Quantum computation of valence two-neutron systems towards solving full nuclear Hamiltonians

@JOINT N3AS – iTHEMS MEETING ON QUANTUM INFORMATION SCIENCE IN MULTIMESSENGER ASTROPHYSICS, Jun 16-18, 2024, RIKEN

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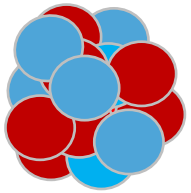
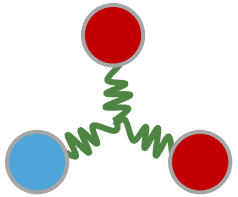
Ref: SY, T. Sato, T. Ogata, T. Naito, M. Kimura, PhysRevC.109.064305 (2024)

Motivations for Quantum Computing in NP(Nuclear Physics)

- strongly interacting protons and neutrons
  (let me consider only "nucleons" dof)



- nuclear force is highly nontrivial



three-nucleon force

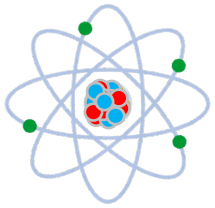
first principle understanding by Lattice QCD
c.f. Ishii, Aoki, Hatsuda, PRL 99, 022001 (2007).

still have very large uncertainty for nuclear structure/reaction(dynamics)

- divergent of the dimension: $10^{16}!$ $10^{19}!!$, $10^{23}!!!$
  most of nuclei cannot be solved in exact manner
  → zoo of nuclear many-body methods
  → need to prepare for "Quantum Computing era" for NP

Difference from other quantum many-body systems

Quantum chemistry:



"99 > % of energy of a molecule in equilibrium

is explained within Hartree-Fock level"

(i.e., single Slater determinant)

rest 1 % is called **correlation energy**:

Møller – Plesset (MP a.k.a MBPT)

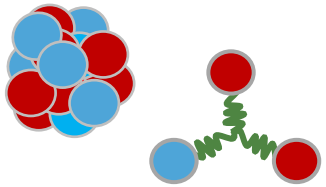
Coupled Cluster Single and Double (CCSD)

CCSD + Triple (CCSDT)

Full Configuration interaction (Full-CI)

accurate but heavy

Nuclear physics:



Interaction is highly non-perturbative

uncertain (many channels, three-nucleon force,..)

^{56}Ni under modern Nuclear Force (Chiral EFT)

HF = - 302.716 MeV

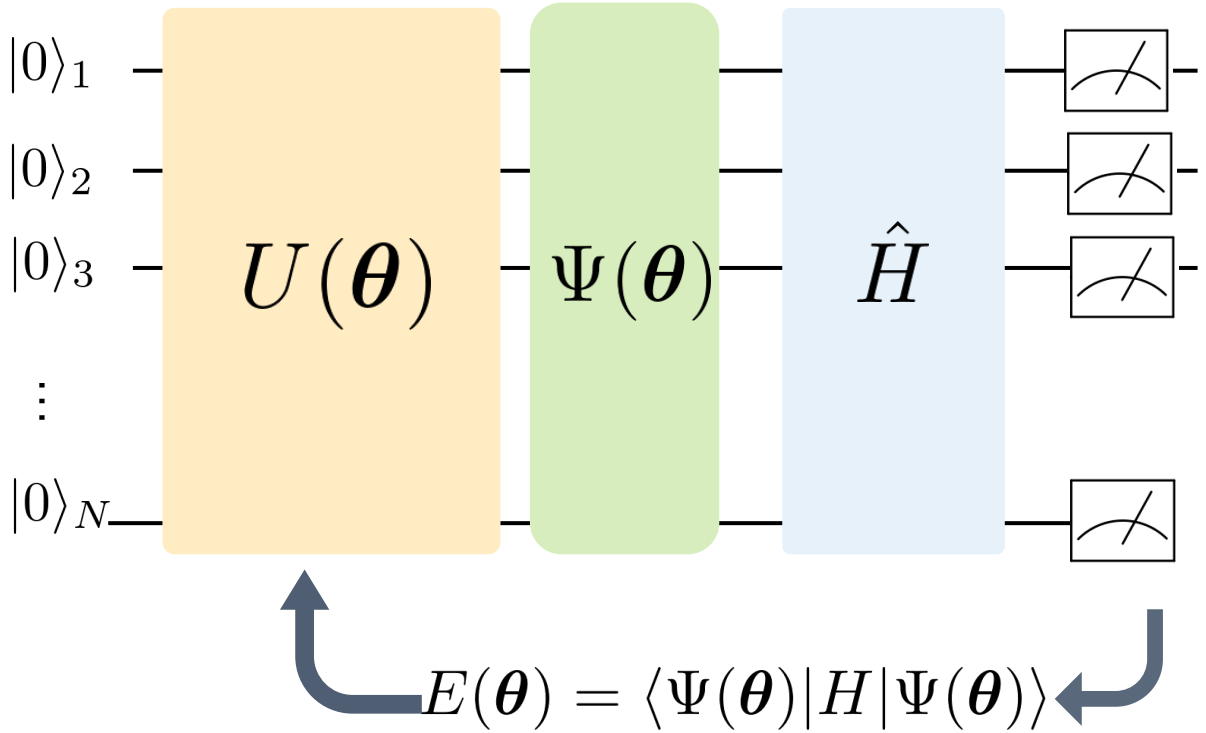
HF + MP2 + MP3 = -473.089 MeV
(MP2 = -152.533, MP3 = -17.716)

~~How dare people say perturbation theory !!~~

c.f. Energy (Exp.) = -483.996 MeV

Variational quantum eigensolver (VQE)

A typical workflow of VQE



1. initialize the qubits
   |00…>, Hartree-Fock, etc.

2. ansatz:
   Operating Unitary gates
   → prepare trial wave functions

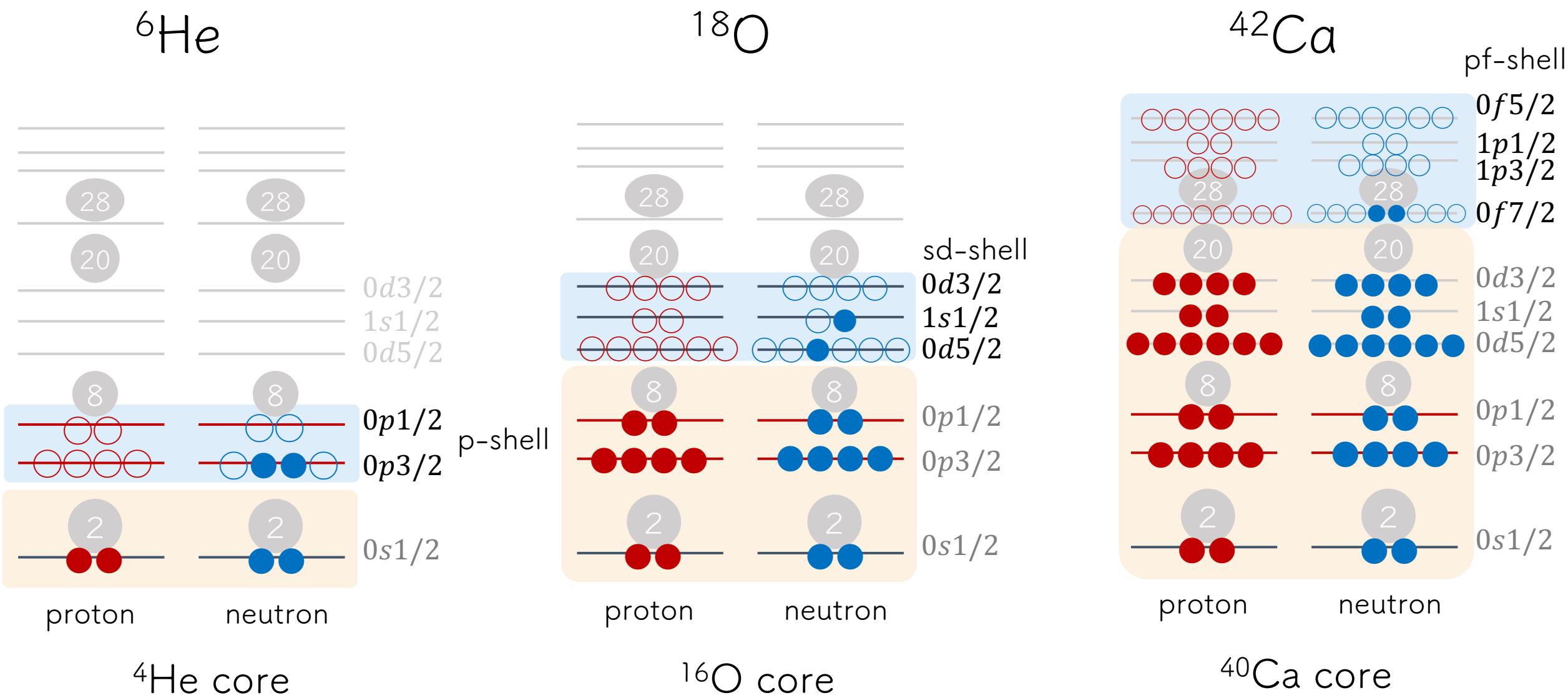
3. Operating Unitary gates (Hamiltonian)
   →measurement → energy

4. Optimize the parameters classically
   to minimize the energy

Popular choice for the ansatz: the unitary coupled cluster (UCC) or its variants

schematics for valence two-neutron systems

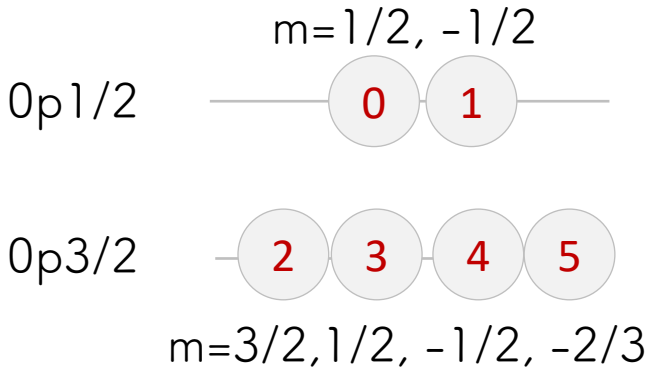
{n, l, j, jz, tz}



blue: valence space, pale orange: inert core

valence two-neutron systems: p shell example

ground state (J=0) can be described only by time-reversal pairs (jz = m & -m)



$|1_0 1_1 0_2 0_3 0_4 0_5\rangle$

$|0_0 0_1 1_2 0_3 0_4 1_5\rangle$

$|0_0 0_1 0_2 1_3 1_4 0_5\rangle$

} Only these have finite amplitude

original Hamiltonian can be rewritten by pair creation/annihilation operators

$$H = \sum_i \varepsilon_i \hat{a}_i^\dagger \hat{a}_i + \frac{1}{4} \sum_{ijkl} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k,$$

$$A_{\tilde{i}}^\dagger = c_i^\dagger c_{\bar{i}}^\dagger, \qquad \left[A_{\tilde{i}}, A_{\tilde{j}}^\dagger\right] = \delta_{\tilde{i}\tilde{j}} \left(1 - N_{\tilde{i}}\right),$$

$$A_{\tilde{i}} = c_{\bar{i}} c_i, \qquad \left[N_{\tilde{i}}, A_{\tilde{j}}^\dagger\right] = 2\delta_{\tilde{i}\tilde{j}} A_{\tilde{j}}^\dagger.$$

$$N_{\tilde{i}} = c_i^\dagger c_i + c_{\bar{i}}^\dagger c_{\bar{i}}.$$

$$H^{\mathrm{pw}} = \sum_i \bar{h}_i A_i^\dagger A_i + \sum_{i \le j} \bar{V}_{ij} A_i^\dagger A_j,$$

$|110000\rangle \rightarrow |100\rangle$

$|001001\rangle \rightarrow |010\rangle$

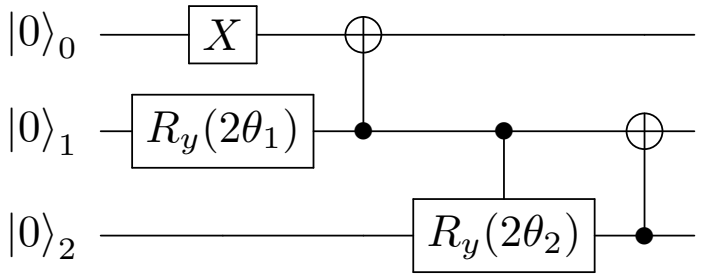
$|000110\rangle \rightarrow |001\rangle$

expressing the "pair" as a single qubit,
# of qubits needed is reduced to half

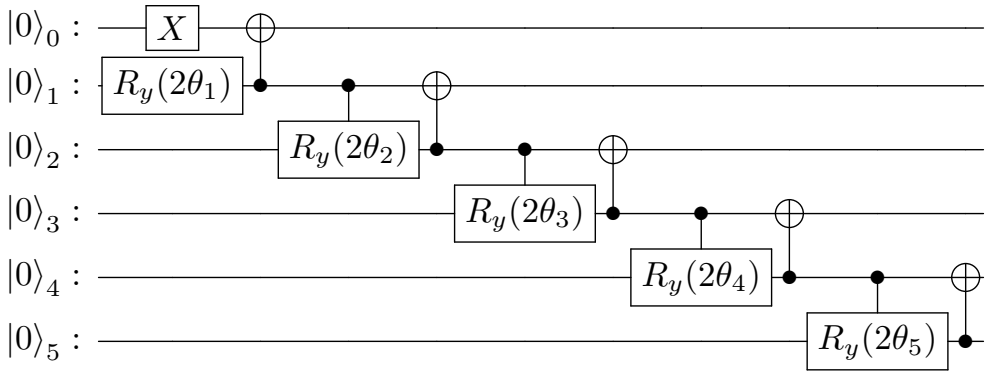
ansatz: circuit for trial wave function

You need only singly occupied configurations
→ ansatz can be expressed by (C-)Ry & CNOTs

^{6}He (3 qubits)



^{18}O (6 qubits)



^{42}Ca (10 qubits)

	# of CNOTs	
	proposed 3N-5	AdaptVQE average(upper)
^{6}He (3 qubits)	4	42 (80)
^{18}O (6 qubits)	13	99 (176)
^{42}Ca (10 qubits)	25	116~304

A. Pérez-Obiol et al., Sci. Rep. 13, 12291 (2023)

Measurement of energy

$$H^{\mathrm{pw}} = \sum_i \bar{h}_i A_i^\dagger A_i + \sum_{i \le j} \bar{V}_{ij} A_i^\dagger A_j, \qquad \hat{H}^{\mathrm{pw}}_{\mathrm{qubit}} = \sum_i \frac{\bar{h}_i + \bar{V}_{ii}}{2} (I - Z_i) + \frac{1}{2} \sum_{i<j} \bar{V}_{ij} (X_i X_j + Y_i Y_j)$$

1st term: Pauli-Z measurement of the ansatz (occupation numbers)

2nd term:

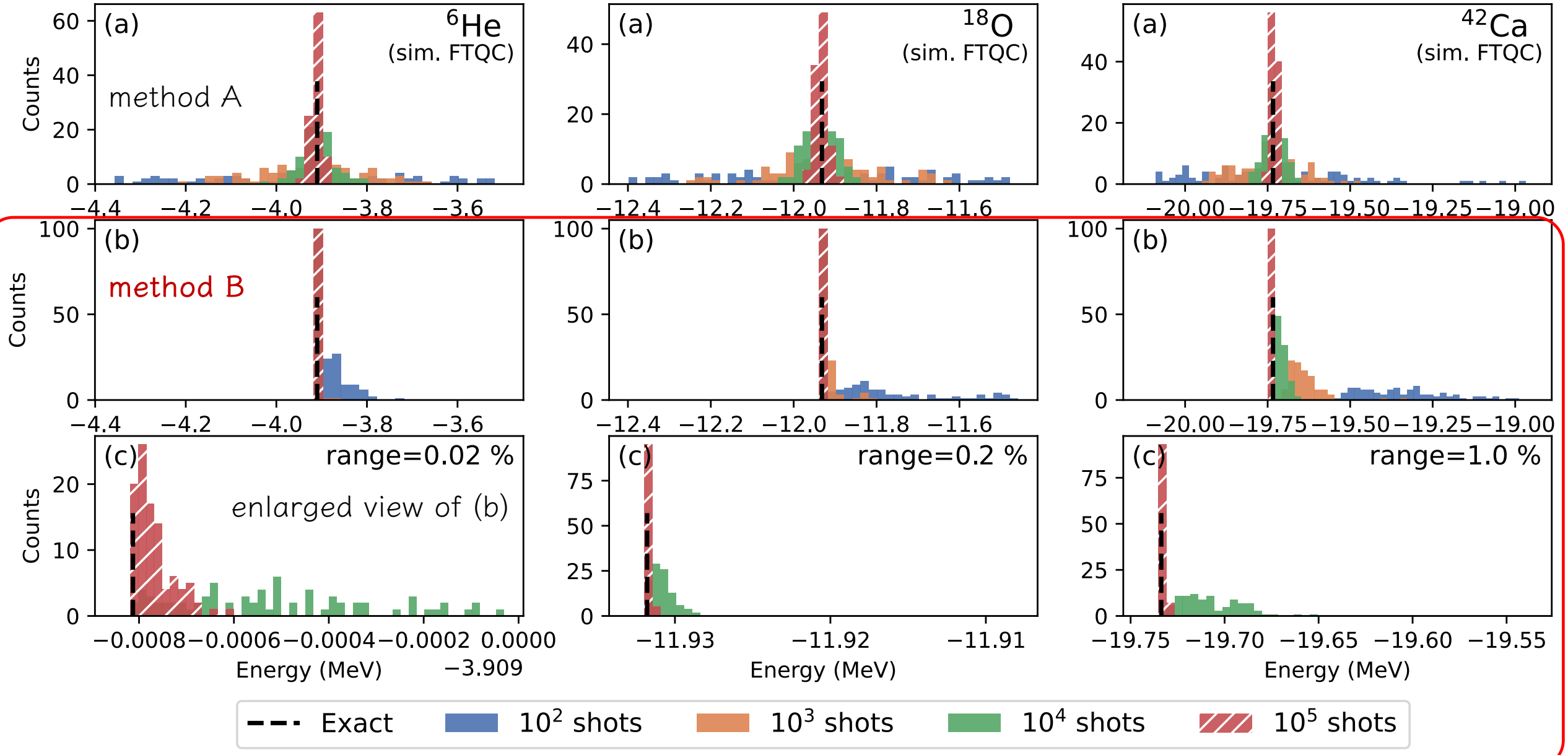
method A: measure expectation value of all Pauli spins (XX, YY)

method B: computational basis sampling (QunaSys&Osaka U. group)

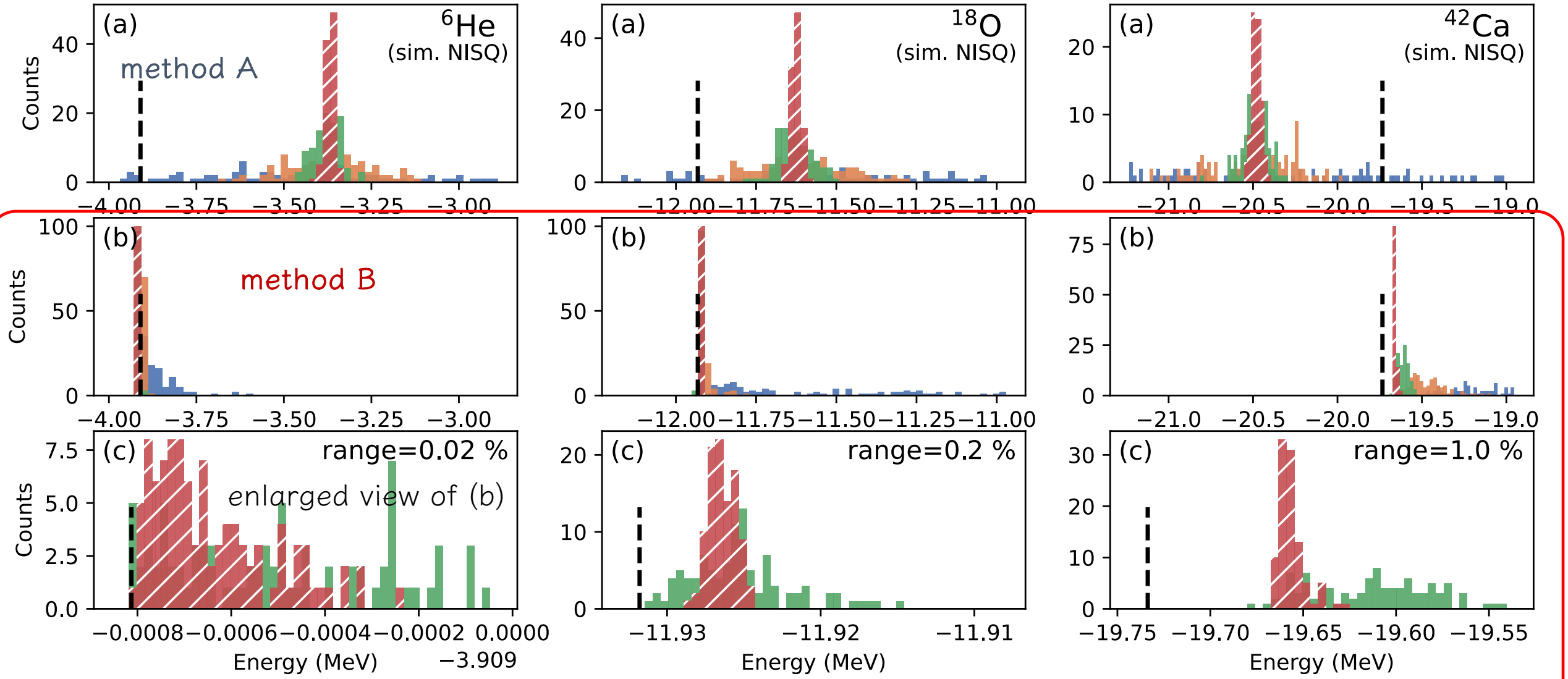
→ variational, only two measurements (ansatz & ansatz + H-gates)

M. Kohda, et al., Phys. Rev. Res. 4, 033173 (2022).

Results: FTQC(noise-free) simulator



Results: NISQ (noisy) simulator



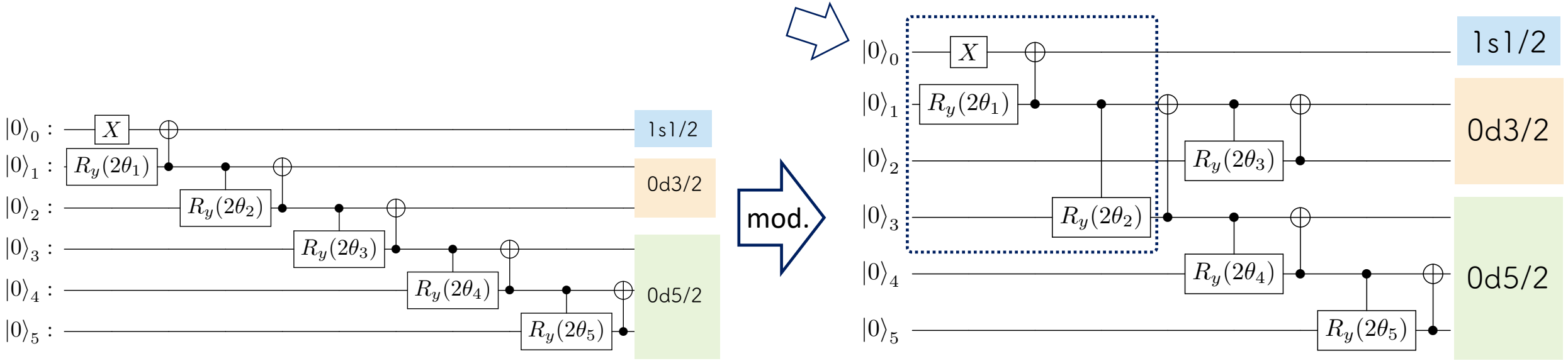
Rearrangement of the ansatz circuit

narrower circuits leads to noise-resilient results

^{18}O (6 qubits)case:

rearrangement of the circuit to the equivalent but shallow circuit

calculating the relative weights of jj-coupling orbitals

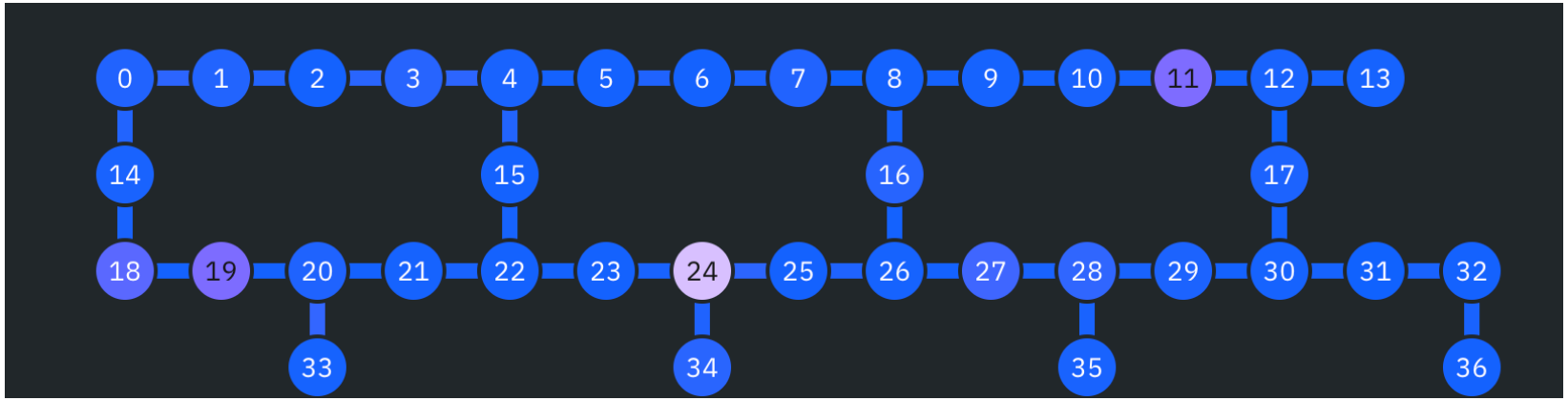


They should give identical results if noise is absent

connectivity of qubits in the hardware is another important factor

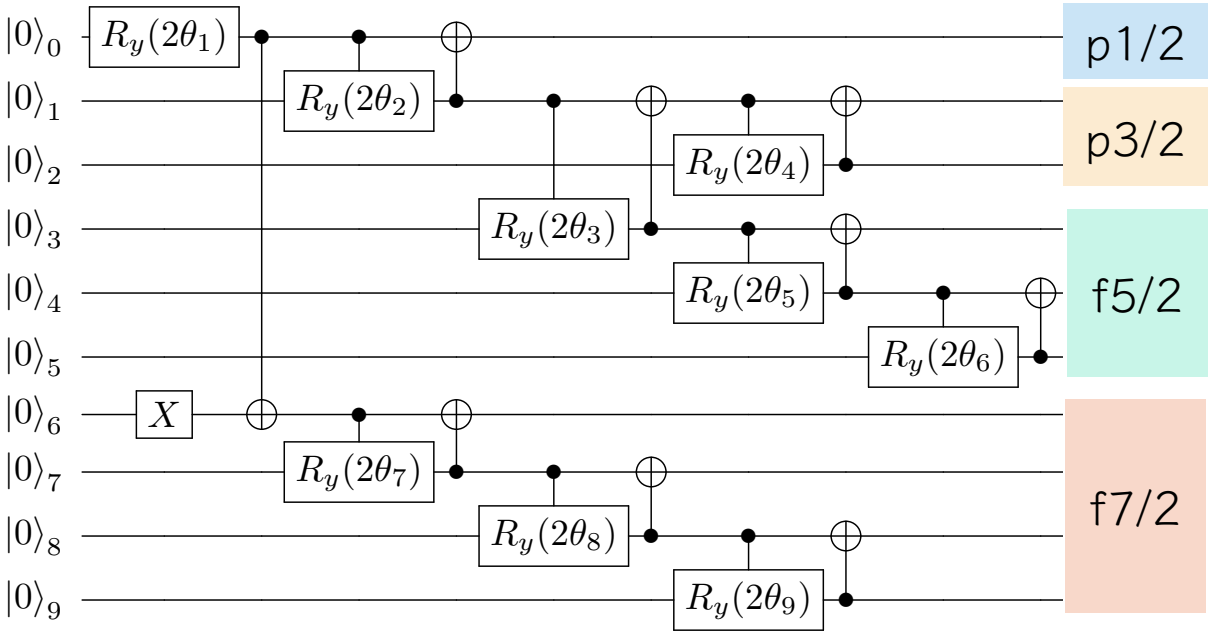
assignment of the qubits on IBMQ devices

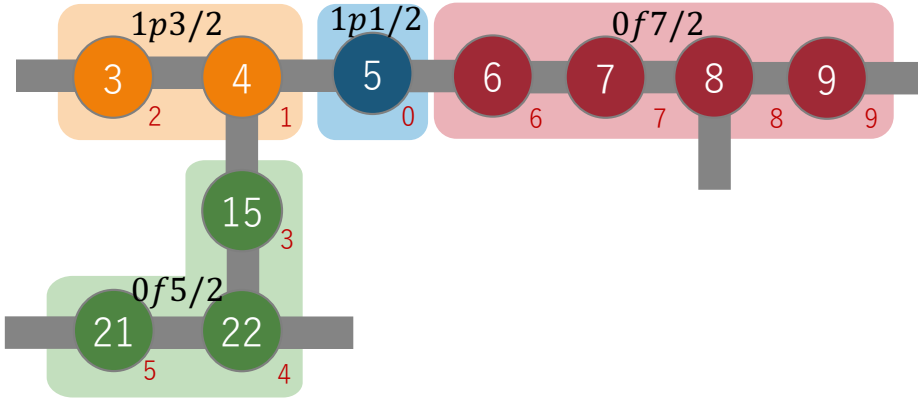
IBM brisbane (127 qubits)



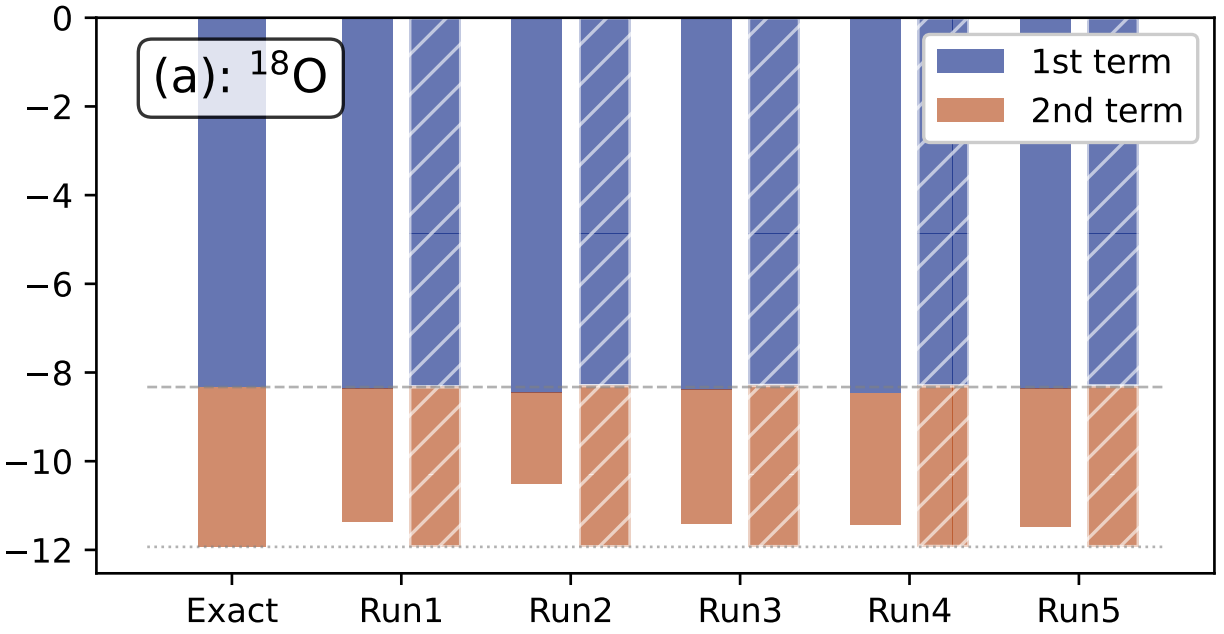
T-connectivity

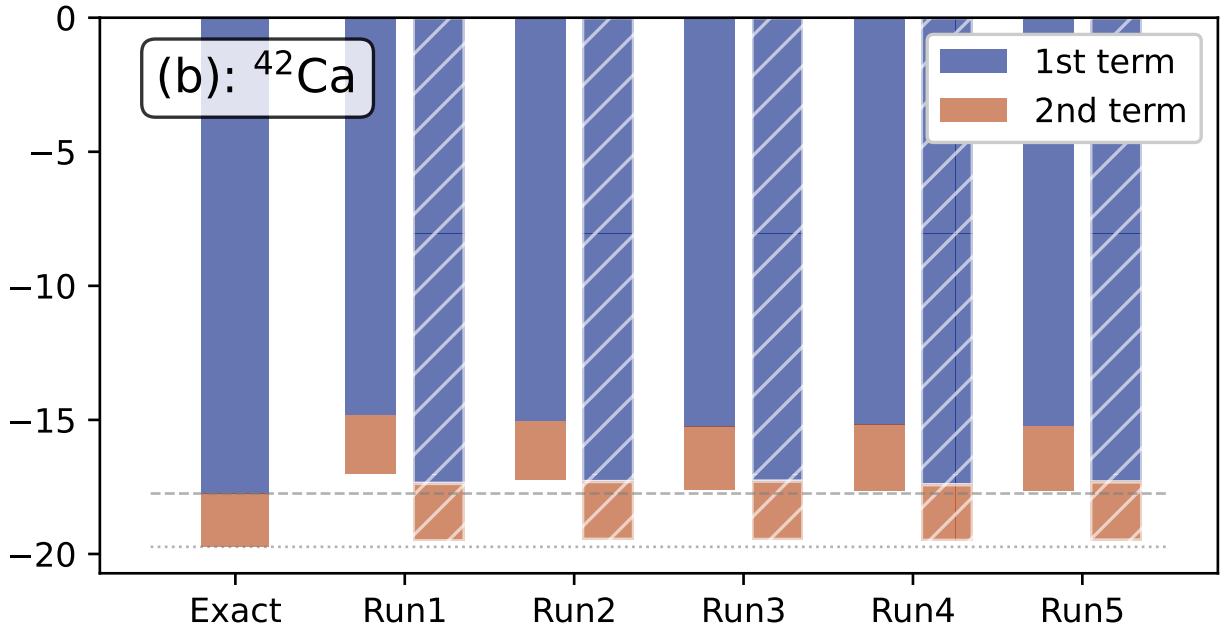
^{42}Ca





Results on real hardware: ibm_brisbane (127 qubits)





Run1-5: different runs

- w/ hatch (//): rearranged

- w/o hatch: original circuit

^{18}O & $^{6}He \rightarrow < 0.1\%$

$^{42}Ca \rightarrow \sim 1\%$

c.f. UCC-type results reported so far

^{6}He ~ 2% PRC 105, 064308 (2022)
^{6}Li ~ 4% PRC 106, 034325 (2022)
^{18}O ~ 3% PRC 108, 064305 (2023)

Summary

SY, T. Sato, T. Ogata, T. Naito, M. Kimura, PhysRevC.109.064305 (2024)

- We explored quantum algorithms for NP on NISQ devices
  - ansatz for valence two neutrons → much fewer CNOTs than UCC
  - accurate: < 0.1% (^{6}He & ^{18}O), ~1%(^{42}Ca)
  - importance of taking care of symmetries, connectivity, etc.
  - parameter optimization: sequential & derivative-free method works fine

see appendix

- TODO (a lot, but some are already in progress!)

  extensions to proton-neutron systems, many-particle systems
  towards driplines ~ input for astrophysics

  not only NISQ algorithms, towards (early-)FTQC

Collaborators & Acknowledgement

Collaborators:

UTokyo: Takeshi Sato, Takumi Ogata

RIKEN iTHEMS: Tomoya Naito

RIKEN Nishina center: Masaaki Kimura

Grant (only for me):

JSPS KAKENHI 22K14030, JGC-Saneyoshi Scholarship Foundation

Typical situation in NP

Full CI: current limitation of the Lanczos method ~ 10^{11} dim.

^{12}C (e.g. Hoyle state)
7 major shell excitation ~ 10^{19} dim. → No-core MCSM

T.Otsuka et al., Nature Comm.**13**:2234 (2022)

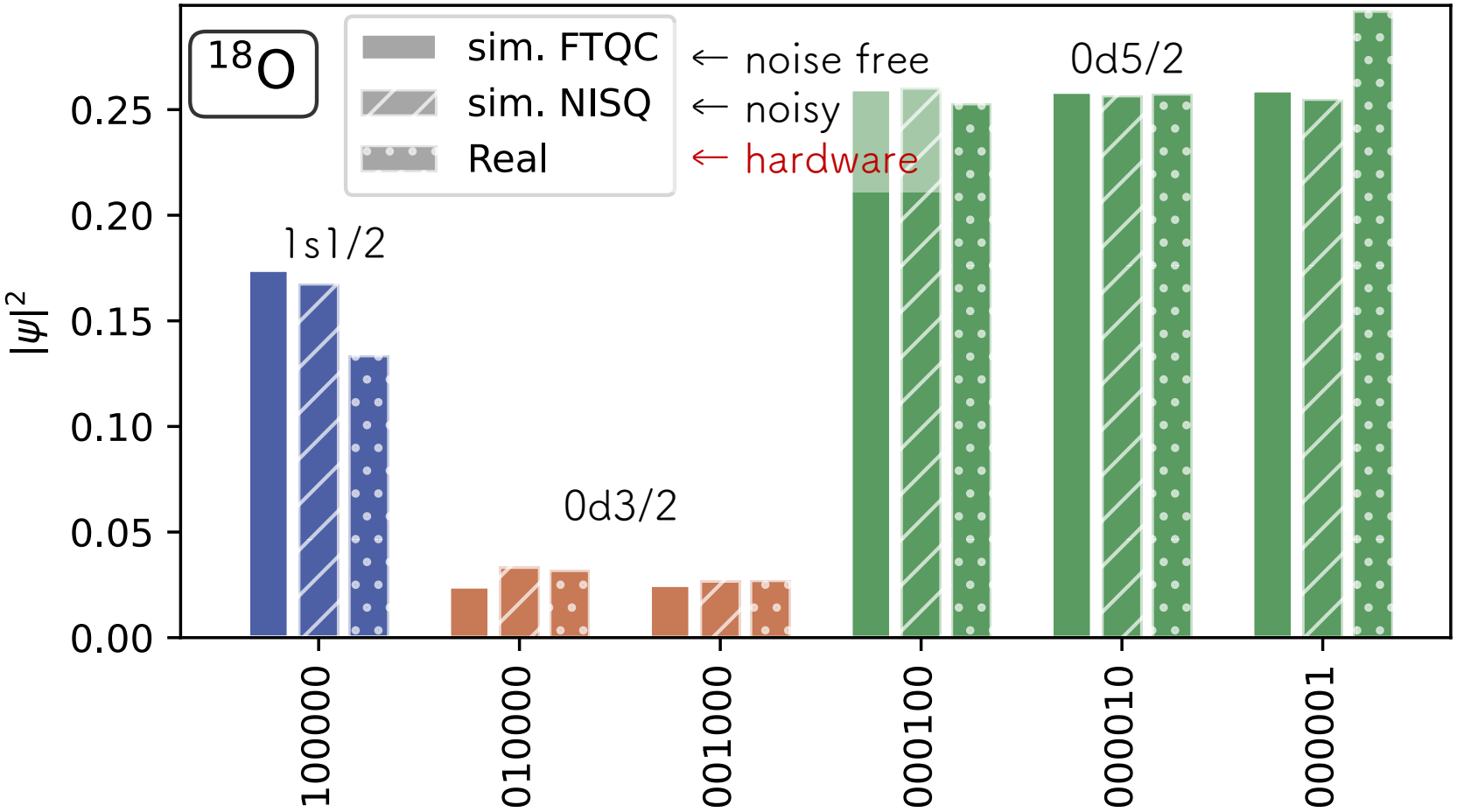
valence CI :

frontiers of neutron-rich nuclei: Ni ~10^{16} or much larger (10^{23}!)

→ CI variants:
Monte Carlo Shell Model (MCSM)
Quasi-vacua Shell Model (QVSM)

T. Togashi et al., PRL 121, 062501 (2018)
N. Shimizu et al., PRC **103**, 014312 (2021)

occupations of pair configurations



Note: the parameters are fixed to the ones giving exact results

for noisy simulator and hardware results, post-selection is done

computational basis sampling

M. Kohda, R. Imai, K. Kanno, K. Mitarai, W. Mizukami, and Y. O. Nakagawa,
Quantum expectation-value estimation by computational basis sampling,
Phys. Rev. Res. 4, 033173 (2022).

$$\langle\psi|H|\psi\rangle = \sum_{m,n=0}^{N} \langle\psi|m\rangle\langle m|H|n\rangle\langle n|\psi\rangle$$

$$= \sum_{m,n=0}^{N} |\langle m|\psi\rangle|^2 \, |\langle n|\psi\rangle|^2 \, \frac{\langle m|H|n\rangle}{\langle m|\psi\rangle\langle\psi|n\rangle}. \qquad (7)$$

$$\langle\psi|X_j \otimes X_k|\psi\rangle = \sqrt{\sigma_j^2\sigma_k^2}\,\mathrm{sgn}\,[\sigma_j\sigma_k], \qquad (8)$$

$$= \sqrt{\langle N_j\rangle\langle N_k\rangle}\,\mathrm{sgn}\,[\langle X_jX_k\rangle] \qquad (9)$$

↑ ansatz plus H-gates on all qubits

↑ equiv. to Z measurement of the ansatz circuit

You just need 2 measurements, ansatz & ansatz + H-gates

Derivative-free & Sequential optimization of the parameters

K. M. Nakanishi, K. Fujii, and S. Todo,
Sequential minimal optimization for quantum-classical hybrid algorithms,
Phys. Rev. Res. 2, 043158 (2020).

$$\mathcal{L}(\boldsymbol{\theta}) = \sum_k w_k \langle\varphi| U^\dagger(\boldsymbol{\theta}) \mathcal{H}_k U(\boldsymbol{\theta}) |\varphi\rangle, \qquad \text{(B1)}$$

= Energy expectation value

Optimizing Ry-gate rotation angle

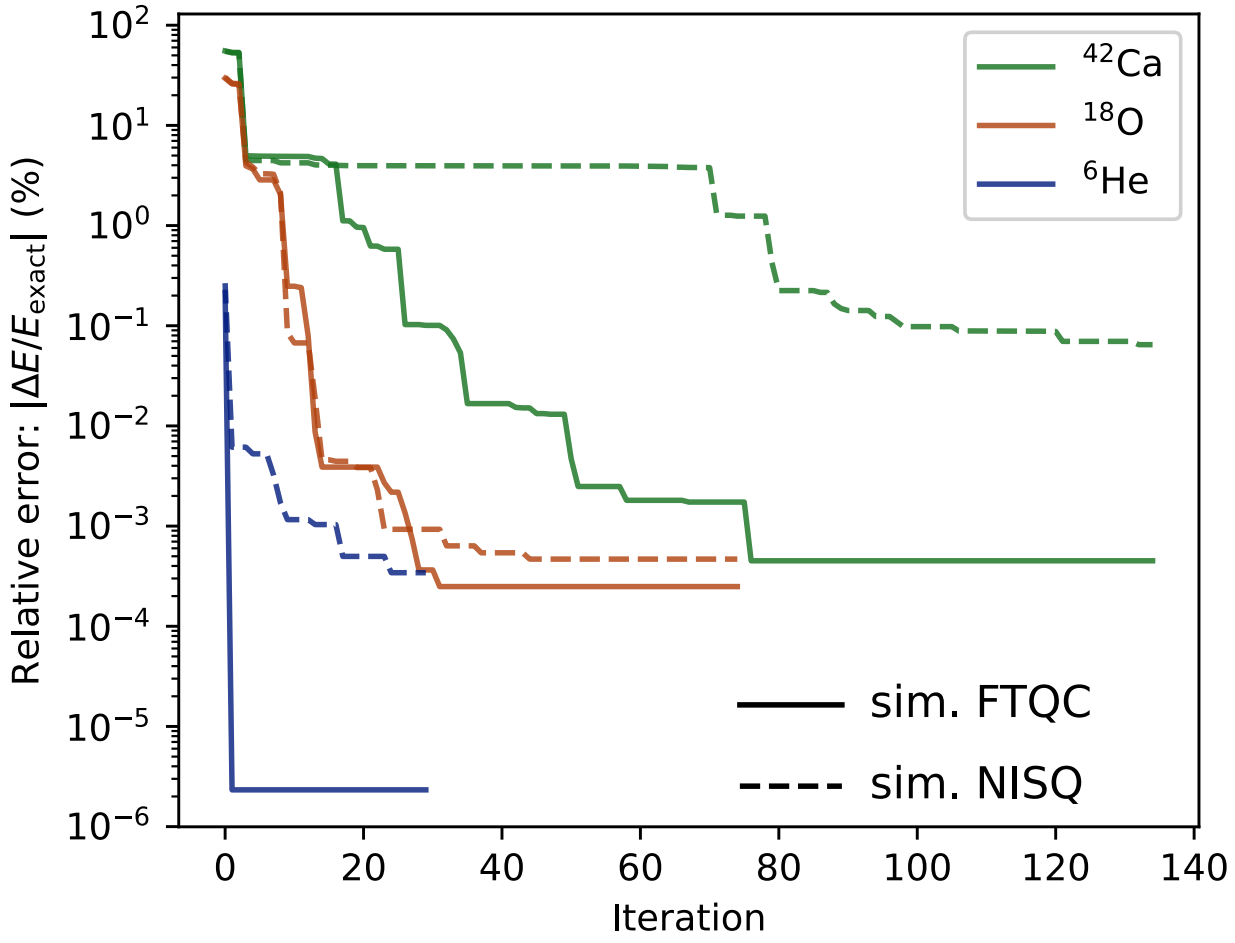
$$\mathcal{L}(\theta_1) = A\cos(\theta_1 - B) + C. \qquad \text{(B2)}$$

Optimizing cRy-gate rotation angle

$$\mathcal{L}(\theta_j) = A\cos\theta_j + B\sin\theta_j + C\cos 2\theta_j + D\sin 2\theta_j + E. \qquad \text{(B3)}$$

Optimization of the circuit parameters

parameters so far are fixed to the ones giving exact results by hand



Using a gradient-free &

sequential optimization technique

we can reproduce the exact ones

← 15sweep for Nq-1 parameters

K. M. Nakanishi, K. Fujii, and S. Todo:
Sequential minimal optimization for quantum-classical hybrid algorithms, Phys. Rev. Res. 2, 043158 (2020).