

Emulators and quantum computing for nuclear structure theory

Nuclear Theory and Nuclear Astrophysics Group,
Sun Yat-sen University, Mar. 28, 2025.



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RIKEN Nishina Center

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My interests

Phenomenology

To understand structure of
e.g. unstable nuclei

Shell-model calc. of
Beta-decays, etc.

Ab initio

nuclear force, 3NF

Full-CI, post-HF, etc.

Uncertainty quantification

To make more “reliable”
predictions

Today, I will focus on these two topics!



Quantum computing

Challenge to the most difficult
quantum many-body systems

Developing software

To interplay with people
from different disciplines

Education for
the next generation

Emulators

To enable us to do “full” UQ
ML applications

Why Emulators/Surrogate models matter?

Condensed matter physics, Quantum Chemistry, Nuclear Physics, etc.

share issues on...

- exponential growth of the size of Hilbert space
- repeating simulations under tons of different params for quantifying uncertainties/inverse problem (e.g. nuclear force)



You may need $10^3\text{-}10^5$ speed up to draw credible intervals

utilizing e.g. MCMC sampling

Review and related works

Colloquium: Eigenvector continuation and projection-based emulators

[Thomas Duguet](#), [Andreas Ekström](#), [Richard J. Furnstahl](#), [Sebastian König](#), and [Dean Lee](#)

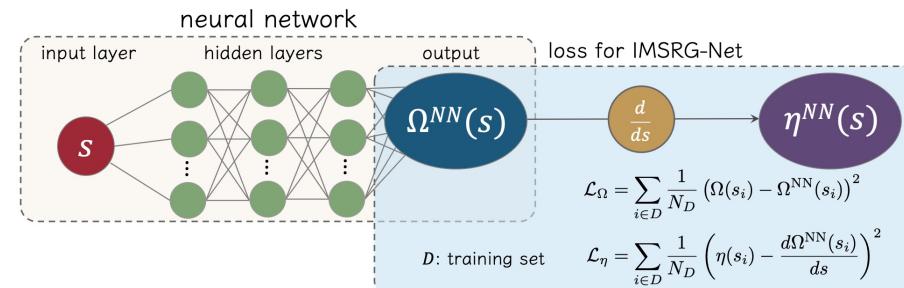
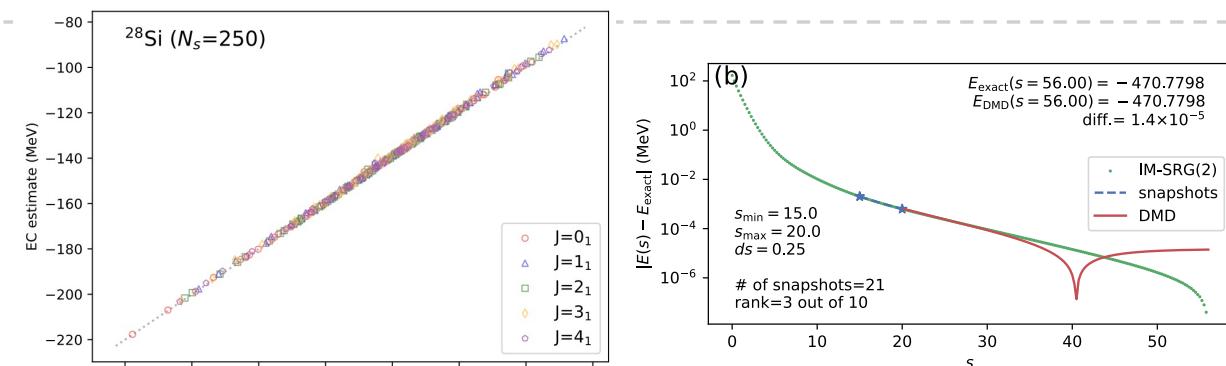
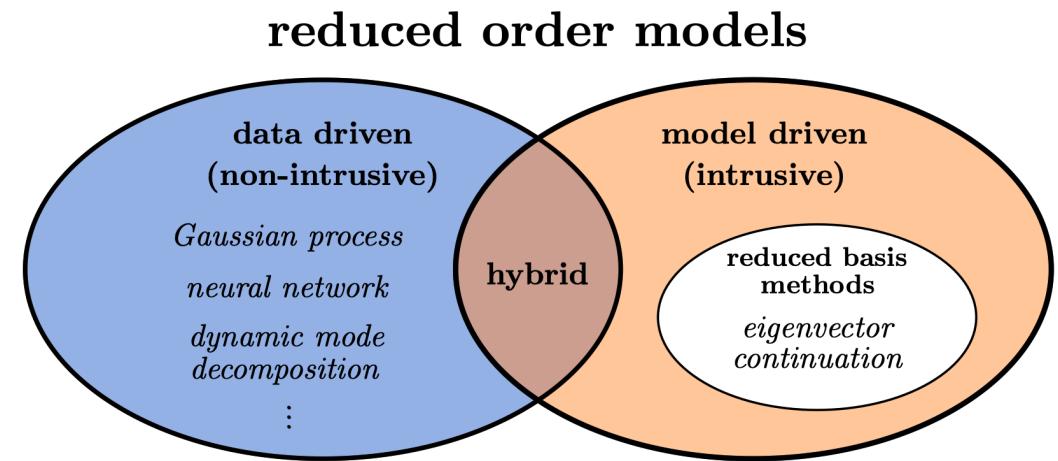
Show more ▾

Rev. Mod. Phys. 96, 031002 – Published 14 August, 2024

DOI: <https://doi.org/10.1103/RevModPhys.96.031002>

From my works...

- Valence-Cl w/ eigenvector continuation
SY & N.Shimizu [PTEP 2022 053D02](#)
- IMSRG w/ physics-informed neural networks
SY [PRC108, 044303 \(2023\)](#)
- IMSRG w/ Dynamic mode decomposition
J. Davidson: [PhD thesis@MSU, 2023](#)
SY [Particles 2025, 8\(1\), 13 \(2025\)](#)



In-medium Similarity Renormalization Group (IMSRG)

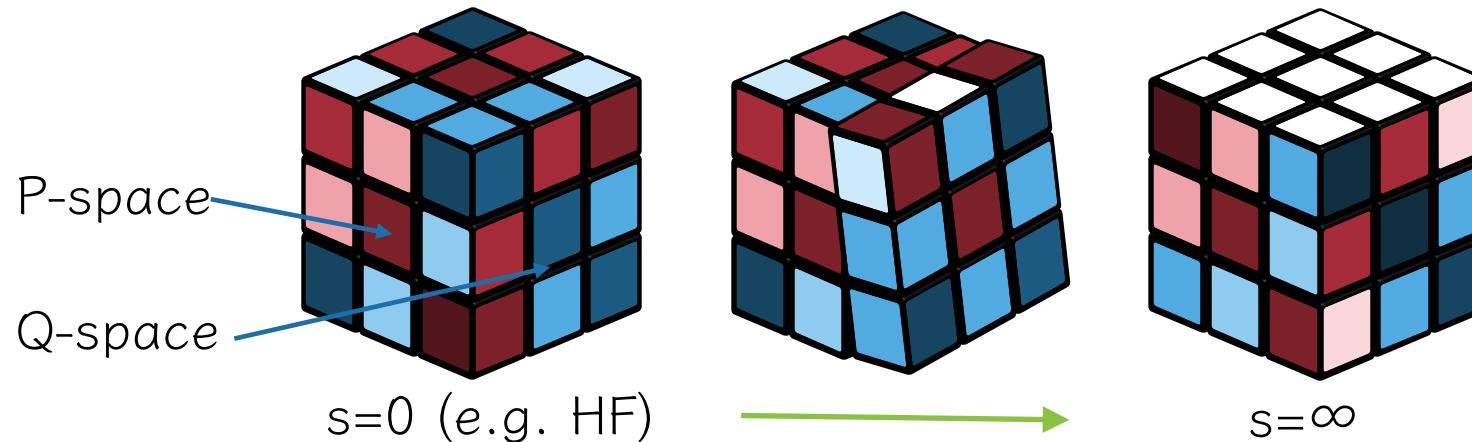
5

IMSRGflow:

K. Tsukiyama, S. K. Bogner, and A. Schwenk, [PRL 106, 222502 \(2011\)](#), [PRC 85, 061304 \(2012\)](#).
S.R.Stroberg et al., [Annu. Rev. Nucl. Part. Sci. 2019. 69:307–362 \(2019\)](#)
T.D.Morris et al., [PRC 92, 034331 \(2015\)](#)

$$\frac{dH(s)}{ds} = [\eta(s), H(s)]$$

P-Q coupling
↓

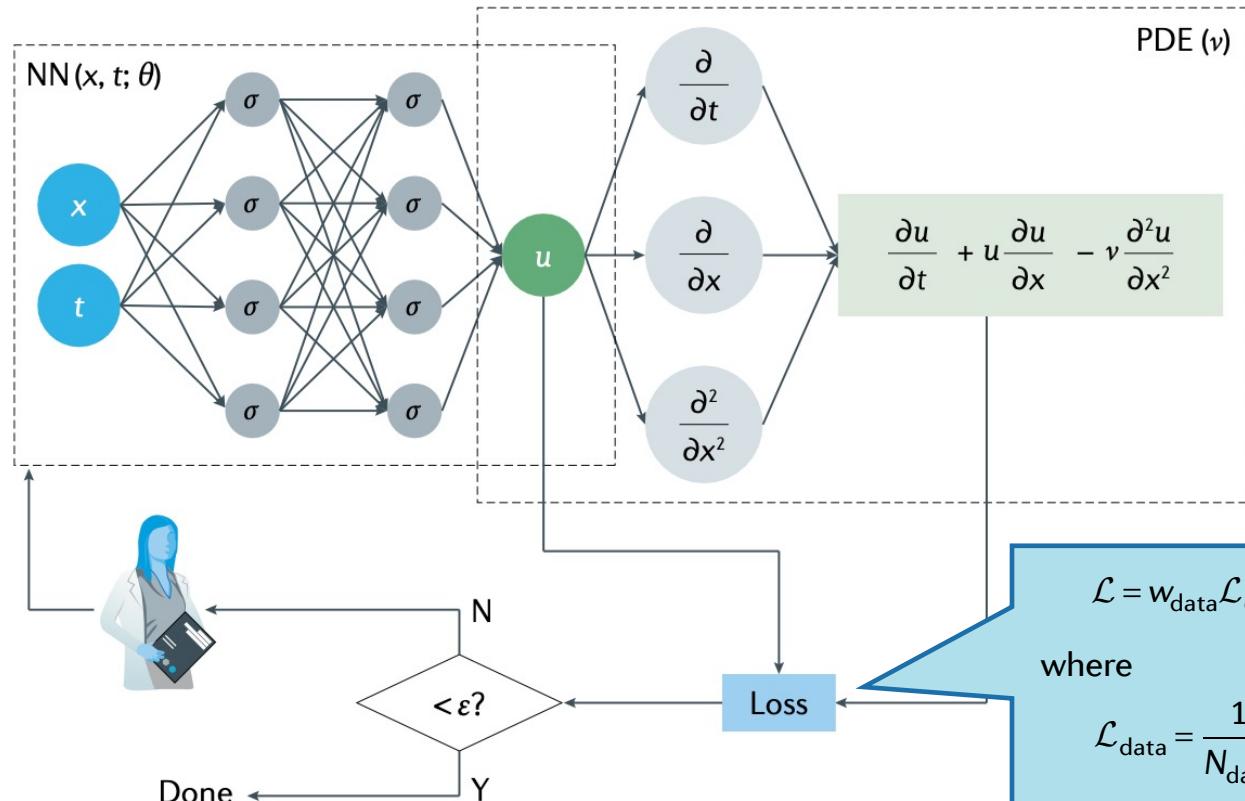


Magnus formulation $U(s) = e^{\Omega(s)}$
 $O(s) = e^{\Omega(s)} O(0) e^{-\Omega(s)}$

$(P, Q) = (\text{hole, particle}) \rightarrow \text{IM-SRG}$ (comparable to CCSD, ADC, etc.)
 $= (\text{valence, others}) \rightarrow \text{Valence space IMSRG}$ (Eff. int./ops. for CI)

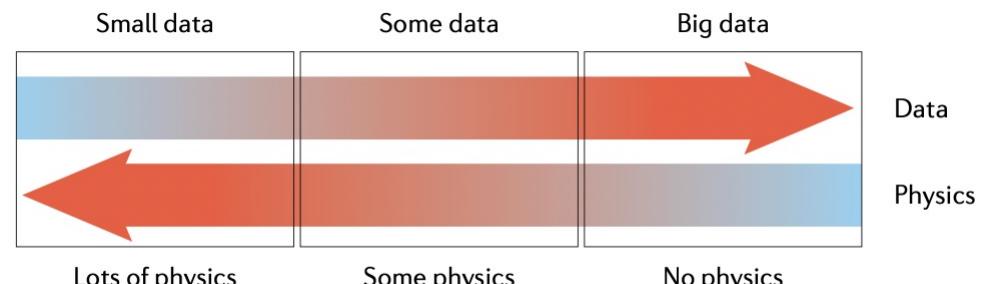
Physics-Informed Neural Networks (PINNs) as an example

Burgers eq. : $\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}$



Ref: [Nature Reviews Physics 3, 422–440 \(2021\)](#)

e.g. Large Language Model



$$\mathcal{L} = w_{\text{data}} \mathcal{L}_{\text{data}} + w_{\text{PDE}} \mathcal{L}_{\text{PDE}},$$

where

$$\mathcal{L}_{\text{data}} = \frac{1}{N_{\text{data}}} \sum_{i=1}^{N_{\text{data}}} (u(x_i, t_i) - u_i)^2 \quad \text{and}$$

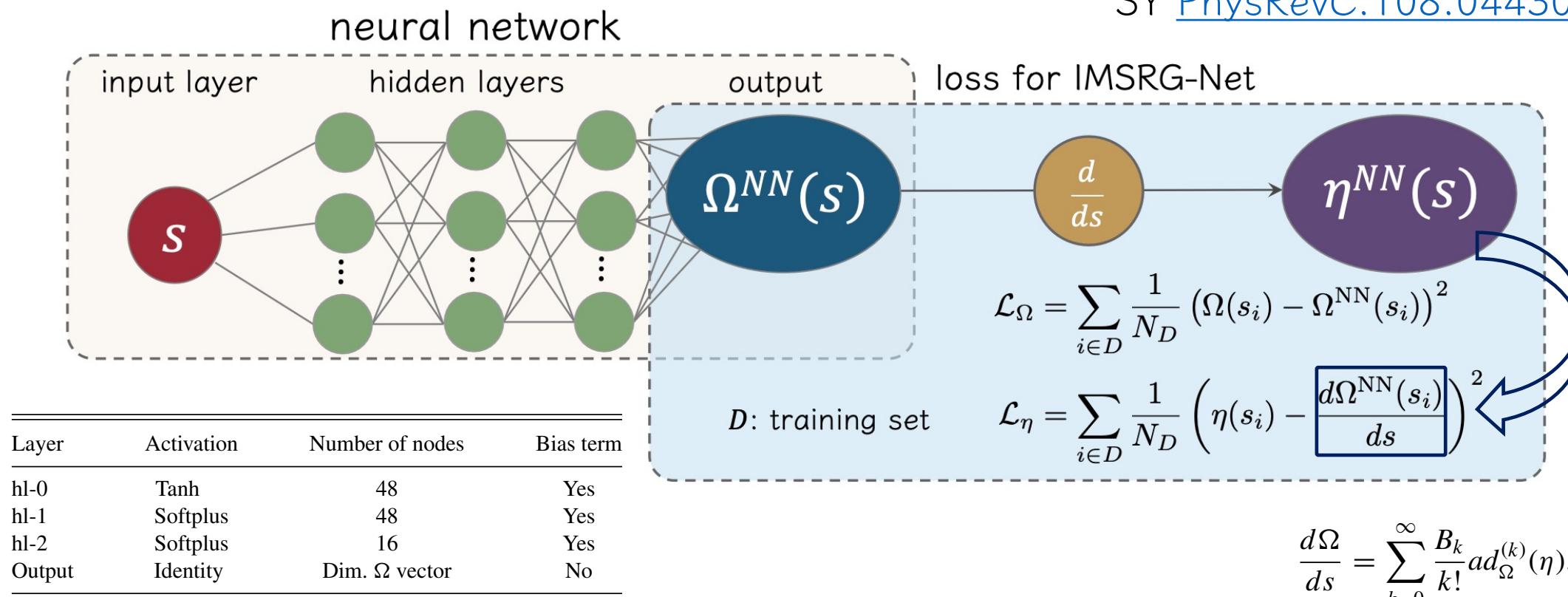
$$\mathcal{L}_{\text{PDE}} = \frac{1}{N_{\text{PDE}}} \sum_{j=1}^{N_{\text{PDE}}} \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} \right)^2 |_{(x_j, t_j)}.$$

“natural” expectation: you want neural networks approximating $u(x, t)$ respecting underlying equation and boundary conditions

IMSRG-Net: PINN-based solver for IMSRG

7

SY [PhysRevC.108.044303 \(2023\)](#)



neural network part is simple Affine layers

$$ad_\Omega^{(k)}(\eta) = [\Omega, ad_\Omega^{(k-1)}(\eta)],$$

$$ad_\Omega^{(0)}(\eta) = \eta, \quad \text{taking leading term}$$

and trained to minimize the sum of loss terms $\mathcal{L} = \mathcal{L}_\Omega + \lambda_\eta \mathcal{L}_\eta$

$$\lambda_\eta = 100$$

Dynamic Mode Decomposition (DMD)

8

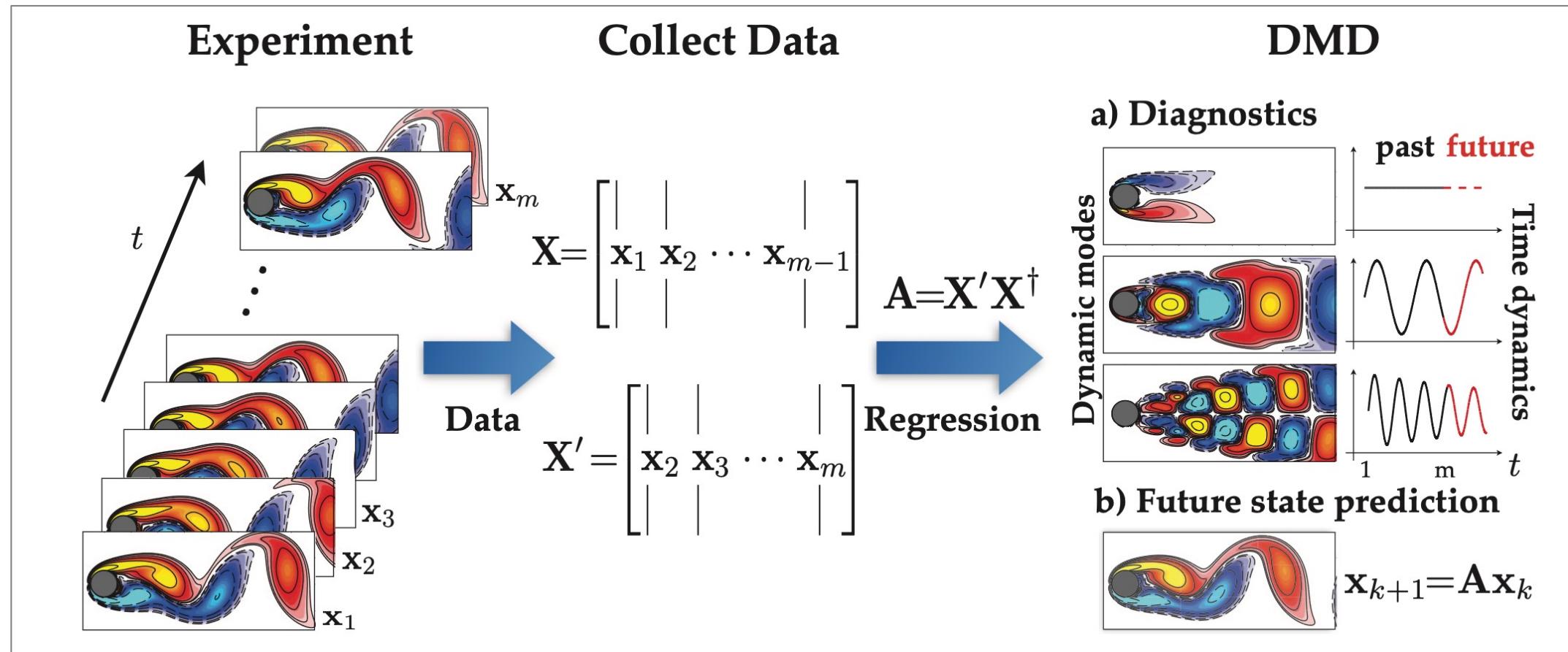


Fig 1.1 from Kutz et al., “[Dynamic Mode Decomposition](#)” SIAM

- various modes are decomposed into “dynamical modes”
- one can reconstruct original snapshots (and make predictions)

DMD algorithms

1.

$$\mathbf{X} \equiv \begin{pmatrix} & D \times N \\ | & & | \\ x_1 & \cdots & x_N \\ | & & | \end{pmatrix}, \mathbf{Y} \equiv \begin{pmatrix} & D \times N \\ | & & | \\ x_2 & \cdots & x_{N+1} \\ | & & | \end{pmatrix} \quad \mathbf{Y} = \mathbf{F}(\mathbf{X}) \rightarrow \mathbf{Y} \approx \mathbf{AX}$$

D (dimension of many-body operator) $> 10^7$ approximating non-linear map F by linear map A
 N (# of snapshots) $\sim 10 - 10^3$?

2. SVD of X $\mathbf{X} = \mathbf{U}\Sigma\mathbf{V}^*$ \rightarrow truncated SVD $\mathbf{X} \approx \mathbf{U}_r\Sigma_r\mathbf{V}_r^\dagger$

3. Compute the matrix A using Moore-Penrose pseudo-inverse of X

$$\mathbf{A} \approx \mathbf{YX}^+ = Y (\mathbf{V}_r \Sigma_r^{-1} \mathbf{U}_r^\dagger)$$

4. Obtain the time evolution linear map in a latent space

$$\tilde{\mathbf{A}} = \mathbf{U}_r^\dagger \mathbf{A} \mathbf{U}_r \approx \mathbf{U}_r^\dagger \mathbf{Y} \mathbf{V}_r \Sigma_r^{-1}$$

k-time step forward can be done in the latent space

encoder

$$\mathbf{A} = \mathbf{U}_r \tilde{\mathbf{A}} \mathbf{U}_r^\dagger$$

decoder

DMD applications to quantum many-body systems

Spin system

transverse-field Ising model

$$H = -J \sum_{\langle i,j \rangle} S_i^z S_j^z - \Gamma \sum_i S_i^x,$$

[Phys. Rev. Research 7, 013085 \(2025\)](#)

Quantum computing

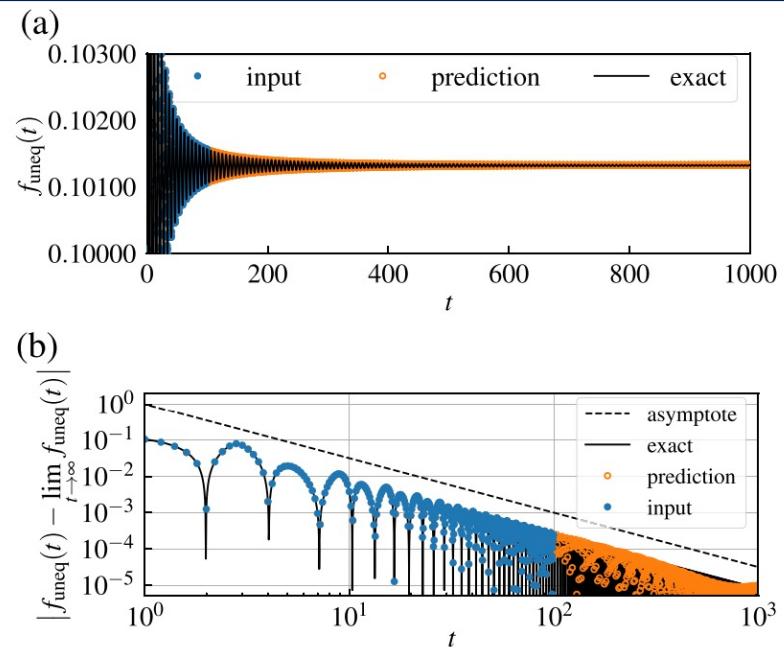
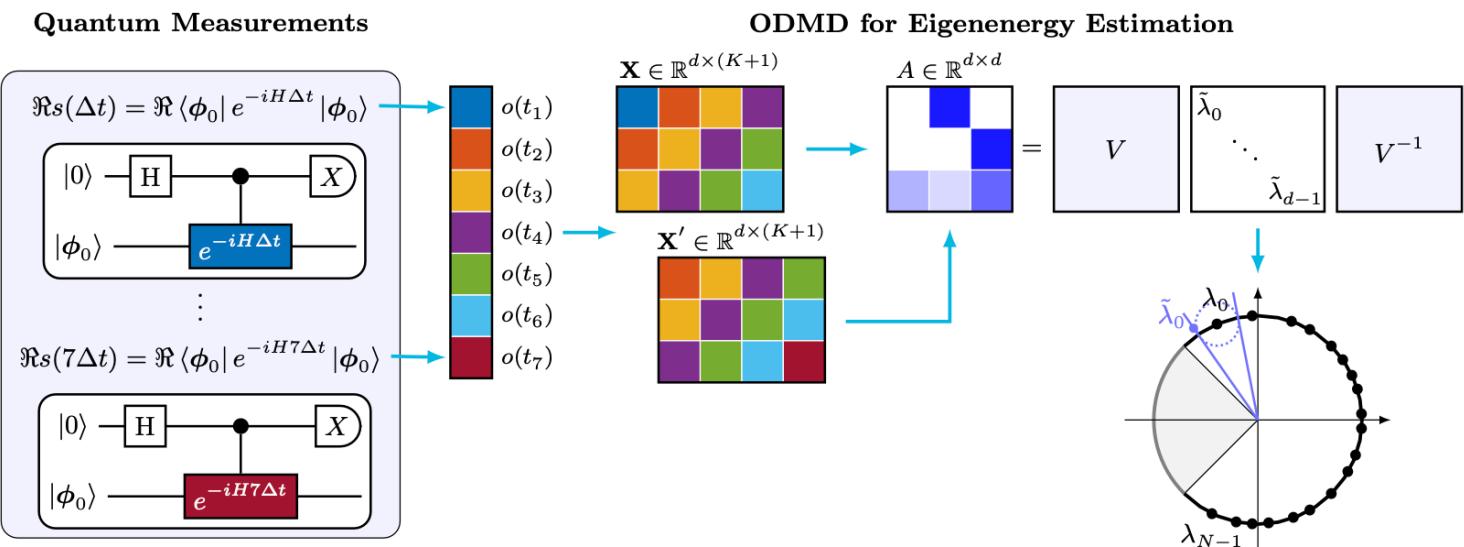


FIG. 8. DMD prediction of the unequal-time onsite transverse spin-spin correlation function in the 1D transverse-field Ising model. We show the time evolution of the absolute value of the correlation function for (a) $t \in [0, 1000]$ and (b) that in the logarithmic scale. The magnified views of the time evolution for (c) $t \in [0, 110]$,

Observable DMD(ODMD):
[arXiv: 2306.01858](#)

Multi-Observable DMD(MODMD):
[arXiv:2409.13691](#)

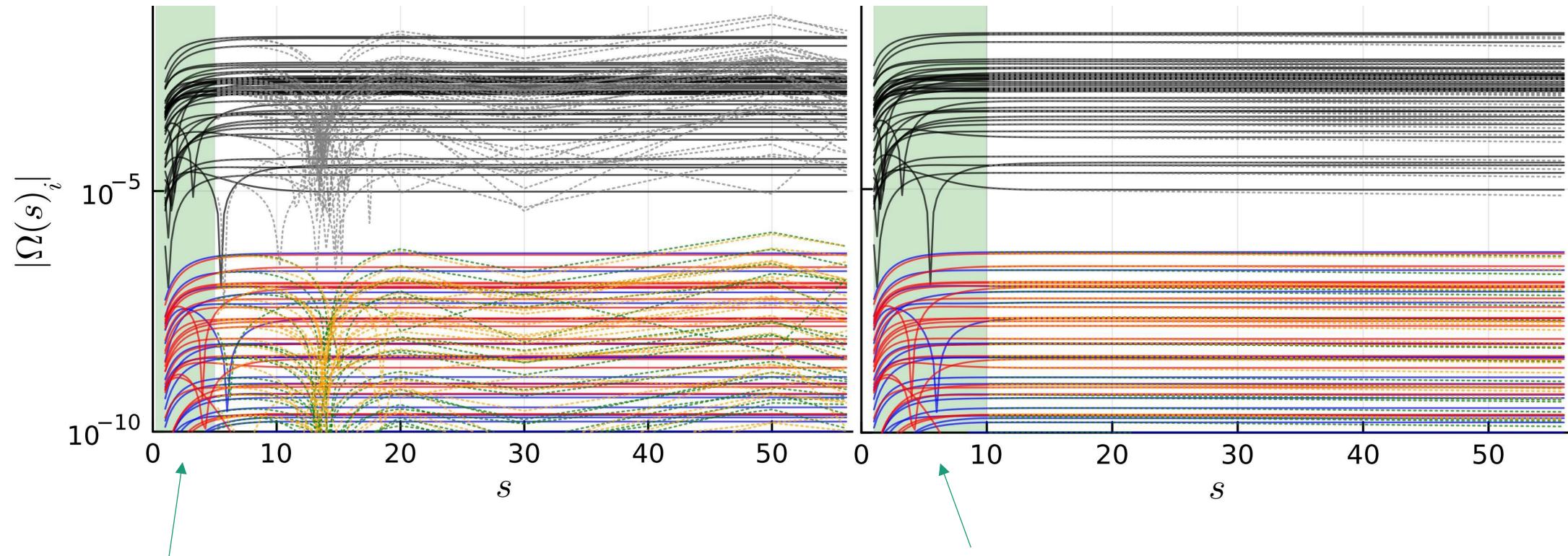
Flow of Magnus operators

11

[Particles 2025, 8\(1\), 13 \(2025\)](#)

^{56}Ni under N3LO + 3NF(lnl)
showing 40 for each (1b, 2bpp, 2bpn)
out of $\sim 10^8$ ($e_{\text{max}}=12$) elements

— 1b
- - - 1b(DMD)
— 2bpp
- - - 2bpp(DMD)
— 2bpn
- - - 2bpn(DMD)



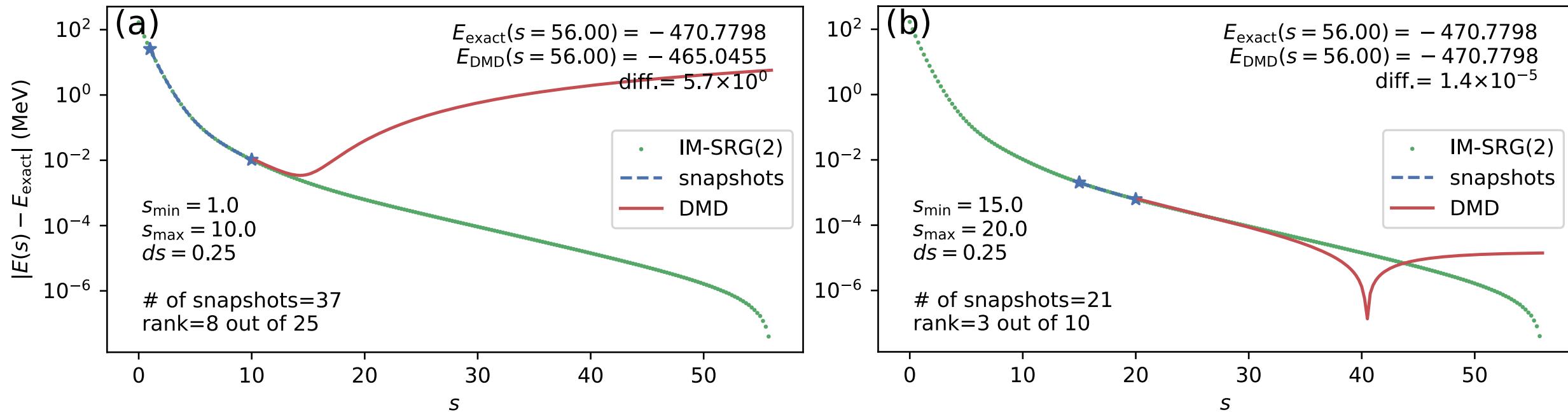
snapshots $s = 0.25 \sim 5$

snapshots $s = 1 \sim 10$
DMD emulation looks nice, but...

Errors on energy estimation

Particles 2025, 8(1), 13 (2025)

12



Using early stage of the snapshots,
only valid for very short term extrapolation

it is nontrivial to take snapshots from where to where

Short summary on emulating IM-SRG

My trials so far:

Physics-Informed Neural Networks (PINNs): [PhysRevC.108.044303 \(2023\)](#)

Dynamic Mode Decomposition (DMD): [Particles 2025, 8\(1\), 13 \(2025\)](#)

For emulating Magnus IMSRG-flow, these are valid only for predicting asymptotic behavior → limited speeding up

Another approach

An Efficient Learning Method to Connect Observables

Hang Yu  ^{1,*} and Takayuki Miyagi  ^{1,†}

¹Center for Computational Sciences, University of Tsukuba, Tsukuba, Ibaraki 305-8577, Japan

Constructing fast and accurate surrogate models is a key ingredient for making robust predictions in many topics. We introduce a new model, the Multiparameter Eigenvalue Problem (MEP) emulator. The new method connects emulators and can make predictions directly from observables to observables. We present that the MEP emulator can be trained with data from Eigenvector Continuation (EC) and Parametric Matrix Model (PMM) emulators. A simple simulation on a one-dimensional lattice confirms the performance of the MEP emulator. Using ²⁸O as an example, we also demonstrate that the predictive probability distribution of the target observables can be easily obtained through the new emulator.

My interests

14

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Developing software

To interplay with people
from different disciplines

Education for
the next generation

Emulators

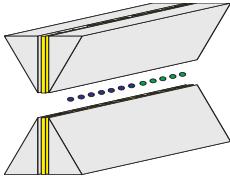
To enable us to do “full” UQ
ML applications

How to realize qubits

Don't ask me details!

15

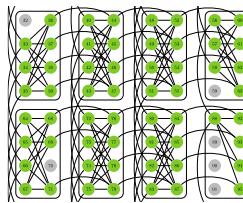
atoms



trapped ions



electron superconducting loops & controlled spin



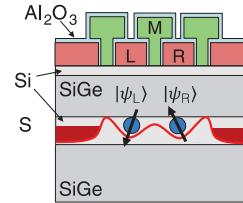
cold atoms



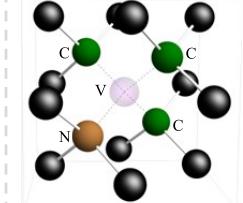
annealing



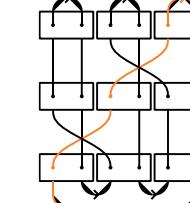
super-conducting



silicon



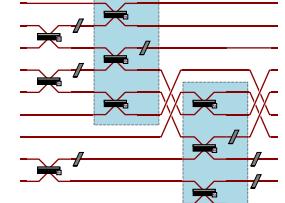
vacancies



topological



photons



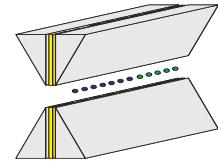
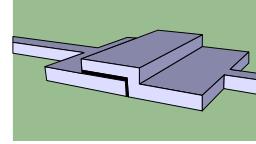
photons



(CC) Olivier Ezratty, 2023 [slide](#)

It may have changed considerably to date!

Brief summary of major qubit types

	atoms	electrons superconducting & spins	photons
	 cold atoms	 trapped ions	 superconducting
qubit size	about 1 μm space between atoms	about 1 μm space between atoms	$(100\mu)^2$
best two qubits gates fidelities	99.5%	99.94%	99.68% (IBM Egret 33 qubits)
best readout fidelity	95%	99.99%	99% (SiGe)
best gate time	$\approx 1 \text{ ns}$	0.1 to 4 μs	20 ns to 300 ns
best T_1	$> 1 \text{ s}$	0.2s-10mn	100-400 μs
qubits temperature	< 1mK 4K for vacuum pump	<1mK 4K cryostat	15mK dilution cryostat
operational qubits	1,180 (Atom Computing)	32 (IonQ and Quantinuum)	433 (IBM) 176 (China)
scalability	up to 10,000	<100	1000s
			millions
			100s
			100s-1M

these are the best figures of merit, but it doesn't mean a single system in a column has them all!

(cc) Olivier Ezratty, 2023. RT = room temperature.

(CC) Olivier Ezratty

Hardware and Software

a very limited list

Quantum Device	Vendor	Qubit Realization Method	Frequently Used Software
IBM Quantum	IBM	Superconducting Qubits	Qiskit
Rigetti Aspen	Rigetti Computing	Superconducting Qubits	Forest SDK, pyQuil
IonQ	IonQ	Trapped Ions	Qiskit, Cirq, Braket (Amazon)
H-series	Quantinuum	Trapped Ions	TKET, Cirq, Qiskit
Xanadu Borealis	Xanadu	Photonic Qubits (Continuous-Variable)	PennyLane, Strawberry Fields

Various SDKs are available, but you may want to use these...



Qiskit

After major update v1.0 (Feb. 2024)...

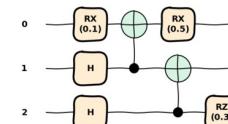
APIs and Docs are terrible



PENNYLANE

Drawing cute circuits

Supporting
OpenFermion, PyTorch



H2→



to benefit from high fidelity of H-series hardware,
mid circuit measurements, etc.

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

1-qubit gates

$$X = HZH$$

$$Y = R_x(-\pi/2)ZR_x(\pi/2)$$

Name	Symbol	Matrix	Name	Symbol	Matrix	Name	Symbol	Matrix
X		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	Y		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$	Z		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard		$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$	Phase		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{bmatrix}$	Universal		$\begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & -e^{i\lambda}\sin\left(\frac{\theta}{2}\right) \\ e^{-i\phi}\sin\left(\frac{\theta}{2}\right) & e^{i(\phi+\lambda)}\cos\left(\frac{\theta}{2}\right) \end{bmatrix}$
X-rotation		$\begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & -i\sin\left(\frac{\theta}{2}\right) \\ -i\sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{bmatrix}$	Y-rotation		$\begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{bmatrix}$	Z-rotation		$\begin{bmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{bmatrix}$

2-qubit gates

Name	Circuit	Matrix	Name	Circuit	Matrix	
CNOT		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$	SWAP		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$	
CZ		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$	fSim		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & -i\sin(\theta) & 0 \\ 0 & -i\sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{bmatrix}$	
a)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & a_{00} & 0 & a_{01} \\ 0 & 0 & 1 & 0 \\ 0 & a_{10} & 0 & a_{11} \end{bmatrix}$	b)		$\begin{bmatrix} a_{00} & 0 & a_{01} & 0 \\ 0 & 1 & 0 & 0 \\ a_{10} & 0 & a_{11} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$	
c)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & a_{00} & a_{01} & 0 \\ 0 & a_{10} & a_{11} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$	d)		$\begin{bmatrix} a_{00} & 0 & 0 & a_{01} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ a_{10} & 0 & 0 & a_{11} \end{bmatrix}$	

Universal gate sets:

{Rx,Ry,Rz,P,CNOT}: commonly used

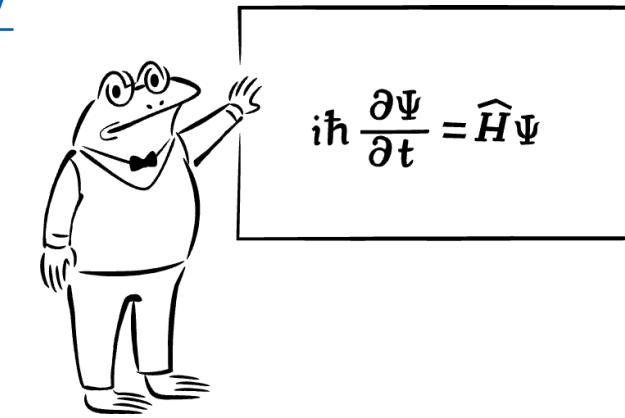
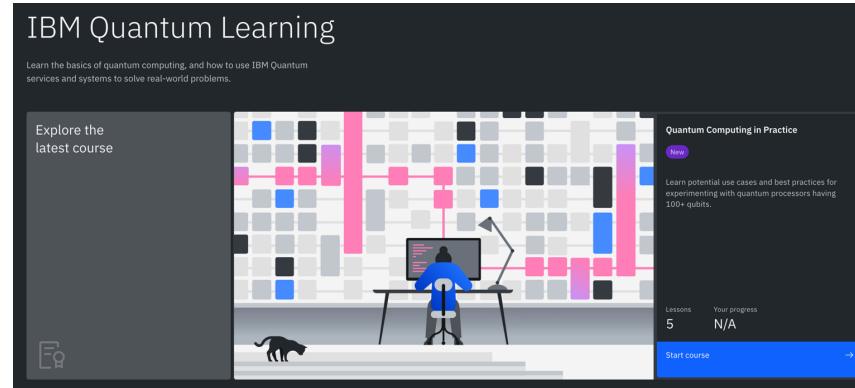
{H,S,T,CNOT}: Clifford set + T gate
T&S are special cases of P

{Toffoli, H}: Toffli = CCNOT

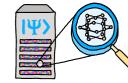
Ref: Edgar Andres Ruiz Guzman
PhD thesis [arXiv:2310.17996](https://arxiv.org/abs/2310.17996)
Paris-Saclay → IBM

Tutorials

IBM Quantum Learning <https://learning.quantum.ibm.com/>

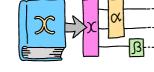


Learn quantum programming with PennyLane
<https://pennylane.ai/qml>



Quantum Computing

Learn how universal computation can be achieved using quantum-mechanical systems.



Quantum Machine Learning

Find out how the principles of quantum computing and machine learning can be united to create something new.



Quantum Chemistry

Study the properties of molecules and materials using quantum computers and algorithms.

And I guess there may be tutorials from Chinese start-up companies

Quantum computing of quantum many-body systems

20

NISQ = Noisy Intermediate-Scale Quantum device

FTQC = Fault-Tolerant Quantum Computer

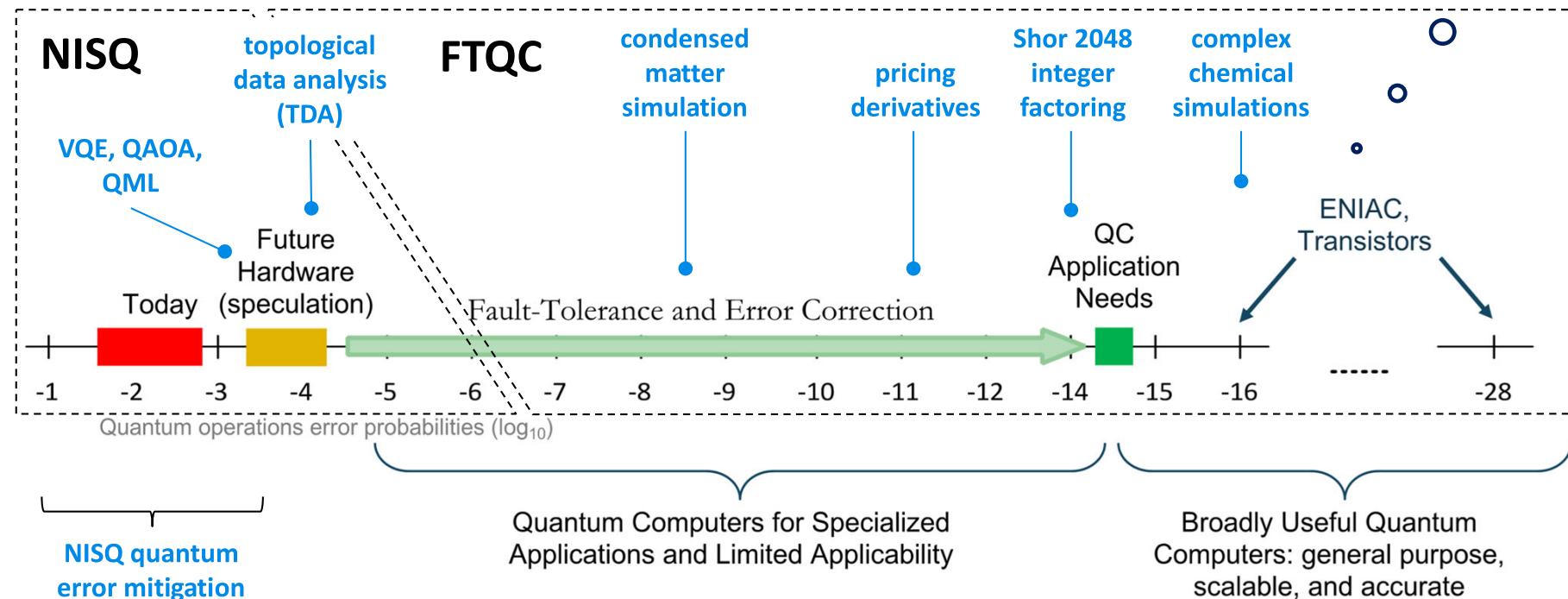
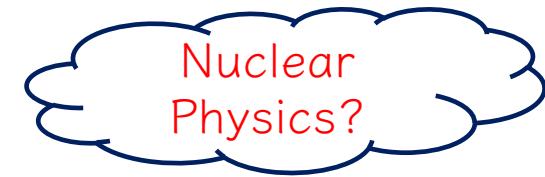


Fig. 18 How NISQ and FTQC may overlap with competition between NISQ and quantum error mitigation extending the capacities of noisy qubits while corrected qubits will enable FTQC and greater depth algorithms. Source: Bert de Jong (Department of Energy) and additions by Ezratty (2023)

[Eur. Phys. J. A \(2023\) 59:94](https://doi.org/10.1140/epja/s10638-023-10638-0)

A NISQ algorithm: Variational Quantum Eigensolver (VQE)

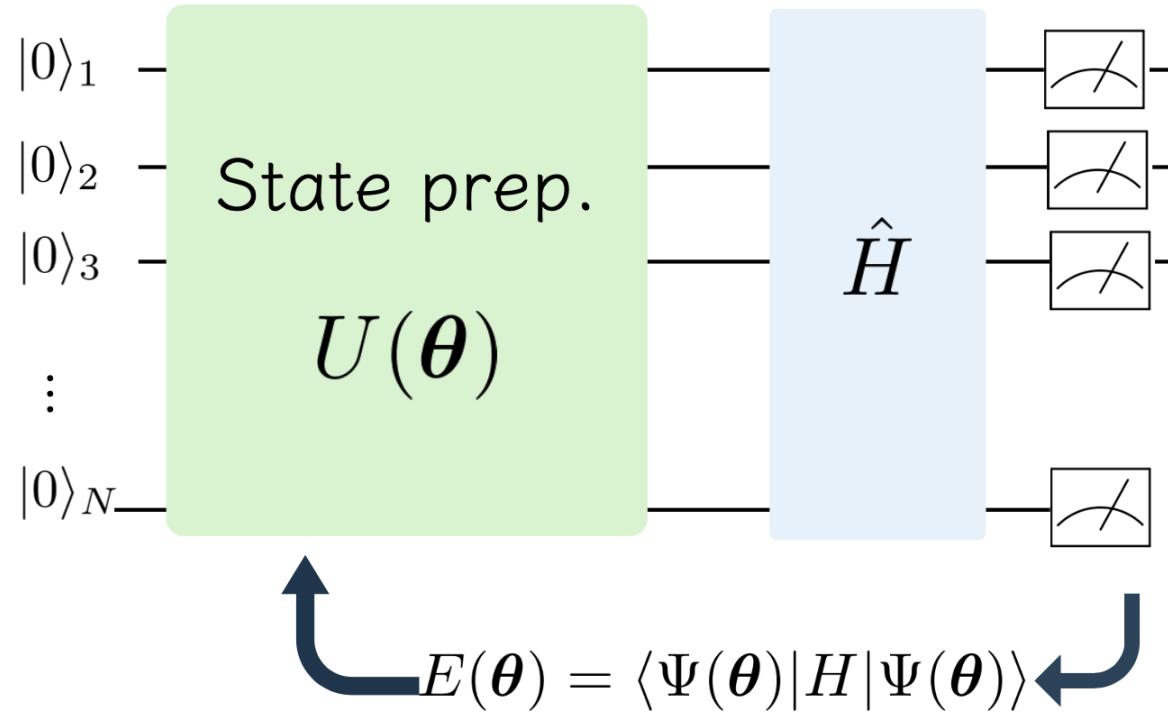
A FTQC algorithm: Quantum Phase Estimation (QPE)

Variational quantum eigensolver (VQE)

21

near-term

A typical workflow of VQE

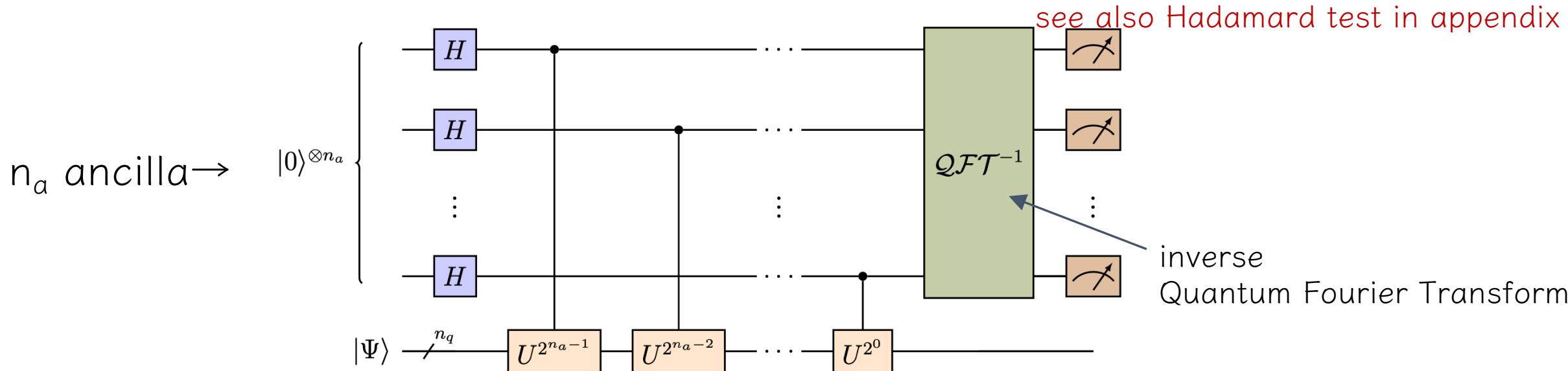


1. initialize the qubits $|00\dots\rangle$, Hartree-Fock, etc.
2. ansatz:
Operating Unitary gates
→ prepare trial wave functions
3. measurement of Hamiltonian
→ energy
4. Optimize the parameters classically
to minimize the energy

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

Quantum Phase Estimation (QPE)

long-term



$$\begin{aligned}
 & |0\rangle^{\otimes n} \otimes |\Psi\rangle \xrightarrow{H^{\otimes n} \otimes I} \frac{1}{\sqrt{2^n}} (|0\rangle + |1\rangle)^{\otimes n} \otimes |\Psi\rangle \\
 & \xrightarrow[\lambda = 2\pi\theta]{\text{controlled } U_s} \frac{1}{\sqrt{2^n}} \left[\left(|0\rangle + e^{2\pi i \theta 2^{n-1}} |1\rangle \right) \otimes \left(|0\rangle + e^{2\pi i \theta 2^{n-2}} |1\rangle \right) \otimes \dots \left(|0\rangle + e^{2\pi i \theta 2^0} |1\rangle \right) \right] \otimes |\Psi\rangle \\
 & = \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} e^{2\pi i \theta k} |k\rangle \otimes |\Psi\rangle \xrightarrow{\mathcal{QFT}^{-1}} \frac{1}{2^n} \sum_{k=0}^{2^n-1} \sum_{x=0}^{2^n-1} \exp \left(2\pi i k \left(\theta - \frac{x}{2^n} \right) \right) |x\rangle \otimes |\Psi\rangle
 \end{aligned}$$

1. You will extract (encode) the information of eigenvalue (as a phase) with n_a ancilla qubits through the controlled unitary gates
2. Using inverse QFT to extract the values of the phases, Error $\sim 2\pi/2^{n_a}$

You will measure integer x , which is distributed around $2^n \theta$

$$\frac{1}{2^n} \sum_{k=0}^{2^n-1} \sum_{x=0}^{2^n-1} \exp\left(2\pi i k \left(\theta - \frac{x}{2^n}\right)\right) |x\rangle \otimes |\Psi\rangle \quad U|\Psi\rangle = e^{i\lambda} |\Psi\rangle = e^{i2\pi\theta} |\Psi\rangle$$

$|\Psi\rangle$ should be either exact or close enough to the exact.

In the latter case, if you expand the trial w.f. by genuine eigen states:

$$|\Psi\rangle = \sum_m c_m |\psi_m^{\text{true}}\rangle$$

→ The probability to measure the eigenvalue of interest is proportional to $|c_m|^2$

How to prepare trial w.f.?

$|\Psi\rangle$ would be highly non-trivial and difficult to prepare in our field

Quantum computing in low-energy NP (not covering all)

Nuclear shell-model simulation in digital quantum computers

A. Pérez-Obiol^{1,5✉}, A. M. Romero^{2,3,5✉}, J. Menéndez^{2,3}, A. Rios^{2,3}, A. García-Sáez^{1,4} &
B. Juliá-Díaz^{2,3}

Scientific Reports (2023) 13:12291

PHYSICAL REVIEW C 106, 034325 (2022)

PHYSICAL REVIEW C 105, 024324 (2022)

Accessing ground-state and excited-state energies in a many-body system after symmetry restoration using quantum computers

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PHYSICAL REVIEW C 107, 044308 (2023)

Quantum computing of the ${}^6\text{Li}$ nucleus via ordered unitary coupled clusters

Oriol Kiss^{1,2,*}, Michele Grossi¹, Pavel Lougovski^{1,3}, Federico Sanchez^{1,2},
Sofia Vallecorsa¹, and Thomas Papenbrock^{1,4,5}

PHYSICAL REVIEW A 108, 032417 (2023)

Quantum computing of the pairing Hamiltonian at finite temperature

Chongji Jiang¹ and Junchen Pei^{1,2,*}

PHYSICAL REVIEW C 105, 064308 (2022)

Demonstration of a quantum-classical coprocessing protocol for simulating nuclear reactions

F. Turro^{1,2,3,*†}, T. Chistolini^{4,*‡}, A. Hashim^{4,5}, Y. Kim^{4,5}, W. Livingston^{4,5}, J. M. Kreikebaum^{4,6}, K. A. Wendt⁷,
J. L. Dubois,⁷ F. Pederiva^{1,2,3}, S. Quaglioni^{1,7}, D. I. Santiago^{1,5}, and I. Siddiqi^{4,5,6}

Nuclear Physics in the Era of Quantum Computing and Quantum Machine Learning

José-Enrique García-Ramos*, Álvaro Sáiz, José M. Arias, Lucas Lamata, and Pedro Pérez-Fernández
arXiv:2307.07332

PHYSICAL REVIEW C 109, 044322 (2024)

Variational approaches to constructing the many-body nuclear ground state for quantum computing

I. Stetcu¹, A. Baroni, and J. Carlson

PHYSICAL REVIEW C 102, 064624 (2020)

Editors' Suggestion

Preparation of excited states for nuclear dynamics on a quantum computer

Alessandro Roggero¹, Chenyi Gu^{1,2}, Alessandro Baroni,³ and Thomas Papenbrock^{1,2,4}

Quantum simulation approach to implementing nuclear density functional theory via imaginary time evolution

Yang Hong Li¹, Jim Al-Khalili¹, and Paul Stevenson¹

Evaluation of phase shifts for non-relativistic elastic scattering using quantum computers

Francesco Turro^{1,*}, Kyle A. Wendt², Sofia Quaglioni^{1,2}, Francesco Pederiva^{3,4}, and Alessandro Roggero^{1,3,4}

arXiv:2407.04155

A NISQ roadmap: ground states of nuclei

valence two neutrons See the appendix

^6He (on ^4He core), ^{18}O (on ^{16}O), ^{42}Ca (on ^{40}Ca)

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

Done!



proton-neutron



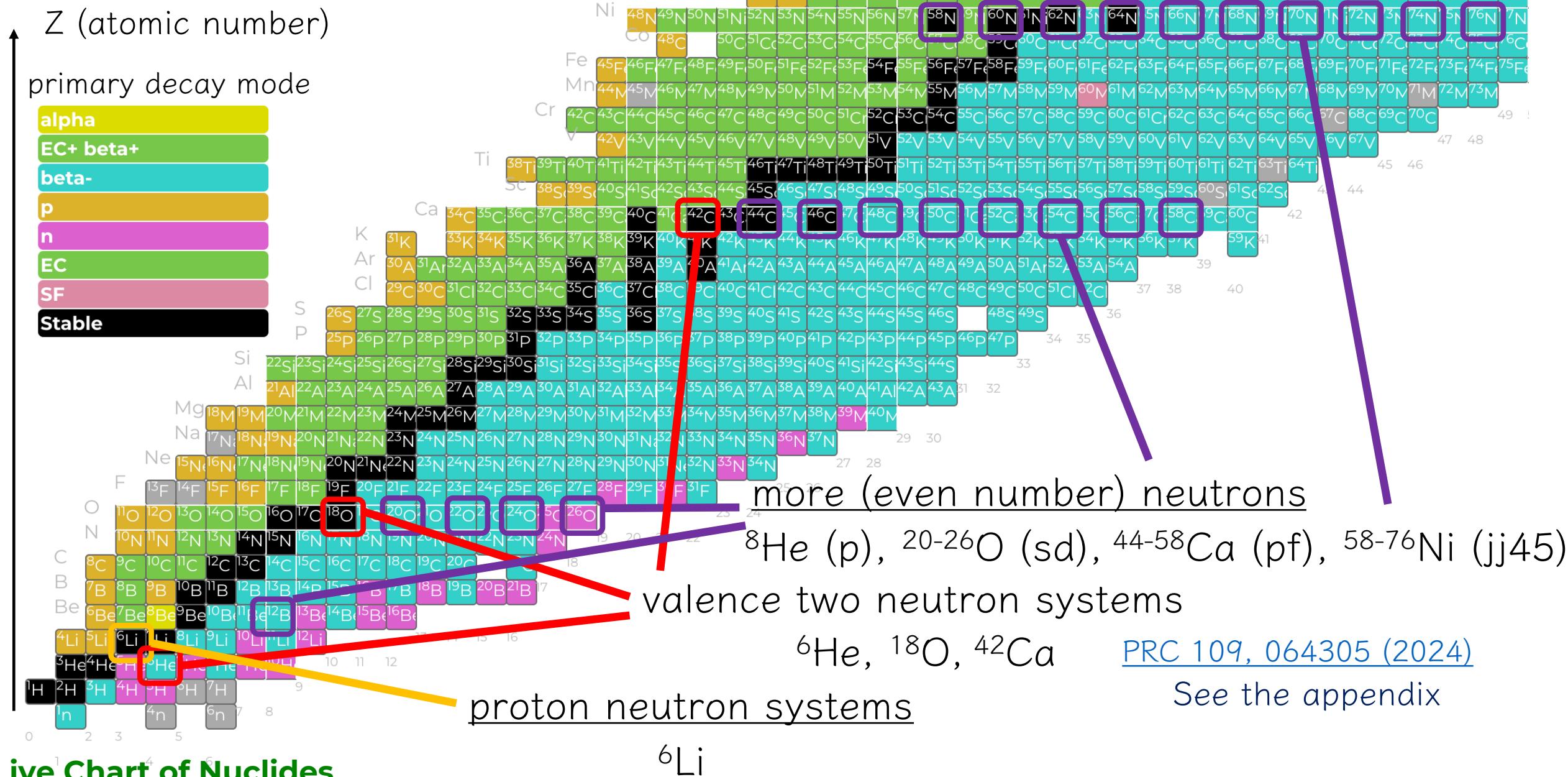
^6Li (on ^4He)

more (even number) neutrons



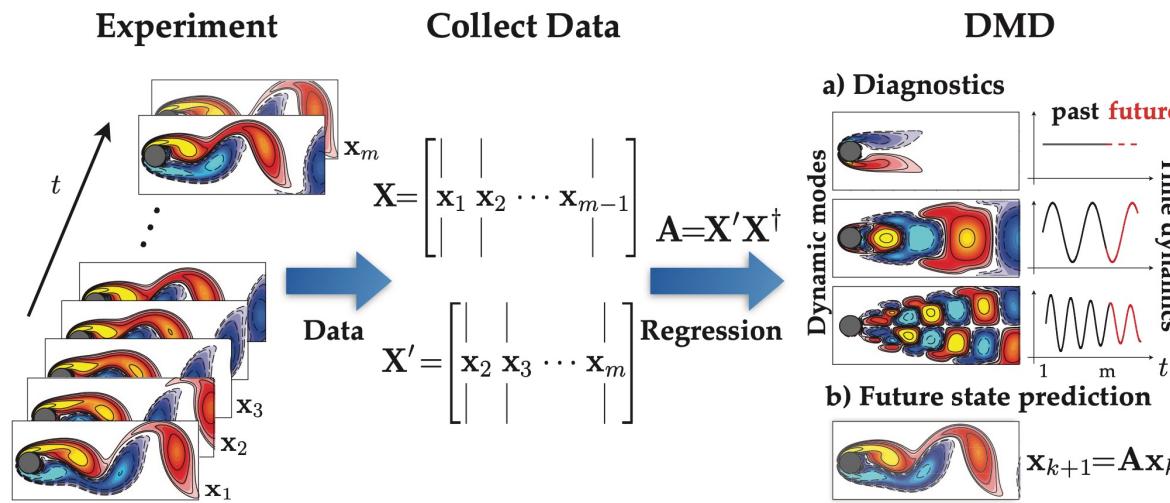
Helium, Oxygen, Calcium, Nickel isotopes

A NISQ roadmap: ground states of nuclei



Observable Dynamic Mode Decomposition

DMD: originally developed in the field of numerical fluid dynamics ~ 2009 (or earlier)



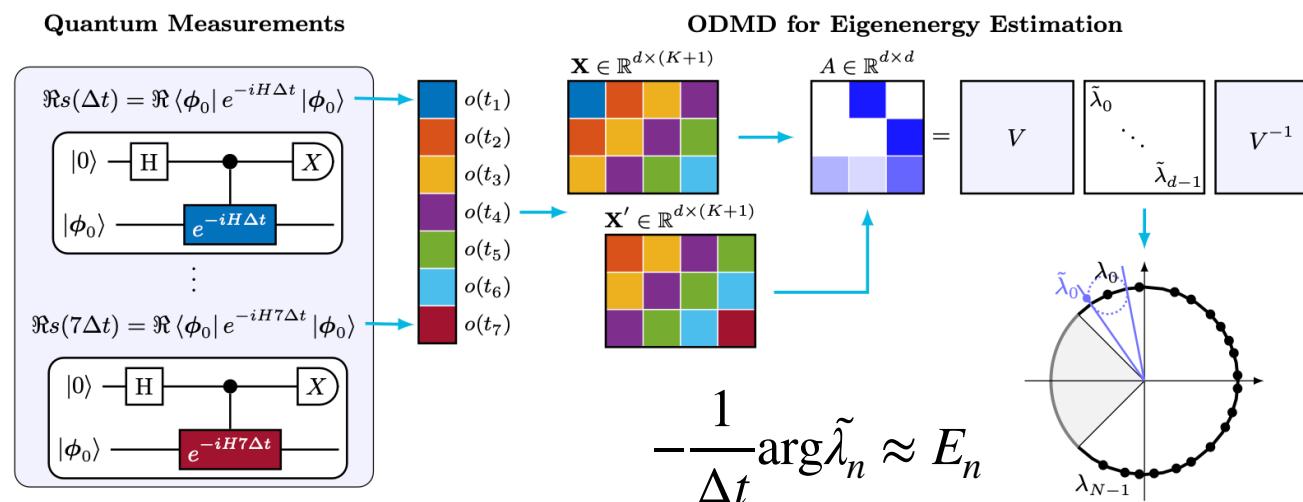
To replace the time evolution by a linear map

$$X \equiv \begin{pmatrix} & & \\ | & \cdots & | \\ x_1 & \cdots & x_N \end{pmatrix}, Y \equiv \begin{pmatrix} & & \\ | & \cdots & | \\ x_2 & \cdots & x_{N+1} \end{pmatrix}$$

$$Y = F(X) \quad \Rightarrow \quad Y \approx AX$$

$$\begin{aligned} A &\approx YX^+ = Y(V_r \Sigma_r^{-1} U_r^\dagger) \\ \tilde{A} &= U_r^\dagger A U_r \approx U_r^\dagger Y V_r \Sigma_r^{-1} \end{aligned}$$

Fig 1.1 from Kutz et al., “Dynamic Mode Decomposition” SIAM



[arXiv:2306.01858](https://arxiv.org/abs/2306.01858) [arXiv:2409.13691](https://arxiv.org/abs/2409.13691)

This $\langle \phi_0 | e^{-iHk\Delta t} | \phi_0 \rangle$ would have information of eigen energies. We may need only overlaps!!

c.f. Quantum Krylov

$$\begin{aligned} N_{kl} &= \langle \Phi_k | \Phi_l \rangle = \langle \Phi_0 | e^{-i(t_l-t_k)H} | \Phi_0 \rangle \\ \tilde{H}_{kl} &= \langle \Phi_k | H | \Phi_l \rangle = \langle \Phi_0 | H e^{-i(t_l-t_k)H} | \Phi_0 \rangle \end{aligned}$$

Summary

Emulators/Surrogate models for IM-IMSRG

tested PINNs&DMD, still need further studies!



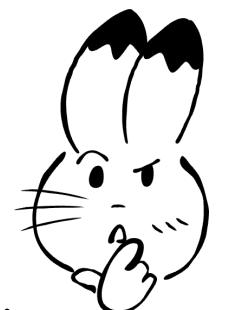
Quantum computing

NISQ applications: w/ UTokyo&RIKEN group

Better ansatz and measurement strategies for n-rich nuclei

Resource estimations : w/ LBNL&Tsukuba

Resources on NISQ/EFTQC/FTQC algorithms for nuclei



Q. Does Quantum computing meet with IM-SRG?

A. We will find out a way, hopefully... Let us consider together.

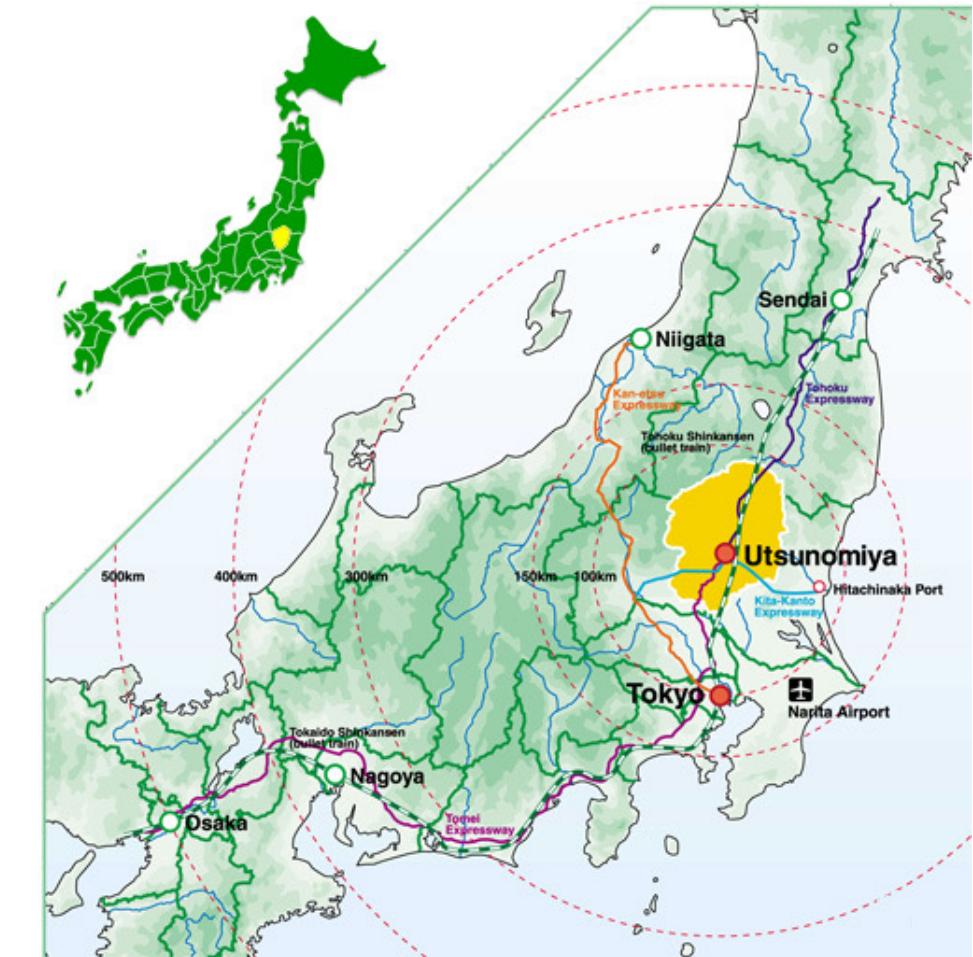
Office of my group

I don't have any students until next year.
This room ↓ is for me collaborators/visitors!
I look forward to your visit, if you want!



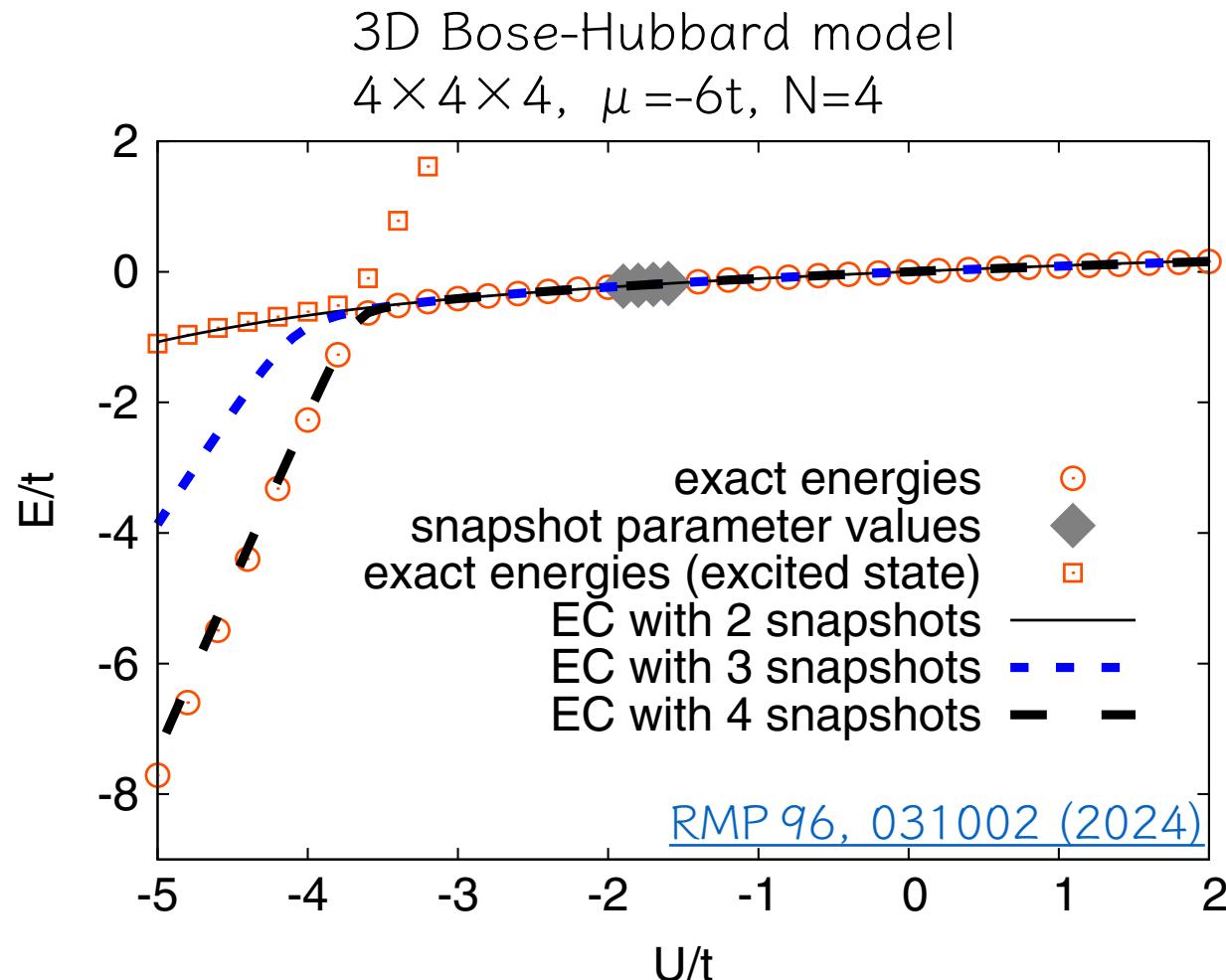
Utsunomiya city (Tochigi prefecture):

Population ~ 520,000 (34th of 1718 cities)
100 km (~ 1 hour) from Tokyo Station



Eigenvector continuation (EC) in a nutshell

30



1. Suppose you have exact eigenstates at some points (taking snapshots)
2. Span the wavefunction by the samples and solve generalized eigen val. prob.

$$\tilde{H}\vec{v} = \lambda N\vec{v},$$
$$\tilde{H}_{i,j} = \langle \psi(\vec{c}_i) | H(\vec{c}_\odot) | \psi(\vec{c}_j) \rangle,$$
$$N_{i,j} = \langle \psi(\vec{c}_i) | \psi(\vec{c}_j) \rangle.$$

$$E(\vec{c}_\odot) \simeq \lambda, \quad |\psi(\vec{c}_\odot)\rangle \simeq \sum_{i=1}^{N_s} v_i |\psi(\vec{c}_i)\rangle \equiv |\psi_{EC}(\vec{c}_\odot)\rangle.$$

↑ a few snapshots are enough to express eigenstates elsewhere

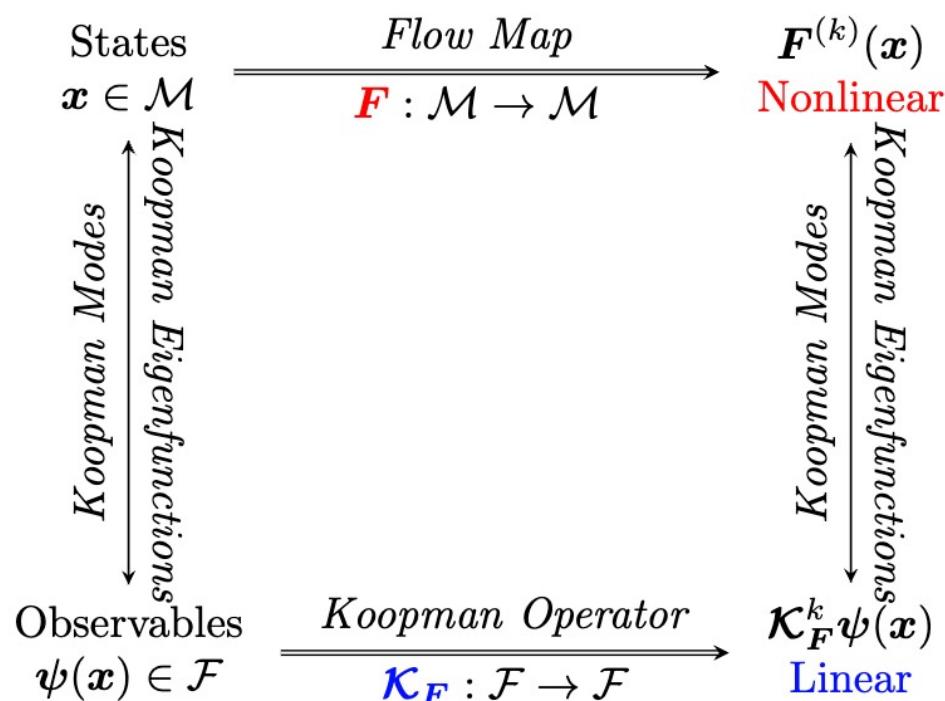
dim. $2^{24} \sim 10^{7.2} \rightarrow 4$ (EC)

That have been proven to be true in many different many-body systems.

Relation/Similarity to Koopman operator and ML

31

Koopman operator



arXiv:2102.02522

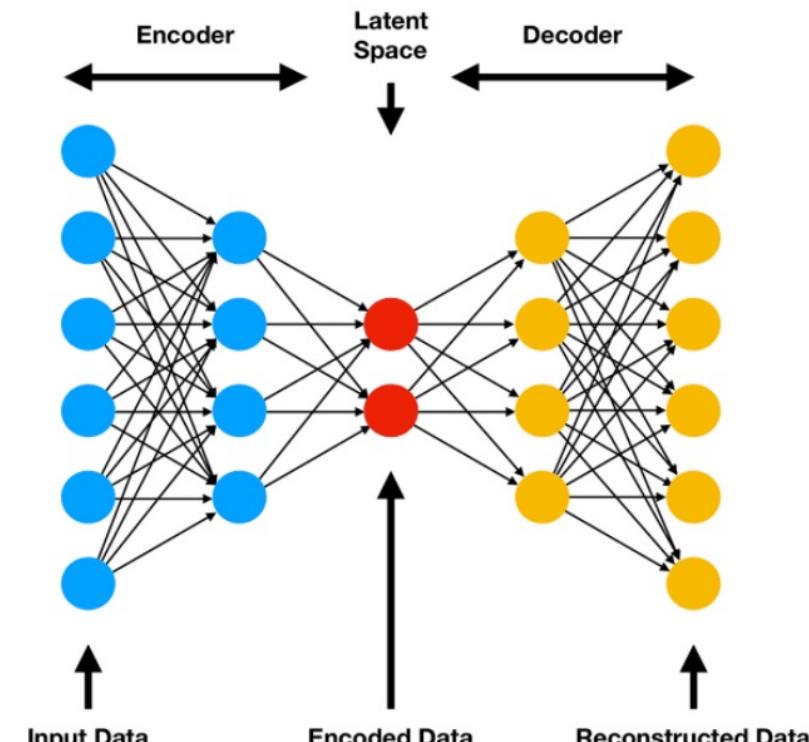
DMD

$$\mathbf{A} = \mathbf{U}_r \tilde{\mathbf{A}} \mathbf{U}_r^\dagger$$

encoder

decoder

Machine Learning



Auto encoder

Fig from a post

Appendix: Quantum computing

Phenomenology

To understand structure of
e.g. unstable nuclei

Shell-model calc. of
Beta-decays, etc.

Ab initio

nuclear force, 3NF

Full-CI, post-HF, etc.

Uncertainty quantification

To make more “reliable”
predictions

Quantum computing

Challenge to the most difficult
quantum many-body systems



Developing software

To interplay with people
from different disciplines

Education for
the next generation

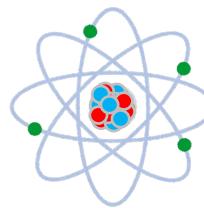
Emulators

To enable us to do “full” UQ
ML applications

Difference from other quantum many-body systems

33

Quantum chemistry:



“ $qq >$ % 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)

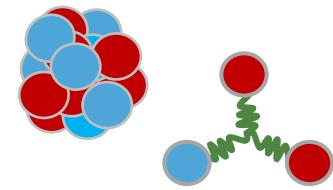
Coupled Cluster Single and Double (CCSD)

CCSD + Triple (CCSDT)

Full Configuration interaction (Full-CI)

accurate but computationally demanding

Nuclear physics:



Interaction is highly non-perturbative & uncertain
many channels, three-nucleon force,...



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

$$\text{HF} = -302.716 \text{ MeV}$$

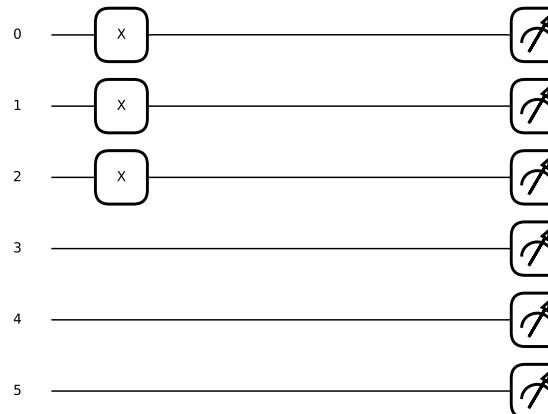
$$\text{HF} + \text{MP2} + \text{MP3} = -473.089 \text{ MeV}$$
$$(\text{MP2} = -152.533, \text{MP3} = -17.716)$$

~~How dare people call it perturbation theory!!~~

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

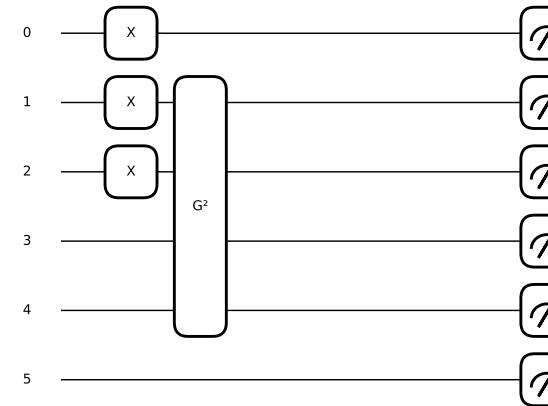
State preparation: mapping of your problems on qubits

Single Slater expression e.g. HF



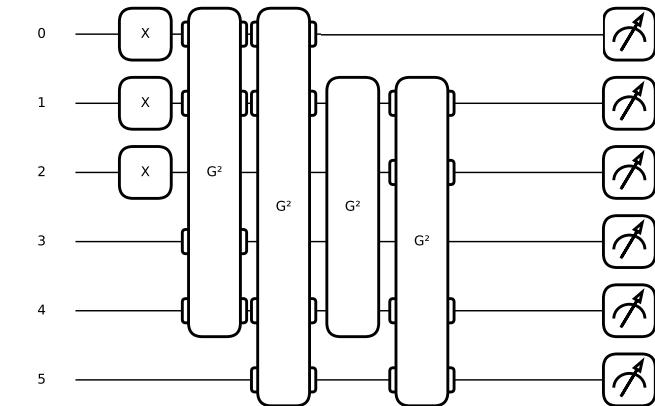
$$|\psi\rangle = |111000\rangle$$

HF + a 2p2h state



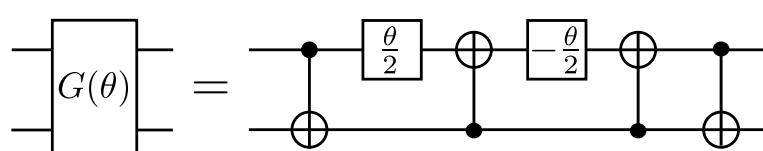
$$|\psi\rangle = \alpha|111000\rangle + \beta|100110\rangle$$

HF + 2p2h states



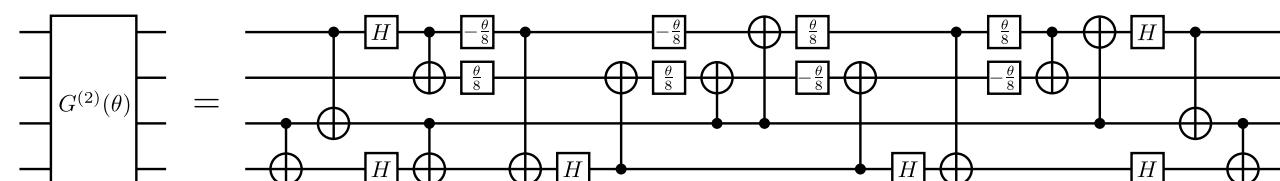
$$|\psi\rangle = \alpha|111000\rangle + \beta|100110\rangle + \gamma|001110\rangle + \dots$$

G = Givens rotation for single excitation



$$\begin{aligned} |00\rangle &\rightarrow |00\rangle, |11\rangle \rightarrow |11\rangle, \\ |01\rangle &\rightarrow \cos\left(\frac{\theta}{2}\right)|01\rangle - \sin\left(\frac{\theta}{2}\right)|10\rangle, \\ |10\rangle &\rightarrow \cos\left(\frac{\theta}{2}\right)|10\rangle + \sin\left(\frac{\theta}{2}\right)|01\rangle, \end{aligned}$$

$G^{(2)}$ = Givens rotation for double excitation



← ↑ symmetry (particle-number conservation)
aware gate operations

Example of trial wavefunction: Coupled Cluster

CC wavefunction: exponential ansatz

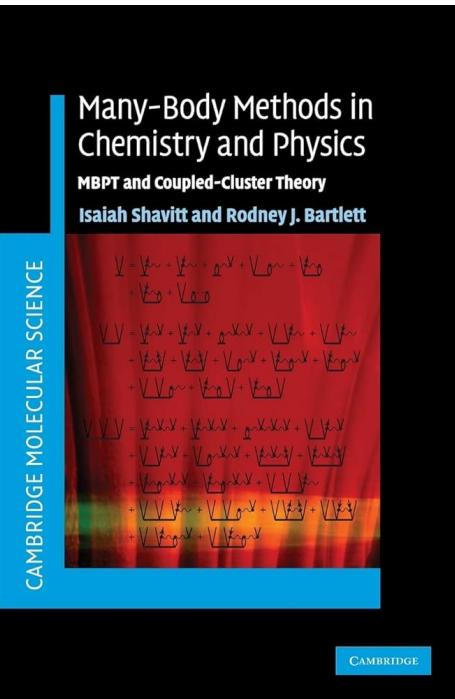
$$|\psi_{\text{CC}}\rangle = e^{\hat{T}} |\text{HF}\rangle \quad \hat{T} = \sum_{k=1}^n \hat{T}_k, \quad \hat{T}_k = \frac{1}{(k!)^2} \sum_{ij\dots}^{\text{occ}} \sum_{ab\dots}^{\text{virt}} t_{ij\dots}^{ab\dots} \tau_{ij\dots}^{ab\dots}, \quad \left. \begin{array}{l} \text{ECS} = \text{HF} \text{ (Brillouin theorem)} \\ \text{CCD} \\ \text{CCSD} \\ \text{CCSD(T)} \\ \text{CCSDT} \\ \vdots \end{array} \right\}$$

$$\tau_{ij\dots}^{ab\dots} = a_a^\dagger a_b^\dagger \dots a_j a_i$$

$$\langle \text{HF} | e^{-\hat{S}} \hat{H} e^{\hat{S}} | \text{HF} \rangle = E$$

$$\langle \mu | e^{-\hat{S}} \hat{H} e^{\hat{S}} | \text{HF} \rangle = 0$$

μ : states have ph-exitations on HF



I. Shavitt and R.J. Bartlett
A bible for MBPT&CC

UCC is Unitary variants of coupled cluster, $S = T - T^\dagger$

not popular in classical computations due to its cost

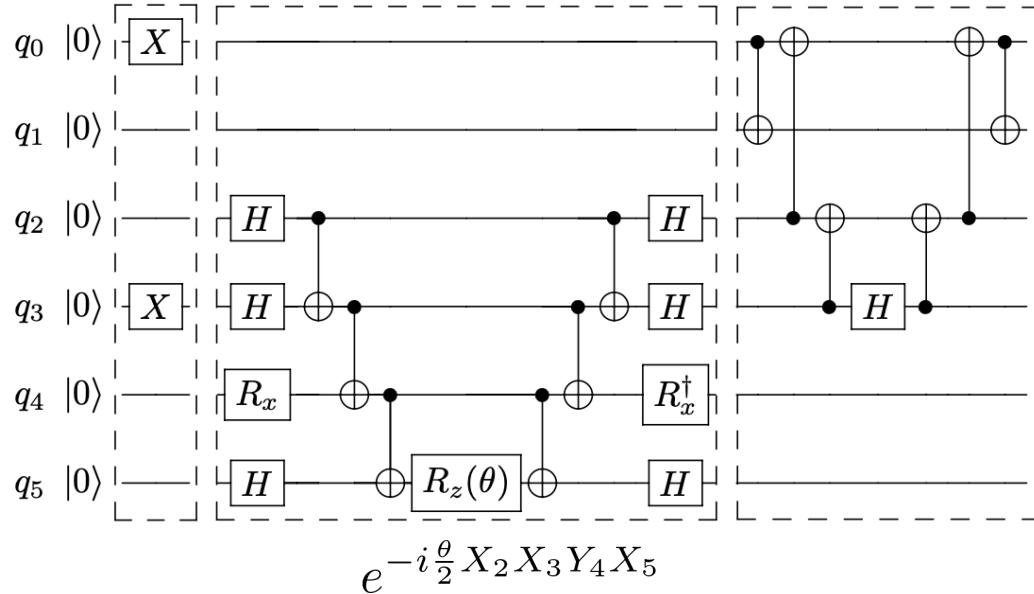
but became Gold standard for Quantum Computing (due to its unitarity)

An example of UCC ansatz

36

[Scientific Reports, 13, 12291 \(2023\)](#)

Exp. of single term for ${}^6\text{Be}$



UCC + Adapt-VQE

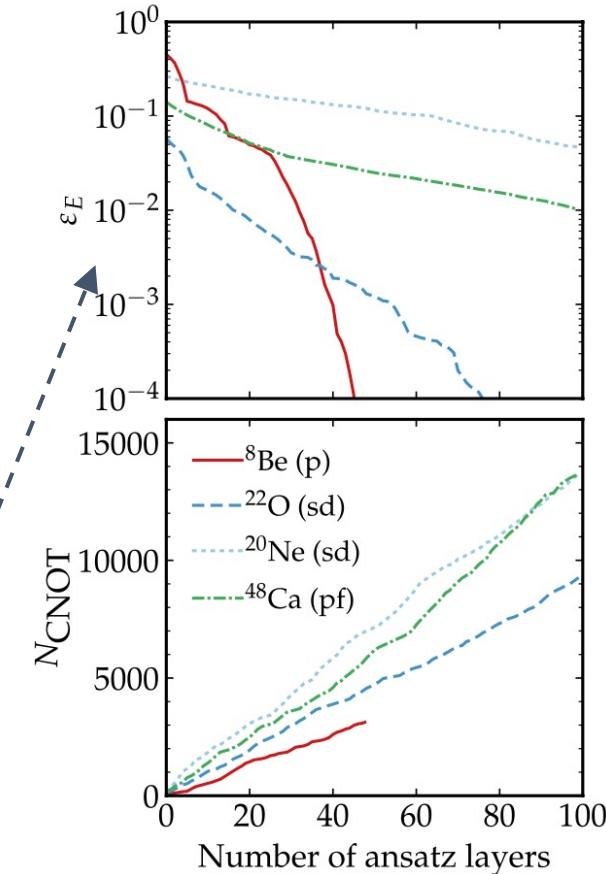
Iterative and variational construction
of exponential ansatz

$$|\psi(\theta)\rangle = \prod_{k=1}^n e^{i\theta_k A_k} |\text{ref}\rangle,$$

$$E = \min_{\theta} \frac{\langle \psi(\theta) | H_{\text{eff}} | \psi(\theta) \rangle}{\langle \psi(\theta) | \psi(\theta) \rangle},$$

A_k is one of the ph excitation operators

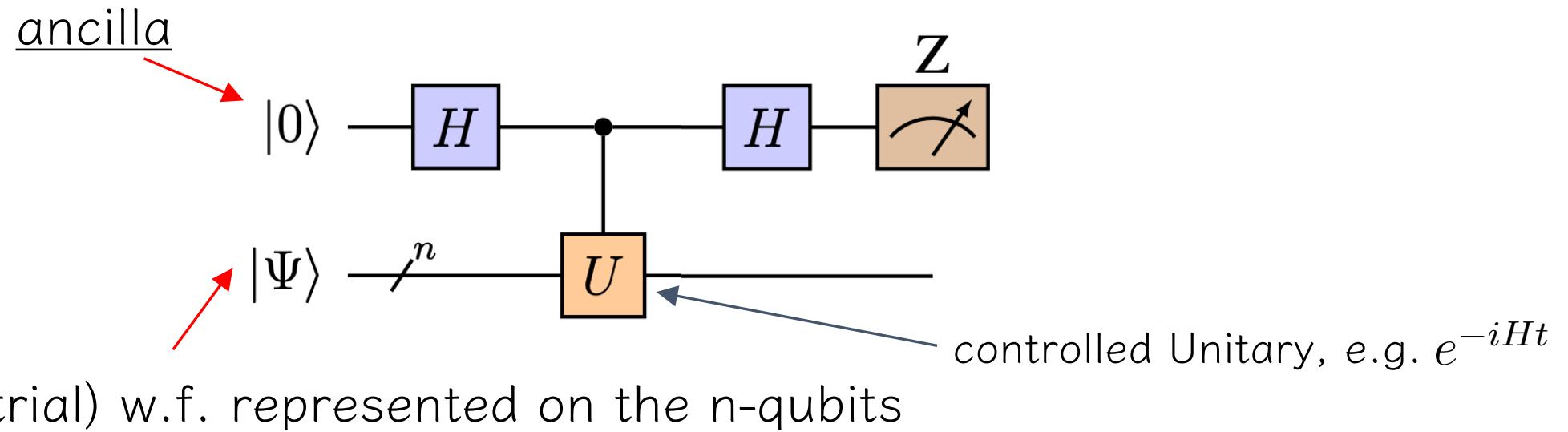
	Fermion operators	Qubit operators
n_p	$a_p^\dagger a_p$	$\frac{1}{2}(1 - Z_p)$
h_{pqrs}	$a_p^\dagger a_q^\dagger a_r a_s + a_r^\dagger a_s^\dagger a_p a_q$	$\frac{1}{8} P_{rs}^{pq} (-X_p X_q X_r X_s + X_p X_q Y_r Y_s - X_p Y_q X_r Y_s - X_p Y_q Y_r X_s - Y_p Y_q Y_r Y_s + Y_p Y_q X_r X_s - Y_p X_q Y_r X_s - Y_p X_q X_r Y_s)$
T_{rs}^{pq}	$i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$	$\frac{1}{8} P_{rs}^{pq} (-X_p Y_q Y_r Y_s - Y_p X_q Y_r Y_s + Y_p Y_q X_r Y_s + Y_p Y_q Y_r X_s + Y_p X_q X_r X_s + X_p Y_q X_r X_s - X_p X_q Y_r X_s - X_p X_q X_r Y_s)$
h_{pq}	$a_p^\dagger a_q + a_q^\dagger a_p$	$\frac{1}{2} \left(\prod_{n=p+1}^{q-1} Z_n \right) (X_p X_q + Y_q Y_p)$
T_{pq}	$i(a_p^\dagger a_q - a_q^\dagger a_p)$	$\frac{1}{2} \left(\prod_{n=p+1}^{q-1} Z_n \right) (Y_p X_q - X_q Y_p)$



To reach 1% error, you may need
10 – 100 layers $\rightarrow 10^3 - 10^4$ CNOTs

c.f. best two-qubits gate fidelity $\sim 99.94\%$
 $0.9994^{1000} \doteq 0.55$, $0.9994^{10000} \doteq 0.002$
no hope w/o error mitigation/correction

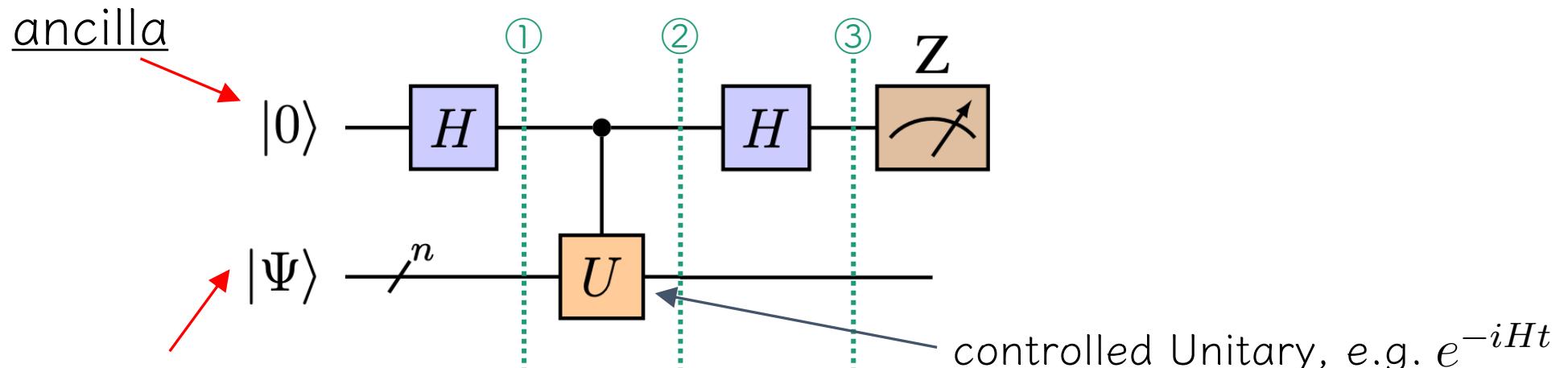
What we want to evaluate $\langle \Psi | U | \Psi \rangle$



Hadamard test

long-term

What we want to evaluate $\langle \Psi | U | \Psi \rangle$



(trial) w.f. represented on the n-qubits

$$\textcircled{1} \rightarrow \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |\Psi\rangle$$

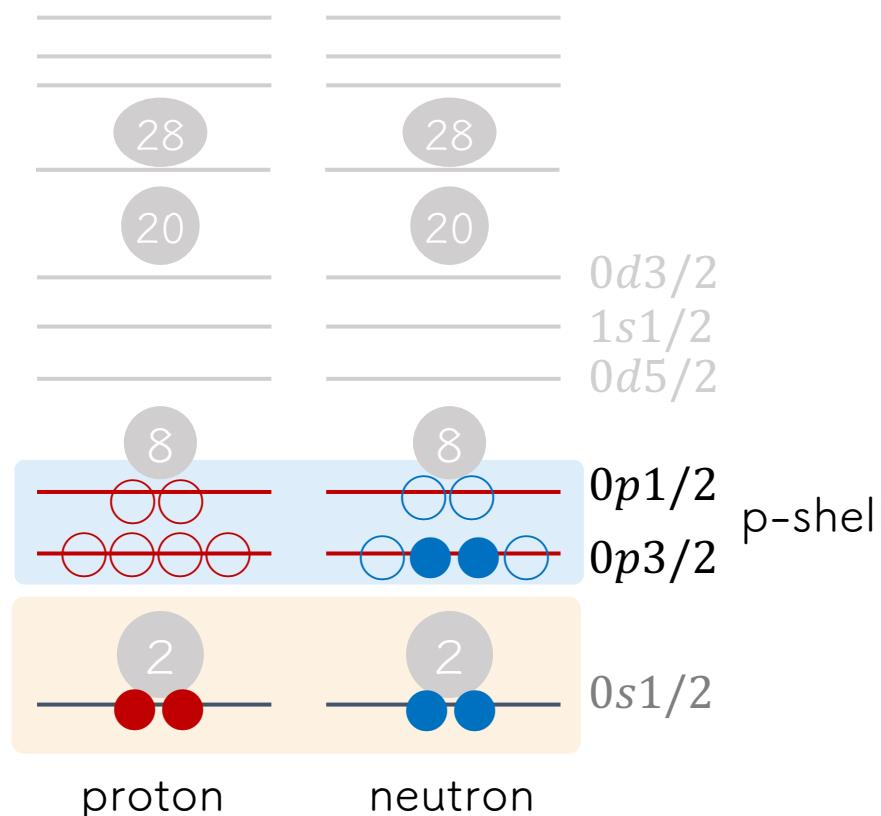
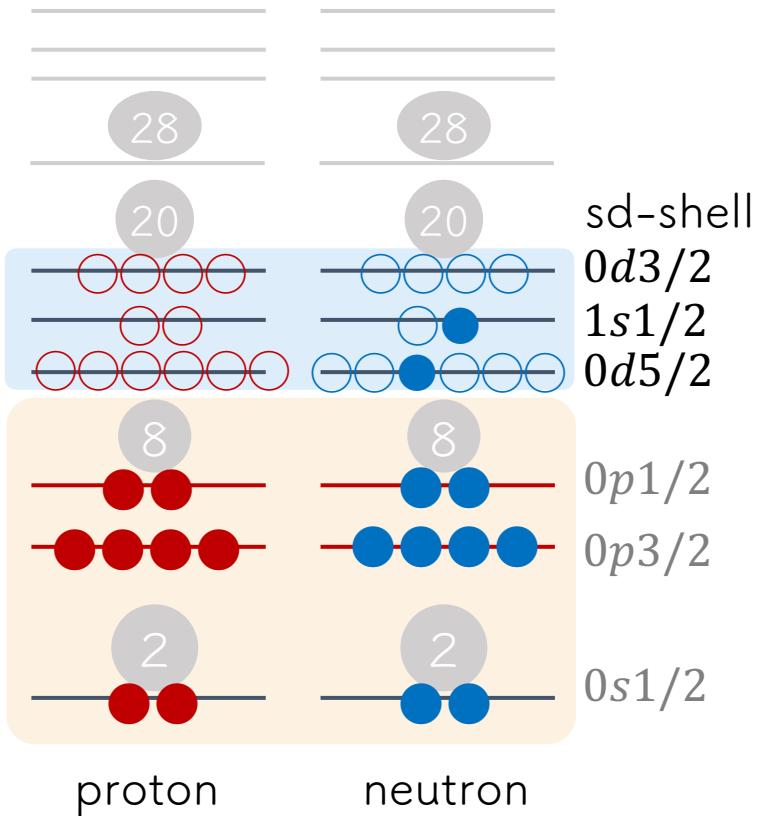
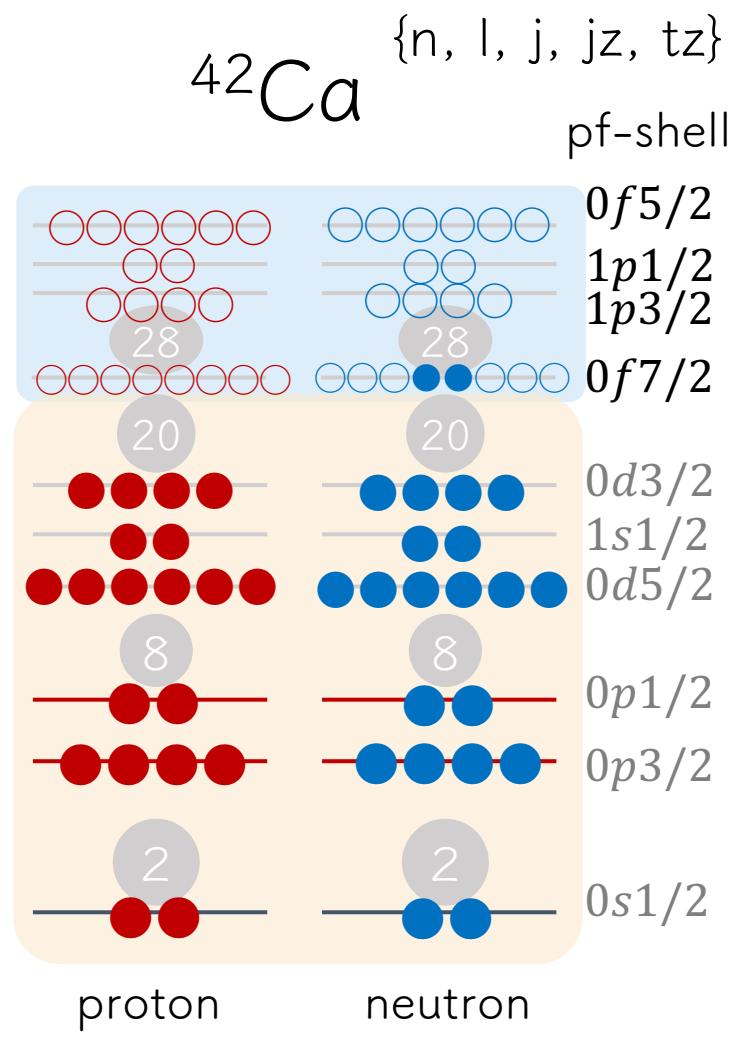
$$\textcircled{2} \rightarrow \frac{1}{\sqrt{2}} |0\rangle \otimes |\Psi\rangle + \frac{1}{\sqrt{2}} |1\rangle \otimes U|\Psi\rangle \quad U|\Psi\rangle = e^{i\lambda} |\Psi\rangle$$

$$\textcircled{3} \rightarrow \frac{|0\rangle + |1\rangle}{2} \otimes |\Psi\rangle + \frac{|0\rangle - |1\rangle}{2} \otimes U|\Psi\rangle \rightarrow \frac{1+e^{i\lambda}}{2} |0\rangle \otimes |\Psi\rangle + \frac{1-e^{i\lambda}}{2} |1\rangle \otimes |\Psi\rangle$$

$$\left. \begin{aligned} P(0) &= \left| \frac{1+e^{i\lambda}}{2} \right|^2 = \frac{1+\cos\lambda}{2} \\ P(1) &= \left| \frac{1-e^{i\lambda}}{2} \right|^2 = \frac{1-\cos\lambda}{2} \end{aligned} \right\}$$

Info. on eigenvalues are encoded as a phase
 → probability to measure ancilla qubits as 0 or 1
 size: $2^n \rightarrow \# \text{ of measurements } M \sim (1/\varepsilon)^n$

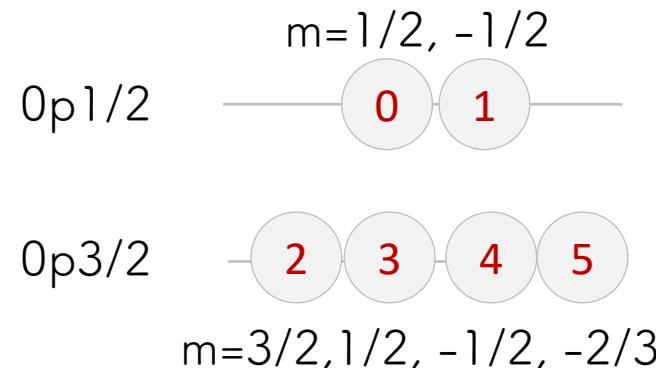
schematics for valence two-neutron systems

 ^6He

 ^{18}O

 ^{42}Ca


blue: valence space (active), pale orange: inert core (inactive)

pair-wise (PW) ansatz: ${}^6\text{He}$ example

ground state ($J=0$) can be described only by time-reversal pairs ($j_z = m \text{ & } -m$)



$$\begin{aligned} |1_0 1_1 0_2 0_3 0_4 0_5\rangle \\ |0_0 1_1 2_0 3_0 4_1 5\rangle \\ |0_0 0_1 2_1 3_1 4_0 5\rangle \end{aligned}$$

Only these have finite amplitude

For more general even nuclei,
PW becomes an approximation

original Hamiltonian can be rewritten by pair creation/annihilation operators

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

$$\begin{aligned} A_{\tilde{i}}^\dagger &= c_i^\dagger c_{\bar{i}}^\dagger, & [A_{\tilde{i}}, A_{\tilde{j}}^\dagger] &= \delta_{\tilde{i}\tilde{j}} (1 - N_{\tilde{i}}), \\ A_{\tilde{i}} &= c_{\bar{i}} c_i, & N_{\tilde{i}} &= c_i^\dagger c_i + c_{\bar{i}}^\dagger c_{\bar{i}}. \quad [N_{\tilde{i}}, A_{\tilde{j}}^\dagger] = 2\delta_{\tilde{i}\tilde{j}} A_{\tilde{j}}^\dagger. \end{aligned}$$

$$H^{\text{PW}} = \sum_{\tilde{i}} \epsilon_{\tilde{i}} N_{\tilde{i}} + \sum_{\tilde{i} < \tilde{j}} \bar{V}_{ij} A_{\tilde{i}}^\dagger A_{\tilde{j}}$$

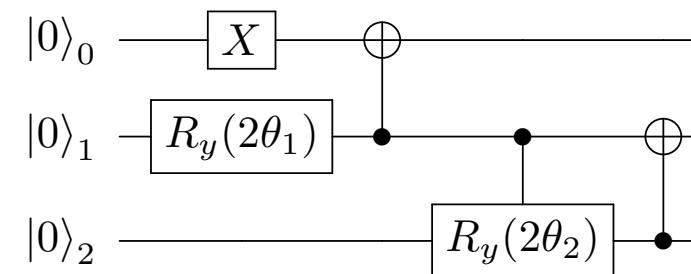
expressing the “pair” as a single qubit,
of qubits needed is reduced to half

$$\left[\begin{array}{l} |1110000\rangle \rightarrow |\overline{1}00\rangle \\ |0011001\rangle \rightarrow |\overline{0}10\rangle \\ |0000110\rangle \rightarrow |\overline{0}01\rangle \end{array} \right]$$

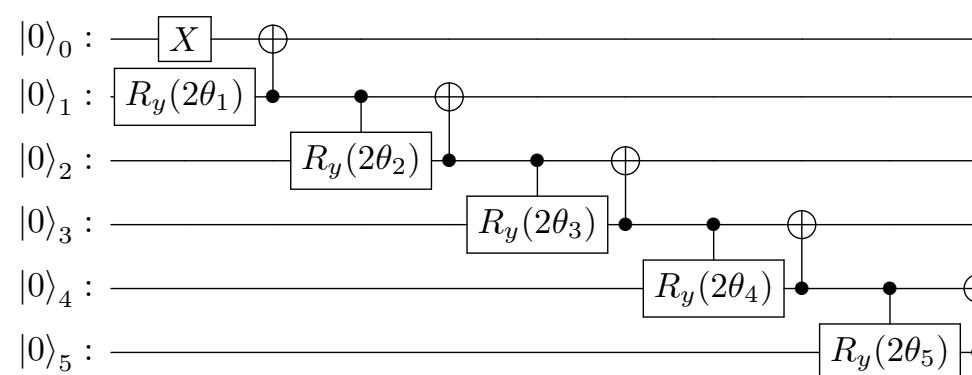
ansatz: circuit for trial wave function

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

	<u># of CNOTs</u>	
	proposed 3N-5	AdaptVQE [Ref] average(upper)
${}^6\text{He}$ (3 qubits)	4	$42 \text{ (80)} \times 2$
${}^{18}\text{O}$ (6 qubits)	13	$qq \text{ (176)} \times 5$
${}^{42}\text{Ca}$ (10 qubits)	25	$116\text{--}304 \times 9$



 The quantum circuit for ${}^6\text{He}$ starts with three qubits in the $|0\rangle_0, |0\rangle_1, |0\rangle_2$ state. It consists of two main parts: a sequence of single-qubit rotations followed by a sequence of CNOT gates. The first part includes an X gate on $|0\rangle_0$, a $R_y(2\theta_1)$ gate on $|0\rangle_1$, and a $R_y(2\theta_2)$ gate on $|0\rangle_2$. The second part consists of CNOT gates between adjacent qubits: C_{01} , C_{12} , and C_{02} .



 The quantum circuit for ${}^{18}\text{O}$ starts with six qubits in the $|0\rangle_0, |0\rangle_1, |0\rangle_2, |0\rangle_3, |0\rangle_4, |0\rangle_5$ state. It follows a similar structure to the ${}^6\text{He}$ circuit, with single-qubit rotations $X, R_y(2\theta_1), R_y(2\theta_2), R_y(2\theta_3), R_y(2\theta_4), R_y(2\theta_5)$ and CNOT gates $C_{01}, C_{12}, C_{23}, C_{34}, C_{45}$.

$\sim 10^3$

similar to the above

Measurement of energy

$$H^{\text{PW}} = \sum_{\tilde{i}} \epsilon_{\tilde{i}} N_{\tilde{i}} + \sum_{\tilde{i} < \tilde{j}} \bar{V}_{ij} A_{\tilde{i}}^\dagger A_{\tilde{j}}$$

$$\hat{H}_{\text{qubit}}^{\text{pw}} = \boxed{\sum_i \frac{\bar{h}_i + \bar{V}_{ii}}{2} (I - Z_i)} + \boxed{\frac{1}{2} \sum_{i < j} \bar{V}_{ij} (X_i X_j + Y_i Y_j)}$$

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)

- post-selection → variational
- only one additional measurement (ansatz + H-gates)

computational basis sampling as a post-selection

Using NISQ devices, you need either post-selection or number projection

$$\begin{aligned} \langle \psi | H | \psi \rangle &= \sum_{m,n=0}^N \langle \psi | m \rangle \langle m | H | n \rangle \langle n | \psi \rangle \\ &= \sum_{m,n=0}^N |\langle m | \psi \rangle|^2 |\langle n | \psi \rangle|^2 \frac{\langle m | H | n \rangle}{\langle m | \psi \rangle \langle \psi | n \rangle}. \end{aligned} \quad (7)$$

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

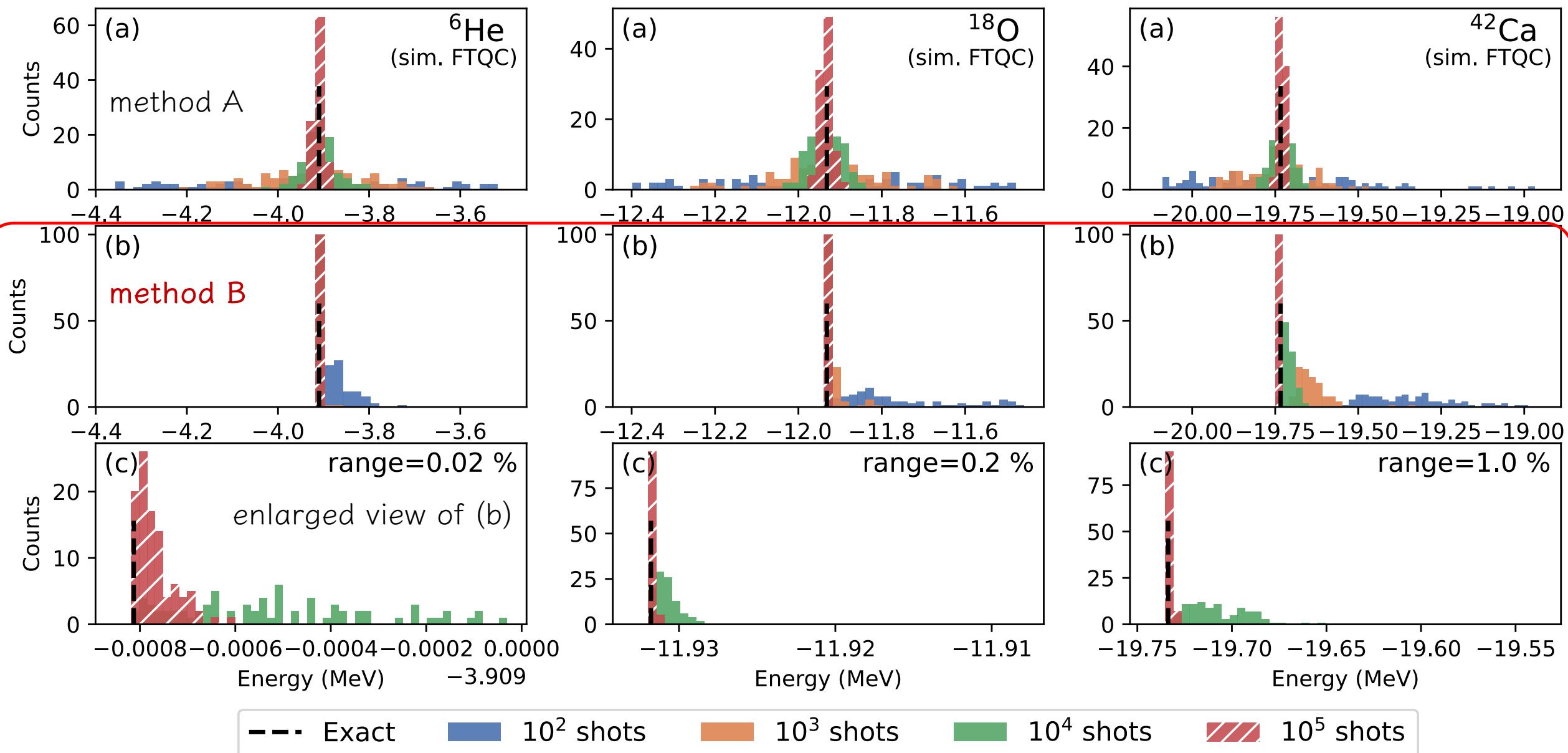
$$= \sqrt{\langle N_j \rangle \langle N_k \rangle} \operatorname{sgn} [\langle X_j X_k \rangle] \quad (9)$$

↑ ansatz plus H-gates on all qubits

↑ equiv. to Z measurement of the ansatz circuit

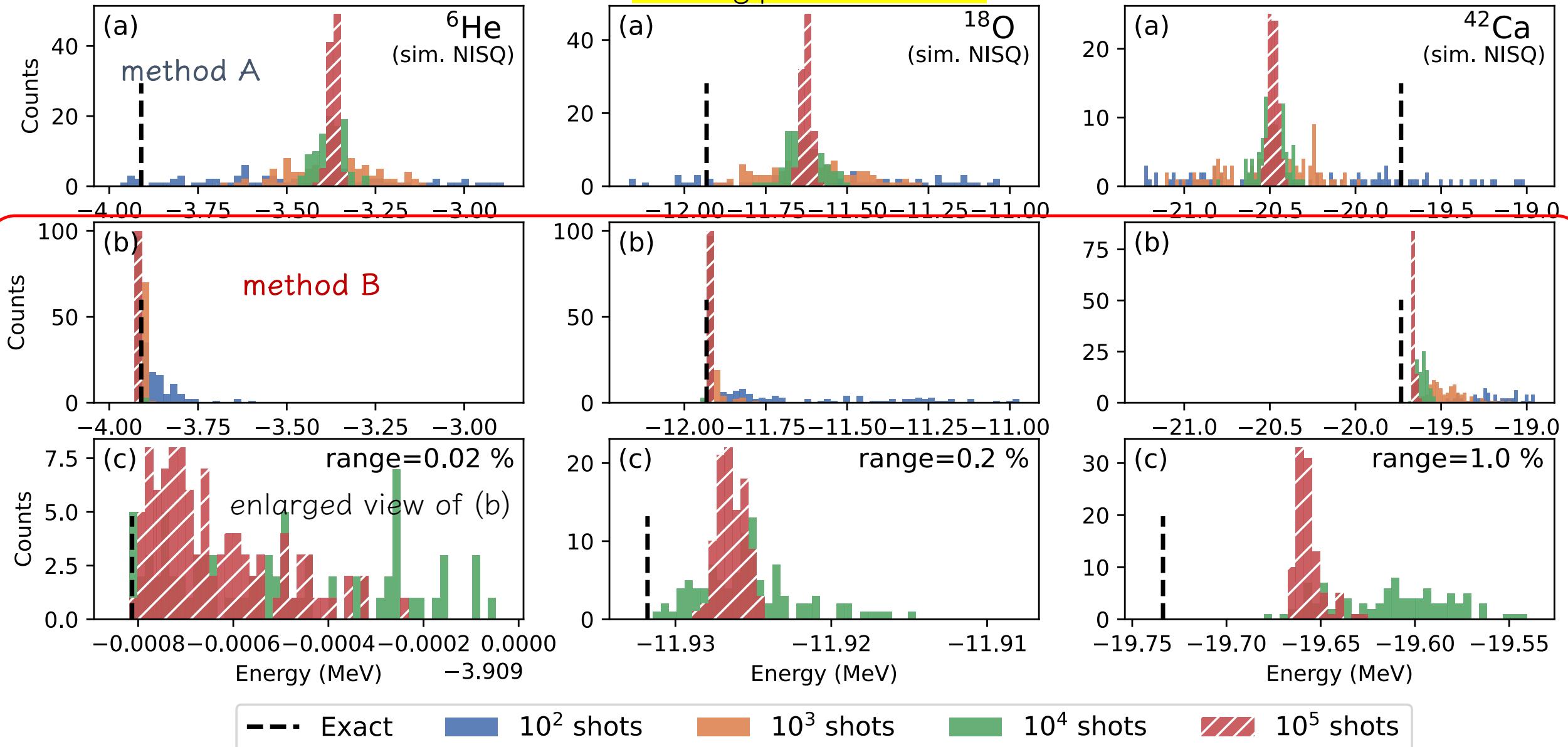
You just need 2 measurements, ansatz & ansatz + H-gates

Results: FTQC(noise-free) simulator



Results: NISQ (noisy) simulator

breaking particle numbers

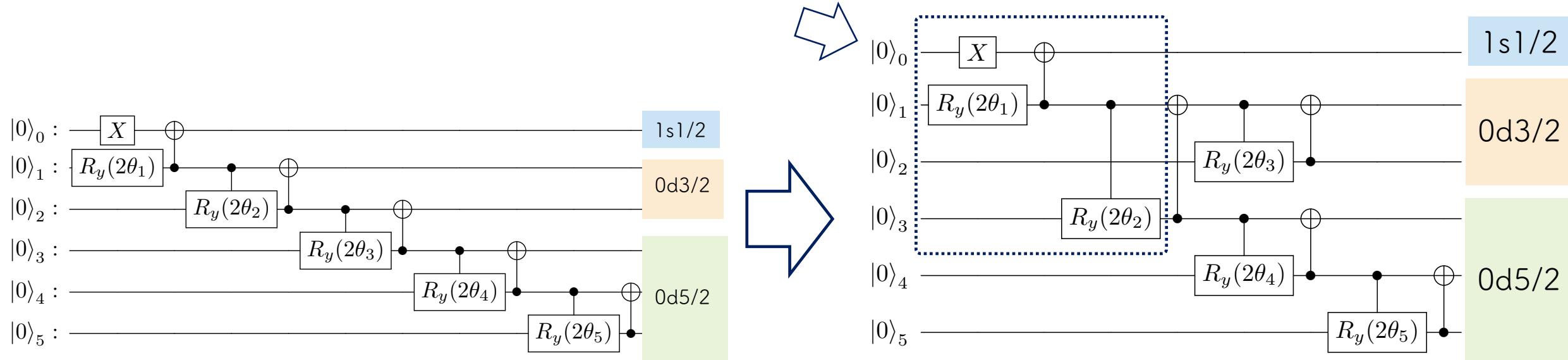


Rearrangement of the ansatz circuit

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

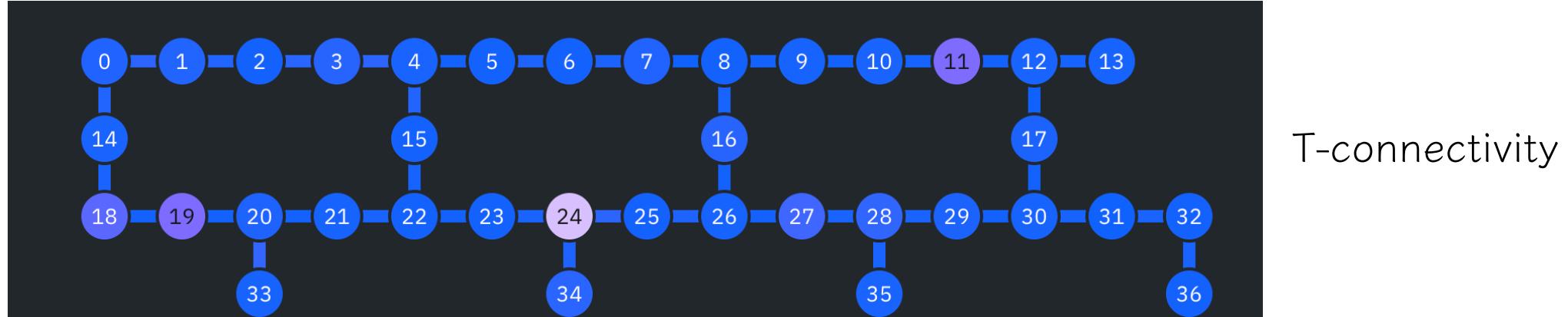


They should give identical results if noise is absent

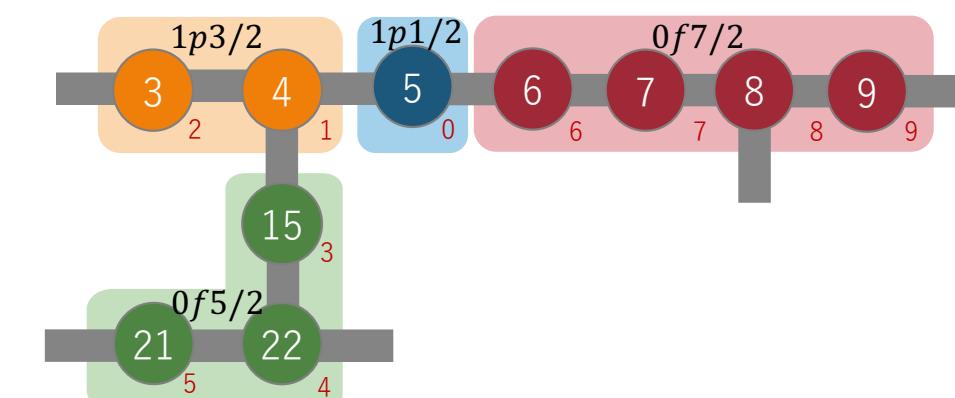
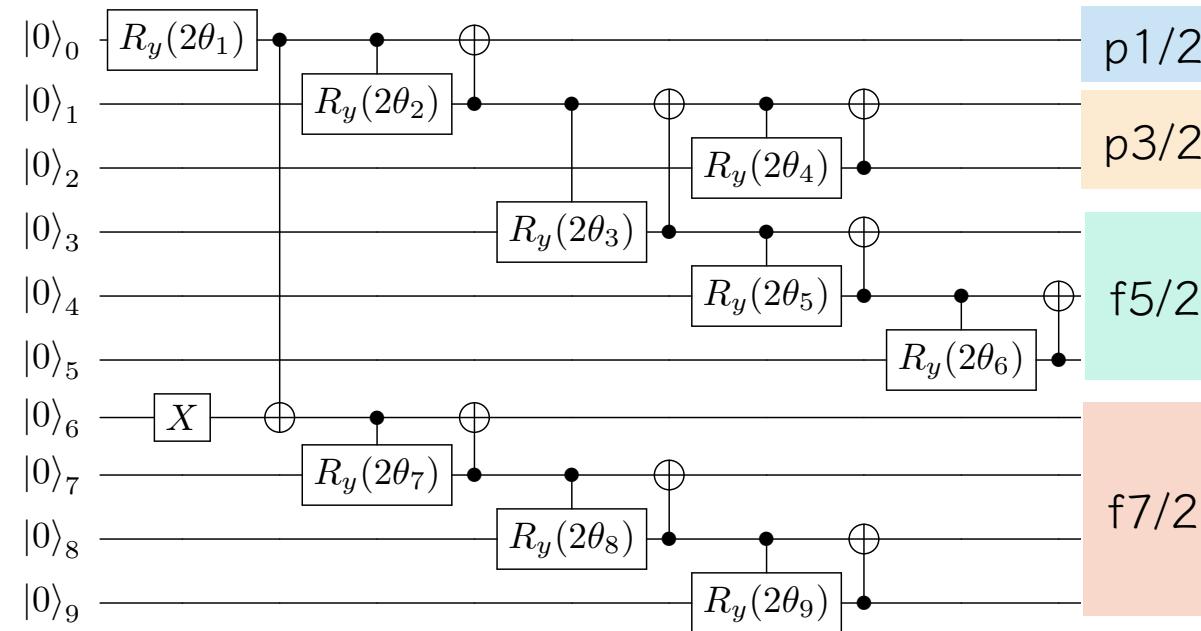
connectivity of qubits in the hardware is another important factor

assignment of the qubits on IBMQ devices

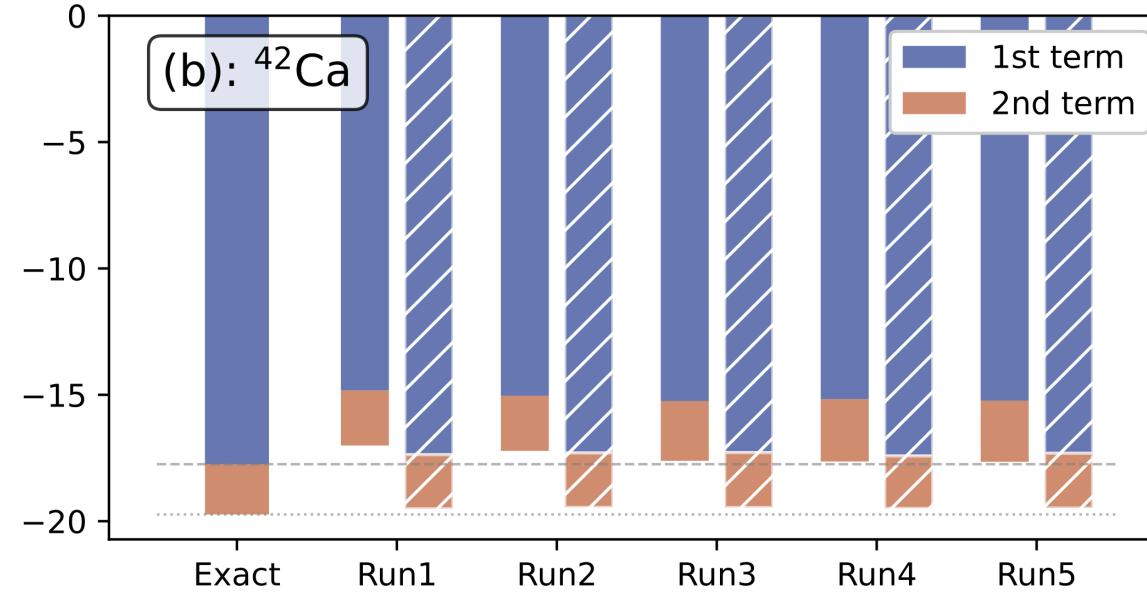
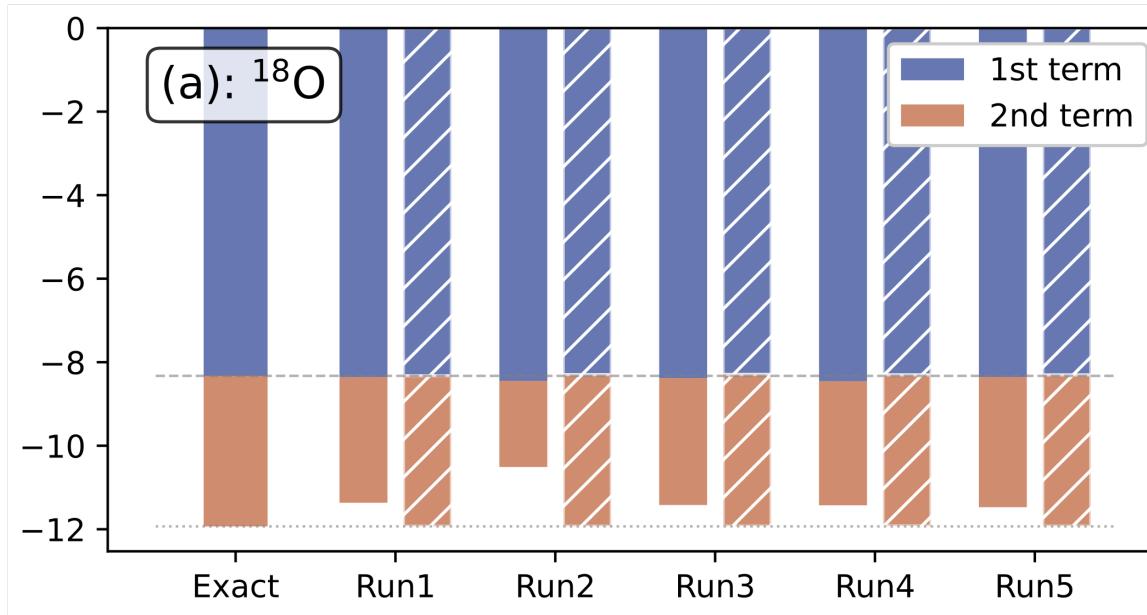
IBM brisbane (127 qubits)



^{42}Ca



Results on real hardware: ibm_brisbane (127 qubits)



Run1-5: different runs

- w/ hatch (//): rearranged
- w/o hatch: original circuit

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

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

c.f. UCC-type results reported so far

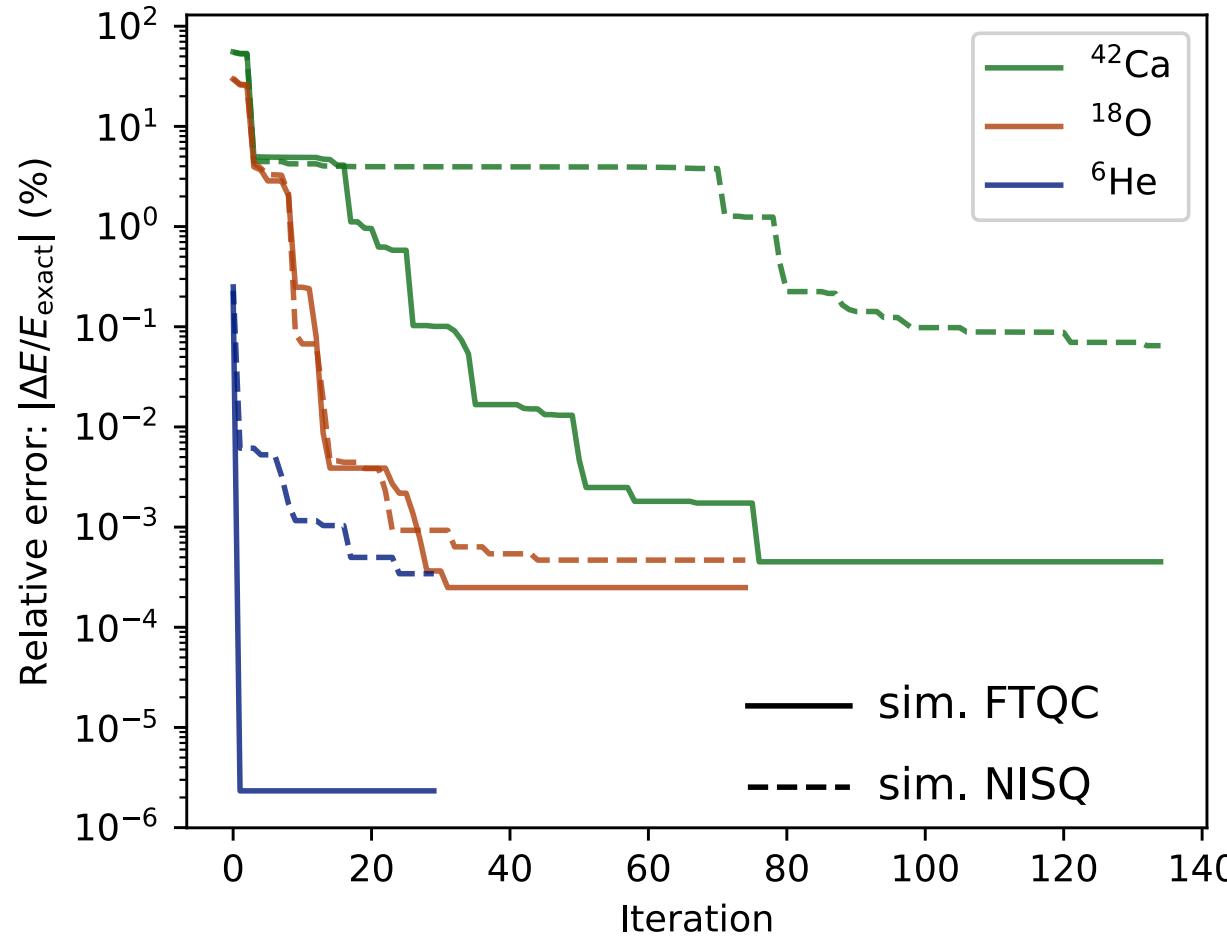
$^6\text{He} \sim 2\% \quad \text{PRC 105, 064308 (2022)}$

$^6\text{Li} \sim 4\% \quad \text{PRC 106, 034325 (2022)}$

$^{18}\text{O} \sim 3\% \quad \text{PRC 108, 064305 (2023)}$

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

Quantum algorithms to solve many-body systems

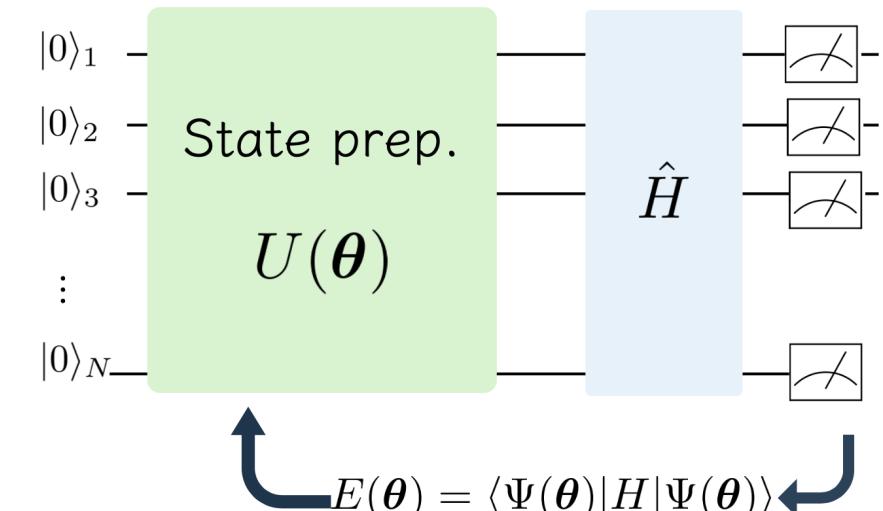
50

Near-term: on NISQ devices

Variational Quantum Eigensolver (VQE):

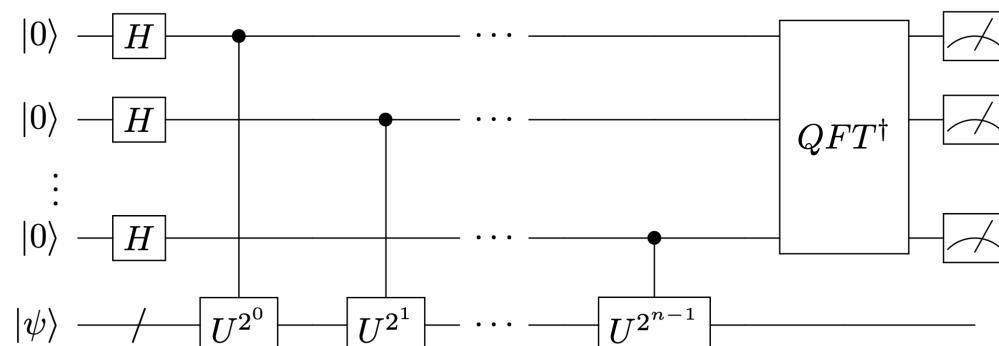
Ansatz (parametric quantum circuits) &
its optimization to get e.g. ground state energy

Long-term: FTQC and Early-FTQC



Quantum Phase Estimation (QPE):

To extract eigenvalues of unitary operations
through (inverse)QFT using ancilla qubits

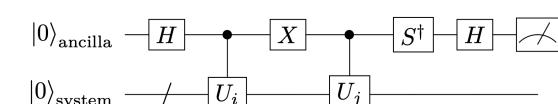
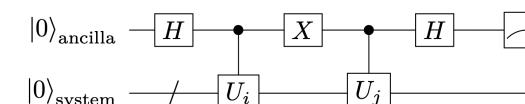


Quantum Krylov subspace methods

Quantum counterpart of e.g. Lanczos method

$$\tilde{H}|\Phi\rangle = EN|\Phi\rangle$$

$$N_{kl} = \langle \Phi_k | \Phi_l \rangle = \langle \Phi_0 | e^{-i(t_l - t_k)H} | \Phi_0 \rangle$$
$$\tilde{H}_{kl} = \langle \Phi_k | H | \Phi_l \rangle = \langle \Phi_0 | H e^{-i(t_l - t_k)H} | \Phi_0 \rangle$$



Appendix: developing software

51

Phenomenology

To understand structure of
e.g. unstable nuclei

Shell-model calc. of
Beta-decays, etc.

Ab initio

nuclear force, 3NF

Full-CI, post-HF, etc.

Uncertainty quantification

To make more “reliable”
predictions

Quantum computing

Challenge to the most difficult
quantum many-body systems



Developing software

To interplay with people
from different disciplines

Education for
the next generation

Emulators

To enable us to do “full” UQ
ML applications

Software development: Julia packages

Aug. 2022~

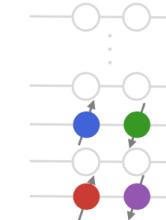


Covering

- Chiral EFT potentials (mainly NN)
- Hartree-Fock & MBPT
- IM-SRG/VS-IMSRG
- Shell model
- Emulators
 - Eigenvector continuation
 - Dynamic mode decomposition

<https://github.com/SotaYoshida/NuclearToolkit.jl>

Feb. 2025~



PairingHamiltonians.jl

To solve a simple model with a bunch of methods:

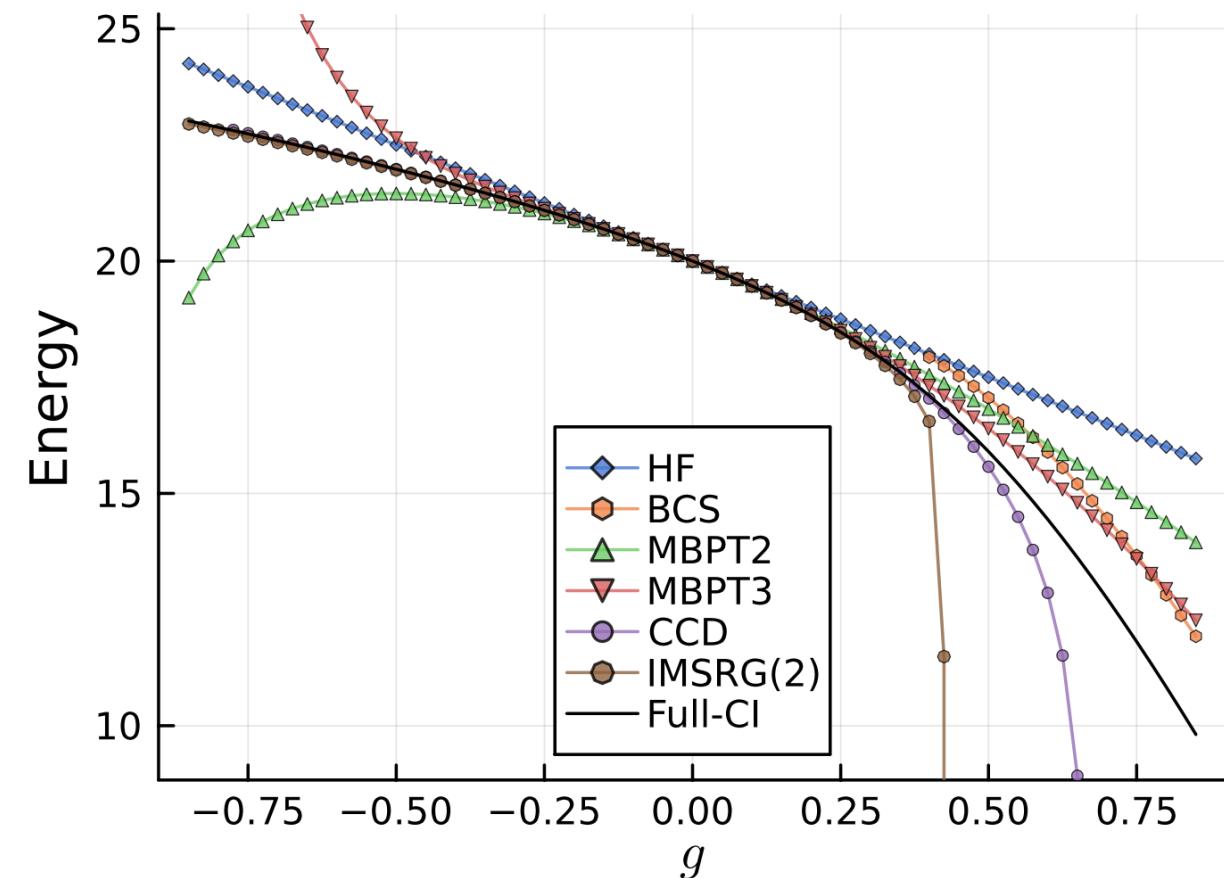
- Full-CI/Exact diagonalization
- Hartree-Fock
- Bardeen-Cooper-Schrieffer (BCS)
- Many-Body Perturbation Theory
- Coupled Cluster
- In-Medium Similarity Renormalization Group
- Eigenvector Continuation

<https://github.com/SotaYoshida/PairingHamiltonians.jl>

$$H_{\text{pair}} = \sum_{i=1}^N \epsilon_i a_i^\dagger a_i - \frac{g}{4} \sum_{ij} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j$$

It is a very simple model,
but a good place

- to learn many-body methods
- as a test ground for e.g.
quantum algorithms



※ I will give a lecture in upcoming [summer school](#) in Japan (in Japanese)
The topic will be solving pairing Hamiltonians with a bunch of methods,
including quantum computing.

My motivations to develop OSS

- Giving tutorials for people from other disciplines, chemistry, computational science, etc.
- Research methods are sometimes “clusterized” (localized) to specific groups



← ~~secret source in Prof. XX's Group~~
secret sauce in Japanese restaurants
(for eel, deep fried pork, etc.)

I am aware that there are some subtleties with sharing the code of nuclear physics, but I think it is important for educations...

We may learn lessons from collective intelligence or co-creation seen in ML community via open-source ML frameworks.