RIKEN-Vancouver Joint Workshop
(August 24 - 25, 2021)

Quantum simulations for quantum many-body systems: Variational quantum algorithms and beyond

Seiji Yunoki (RIKEN)

- K. Seki, T. Shirakawa & S. Yunoki, Phys. Rev. A **101**, 052340/1-15 ('20).
- T. Shirakawa, K. Seki & S. Yunoki, Phys. Rev. Research **3**, 013004/1-32 ('21).
- K. Seki & S. Yunoki, PRX Quantum **2**, 010333/1-45 ('21).

RIKEN QUANTUM COMPUTING

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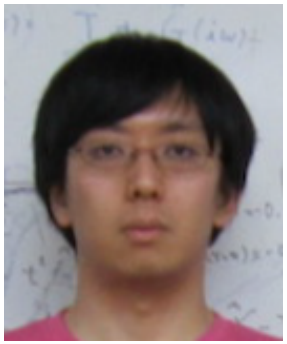
Collaborators



Kazuhiro Seki
(Researcher at RQC)

Tomonori Shirakawa
(Senior Researcher at R-CCS & RQC)

- **K. Seki**, **T. Shirakawa** & S. Yunoki, Phys. Rev. A **101**, 052340/1-15 ('20).
- **T. Shirakawa**, **K. Seki** & S. Yunoki, Phys. Rev. Research **3**, 013004/1-32 ('21).
- **K. Seki** & S. Yunoki, PRX Quantum **2**, 010333/1-45 ('21).

RIKEN QUANTUM COMPUTING

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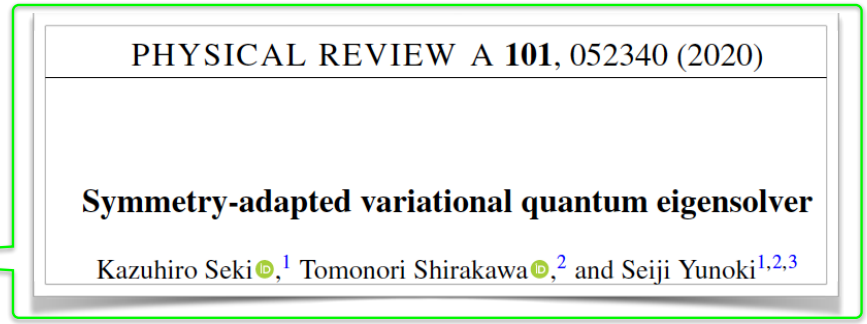
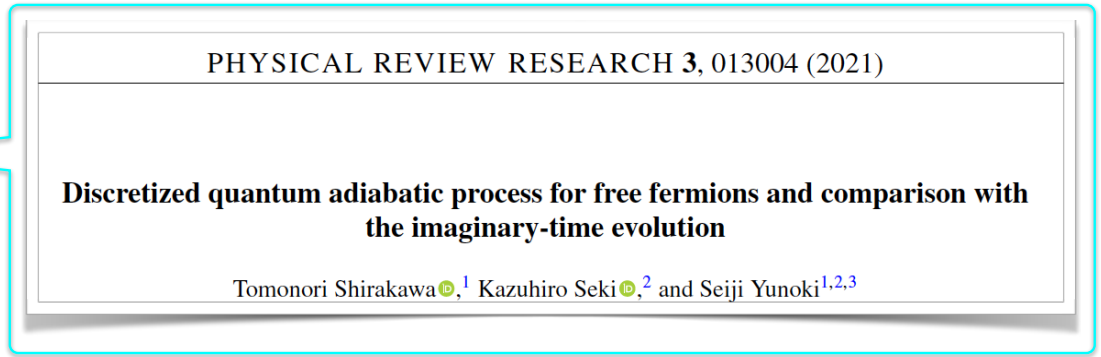
  - quantum simulation in NISQ devices
  - variational quantum algorithms: VQE etc.
- Symmetry-adapted VQE
  - less number of variational parameters
  - shallow circuit depth
- QAOA
  - discretized quantum adiabatic process
  - no prior knowledge for a better circuit structure
- Quantum power method
  - no prior knowledge for a better circuit structure
  - no variational parameters
- Summary


PHYSICAL REVIEW A **101**, 052340 (2020)

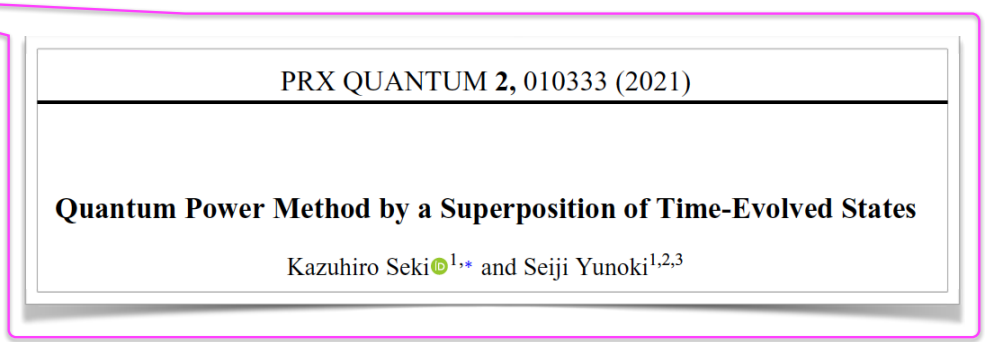
Symmetry-adapted variational quantum eigensolver

Kazuhiro Seki,[1] Tomonori Shirakawa,[2] and Seiji Yunoki[1,2,3]


PHYSICAL REVIEW RESEARCH **3**, 013004 (2021)

Discretized quantum adiabatic process for free fermions and comparison with the imaginary-time evolution

Tomonori Shirakawa,[1] Kazuhiro Seki,[2] and Seiji Yunoki[1,2,3]


PRX QUANTUM **2**, 010333 (2021)

Quantum Power Method by a Superposition of Time-Evolved States

Kazuhiro Seki[1,*] and Seiji Yunoki[1,2,3]

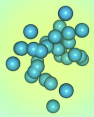
Introduction

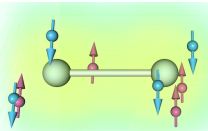
Quantum simulation in quantum computer

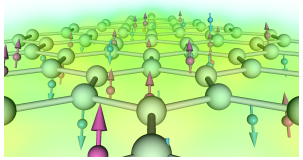
R. P. Feynman, Int. J. Theor. Phys. **21**, 467 (1982).

Richard P. Feynman

"…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…"



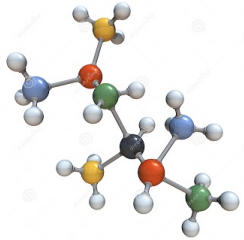




classical computer

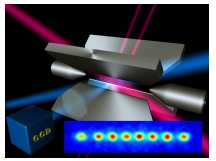
exponentially large
resource required

quantum materials



exponentially large
degrees of freedom

other quantum systems



exponentially large
resource available

Simulating a quantum system by using other quantum systems

Quantum simulation in Noisy Intermediate-Scale Quantum (NISQ) devices

Quantum **2**, 79 ('18)

John Preskill

Quantum Computing in the NISQ era and beyond

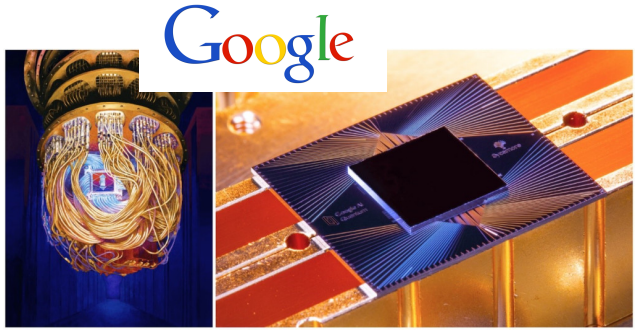
John Preskill

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

30 July 2018

Noisy Intermediate-Scale Quantum (NISQ) technology will be available in the near future. Quantum computers with 50-100 qubits may be able to perform tasks which surpass the capabilities of today's classical digital computers, but noise in quantum gates will limit the size of quantum circuits that can be executed reliably. NISQ devices will be useful tools for exploring many-body quantum physics, and may have other useful applications, but the 100-qubit quantum computer will not change the world right away — we should regard it as a significant step toward the more powerful quantum technologies of the future. Quantum technologists should continue to strive for more accurate quantum gates and, eventually, fully fault-tolerant quantum computing.

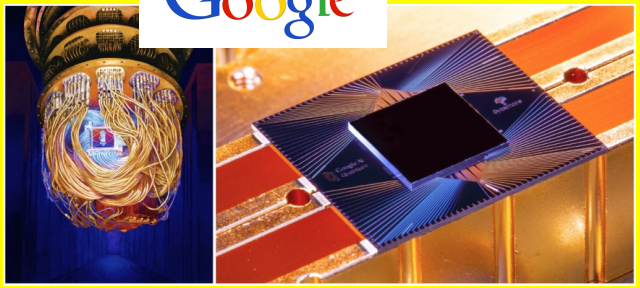
50~100 qubits without fault tolerant



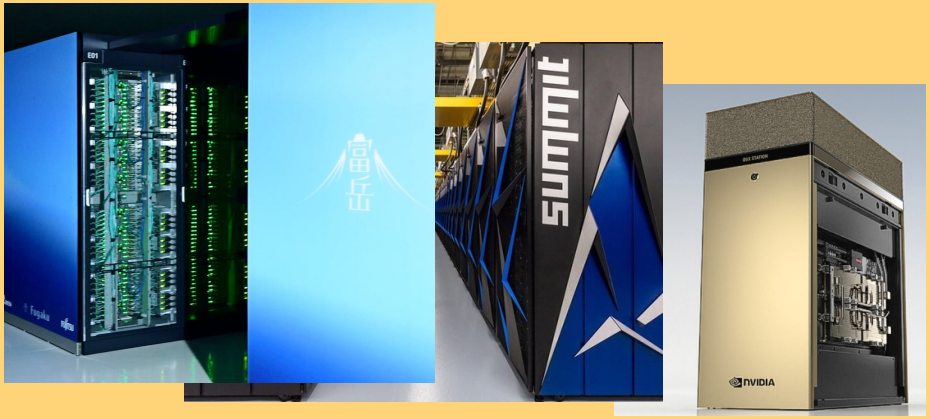
Can we do something interesting in NISQ devices !!??

Quantum-classical hybrid scheme

quantum computer



classical computer



describe a quantum state

pre/post processing
less demanding tasks
....

Variational quantum eigenvalue solver (VQE)

A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik & J. L. O'Brien, Nat. Commun. **5**, 4213 ('14)

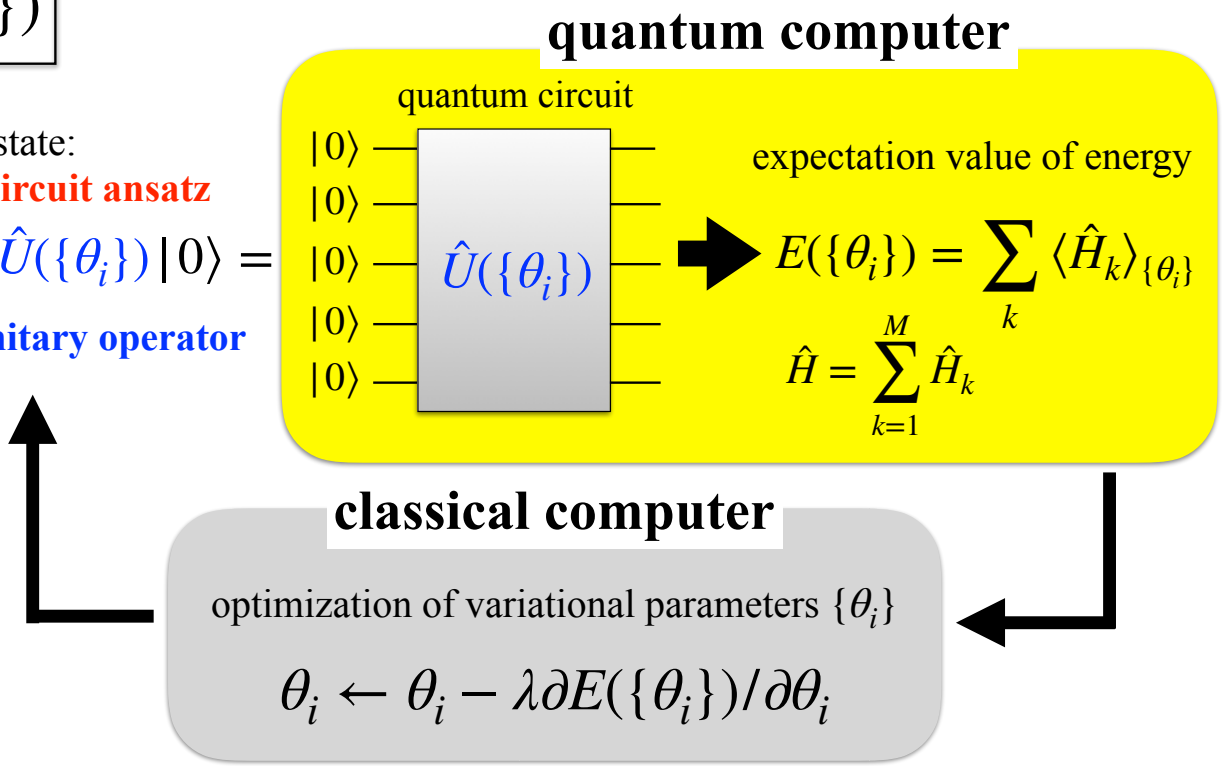
$$\hat{H}|\Psi(\{\theta_i\})\rangle = E(\{\theta_i\})|\Psi(\{\theta_i\})\rangle$$

variational quantum state:

parametrized circuit ansatz

$$|\Psi(\{\theta_i\})\rangle = \hat{U}(\{\theta_i\})|0\rangle =$$

unitary operator



N: number of qubits

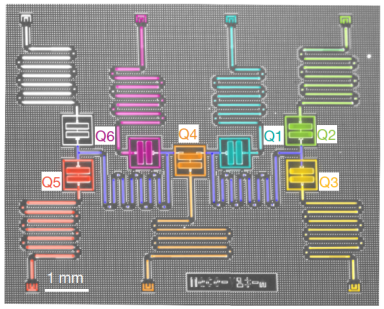
$|\Psi(\{\theta_i\})\rangle$: 2^N dimensional vector
(variational state)

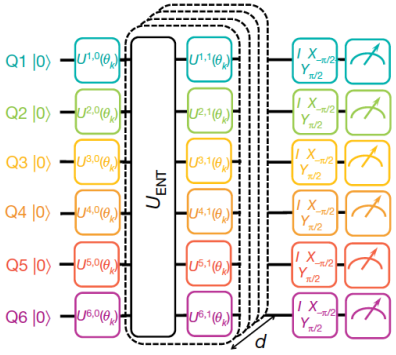
$\{\theta_i\}$: poly(N) dimensional vector
(variational parameters)

Efficient parametrization of
a variational state is crucial

Hardware efficient VQE by IBM

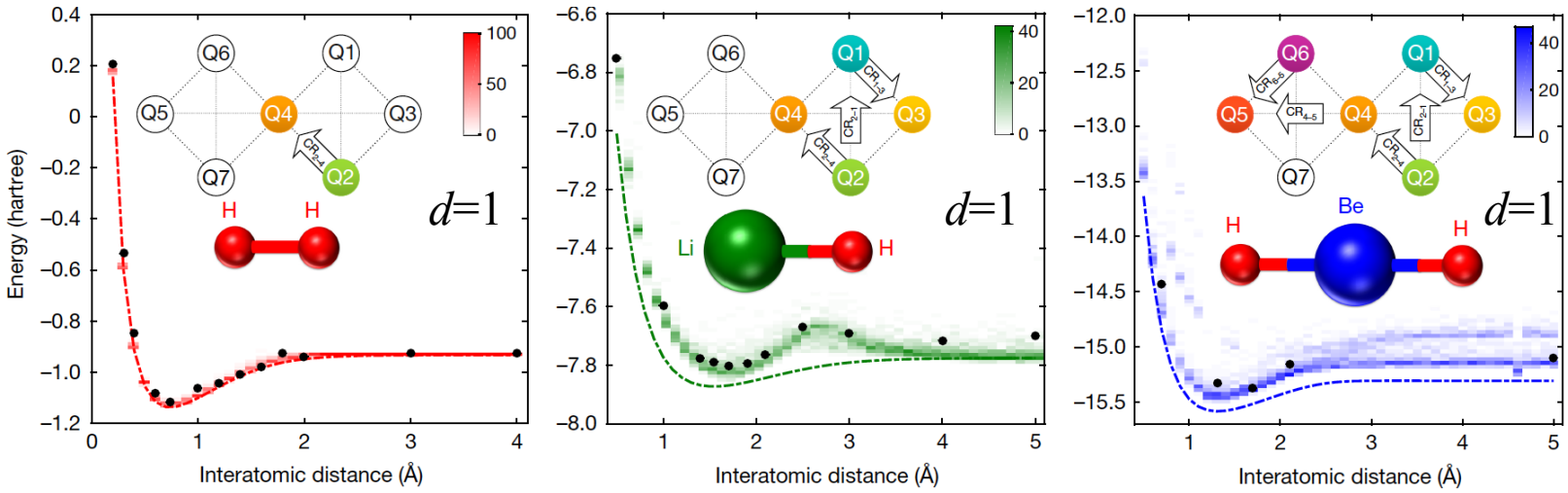
A. Kandala, A. Mezzacapo, K. Temme, M. Takita, M. Brink, J. M. Chow & J. M. Gambetta, Nature **549**, 242 ('17)





$$|\Phi(\boldsymbol{\theta})\rangle = \prod_{q=1}^{N} [U^{q,d}(\boldsymbol{\theta})] \times U_{\mathrm{ENT}} \times \prod_{q=1}^{N} [U^{q,d-1}(\boldsymbol{\theta})] \times \cdots \times U_{\mathrm{ENT}} \times \prod_{q=1}^{N} [U^{q,0}(\boldsymbol{\theta})] |00\ldots0\rangle$$

U_{ENT}: cross resonance gates that can realize $[ZX]^b$
cf. CNOT=$[ZI]^{-1/2}[ZX]^{1/2}[IX]^{-1/2}$
($[ZX]^{1/2}$ sandwiched by single-qubit rotations)
Rigetti and Devoret, PRB '10

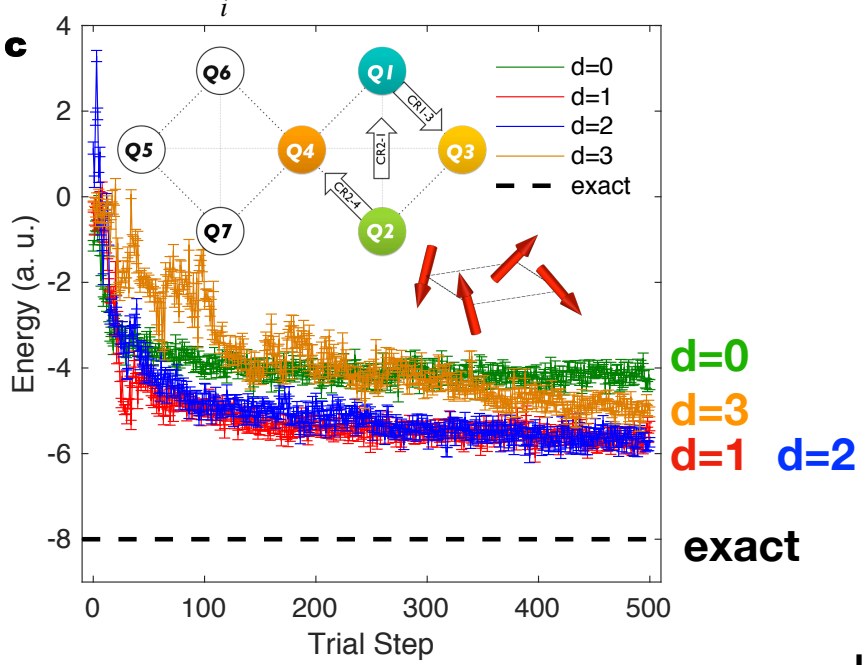


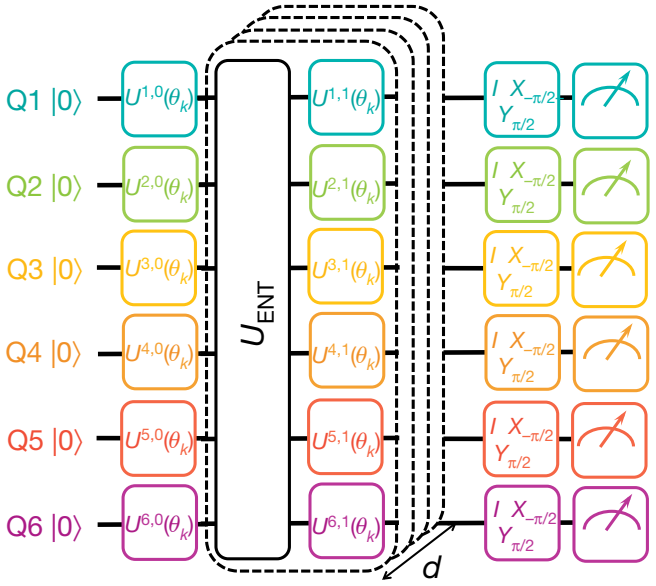
Hardware efficient VQE by IBM

A. Kandala, A. Mezzacapo, K. Temme, M. Takita, M. Brink, J. M. Chow & J. M. Gambetta, Nature **549**, 242 ('17)

4-site S=1/2 Heisenberg model: experiment

$$H = J \sum_i S_i \cdot S_{i+1}$$





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cf. CNOT=$[ZI]^{-1/2}[ZX]^{1/2}[IX]^{-1/2}$
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Rigetti and Devoret, PRB '10

Symmetry-adapted VQE

- A system described by Hamiltonian H has its own symmetry
  - point group symmetry, translational symmetry, spin rotational symmetry, ⋯
- A parametrized circuit inherently breaks the symmetry of H

■ K. Seki, T. Shirakawa & S. Yunoki, Phys. Rev. A **101**, 052340/1-15 (’20).

Projection operator to restore symmetry

■ **Projection operator $\hat{P}_l^{(\gamma)}$ onto the γ irreducible representation with the l-th entry:**

$$\hat{P}_l^{(\gamma)} = \frac{d_\gamma}{|\mathcal{G}|} \sum_{\hat{g}\in\mathcal{G}} [\bar{D}^{(\gamma)}(\hat{g})]^*_{ll} \hat{g}$$

a sum of unitaries

$\hat{g}$: symmetry operator s. t. $\hat{g}\hat{H}\hat{g}^{-1} = \hat{H}$: **unitary**

but $\hat{P}_l^{(\gamma)}$ is not unitary

■ **Symmetry adapted state:**

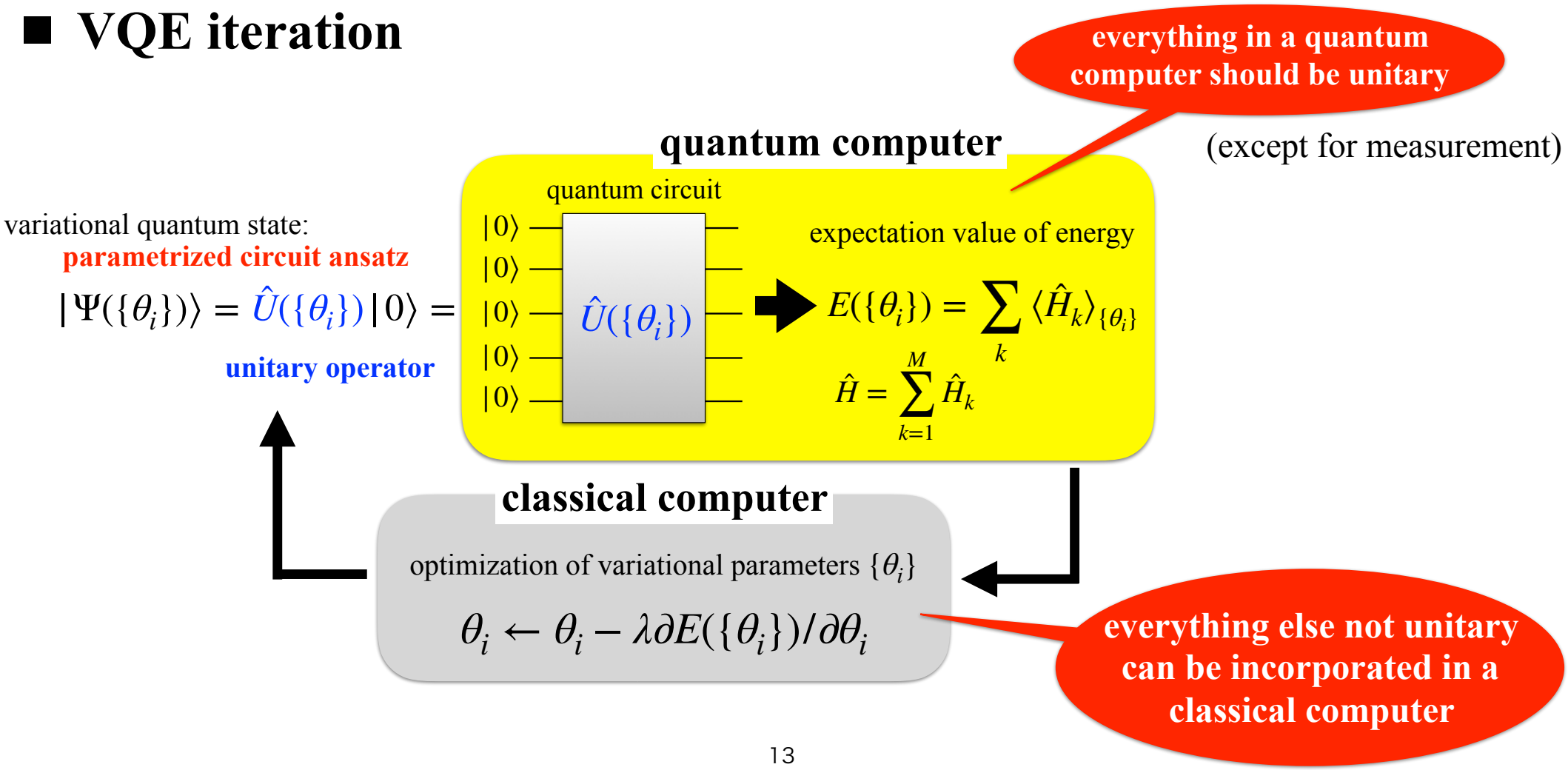
Symmetry-broken state

$$|\psi_l^{(\gamma)}\rangle \sim \hat{P}_l^{(\gamma)} |\psi\rangle$$

$$|\psi_l^{(\gamma)}\rangle = \frac{\hat{P}_l^{(\gamma)} |\psi\rangle}{\sqrt{\langle\psi| \hat{P}_l^{(\gamma)} |\psi\rangle}}$$

Simple idea of how to treat non-unitary operation

■ VQE iteration



S=1/2 antiferromagnetic Heisenberg model (J>0)

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

$\hat{X}_i, \hat{Y}_i, \hat{Z}_i$: Pauli matrices

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

The ground state:

- Total spin $S = 0$ (spin singlet)
- Total momentum $q = 0$ (spatially symmetric)

Marshall '55
Lieb and Mattis '62

Our strategy:
1. Make a spin-symmetric circuit Ansatz which may break the spatial symmetry
2. Restore the spatial symmetry by applying a non-unitary projection operator

RVB-type wave function

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

Exponential-SWAP gates

$$\hat{\mathcal{U}}(\boldsymbol{\theta}) = \prod_{\langle ij\rangle} \hat{U}_{ij}(\theta_{ij})$$

$$\hat{U}_{ij}(\theta) = \exp\left(-\mathrm{i}\theta\hat{\mathcal{P}}_{ij}/2\right) = \hat{I}\cos\frac{\theta}{2} - \mathrm{i}\hat{\mathcal{P}}_{ij}\sin\frac{\theta}{2}$$

$\boldsymbol{\theta}$: variational parameters

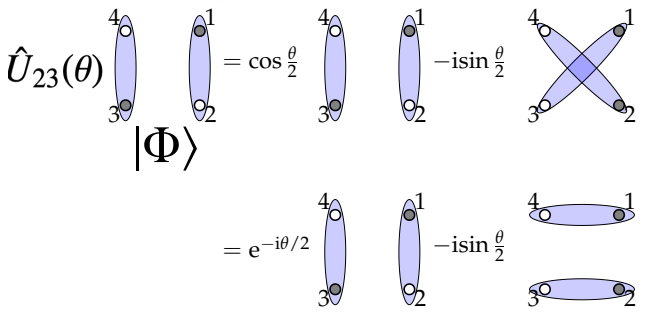
Singlet product state

$$|\Phi\rangle = \bigotimes_{i\in 2\mathbb{Z}+1} |[i, i+1]\rangle$$

$|[i, j]\rangle$: spin-singlet state

$$|[i, j]\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_i|1\rangle_j - |1\rangle_i|0\rangle_j\right)$$

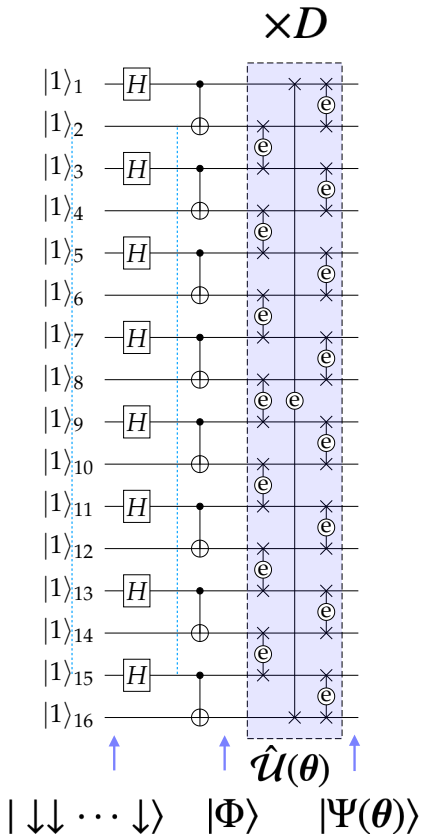
example: N=4



$|\Psi(\theta)\rangle$ represents a linear combination of dimer coverings.

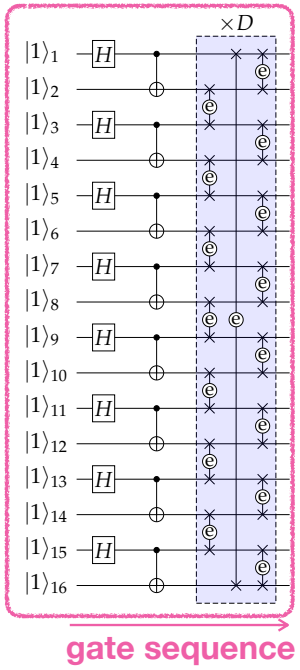
→**Resonating-valence-bond** (**RVB**)-type wave function

Quantum circuit



RVB-type wave function on a quantum circuit

Quantum circuit



"Physical" interpretation

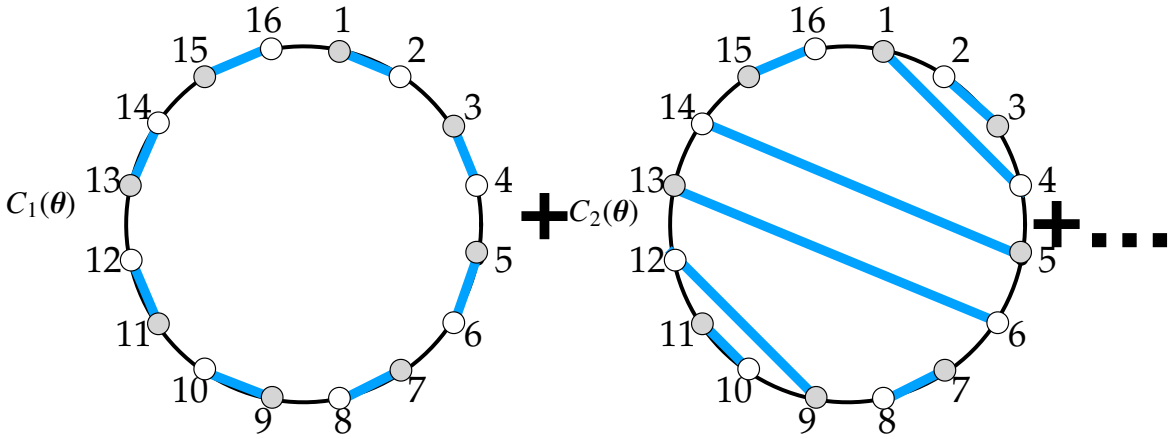
$|0\rangle_i$: spin ↑ associated with ith site

$|1\rangle_i$: spin ↓ associated with ith site

Resonating valence-bond (RVB)-type state

= a superposition of many singlet-pair-product states

cf. spin liquids



Restoring translation symmetry by projection operator

Symmetry-broken state

Symmetry-restored state → $|\Psi_q(\theta)\rangle = \dfrac{\hat{P}_q|\Psi(\theta)\rangle}{\sqrt{\langle\Psi(\theta)|\hat{P}_q|\Psi(\theta)\rangle}}$ where

Projection operator: $\hat{P}_q = \dfrac{1}{|\mathcal{G}|}\sum_{n\in\mathcal{G}}[\chi^{(q)}(\hat{T}_n)]^*\hat{T}_n$ ← Sum of unitaries

$\hat{T}_n$: translation operator s. t. $\hat{T}_n\hat{H}\hat{T}_n^{-1} = \hat{H}$: **unitary**

$\chi^{(q)}(\hat{T}_n) = \exp(-\mathrm{i}qn)$: character of $\hat{T}_n$

$[\hat{H}, \hat{T}_n] = 0 \quad [\hat{H}, \hat{P}_q] = 0$

$\hat{P}_q^2 = \hat{P}_q$

Variational energy w.r.t. the symmetry-restored state

$$E_q(\theta) = \langle\Psi_q(\theta)|\hat{H}|\Psi_q(\theta)\rangle = \frac{\langle\Psi(\theta)|\hat{H}\hat{P}_q|\Psi(\theta)\rangle}{\langle\Psi(\theta)|\hat{P}_q|\Psi(\theta)\rangle}$$

evaluate these matrix elements with quantum computers

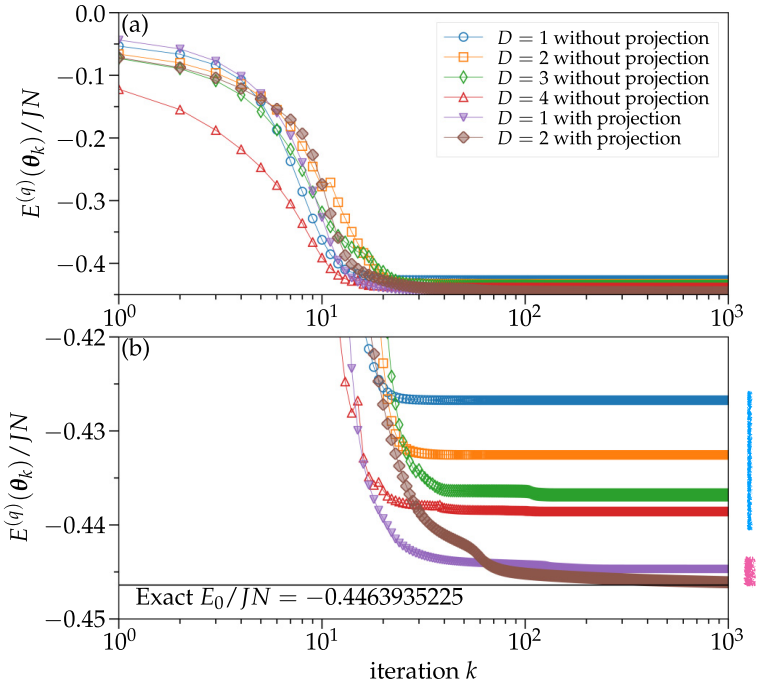
Ground-state energy and fidelity

K. Seki, T. Shirakawa & S. Yunoki, Phys. Rev. A **101**, 052340 ('20).

■**S=1/2 Heisenberg ring with 16 sites**

Parameter optimization: natural gradient descent

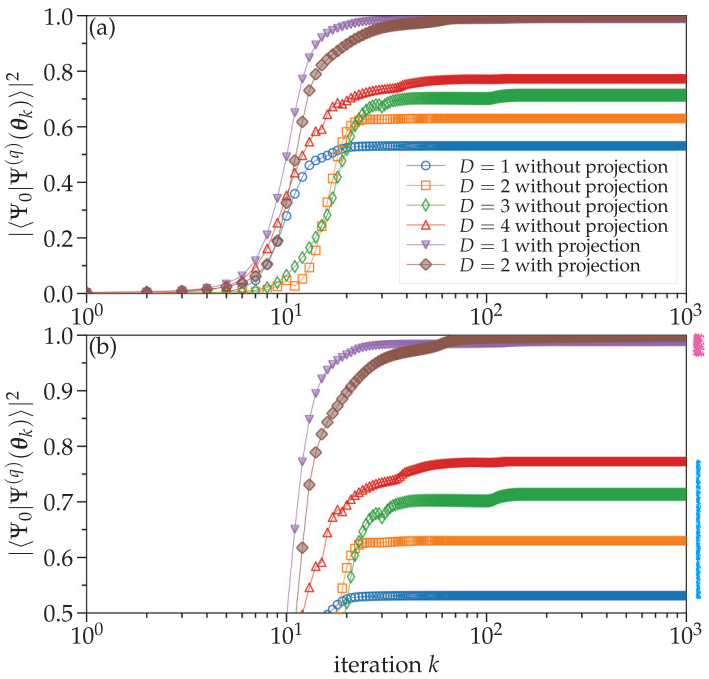
Energy



D=1,2,3,4 without sym.

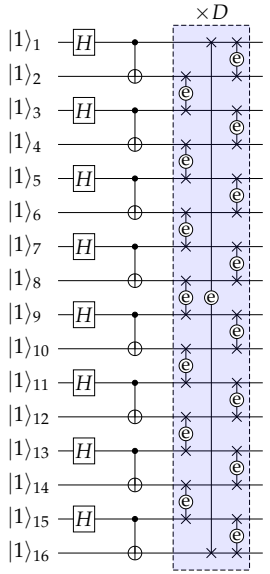
with sym. D=1,2

Fidelity



with sym. D=1,2

without sym. D=1,2,3,4

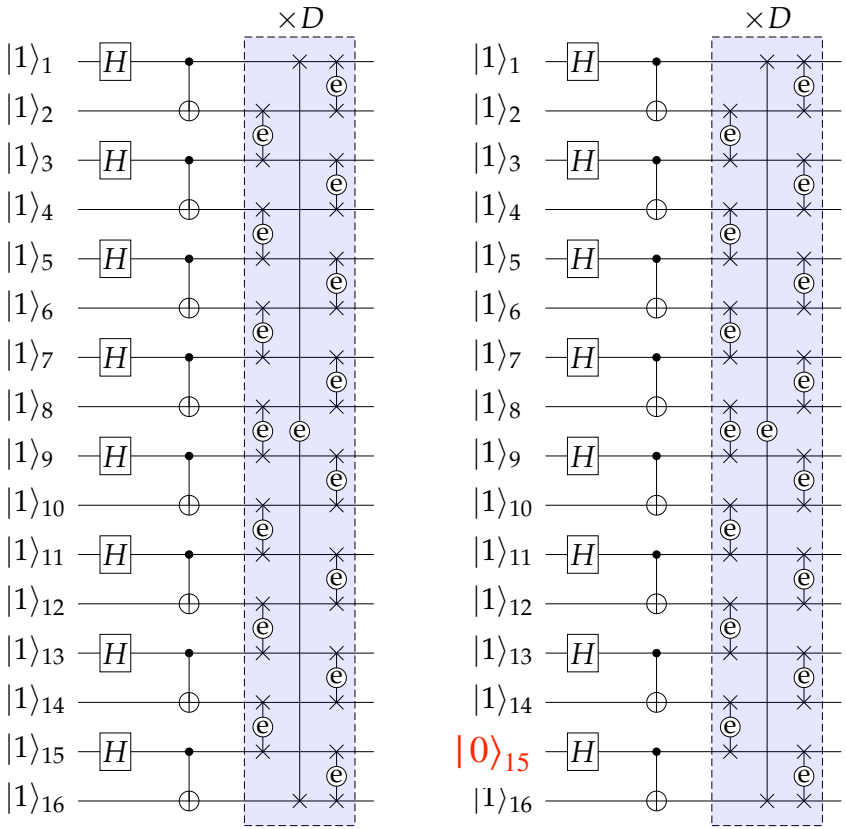


D: # of layers

Substantial improvement with much less # of layers D !!

Excited states with S=1

- **Same circuit structure except for a single input qubit**

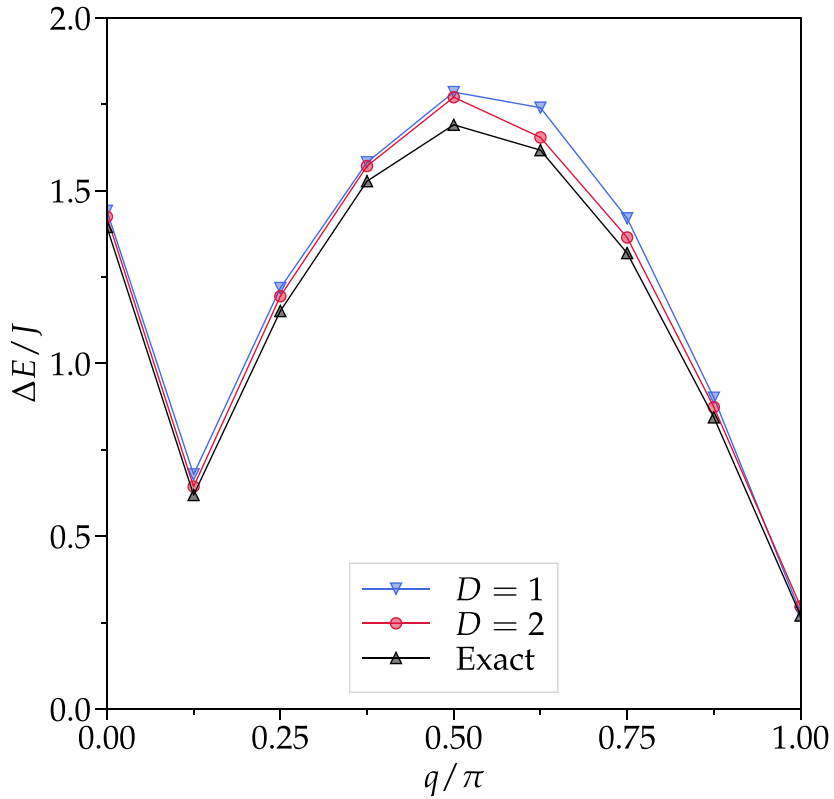


ground state $\chi^{(q)}(\hat{T}_n) = 1$

excited state (S=1 & momentum q) $\chi^{(q)}(\hat{T}_n) = \exp(iqn)$

K. Seki, T. Shirakawa & S. Yunoki, Phys. Rev. A **101**, 052340 ('20).

Lowest excitation energy with S=1 at different q

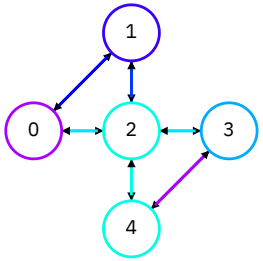


Experiment with a quantum device

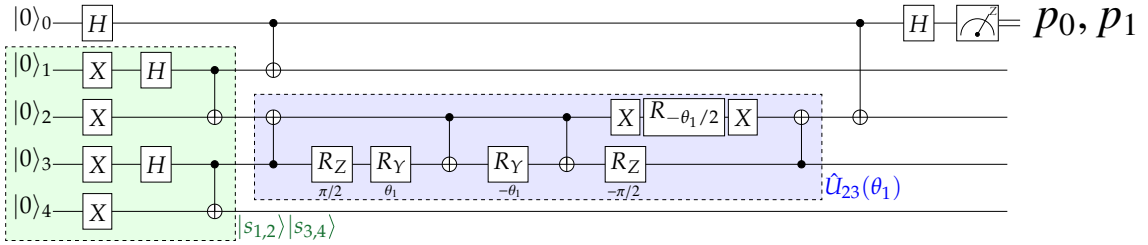
■ **S=1/2 Heisenberg ring with 4 sites**

K. Seki, T. Shirakawa & S. Yunoki, Phys. Rev. A **101**, 052340 ('20).

ibmq_5_yorktown



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



Exact $E_0/J = -2$

Estimated $E_0/J = -2.00682(1647)$

$p_0 - p_1 = \mathrm{Re}\langle\Psi_0|\hat{X}_1\hat{X}_2|\Psi_0\rangle$

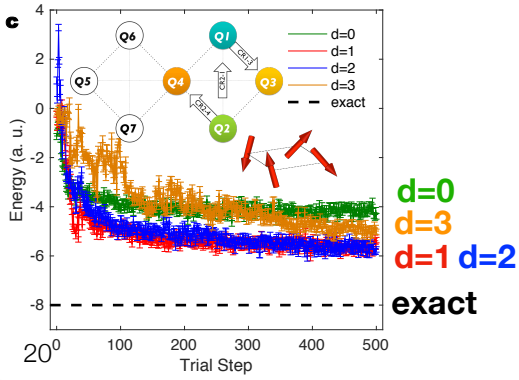
Sample	$p_0(\%)$	$p_1(\%)$	$\mathrm{Re}\langle\Psi_0\|\hat{X}_1\hat{X}_2\|\Psi_0\rangle$
1	15.430	84.570	-0.69140
2	17.969	82.031	-0.64062
3	15.625	84.375	-0.68750
4	16.309	83.691	-0.67382
5	16.016	83.984	-0.67968
6	15.430	84.570	-0.69140
7	17.578	82.422	-0.64844
8	18.457	81.543	-0.63086
9	17.090	82.910	-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

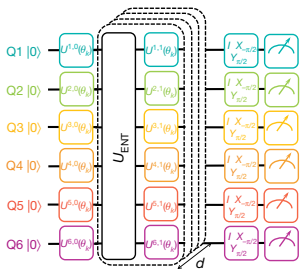
data taken on April 6, 2020 (EST)

Exact energy is obtained within the statistical error !!

vs.

Hardware efficient VQE by IBM





Kandala et al., Nature '17

Quantum circuit ansatz based on quantum adiabatic process

- **Quantum approximate optimization algorithm (QAOA)**
- **A guiding principle of designing a quantum circuit ansatz**

- T. Shirakawa, K. Seki & S. Yunoki, Phys. Rev. Research **3**, 013004/1-32 (’21).

Discretized quantum adiabatic process

■ quantum adiabatic process

$$\hat{\mathscr{H}}(\tau) = s_{\rm i}(\tau)\hat{\mathscr{H}}_{\rm i} + s_{\rm f}(\tau)\hat{\mathscr{H}}_{\rm f}$$

where scheduling functions satisfy

$$s_{\rm i}(\tau_{\rm i}) = s_{\rm f}(\tau_{\rm f}) = 1$$

$$s_{\rm i}(\tau_{\rm f}) = s_{\rm f}(\tau_{\rm i}) = 0$$

$$\hat{\mathscr{H}}(\tau_{\rm i}) = \hat{\mathscr{H}}_{\rm i}, \hat{\mathscr{H}}(\tau_{\rm f}) = \hat{\mathscr{H}}_{\rm f}$$

The final state $|\psi(\tau_{\rm f})\rangle$ at $\tau = \tau_{\rm f}$ is

$$|\psi(\tau_{\rm f})\rangle = \hat{\mathscr{U}}(\tau_{\rm f}, \tau_{\rm i})|\psi_{\rm i}\rangle$$

where $|\psi_{\rm i}\rangle$ is the ground state of $\hat{\mathscr{H}}_{\rm i}$ and

$$\hat{\mathscr{U}}(\tau_{\rm f}, \tau_{\rm i}) = T_\tau {\rm e}^{-{\rm i}\int_{\tau_{\rm i}}^{\tau_{\rm f}} \hat{\mathscr{H}}(\tau)d\tau}$$

The final state $|\psi(\tau_{\rm f})\rangle$ is the ground state of $\hat{\mathscr{H}}_{\rm f}$, provided $T = \tau_{\rm f} - \tau_{\rm i}$ is large.

■ discretized quantum adiabatic process

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

and $\hat{\mathscr{H}}_{\rm i} = \hat{\mathscr{V}}_1$

The time-evolution operator is

$$\hat{\mathscr{U}}(\tau_{\rm f}, \tau_{\rm i}) = \lim_{M\to\infty} \hat{\mathscr{U}}_d(\theta_M)\hat{\mathscr{U}}_d(\theta_{M-1})\cdots\hat{\mathscr{U}}_d(\theta_1)$$

where

$$\hat{\mathscr{U}}_d(\theta_m) = {\rm e}^{-{\rm i}\theta_1^{(m)}\hat{\mathscr{V}}_1}{\rm e}^{-{\rm i}\theta_2^{(m)}\hat{\mathscr{V}}_2}$$

$$\left.\begin{aligned}\theta_1^{(m)} &= [s_{\rm i}(\tau_m) + s_{\rm f}(\tau_m)]\delta\tau \\ \theta_2^{(m)} &= s_{\rm f}(\tau_m)\delta\tau\end{aligned}\right\}$$: linear scheduling

with

$$\delta\tau = (\tau_{\rm f} - \tau_{\rm i})/M$$

$$\tau_m = \tau_{\rm i} + m\delta\tau$$

- Set M to be finite
- **Consider $\{\theta_1^{(m)}, \theta_2^{(m)}\}$ as variational parameters**

Quantum circuit inspired by quantum adiabatic process

■ Discretized quantum adiabatic process (DQAP) ansatz

$$\hat{\mathscr{H}} = \hat{\mathscr{V}}_1 + \hat{\mathscr{V}}_2 \,(=\hat{\mathscr{H}}_{\rm f}),\ \text{where}\ [\hat{\mathscr{V}}_1, \hat{\mathscr{V}}_2] \neq 0,$$

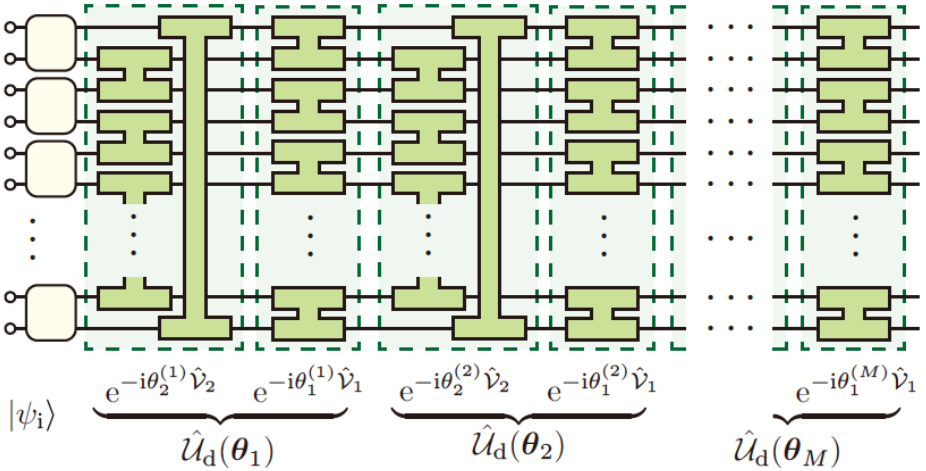
ground state of $\hat{\mathscr{V}}_1\,(=\hat{\mathscr{H}}_{\rm i})$

$$|\psi_M(\{\theta_p^{(m)}\})\rangle = \hat{\mathscr{U}}_d(\boldsymbol{\theta}_M)\hat{\mathscr{U}}_d(\boldsymbol{\theta}_{M-1})\cdots\hat{\mathscr{U}}_d(\boldsymbol{\theta}_1)\,|\psi_{\rm i}\rangle$$

where

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

determine $\{\theta_1^{(m)}, \theta_2^{(m)}\}$ so as to minimize the variational energy



> (almost) No ambiguity in circuit structure

> QAOA for a quantum state preparation

Ho & Hsieh, SciPost Phys. **6**, 29 ('19).
Mbeng, Fazio & Santoro, arXiv:1906.08948.
Mbeng, Fazio & Santoro, arXiv:1911.12259.
Wauters, Mbeng & Santoro, arXiv:2003.07419.

> Digitized adiabatic quantum commuting

R. Brends, et.al., Nat. Commun. **6**, 7654 ('15).
R. Barends, et.al., Nature **534**, 222 ('16).

■ In quantum approximate optimization algorithm (QAOA) for combinatorial optimization problems, $\hat{\mathscr{H}}$ is a classical Ising model (Farhi et al., arXiv:1411.4028).

DQAP ansatz for 1D free fermions

1D spinless free fermions with L sites at half filling

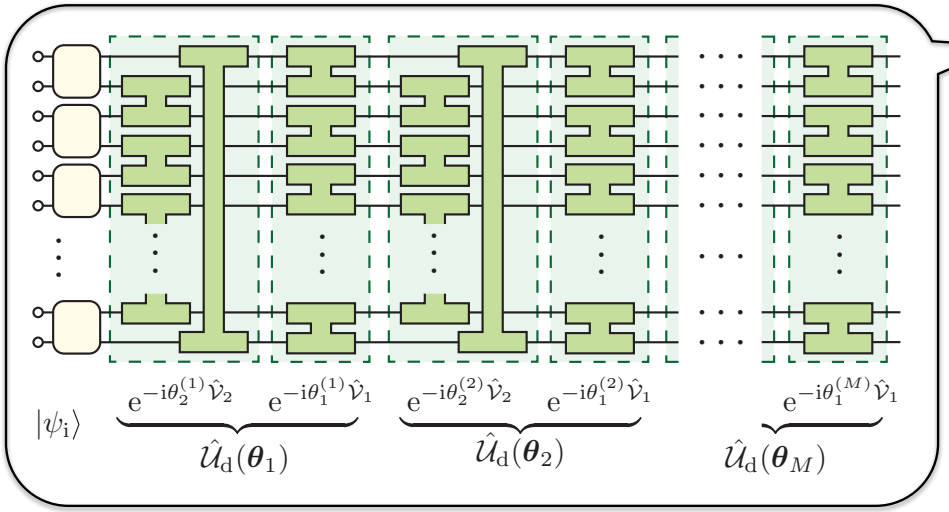
T. Shirakawa, K. Seki & S. Yunoki, Phys. Rev. Research **3**, 013004 ('21).

$$\mathcal{H} = -t\sum_{x=1}^{L-1}(\hat{c}_{x+1}^\dagger \hat{c}_x + \hat{c}_x^\dagger \hat{c}_{x+1}) - t\gamma(\hat{c}_1^\dagger \hat{c}_L + \hat{c}_L^\dagger \hat{c}_1) = \hat{\mathcal{V}}_1 + \hat{\mathcal{V}}_2$$

"even" bond: $\mathcal{V}_1 = -t\sum_{x=1}^{L/2}(\hat{c}_{2x}^\dagger \hat{c}_{2x-1} + \hat{c}_{2x-1}^\dagger \hat{c}_{2x})$

$$\gamma = \begin{cases} 1 & \text{periodic} \\ -1 & \text{anti-periodic} \end{cases}$$

"odd" bond: $\mathcal{V}_2 = -t\sum_{x=1}^{L/2-1}(\hat{c}_{2x+1}^\dagger \hat{c}_{2x} + \hat{c}_{2x}^\dagger \hat{c}_{2x+1}) - \gamma t(\hat{c}_1^\dagger \hat{c}_L + \hat{c}_L^\dagger \hat{c}_1)$



$$|\psi_M(\boldsymbol{\theta})\rangle = \hat{\mathcal{U}}_M(\boldsymbol{\theta})\,|\psi_{\rm i}\rangle$$

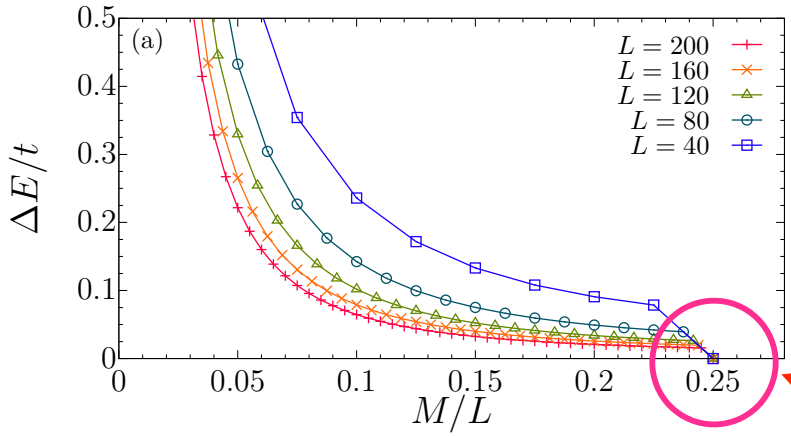
$$\hat{\mathcal{U}}_M(\boldsymbol{\theta}) = \hat{\mathcal{U}}_d(\boldsymbol{\theta}_M)\hat{\mathcal{U}}_d(\boldsymbol{\theta}_{M-1})\cdots\hat{\mathcal{U}}_d(\boldsymbol{\theta}_1)$$

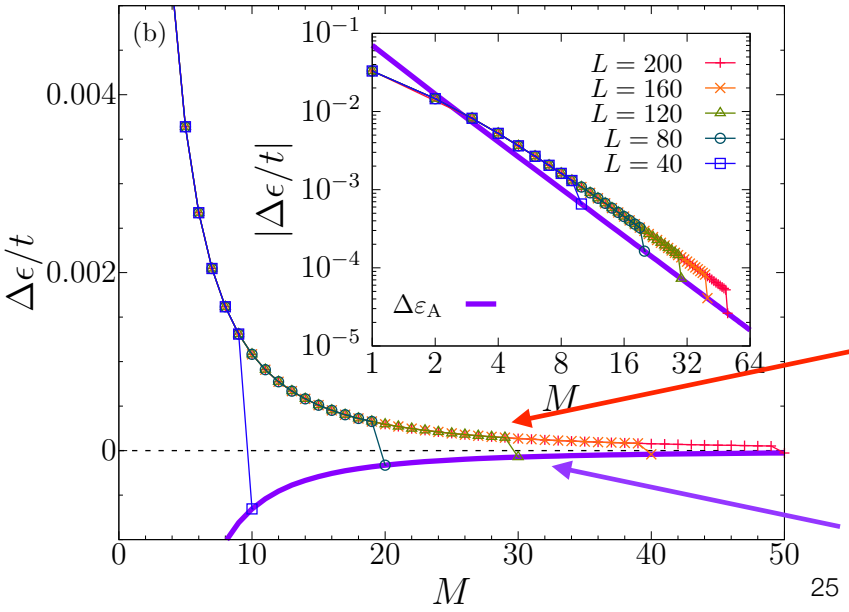
$$\boldsymbol{\theta} = \{\boldsymbol{\theta}_m\}_{m=1}^M$$

$$\boldsymbol{\theta}_m = \{\theta_1^{(m)}, \theta_2^{(m)}\}$$

→ variational parameters

Ground state energy





T. Shirakawa, K. Seki & S. Yunoki, Phys. Rev. Research **3**, 013004 ('21).

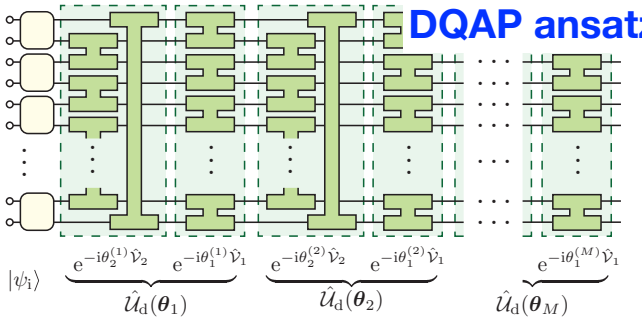
$$\Delta E = E(\boldsymbol{\theta}) - E_{\rm exact}(L)$$

$$E(\boldsymbol{\theta}) = \langle \psi_M(\boldsymbol{\theta}) \,|\, \hat{\mathscr{H}} \,|\, \psi_M(\boldsymbol{\theta}) \rangle$$

$E_{\rm exact}(L)$: exact ground state energy for system size L

exact ground state at *M=L/4*

DQAP ansatz



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

states $|\psi_M(\boldsymbol{\theta})\rangle$ with $M < L/4$ are independent of system size L

purple line: $E_{\rm exact}(L)/L - \lim_{L\to\infty} E_{\rm exact}/L$ with $M = L/4$

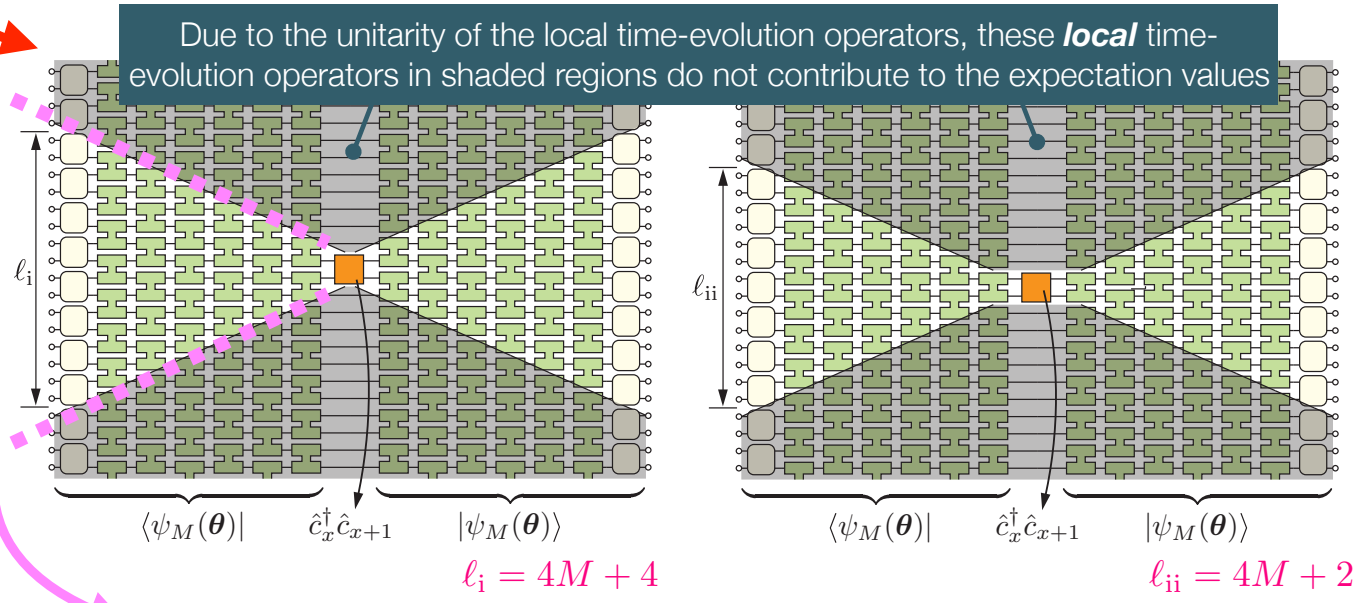
Causality cone and Lieb-Robinson bound

$$E(\boldsymbol{\theta}) = \langle \psi_M(\boldsymbol{\theta}) \,|\, \hat{\mathscr{H}} \,|\, \psi_M(\boldsymbol{\theta}) \rangle$$

$$\hat{\mathscr{H}} = \sum_{k=1}^{L/2} (\hat{\mathscr{V}}_1^{(k)} + \hat{\mathscr{V}}_2^{(k)})$$

$$\hat{\mathscr{V}}_1^{(k)} = -t\left(\hat{c}_{2k}^\dagger \hat{c}_{2k-1} + \mathrm{h.c}\right) \qquad \hat{\mathscr{V}}_2^{(k)} = -t\left(\hat{c}_{2k+1}^\dagger \hat{c}_{2k} + \mathrm{h.c}\right)$$

T. Shirakawa, K. Seki & S. Yunoki, Phys. Rev. Research **3**, 013004 ('21).



causality cone set by **Lieb-Robinson bound**

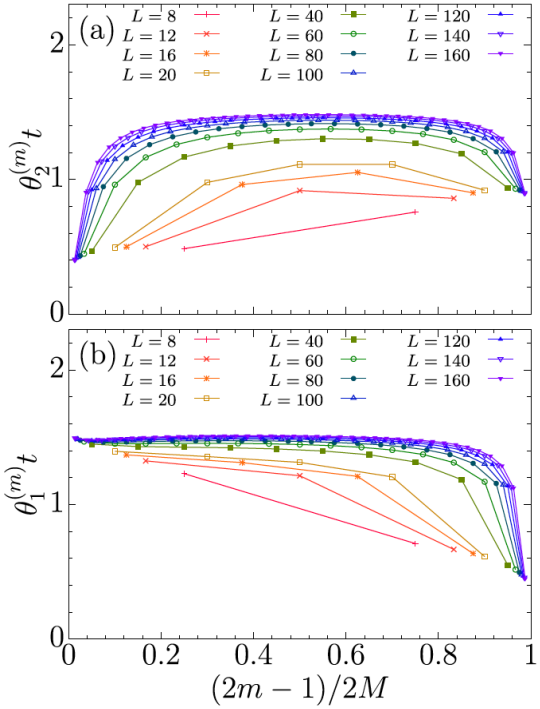
M=L/4 corresponds to the point where the causality-cone exceeds the system size *L*.

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

Total time necessarily to reach the exact GS

T. Shirakawa, K. Seki & S. Yunoki, Phys. Rev. Research **3**, 013004 ('21).

- **optimized variational parameters for M=L/4 (exact solution)**

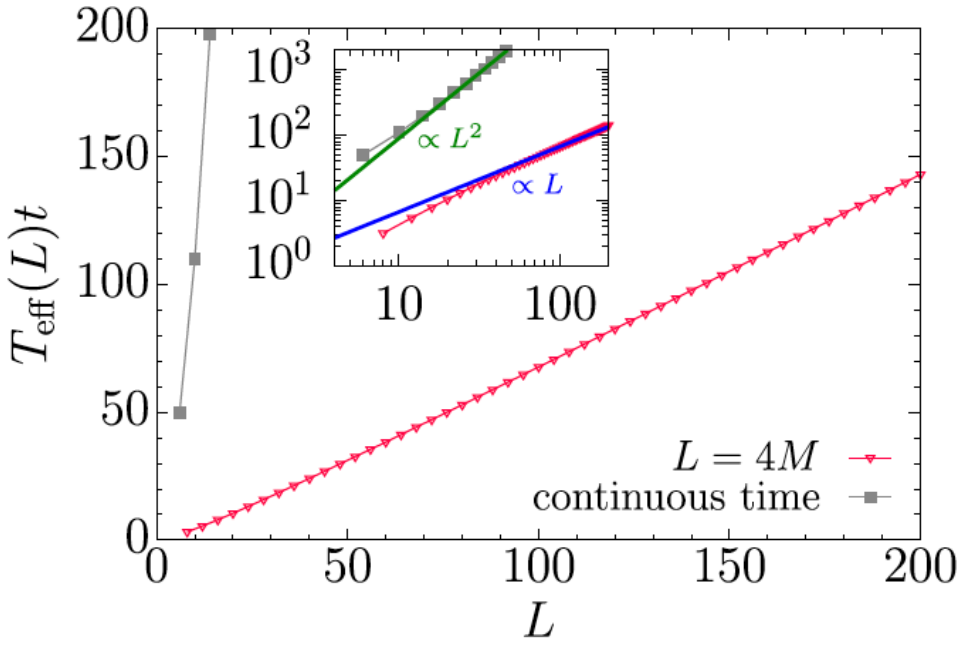


Effective total evolution time:

$$T_{\rm eff}(L) = \sum_{m=1}^{M} (\theta_1^{(m)} + \theta_2^{(m)})$$

- **Total evolution time: continuous time QAP vs. discretized QAP**

1D free spineless fermions: minimum gap ~ 1/L. The adiabatic theorem thus tells us that the evolution time necessary to obtain the exact GS is ~ L^2.



Polynomial speedup over the continuous time quantum adiabatic calculation

Imaginary-time evolution

T. Shirakawa, K. Seki & S. Yunoki, Phys. Rev. Research **3**, 013004 ('21).

$$|\psi_M(\boldsymbol{\theta})\rangle = \mathrm{e}^{-\mathrm{i}\theta_1^{(M)}\hat{\mathscr{V}}_1}\mathrm{e}^{-\mathrm{i}\theta_2^{(M)}\hat{\mathscr{V}}_2}\cdots\mathrm{e}^{-\mathrm{i}\theta_1^{(1)}\hat{\mathscr{V}}_1}\mathrm{e}^{-\mathrm{i}\theta_2^{(1)}\hat{\mathscr{V}}_2}|\psi_\mathrm{i}\rangle$$

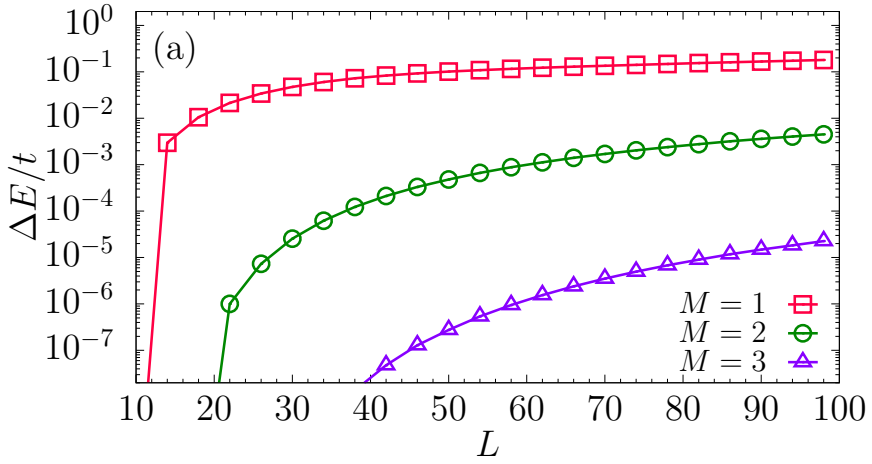
$\{\theta_1^{(m)}, \theta_2^{(m)}\}_{m=1}^{M}$: variational parameters

$$\longrightarrow \quad |\phi_M(\boldsymbol{\tau})\rangle = \mathrm{e}^{-\tau_1^{(M)}\hat{\mathscr{V}}_1}\mathrm{e}^{-\tau_2^{(M)}\hat{\mathscr{V}}_2}\cdots\mathrm{e}^{-\tau_1^{(1)}\hat{\mathscr{V}}_1}\mathrm{e}^{-\tau_2^{(1)}\hat{\mathscr{V}}_2}|\psi_\mathrm{i}\rangle$$

$\{\tau_1^{(m)}, \tau_2^{(m)}\}_{m=1}^{M}$: variational parameters

$$E(\boldsymbol{\tau}) = \langle\phi_M(\boldsymbol{\tau})|\hat{\mathscr{H}}|\phi_M(\boldsymbol{\tau})\rangle$$

$$\Delta E = E(\boldsymbol{\tau}) - E_\mathrm{exact}(L)$$



exponentially fast convergence with *M*

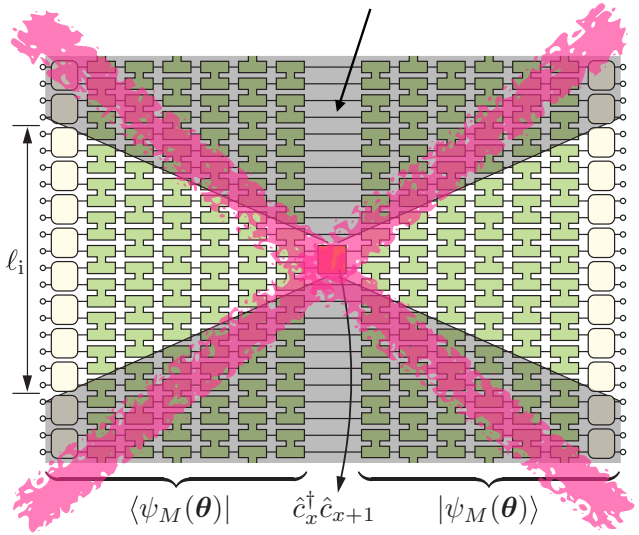
Only M=3 layers are enough for the ground state with $L \leq 100$

Imaginary-time evolution

T. Shirakawa, K. Seki & S. Yunoki, Phys. Rev. Research **3**, 013004 ('21).

$$|\phi_M(\boldsymbol{\tau})\rangle = \mathrm{e}^{-\tau_1^{(M)}\hat{\mathscr{V}}_1}\mathrm{e}^{-\tau_2^{(M)}\hat{\mathscr{V}}_2}\cdots\mathrm{e}^{-\tau_1^{(1)}\hat{\mathscr{V}}_1}\mathrm{e}^{-\tau_2^{(1)}\hat{\mathscr{V}}_2}|\psi_{\mathrm{i}}\rangle$$

no cancellation of the imaginary time evolution operators



There is **no causality cone** and **no Lieb-Robinson bound** because of the **non-unitary** of the local imaginary-time evolution operators

Non-locality due to the non-unitarity imaginary-time evolution

How can we implement the **non-unitary** imaginary-time evolution and the **unnormalized** state $|\phi_M(\boldsymbol{\tau})\rangle$?

Quantum power method

- Imaginary time evolution (e.g., QMC): $\lim_{\beta\to\infty} \mathrm{e}^{-\beta\hat{H}}|\phi_0\rangle \to |\Psi_{\mathrm{GS}}\rangle$
- Power method: $\lim_{n\to\infty} (\lambda - \hat{H})^n |\phi_0\rangle \to |\Psi_{\mathrm{GS}}\rangle$

■ K. Seki & S. Yunoki, PRX Quantum **2**, 010333/1-45 ('21).

Matrix power

$$|\psi\rangle \qquad \hat{H}|\psi\rangle \qquad \hat{H}^2|\psi\rangle \qquad \ldots \qquad \hat{H}^n|\psi\rangle$$

In classical computation of quantum many (*N*)-body systems,

matrix powers have various applications such as

- **Krylov-subspace methods (e.g., Lanczos)**
- **Polynomial expansion methods (e.g., Chebyshev)**
- **Moment and cumulant methods (e.g., high-temperature expansion)**

the dimension of vectors increases exponentially in *N*

Quantum evaluation of $\langle H^n \rangle$?

$$\langle\psi|\hat{H}^n|\psi\rangle = \langle\psi|\left(\sum_i h_i \hat{P}_i\right)^n|\psi\rangle$$

# of measurements increases exponentially in *n* or 4^N

Direct treatment of H^n?

H^n is not unitary !!

Our strategy:
Approximate H^n by a linear combination of unitaries

Approximated Hamiltonian power

K. Seki & S. Yunoki, PRX Quantum **2**, 010333 ('21).

Main idea

$$\hat{\mathcal{H}}^n = \mathrm{i}^n \left. \frac{\mathrm{d}^n \hat{U}(t)}{\mathrm{d}t^n} \right|_{t=0} \quad \text{where} \quad \hat{U}(t) = \mathrm{e}^{-\mathrm{i}\hat{\mathcal{H}}t}$$

in a time-discretized form, e.g.,

$$\hat{\mathcal{H}}^1 \approx \frac{\mathrm{i}}{\Delta_\tau}\left[\hat{U}\left(\frac{\Delta_\tau}{2}\right) - \hat{U}\left(-\frac{\Delta_\tau}{2}\right)\right]$$

$$\hat{\mathcal{H}}^2 \approx \frac{\mathrm{i}^2}{\Delta_\tau^2}\left[\left[\hat{U}\left(\frac{\Delta_\tau}{2}\right)\right]^2 - 2\hat{I} + \left[\hat{U}\left(-\frac{\Delta_\tau}{2}\right)\right]^2\right]$$

$$\vdots$$

H^n **is approximated by a linear combination of (n+1) unitaries**

Approximated Hamiltonian power

K. Seki & S. Yunoki, PRX Quantum **2**, 010333 ('21).

$$\hat{\mathcal{H}}^n = \mathrm{i}^n \left.\frac{\mathrm{d}^n \hat{U}(t)}{\mathrm{d}t^n}\right|_{t=0} \quad \text{where} \quad \hat{U}(t) = \mathrm{e}^{-\mathrm{i}\hat{\mathcal{H}}t}$$

central finite difference approximation

$$\hat{\mathcal{H}}^n = \hat{\mathcal{H}}^n(\Delta_\tau) + O(\Delta_\tau^2) \quad \text{where}$$

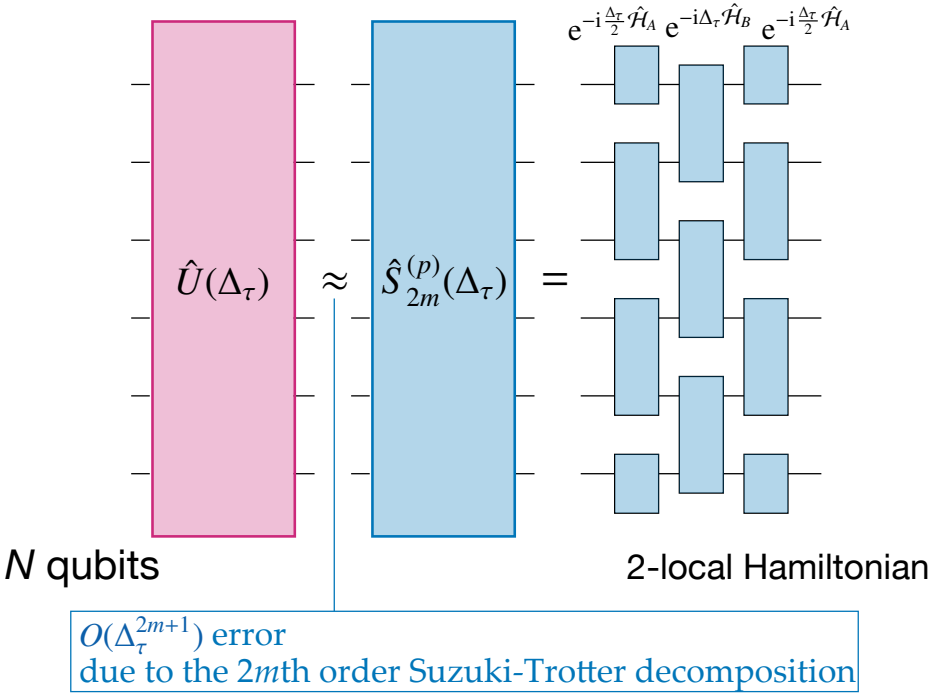
$$\hat{\mathcal{H}}^n(\Delta_\tau) = \sum_{k=0}^{n} c_{n,k} \left[\hat{U}\left(\frac{\Delta_\tau}{2}\right)\right]^{n-2k} \qquad c_{n,k} = \frac{\mathrm{i}^n}{\Delta_\tau^n}(-1)^k \binom{n}{k}$$

Symmetric Suzuki-Trotter approximation

$$\hat{\mathcal{H}}^n = \hat{\mathcal{H}}^n_{\mathrm{ST}}(\Delta_\tau) + O(\Delta_\tau^2) + O(\Delta_\tau^{2m}) \quad \text{where}$$

$$\hat{\mathcal{H}}^n_{\mathrm{ST}}(\Delta_\tau) = \sum_{k=0}^{n} c_{n,k} \left[\hat{S}^{(p)}_{2m}\left(\frac{\Delta_\tau}{2}\right)\right]^{n-2k}$$

***H*ⁿ is approximated by a sum of (n+1) unitaries**

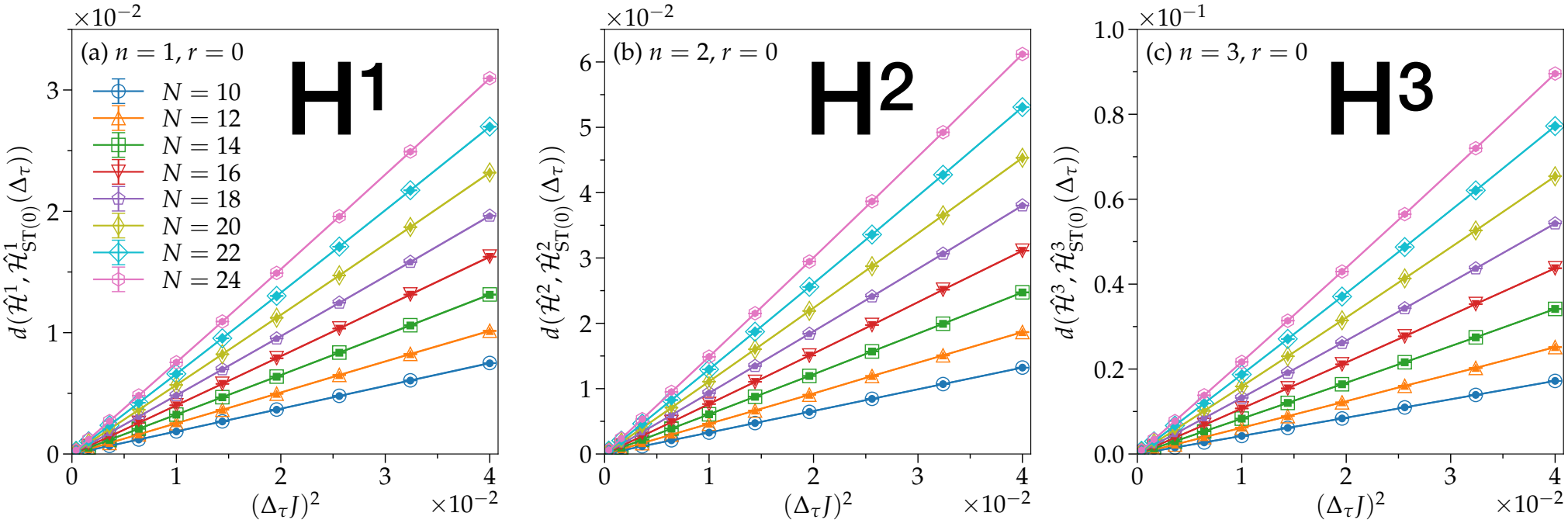


number of the gates: *k*-local Hamiltonian
~ O(*knN*) for spin models
~ O(*knN* log*N*) for fermionic models

Time-discretization error in approximated H^n

K. Seki & S. Yunoki, PRX Quantum **2**, 010333 ('21).

H: 1D S=1/2 Heisenberg model



operator distance

$$d(\hat{A}, \hat{B}) = \sqrt{1 - \frac{\left|\left\langle \hat{A}, \hat{B} \right\rangle_{\mathrm{F}}\right|}{\left\|\hat{A}\right\|_{\mathrm{F}} \left\|\hat{B}\right\|_{\mathrm{F}}}}$$

Time-discretization error is well controlled

Time-discretization error in approximated H^n

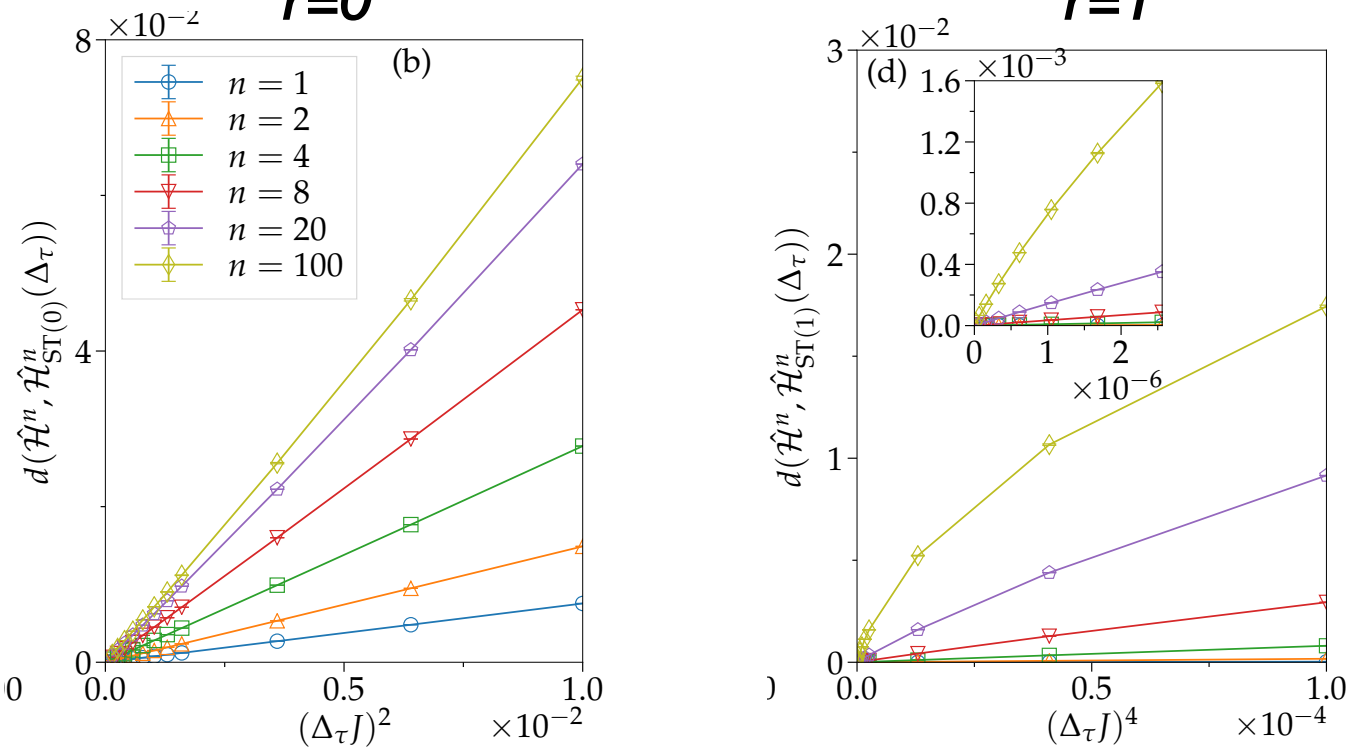
K. Seki & S. Yunoki, PRX Quantum **2**, 010333 ('21).

***N*=24 fixed**

r=0

H: 1D S=1/2 Heisenberg model

r=1



operator distance

$$d(\hat{A}, \hat{B}) = \sqrt{1 - \frac{\left|\left\langle \hat{A}, \hat{B} \right\rangle_{\mathrm{F}}\right|}{\left\|\hat{A}\right\|_{\mathrm{F}} \left\|\hat{B}\right\|_{\mathrm{F}}}}$$

Error is well controlled even for quite large power (n=100)

Application: Krylov-subspace diagonalization

Rayleigh-Ritz technique

Approximate the ground state of H within a subspace $\mathcal{U}_n = \mathrm{span}\left(|u_1\rangle, |u_2\rangle, \cdots, |u_n\rangle\right)$

$$|\Psi_0\rangle \approx \sum_{i=1}^{n} v_i |u_i\rangle$$

where v_i can be obtained by solving the generalized eigenvalue equation

$$\boldsymbol{H}\boldsymbol{v} = \boldsymbol{S}\boldsymbol{v}\epsilon \qquad [\boldsymbol{H}]_{ij} = \langle u_i|\hat{\mathcal{H}}|u_j\rangle \qquad [\boldsymbol{S}]_{ij} = \langle u_i|u_j\rangle$$

A relevant choice of the subspace: Krylov subspace

reference state(s)

Choose $\boldsymbol{U}_n$ as a Krylov subspace $\mathcal{U}_n = \mathcal{K}_n(\hat{H}, |\psi\rangle) = \mathrm{span}\left(|\psi\rangle, \hat{H}|\psi\rangle, \cdots, \hat{H}^{n-1}|\psi\rangle\right)$

Then we have

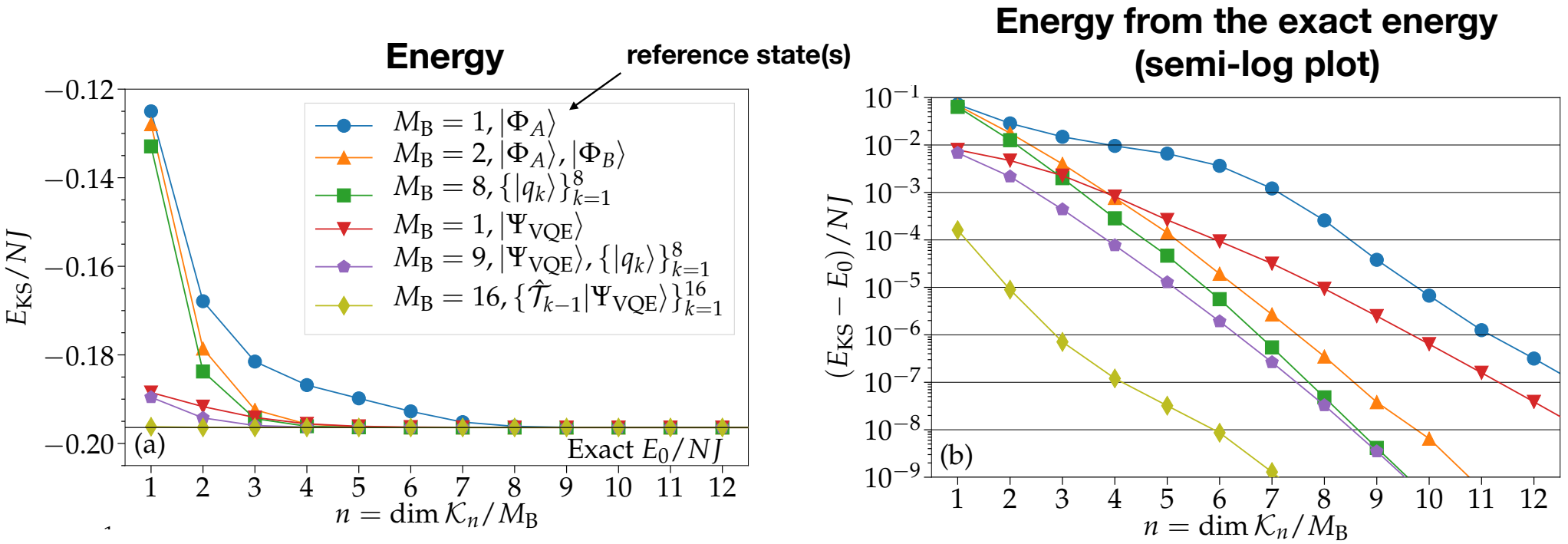
$$\boldsymbol{H}\boldsymbol{v} = \boldsymbol{S}\boldsymbol{v}\epsilon \quad [\boldsymbol{H}]_{ij} = \langle\psi|\hat{\mathcal{H}}^{i+j-1}|\psi\rangle \quad [\boldsymbol{S}]_{ij} = \langle\psi|\hat{\mathcal{H}}^{i+j-2}|\psi\rangle$$

quantum-power method

Application: Krylov-subspace diagonalization

K. Seki & S. Yunoki, PRX Quantum **2**, 010333 ('21).

1D S=1/2 Heisenberg model (L=16 and $\Delta\tau J$=0.05 with Richardson extrapolation)



Krylov subspace: $\mathcal{U}_n = \mathcal{K}_n(\hat{H}, |\psi\rangle) = \mathrm{span}\left(|\psi\rangle, \hat{H}|\psi\rangle, \cdots, \hat{H}^{n-1}|\psi\rangle\right)$

Energy converges exponentially in *n*

Use of multiple initial (reference) states helps the better convergence

Summary

- Quantum-classical hybrid scheme is a promising approach for simulating quantum many-body systems in NISQ devices

- We want to go beyond a quantum variational approach
  - parameter optimization in a classical computer
  - no knowledge of a quantum circuit structure

- Symmetry-adapted VQE scheme
  - non-unitarity treated as post-processing in a classical computer
  - shallow circuit with less number of gates

- Circuit construction based on discretized quantum adiabatic process
  - no prior knowledge required for a better circuit
  - requires variational parameter optimization

- Quantum power method
  - no variational parameters & no prior knowledge for a better circuit