lim_{L \to \infty} E_{exact}(L)/L + \lim_{L \to \infty} E_{exact$$





Causality cone and Lieb-Robinson bound Reco R



M = L/4 corresponds to the point where the causality-cone exceeds the system size L.



T. Shirakawa, K. Seki & S. Yunoki, Phys. Rev. Research 3, 013004 (2021)

causality cone set by Lieb-Robinson bound

The DQAP ansatz can provide the circuit with the minimum number of depths (M=L/4) to describe the exact ground state





Quantum simulation for spin-1/2 Heisenberg model

K. Seki, T. Shirakawa & S. Yunoki, Phys. Rev. A 101, 052340 (2020)





$$\hat{\mathcal{H}} = \frac{J}{4} \sum_{\langle i,j \rangle} \left(\hat{X}_i \hat{X}_j + \hat{Y}_i \hat{Y}_j + \hat{Z}_i \hat{Z}_j \right) = \frac{J}{2} \sum_{\langle i,j \rangle} \left(\hat{\mathcal{P}}_{ij} - \frac{\hat{I}}{2} \right)$$

 $\hat{X}_i, \hat{Y}_i, \hat{Z}_i$: Pauli matrices $|\hat{\mathcal{P}}_{ij}|$: Permutation (SWAP)

In 1D

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

$$\hat{H}_{1} = \frac{J}{2} \sum_{i: \text{ odd}} \left(\hat{P}_{i,i+1} - \frac{\hat{I}}{2} \right), \ \hat{H}_{2} = \frac{J}{2} \sum_{i: \text{ even}} \left(\hat{P}_{i,i+1} - \frac{\hat{I}}{2} \right)$$

DQAP ansatz:

 $|\psi_{M}(\{\theta_{1}^{(m)},\theta_{2}^{(m)}\})\rangle = \hat{\mathcal{U}}_{d}(\boldsymbol{\theta}_{M})\hat{\mathcal{U}}_{d}(\boldsymbol{\theta}_{M-1})$

$$\hat{\mathcal{U}}_d(\boldsymbol{\theta}_m) = \mathrm{e}^{-\mathrm{i}\theta_1^{(m)}\hat{H}_1}\mathrm{e}^{-\mathrm{i}\theta_2^{(m)}\hat{H}_2}$$

(ESWAP circuit ansatz)

S = 1/2 antiferromagnetic Heisenberg model

K. Seki, T. Shirakawa & S. Yunoki, Phys. Rev. A 101, 052340 (2020)

) operator s.t.
$$\hat{\mathcal{P}}_{ij}|a\rangle_i|b\rangle_j = |b\rangle_i|a\rangle_j$$

$$)\cdots \hat{\mathcal{U}}_{d}(\boldsymbol{\theta}_{1}) | \boldsymbol{\psi}_{i} \rangle$$

singlet product

state: GS of \hat{H}_1

$$e^{-i\theta_2^{(m)}\hat{H}_2} = \prod_{i=1}^{\infty} e^{-i\theta_2^{(m)}\hat{P}_{i,i+1}/2}$$

i:even





RVB-type parametrized circuit ansatz

- Resonating valence bond (RVB) state
 - Represent any spin state
 - Magnetic order / topological order / valence bond solid . . .
- DQAP ansatz constructs RVB states
 - $|\Phi\rangle$ represents a nearest neighboring dimer covering
 - $|\Psi(\theta)\rangle$ represents a linear combination of dimer coverings

$$|\Psi(\theta)\rangle = \hat{\mathcal{U}}(\theta)|\Phi\rangle$$

Exponential-SWAP gates
$$\hat{\mathcal{U}}(\theta) = \prod_{\langle ij \rangle} \hat{\mathcal{U}}_{ij}(\theta_{ij})$$
$$\hat{\mathcal{U}}_{ij}(\theta) = \exp(-i\theta\hat{\mathcal{P}}_{ij}/2)$$
$$= \hat{I}\cos\frac{\theta}{2} - i\hat{\mathcal{P}}_{ij}\sin\frac{\theta}{2}$$
$$|[i, j]\rangle : \text{spin}$$
$$|[i, j]\rangle = \frac{1}{\sqrt{2}}$$

K. Seki, T. Shirakawa & S. Yunoki, Phys. Rev. A 101, 052340 (2020)



P. W. Anderson, Mater. Res. Bull. 8, 153 (1973)







 $|[i, i + 1]\rangle$

n-singlet state

 $\frac{1}{\sqrt{2}}\left(|0\rangle_{i}|1\rangle_{j}-|1\rangle_{i}|0\rangle_{j}\right)$







Experiment with a quantum device

S=1/2 Heisenberg ring with 4 sites

ibmq_5_yorktown





each sample contains 1,024 measurements

Sample	$p_0(\%)$	$p_1(\%)$	$Re\langle \Psi_0 \hat{X}_1 \hat{X}_2 \Psi_0 \rangle$	
1	15.430	84.570	-0.69140	
2	17.969	82.031	-0.64062	
3	15.625	84.375	-0.68750	
4	16.309	83.691	-0.67382	
5	16.016	83.984	-0.67968	
6	15.430	84.570	-0.69140	
7	17.578	82.422	-0.64844	
8	18.457	81.543	-0.63086	
9	17.090	82.910	-0.65820	
10	17.969	82.031	-0.64062	
11	16.602	83.398	-0.66796	
12	17.090	82.910	-0.65820	
13	16.992	83.008	-0.66016	
14	15.527	84.473	-0.68946	
15	16.113	83.887	-0.67774	
16	14.648	85.352	-0.70704	
Mean	16.553(274)	83.447(274)	-0.66894(549)	
Ideal	16.667	83.333	-0.66667	standard error

data taken on April 6, 2020 (EST) of the mean

RVB-type circuit ansatz catches the physics!!

K. Seki, T. Shirakawa & S. Yunoki, Phys. Rev. A 101, 052340 (2020)

Quantum circuit for evaluating the spin correlation function $\operatorname{Re}\langle\Psi_0|\hat{X}_1\hat{X}_2|\Psi_0\rangle$







ESWAP circuit state breaks the translational symmetry, but can be restored by:

 $\hat{P}^{(q)}|\psi(\vec{\theta})\rangle = \frac{\hat{P}^{(q)}|\psi(\vec{\theta})\rangle}{\sqrt{\langle\psi(\vec{\theta})|\hat{P}^{(q)}|\psi(\vec{\theta})\rangle}}$

Energy expectation value:

$$E^{(q)}(\vec{\theta}) = \frac{\langle \psi(\vec{\theta}) | \hat{H}\hat{P}^{(q)} | \psi(\vec{\theta}) \rangle}{\langle \psi(\vec{\theta}) | \hat{P}^{(q)} | \psi(\vec{\theta}) \rangle} = \frac{\sum_{n=0}^{N-1} \chi^{(q)}}{\sum_{n=0}^{N-1} \chi^{(q)}}$$

Variational energy per site for **16-site Heisenberg model:**

$$-0.42 - 0.43 - 0.43 - 0.44 - 0.44 - 0.45 -$$

Symmetry-adapted VQE

K. Seki, T. Shirakawa & S. Yunoki, Phys. Rev. A 101, 052340 (2020)







Quantum simulation for topological order state

R.-Y. Sun, T. Shirakawa & S. Yunoki, Phys. Rev. B 107, L041109 (2023)

See Poster 70







Toric code model in a magnetic field

• Toric code model

$$H_{\rm TC} = -\sum_{s} A_s - \sum_{p} B_p$$

- Exactly solvable
- Intrinsic topological order / equally-weighted quantum loop ($|1\rangle$) gas
- OBC ground state

$$- |\Psi_0\rangle = \prod_{p=1}^{N_p} \left(\frac{1}{\sqrt{2}}I_p + \frac{1}{\sqrt{2}}B_p\right) |00\cdots0\rangle$$

- Realizable on real quantum devices with high fidelity
 - Only need Hadamard gate and CNOT gate
- Toric code in a magnetic field

$$H_{\text{TCM}}(x) = (1 - x)H_{\text{TC}} - x\sum_{i=1}^{N} \sigma_i^z$$

- Non-exactly solvable
- Topological order to ferromagnetic order: $x_c \sim 0.25$

R.-Y. Sun, T. Shirakawa & S. Yunoki, Phys. Rev. B 107, L041109 (2023)



Goal: simulate the ground state of $H_{\text{TCM}}(x)$ on quantum computer





Parametrized loop gas circuit (PLGC)

- To simulate loop gas with loop tensions
 - Design a parametrized circuit to represent weightadjustable quantum loop gas
- Dope parameter

$$H|0\rangle = R_y(\pi/2)|0\rangle$$

$$R_{y}(\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$$

- Replace Hadamard gate with Rotation-y gate
- Number of parameters: N_p
- Realizable on real quantum devices
 - Rotation-y gate can be realized with high fidelity
 - With the same complexity

R.-Y. Sun, T. Shirakawa & S. Yunoki, Phys. Rev. B 107, L041109 (2023)













- Ground state energy by VQE calculations with PLGC
 - Difference difference with the numerical exact energy $< 10^{-2}$
 - Keep the accuracy for arbitrary magnetic field strength
 - Keep the accuracy in the systems with varying sizes
- Observing topological quantum phase transition
 - Magnetization:

$$\langle m_z \rangle = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i^z \rangle$$
 Entangle entropy subsys

Topological entanglement entropy (TEE):

$$S_{\text{topo}} = S_{\text{A}} + S_{\text{B}} + S_{\text{C}} - S_{\text{AB}} - S_{\text{BC}} - S_{\text{AC}} + S_{\text{BC}} - S_{\text{AC}} + S_{\text{BC}} - S_{\text{AC}} + S_{\text{BC}} - S_{\text{AC}} + S_{\text{BC}} - S_{\text{AC}} + S_{\text{BC}} - S_{\text{AC}} + S_{\text{$$

VQE calculations are consistent with numerical exact results

VQE simulation using PLGC





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VQE simulation using PLGC









- Quantum computing provides a new way to study correlated quantum many-body systems
 - Quantum simulation: simulate quantum system of interest by another controllable quantum system
- We are in the NISQ era
 - Noisy quantum devices with quantum-classical hybrid algorithms
 - Apply to quantum many-body physics: variational quantum eigensolver (VQE, promising but with challenges)
- VQE study of correlated quantum many-body systems
 - Discretized quantum adiabatic process (DQAP) ansatz provides the exact ground state with L/4 depths: PRResearch 3, 013004 (2021)
 - RVB-type circuit ansatz (emerged from DQAP) catches the ground state of Heisenberg model; Broken symmetry can be restored by post processing (symmetry-adapted VQE): PRA 101, 052340 (2020)
 - Real-device-realizable PLGC ansatz describes the topological order in non-exactly solvable cases and can go through the phase transition: PRB 107, L041109 (2023)

Thanks for your attention!

Summary

