

量子計算機による核子多体系計算

核力・ハドロン間相互作用と量子多体計算の進展
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◆ カイラル核力に依拠した構造・反応計算の進展



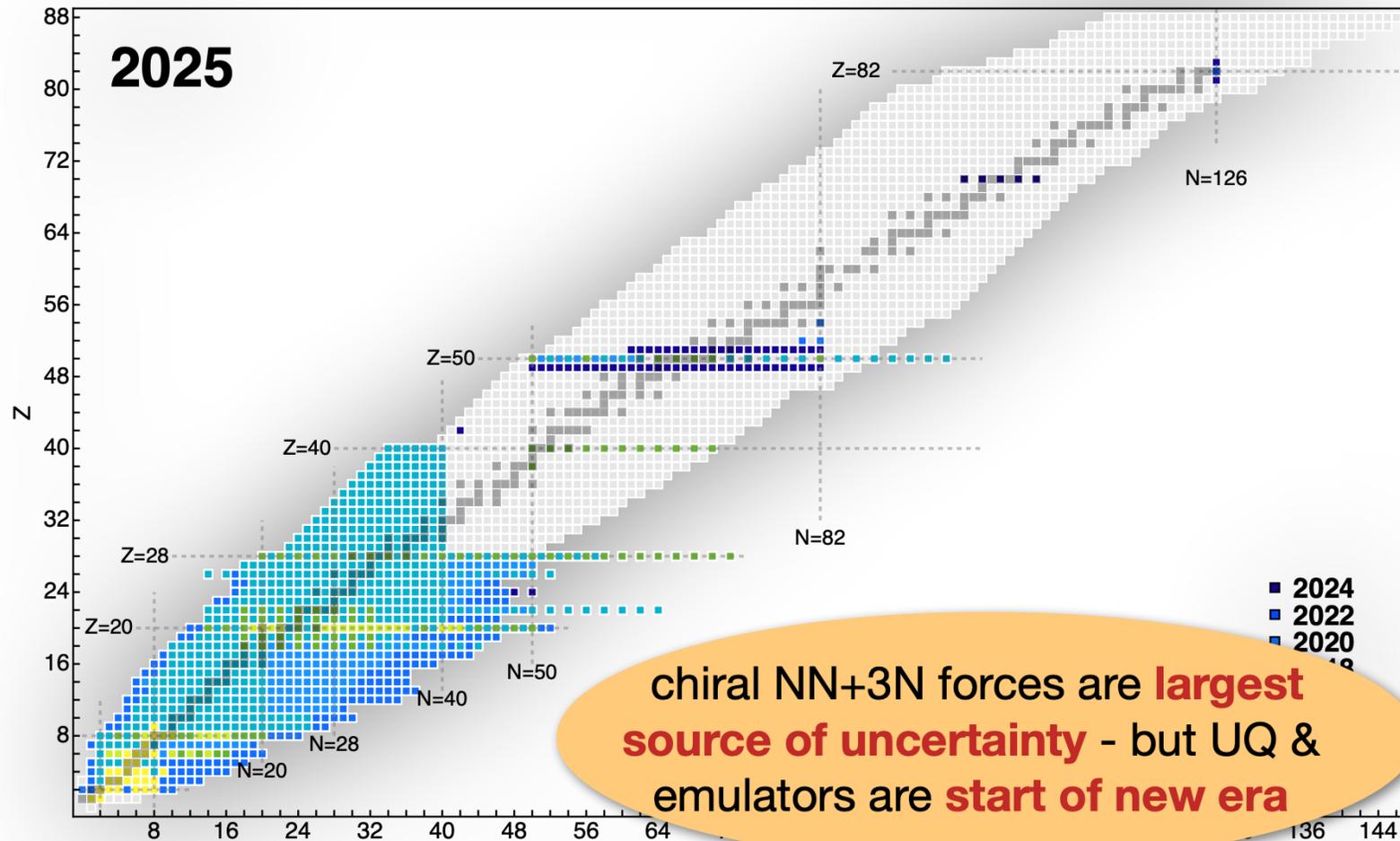
◆ 量子計算

- 概要
- NISQ application SY et al. [PRR 8, 013134 \(2026\)](#)
- FTQCにむけたリソース推定/ソフトウェア開発

核力に依拠した核構造計算の到達領域

post-HF (CC/IM-SRG/etc.): 基底状態の束縛エネルギー/半径 → ^{132}Sn , ^{208}Pb 領域へ

Eff. Ops.: 開殻のスペクトル, EM/GT遷移, etc. → valence CI costが律速, O近傍driplineやNi領域へ



H. Hergert - 2025 Workshop on Progress in Ab Initio Nuclear Theory (PAINT), TRIUMF, Vancouver, Feb 26, 2025

←この図だけでも、

- Green's function Monte Carlo
- No-Core Shell Model
- post-HF (CC/IMSRG)
- post-HF + shell model
SMCC, VS-IMSRG, etc.

などなど、手法は様々

Courtesy of H. Hergert, [PAINT2025](#)

カイラル核力と基底状態の構造計算の歩み

2015 NNLOsat: NNLOまでのNN+3NFのLECsをtriton - Oxygen isotopeでfix

A. Ekström et al. [PRC 91, 051301\(R\) \(2015\)](#)
Erratum [PRC 109, 059901 \(2024\)](#)

2011 EM1.8/2.0: K. Hebeler et al. [Phys. Rev. C 83, 031301\(R\)](#)

NN (SRG-evolved) + bare 3NF, 元はmatterの計算に関する論文
→ 後にmagic interactionと呼ばれるように。

2017 中重核の系統的なIM-SRG計算:

J. Simonis et al. [Phys. Rev. C 96, 014303](#)

2020 NN+3NF (lnl) ※local-nonlocalの略

V. Soma et al. [Phys. Rev. C 101, 014318](#) ⇨

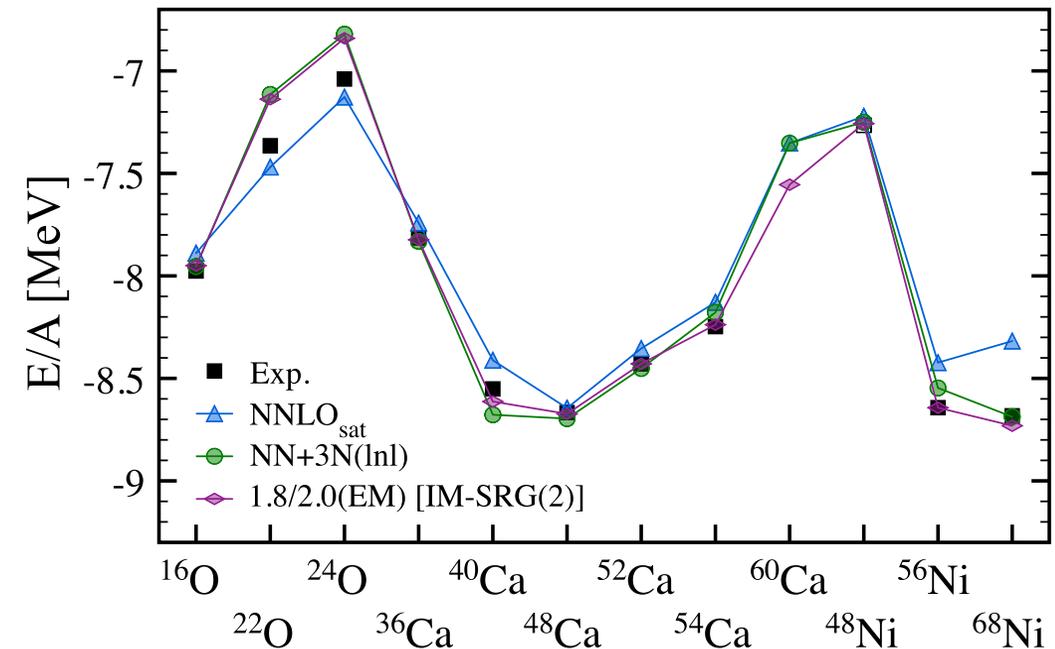
2015~2020 「Saturation propertyが重要」

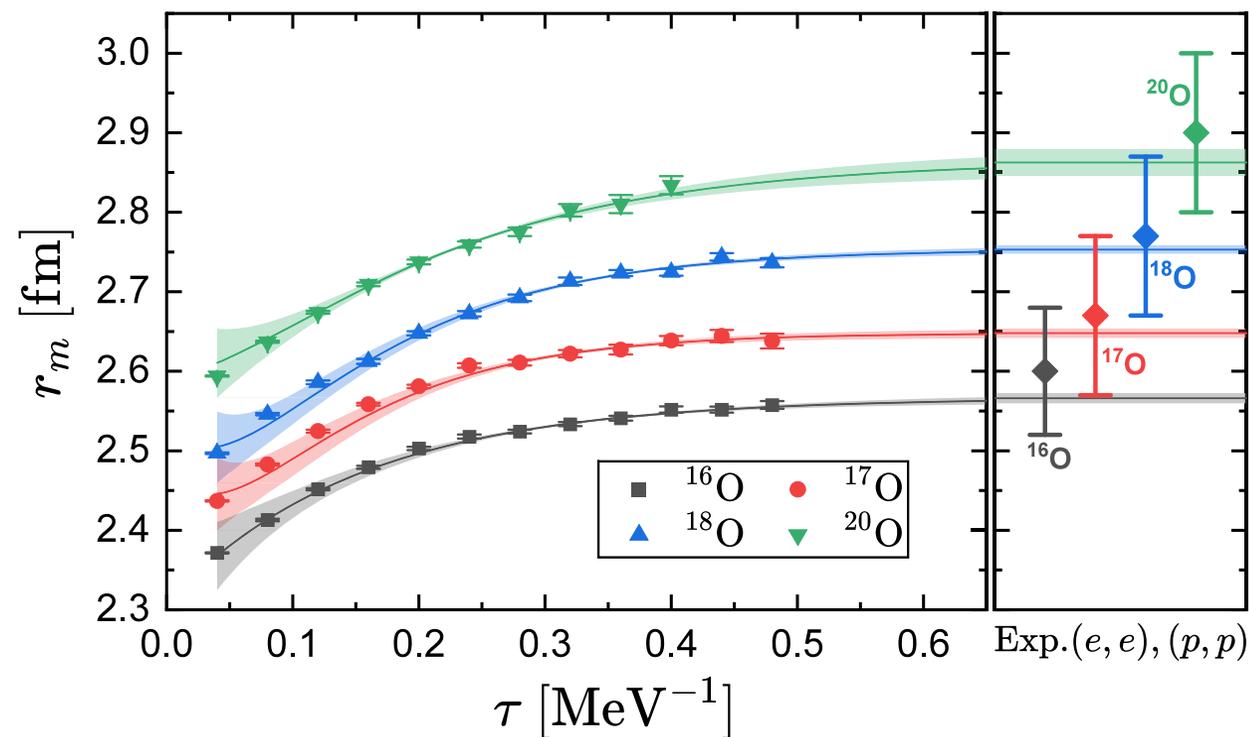
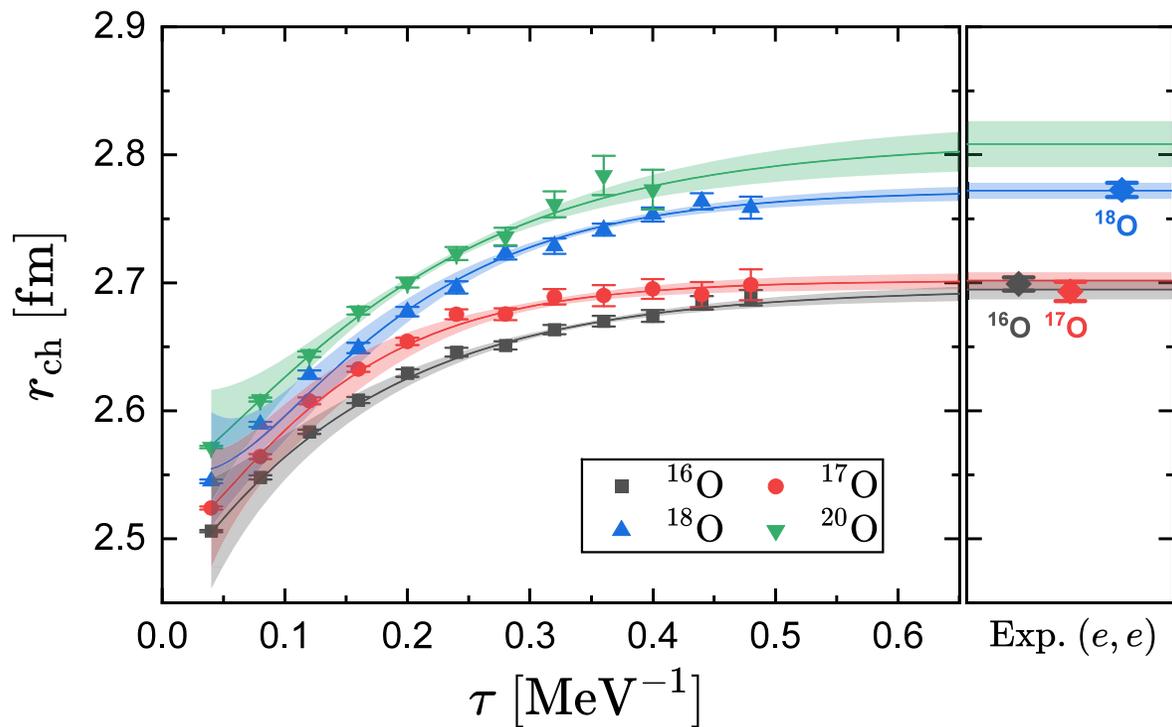
→ 2020~ 「3NFのnon-local regulatorが重要」

	Two-nucleon force	Three-nucleon force	Four-nucleon force
LO (Q^0)		—	—
NLO (Q^1)		—	—
N^2 LO (Q^2)			—
N^3 LO (Q^3)			
N^4 LO (Q^4)			

FIGURE 2 | Hierarchy of nuclear forces at increasing orders in chiral expansion in the Weinberg scheme. Solid and dashed lines refer to nucleons and pions, respectively. Solid dots, filled circles, filled squares, filled diamonds, and open squares refer to vertices from the Lagrangian in Equation (1) of dimension $\Delta = 0, 1, 2, 3,$ and 4, respectively.

E. Epelbaum [Front. Phys. 8:98](#).





- 酸素同位体の荷電半径を説明& ^{20}O の予言
 “A challenge for Nuclear forces” [PRL117, 052501 \(2016\)](#)
- matter radiusの測定に言及できる精度
 ※ e/p弾性散乱 vs I/CC

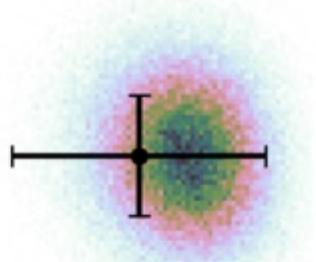
	^{16}O	^{17}O	^{18}O	^{20}O
r_{ch} [NLEFT]	2.704(17)	2.709(15)	2.768(17)	2.810(32)
Exp. (e, e)	2.699(5)	2.693(8)	2.776(2)	
r_m [NLEFT]	2.576(17)	2.651(14)	2.744(19)	2.863(33)
Exp. (e, e), (p, p)	2.60(8)	2.67(10)	2.77(10)	2.90(10)
Exp. σ_I	2.54(2)	2.59(5)	2.61(8)	2.69(3)
Exp. σ_{cc}	2.57(2)		2.64(8)	2.71(3)

c.f. wavefunction matching [Nature volume 630, pages59–63 \(2024\)](#)

Uncertainty quantification (UQ) /不定性評価

- 相互作用由来の統計誤差
- EFT truncation, many-body trunc.
- etc.

理論の予測は"点"から、これまで蓄積した知識を反映した分布(信頼区間)へ



B. D. Carlsson et al. [Phys. Rev. X 6, 011019 \(2016\)](#)

Surrogate models/Emulators

UQには、 10^4 通りのinputなど異なるsetupで計算する必要がある

high-fidelityな計算方法で、
~1%のerrorを許してでも
3-5桁の高速化がしたい

代表例:

- Eigenvector continuation
≡ Reduced basis methods
T. Duguet et al.

[Rev. Mod. Phys. 96, 031002 \(2024\)](#)

- Data-driven approaches (e.g. ML)

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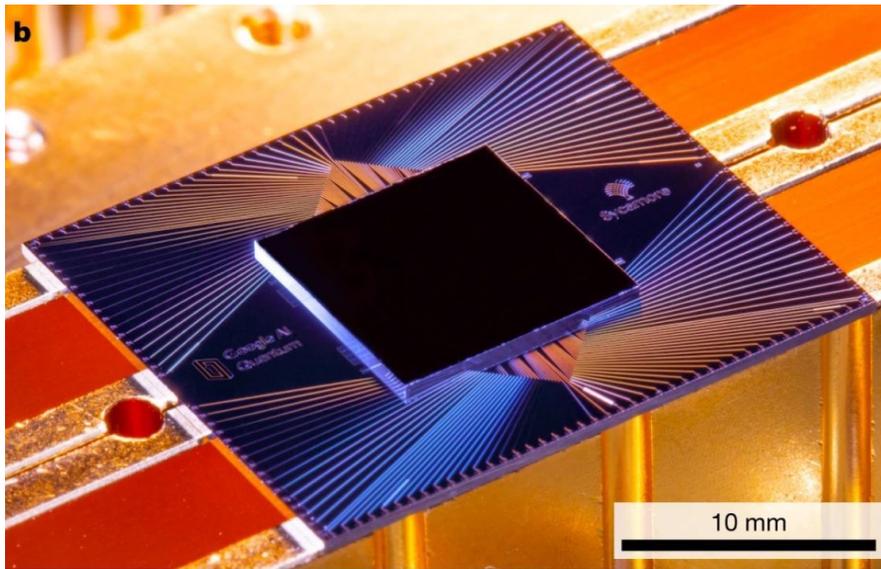
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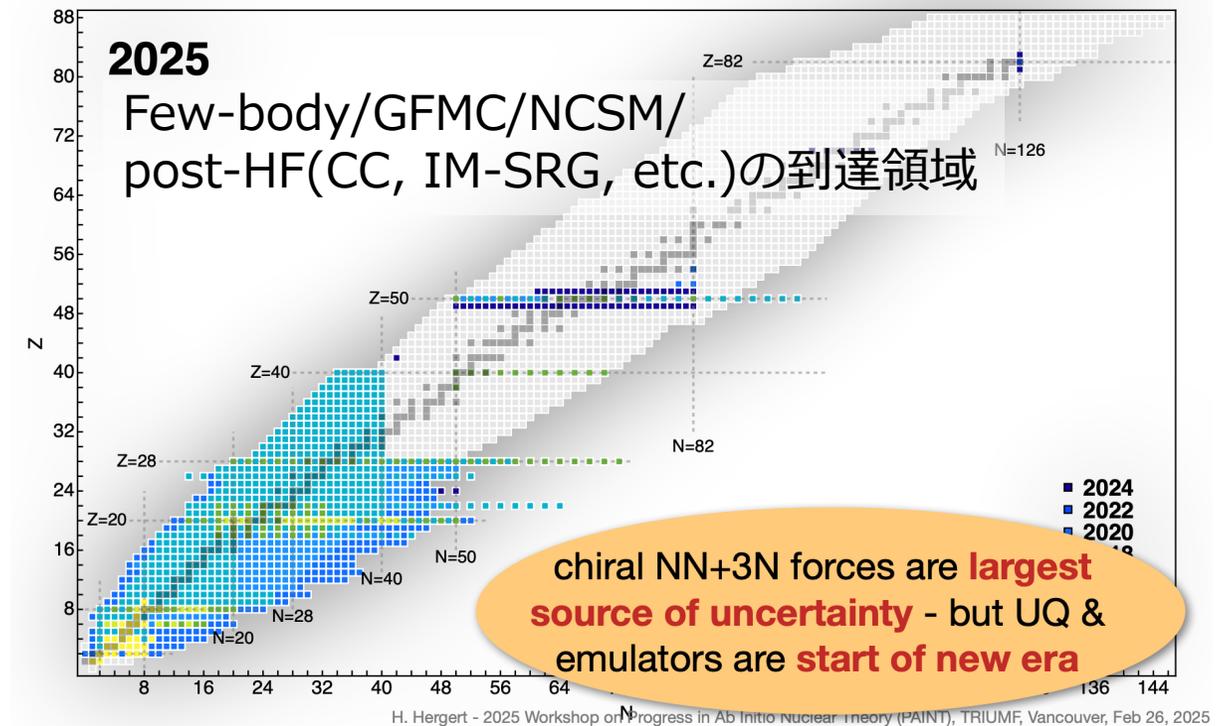
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量子計算機は、核構造・反応計算の到達領域・理解を塗り替えるか？



Google team, Nature 574 505 (2019)



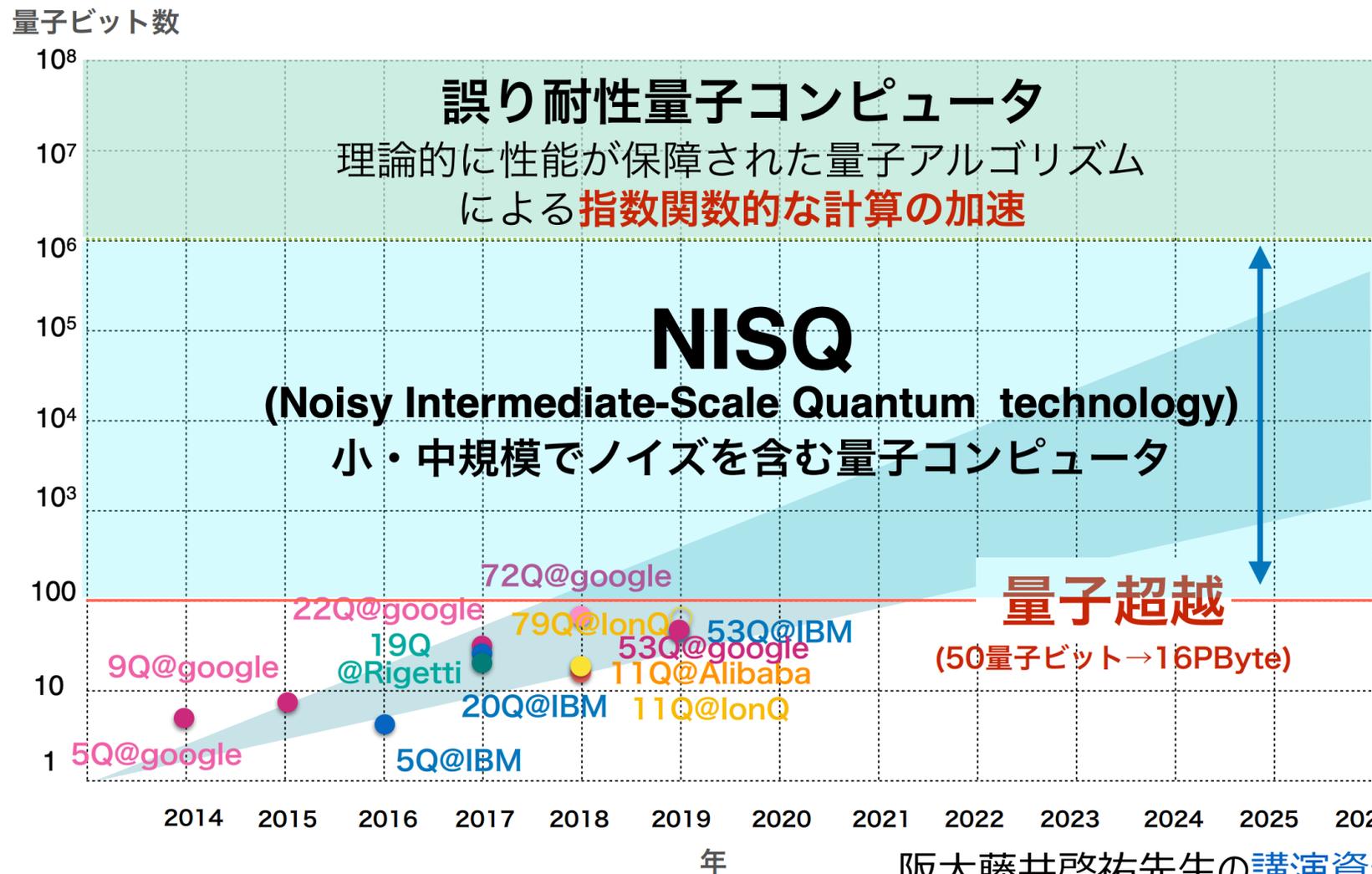
Courtesy of H. Hergert, [PAINT2025](#)

私の立場は「現状まだ分からないが、分野として誤り訂正を有した量子計算機の到来に備えておくべきであろう」

NISQからFTQCへ

NISQ = Noisy Intermediate-Scale Quantum device

FTQC = Fault-Tolerant Quantum Computer

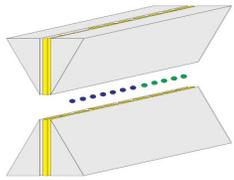


How to realize qubits

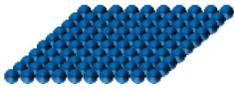
atoms

electron superconducting loops & controlled spin

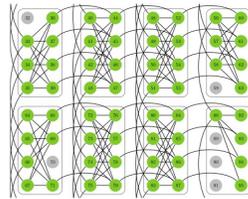
photons



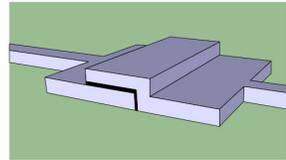
trapped ions



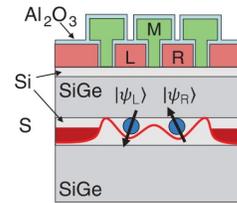
cold atoms



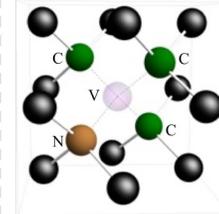
annealing



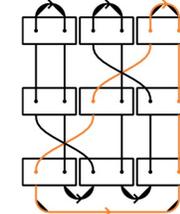
super-conducting



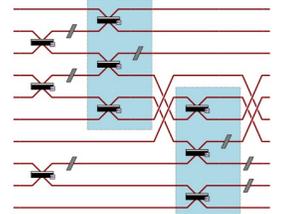
silicon



vacancies



topological



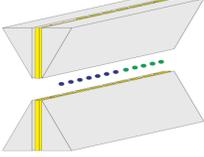
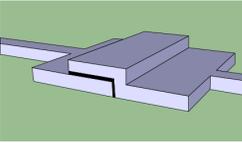
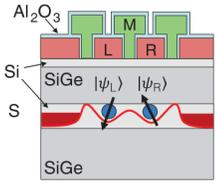
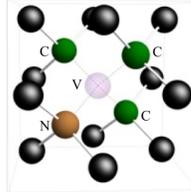
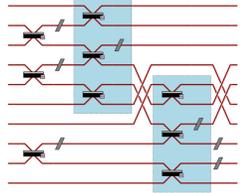
photons



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

Note: may be outdated due to extremely rapid development of technology and market

Major qubit types

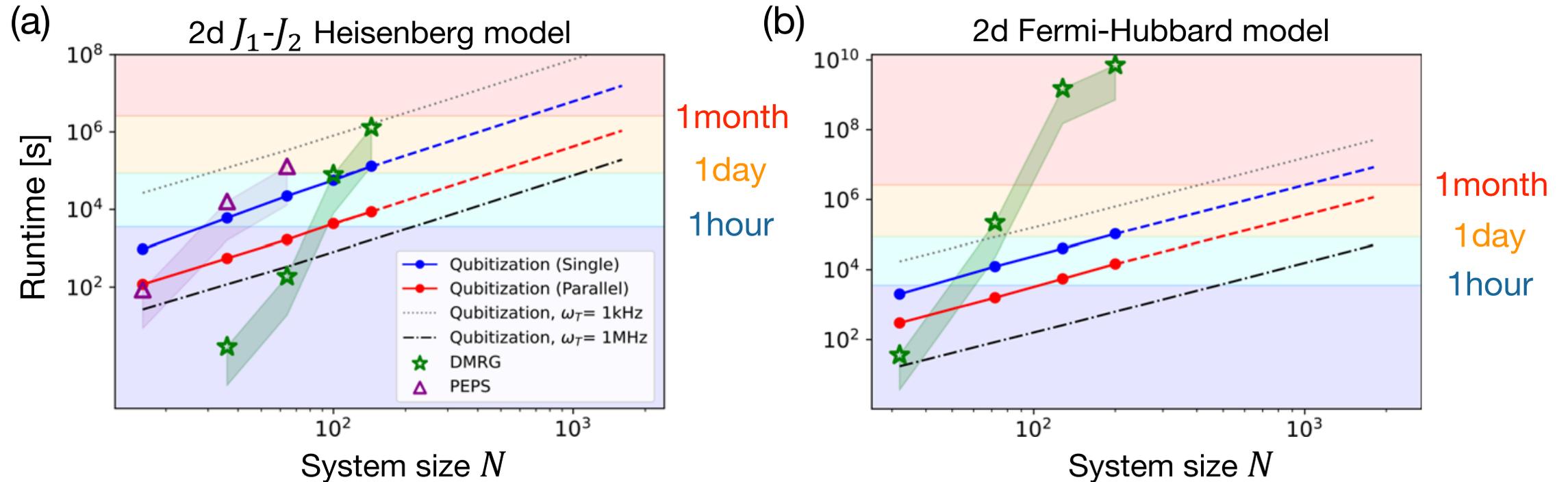
	atoms		electrons superconducting & spins			photons
						
	cold atoms	trapped ions	superconducting	silicon	NV centers	photons
qubit size	about 1 μm space between atoms	about 1 μm space between atoms	$(100\mu)^2$	$(100\text{nm})^2$	$<(100\text{nm})^2$	nanophotonics waveguides lengths, MZI, PBS, etc
best two qubits gates fidelities	99.5%	99.94%	99.68% (IBM Egret 33 qubits)	>99% (SiGe)	99.2%	98%
best readout fidelity	95%	99.99%	99.4%	99% (SiGe)	98%	50%
best gate time	≈ 1 ns	0.1 to 4 μs	20 ns to 300 ns	≈ 5 μs	10-700 ns	<1 ns
best T_1	> 1 s	0,2s-10mn	100-400 μs	20-120 μs	2.4 ms	∞ & time of flight
qubits temperature	< 1mK 4K for vacuum pump	<1mK 4K cryostat	15mK dilution cryostat	100mK-1K dilution cryostat	4K to RT	RT 4K-10K cryostats for photons gen. & det.
operational qubits	1,180 (Atom Computing)	32 (IonQ and Quantinuum)	433 (IBM) 176 (China)	12 (Intel) in SiGe	5 (Quantum Brilliance)-10	216 modes GBS (Xanadu)
scalability	up to 10,000	<100	1000s	millions	100s	100s-1M

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

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

(CC) Olivier Ezratty

量子優位性が期待されるアプリケーションは？



Quantum Phase Estimation with “Qubitization”

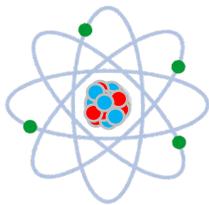
N. Yoshioka et al. [npj Quantum Info. 10, 45 \(2024\)](#)

計算量/計算理論としての優位性のほか、runtime上の優位性も重要

量子優位性の達成には、精緻なリソース推定&課題設計が不可欠

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)

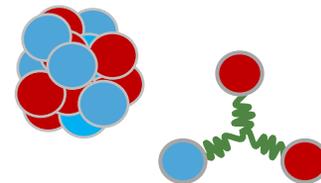
accurate but computationally demanding



Solve

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi$$

Nuclear physics:



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



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

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

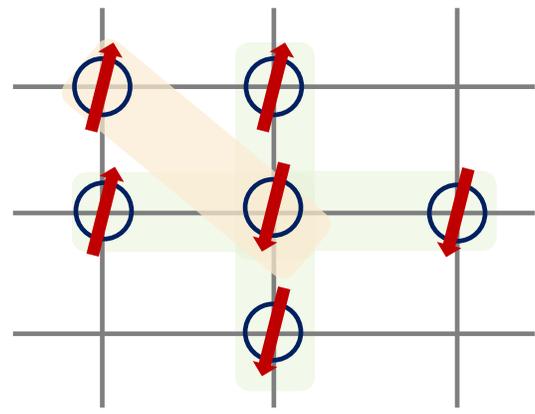
$$\text{HF} + \text{MP2} + \text{MP3} = -473.089 \text{ MeV}$$

(MP2 = -152.533, MP3 = -17.716)

$$\text{c.f. Energy (Exp.)} = -483.996 \text{ MeV}$$

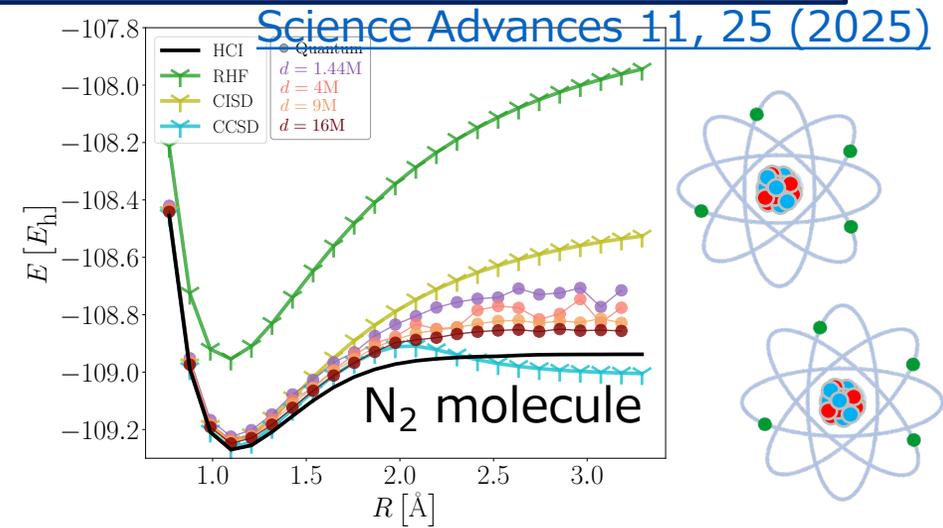
Similar discussion in a different way

Condensed matter (spin systems)



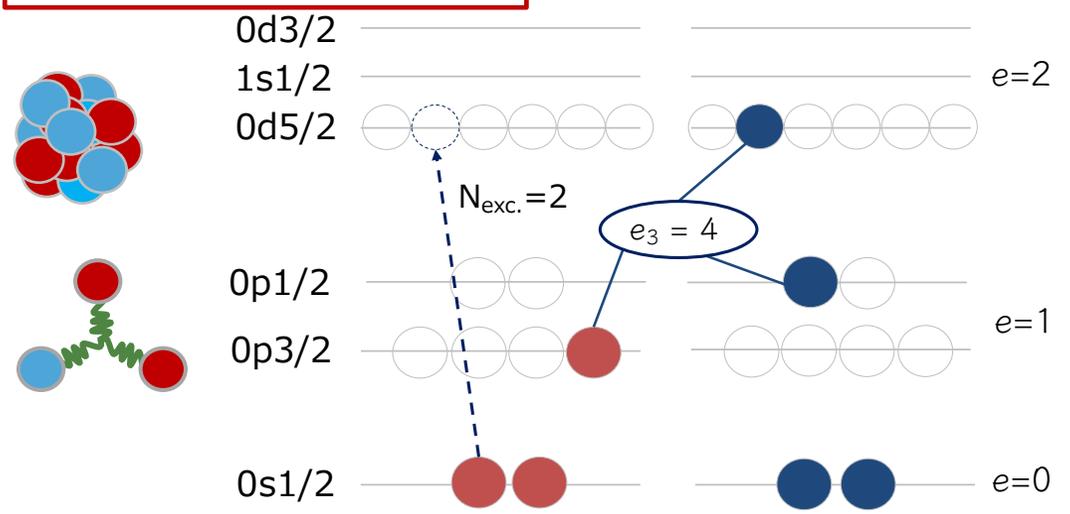
$$\hat{H} = -t \sum_{i,\sigma} \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{i+1,\sigma} + \hat{c}_{i+1,\sigma}^\dagger \hat{c}_{i,\sigma} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Chemistry (electronic system)



$$\hat{H} = E_0 + \sum_{pr\sigma} h_{pr} \hat{a}_{p\sigma}^\dagger \hat{a}_{r\sigma} + \sum_{prqs\sigma\tau} \frac{(pr|qs)}{2} \hat{a}_{p\sigma}^\dagger \hat{a}_{q\tau}^\dagger \hat{a}_{s\tau} \hat{a}_{r\sigma}$$

Nuclear system

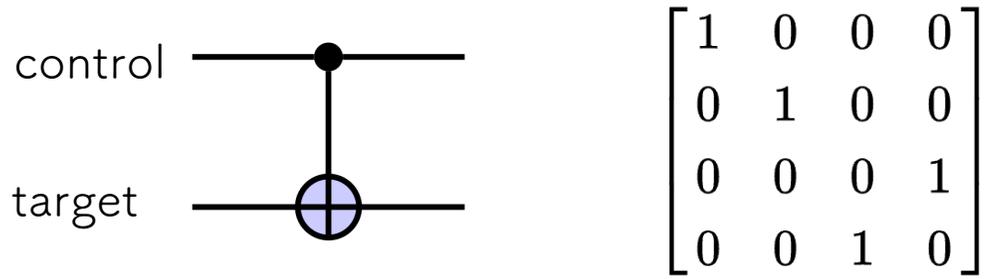


- almost all-to-all connectivity
- proton/neutron dof.
- Three Nucleon Force

ボトルネックとなる量子ゲート

NISQ \Rightarrow 2-qubit ゲート (例: CNOT)

If control qubit is $|1\rangle$, apply NOT on target



on $|00\rangle, |01\rangle, |10\rangle, |11\rangle$



1000 CNOTs in your circuit?

Even with "three-nine" accuracy... $(0.999)^{1000} \sim 0.37$ you will get noisy outcome!!

FTQC \Rightarrow 非-Clifford ゲート (典型的にはT-gate)

Arbitrary Rz rotation can be approximated by ~ 100 T-gates with $\varepsilon = 10^{-10}$

N.J. Ross and P. Selinger: [Quantum Information and Computation 16\(11-12\):901-953, 2016](#)

NISQ/FTQCのそれぞれの問題設定でリソース推定/検証が不可欠

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◆ 量子計算

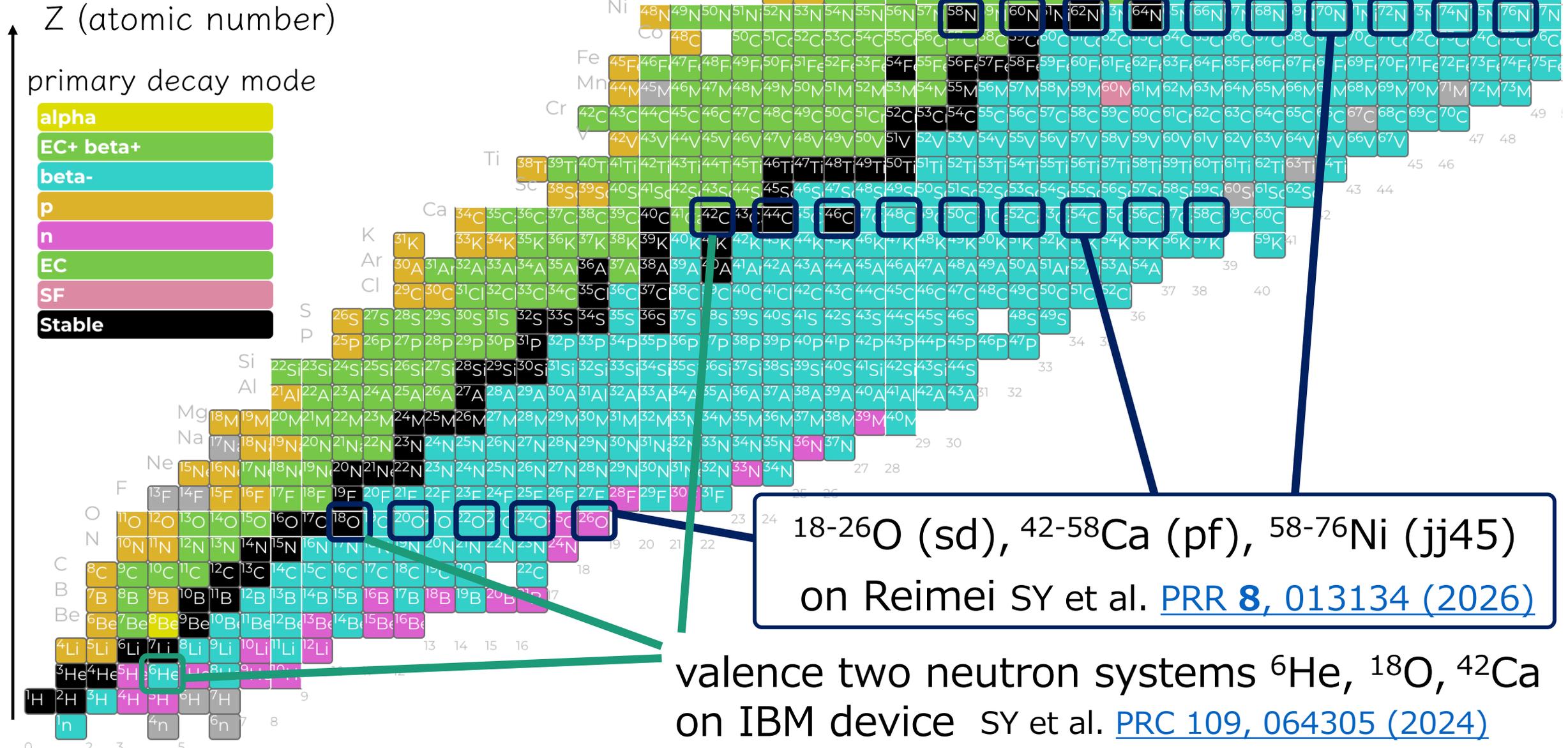
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Target: core + valence neutron system



殻模型計算の相互作用を使用
ラップトップでも10秒もあれば対角化できるが...

Q. より効率的な状態作成の方法はないか？

long-termの量子アルゴリズムでは、真の波動関数と overlap さえもっていれば、“やりよう”がある

Fermion自由度を $v=0$ pairの自由度に畳む

→ **DOCI**: ペア自由度の対角化

→ **pUCCD**: ペア自由度のCoupled Cluster

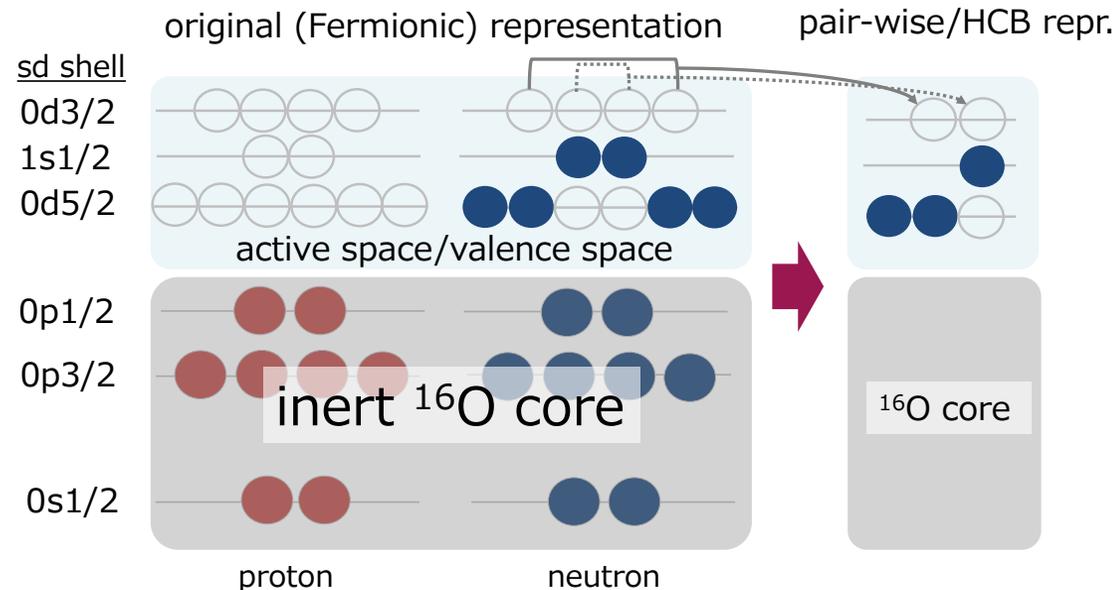
$$|\psi_{\text{pUCCD}}\rangle = \exp(T - T^\dagger) |\text{ref.}\rangle \equiv U |\text{ref.}\rangle$$

$$U = \exp \left[\sum_{hp} t_h^p (A_p^\dagger A_h - A_h^\dagger A_p) \right], \quad U_{\text{qubit}} = \exp \left[\sum_{p,q} \frac{it_h^p}{2} (X_p Y_h - Y_p X_h) \right],$$

$$\approx \prod_{p,h} \exp \left[\frac{it_h^p}{2} (X_p Y_h - Y_p X_h) \right].$$

↑ ペアのp-h励起

c.f. 電子系ではspin up/downをpairにとる

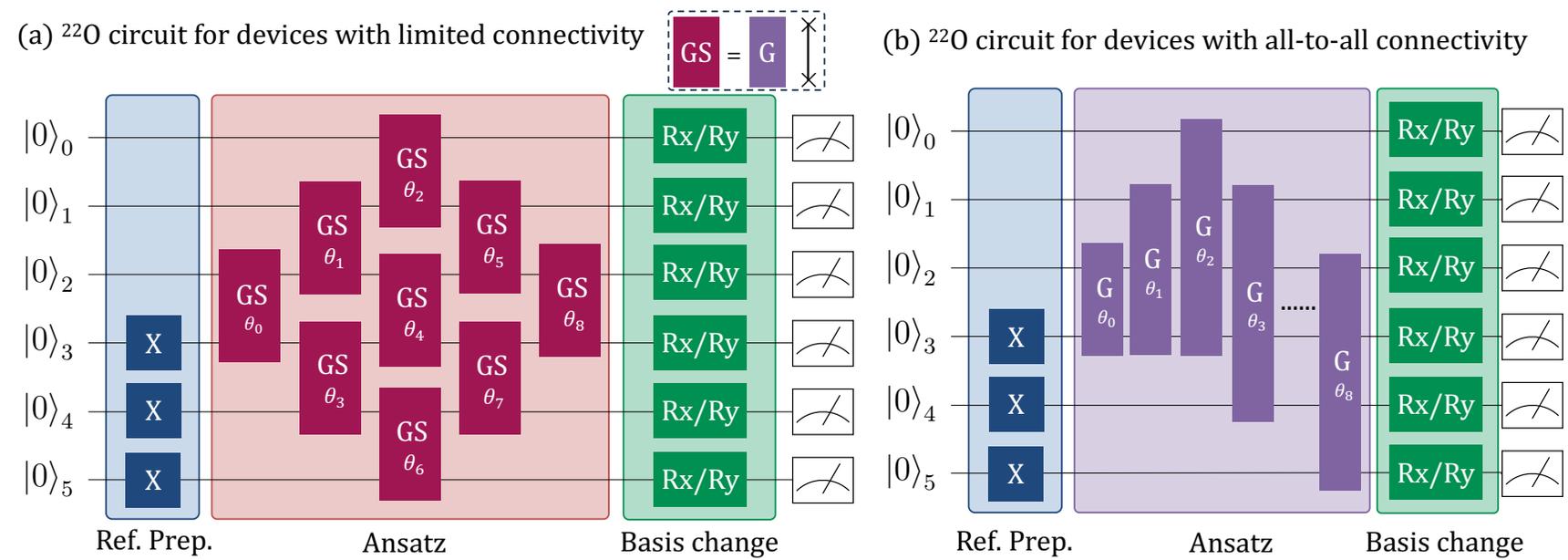


Nucleus	N_q	Dimensions			
		Fermionic/HCB	FCI	UCCD ($v=0$)	pUCCD
$^{18}\text{O}, ^{26}\text{O}$	12/6		14	5	5
$^{20}\text{O}, ^{24}\text{O}$			81	14	8
^{22}O			142	19	9
$^{42}\text{Ca}, ^{58}\text{Ca}$	20/10		30	9	9
$^{44}\text{Ca}, ^{56}\text{Ca}$			565	44	16
$^{46}\text{Ca}, ^{54}\text{Ca}$			3952	119	21
$^{48}\text{Ca}, ^{52}\text{Ca}$			12 022	209	24
^{50}Ca			17 276	251	25
$^{58}\text{Ni}, ^{76}\text{Ni}$	22/11		19	10	10
$^{60}\text{Ni}, ^{74}\text{Ni}$			365	54	18
$^{62}\text{Ni}, ^{72}\text{Ni}$			3103	164	24
$^{64}\text{Ni}, ^{70}\text{Ni}$			12 240	329	28
$^{66}\text{Ni}, ^{68}\text{Ni}$			23 884	461	30

≡ DOCI

Pair Unitary Coupled Cluster Doubles (pUCCD)

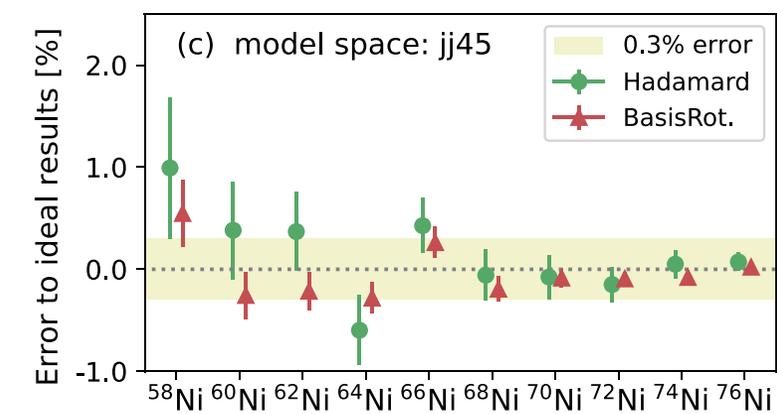
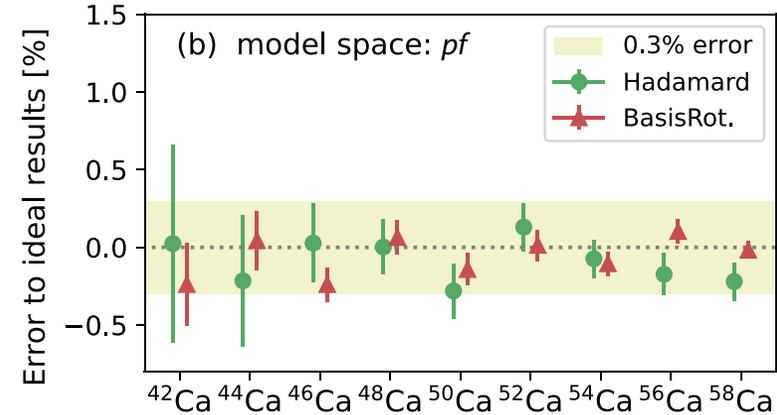
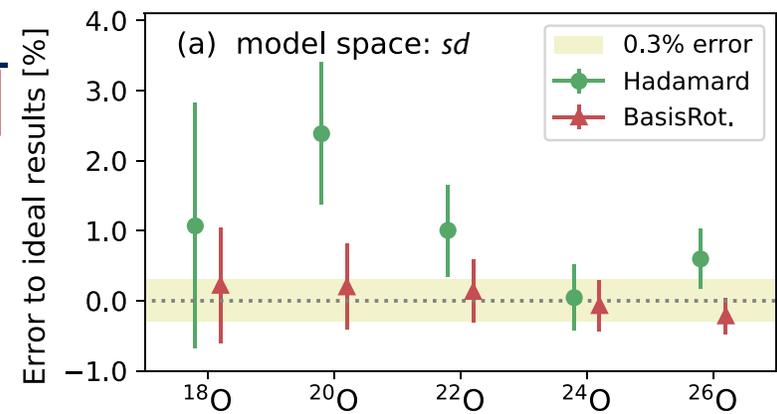
例: ^{22}O をsd shellで考える... 12軌道に6バレンス中性子 \Rightarrow 6ペア軌道に3ペア占有



- particle-hole間の励起は上のような $N_p \times N_h$ 個のGivens rotationで表現
 - ※ connectivity(超伝導方式)を意識した、最近接量子ビットの演算のみ
 - 右は、all-to-all (イオンラップ)で実行可能な回路
- 回路のパラメータ \equiv CC amplitudesは古典最適化済 (量子でも可能)

理研&Quantinuum 黎明での結果

Nuclide	Ideal pUCCD	Hadamard → <XX>測定	<XX+YY>を対角化する基底変換
¹⁸ O	-11.932	-11.802 (1.1 × 10 ⁰ %)	-11.893 (3.3 × 10 ⁻¹ %)
²⁰ O	-22.939	-22.383 (2.4 × 10 ⁰ %)	-22.854 (3.7 × 10 ⁻¹ %)
²² O	-33.924	-33.560 (1.1 × 10 ⁰ %)	-33.829 (2.8 × 10 ⁻¹ %)
²⁴ O	-41.021	-40.985 (8.8 × 10 ⁻² %)	-41.027 (1.5 × 10 ⁻² %)
²⁶ O	-40.869	-40.613 (6.3 × 10 ⁻¹ %)	-40.940 (1.8 × 10 ⁻¹ %)
⁴² Ca	-19.734	-19.727 (3.6 × 10 ⁻² %)	-19.775 (2.1 × 10 ⁻¹ %)
⁴⁴ Ca	-38.462	-38.540 (2.0 × 10 ⁻¹ %)	-38.424 (9.9 × 10 ⁻² %)
⁴⁶ Ca	-56.440	-56.414 (4.7 × 10 ⁻² %)	-56.565 (2.2 × 10 ⁻¹ %)
⁴⁸ Ca	-73.556	-73.538 (2.5 × 10 ⁻² %)	-73.489 (9.1 × 10 ⁻² %)
⁵⁰ Ca	-84.921	-85.135 (2.5 × 10 ⁻¹ %)	-85.007 (1.0 × 10 ⁻¹ %)
⁵² Ca	-95.190	-95.038 (1.6 × 10 ⁻¹ %)	-95.149 (4.3 × 10 ⁻² %)
⁵⁴ Ca	-102.557	-102.622 (6.3 × 10 ⁻² %)	-102.648 (8.8 × 10 ⁻² %)
⁵⁶ Ca	-104.462	-104.620 (1.5 × 10 ⁻¹ %)	-104.325 (1.3 × 10 ⁻¹ %)
⁵⁸ Ca	-106.666	-106.885 (2.0 × 10 ⁻¹ %)	-106.668 (1.7 × 10 ⁻³ %)
⁵⁸ Ni	-21.447	-21.207 (1.1 × 10 ⁰ %)	-21.291 (7.3 × 10 ⁻¹ %)
⁶⁰ Ni	-40.961	-40.752 (5.1 × 10 ⁻¹ %)	-40.992 (7.4 × 10 ⁻² %)
⁶² Ni	-59.013	-58.703 (5.2 × 10 ⁻¹ %)	-59.015 (4.5 × 10 ⁻³ %)
⁶⁴ Ni	-75.687	-76.027 (4.5 × 10 ⁻¹ %)	-75.765 (1.0 × 10 ⁻¹ %)
⁶⁶ Ni	-91.059	-90.552 (5.6 × 10 ⁻¹ %)	-90.695 (4.0 × 10 ⁻¹ %)
⁶⁸ Ni	-105.237	-105.169 (6.5 × 10 ⁻² %)	-105.288 (4.8 × 10 ⁻² %)
⁷⁰ Ni	-118.215	-118.189 (2.2 × 10 ⁻² %)	-118.158 (4.8 × 10 ⁻² %)
⁷² Ni	-130.379	-130.511 (1.0 × 10 ⁻¹ %)	-130.397 (1.3 × 10 ⁻² %)
⁷⁴ Ni	-141.694	-141.565 (9.1 × 10 ⁻² %)	-141.715 (1.5 × 10 ⁻² %)
⁷⁶ Ni	-152.103	-151.986 (7.7 × 10 ⁻² %)	-152.054 (3.2 × 10 ⁻² %)



Ideal simulationの~0.1%精度で実機測定できている

※図の統計誤差はブートストラップで評価 [PRR 8, 013134 \(2026\)](#)

◆ カイラル核力に依拠した構造・反応計算の進展

◆ 量子計算

- 概要

- NISQ application SY et al. [PRR 8, 013134 \(2026\)](#)

- FTQCにむけたリソース推定/ソフトウェア開発



FTQCに向けたリソース推定のためのsetup

Model spaces: HO with emax truncation

- valence space: $p, sd, pf, sdpf, pfsdg, \dots$
- No core space: NN-only and NN+3NF

Quantum algorithms and counting rule:

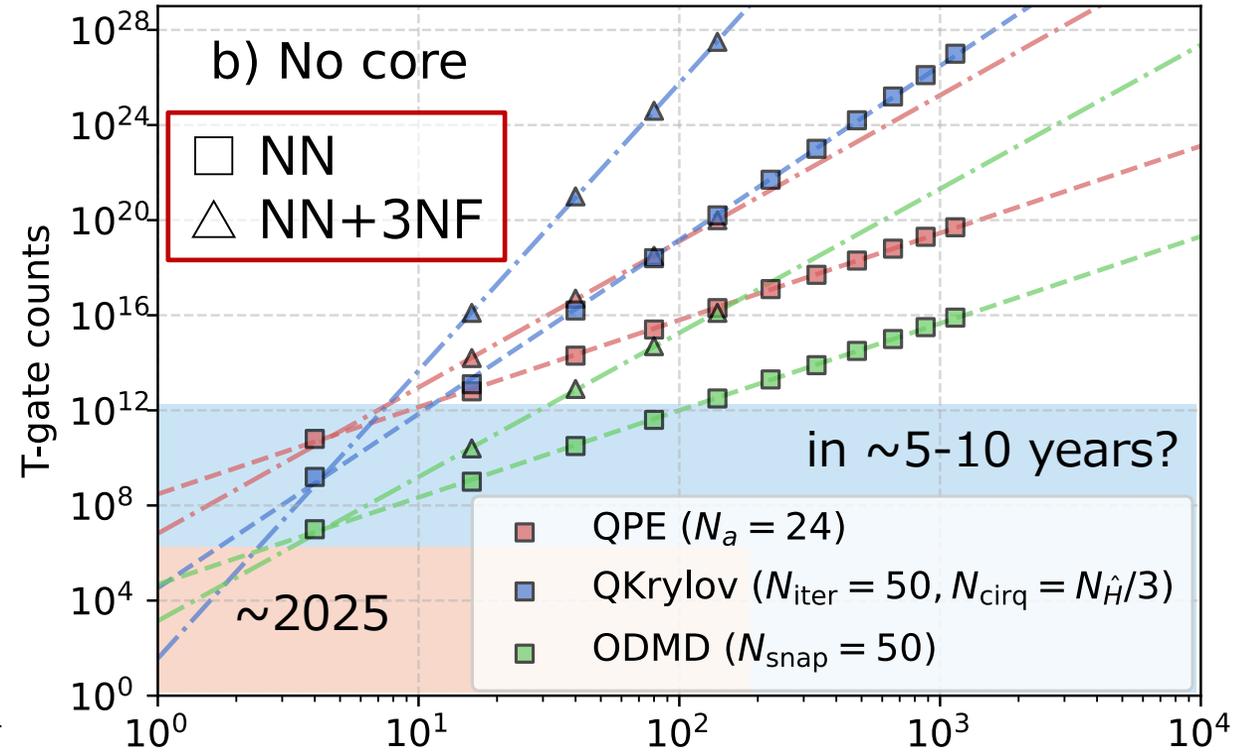
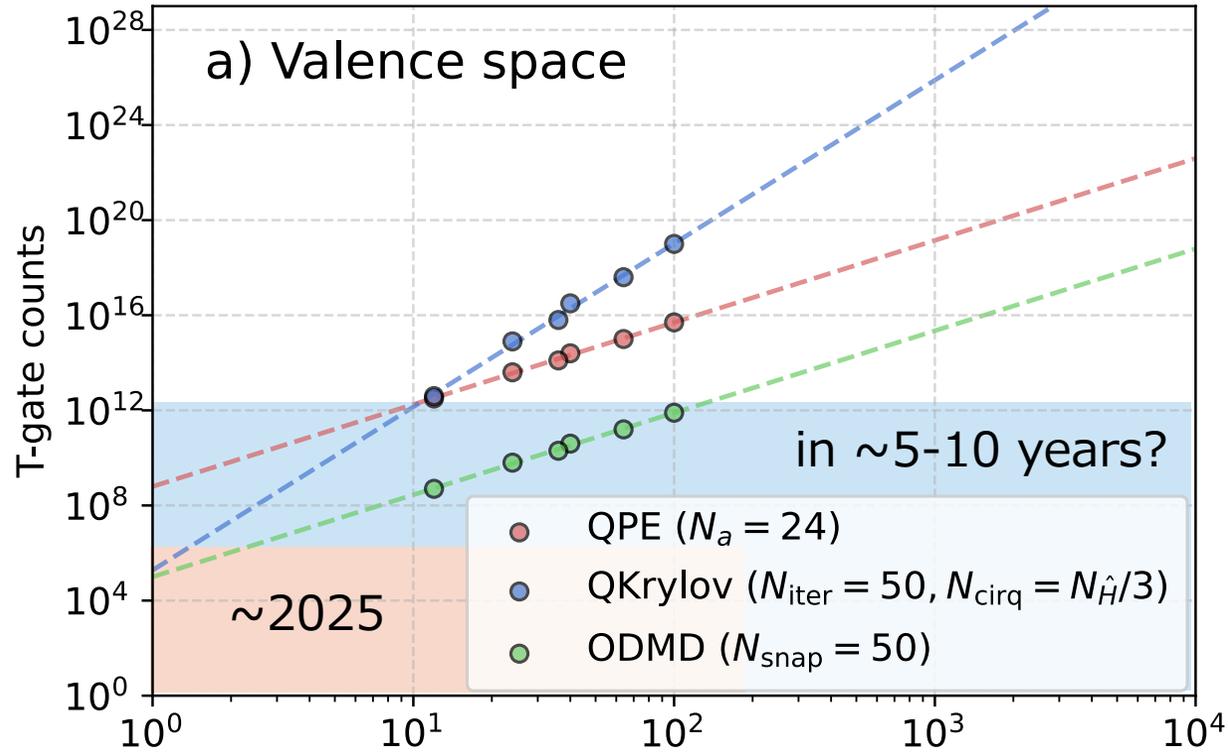
- (Early-)FTQC algorithms: QPE, QKrylov, Observable DMD
- Single Trotter controlled-unitaries
w/o any \doteq assuming all-to-all connectivity of qubits
- Toffoli (CCX) \Leftrightarrow 4 T-gates and $Rz \Leftrightarrow$ 100 T-gates

[PRA 87, 022328 \(2013\)](#)

[Quant. Info. Comp. 16\(11-12\):901-953, 2016](#)

For NISQ application (valence shell model with Adapt-VQE +UCC),
please refer to the paper by Barcelona group [Sci. Rep. 13, 12291 \(2023\)](#)

Resource estimation for Nuclear CI w/ FTQC algorithms



横軸=qubit数: 1 粒子基底(調和振動子 $\{n, l, j, j_z, t_z\}$)の数

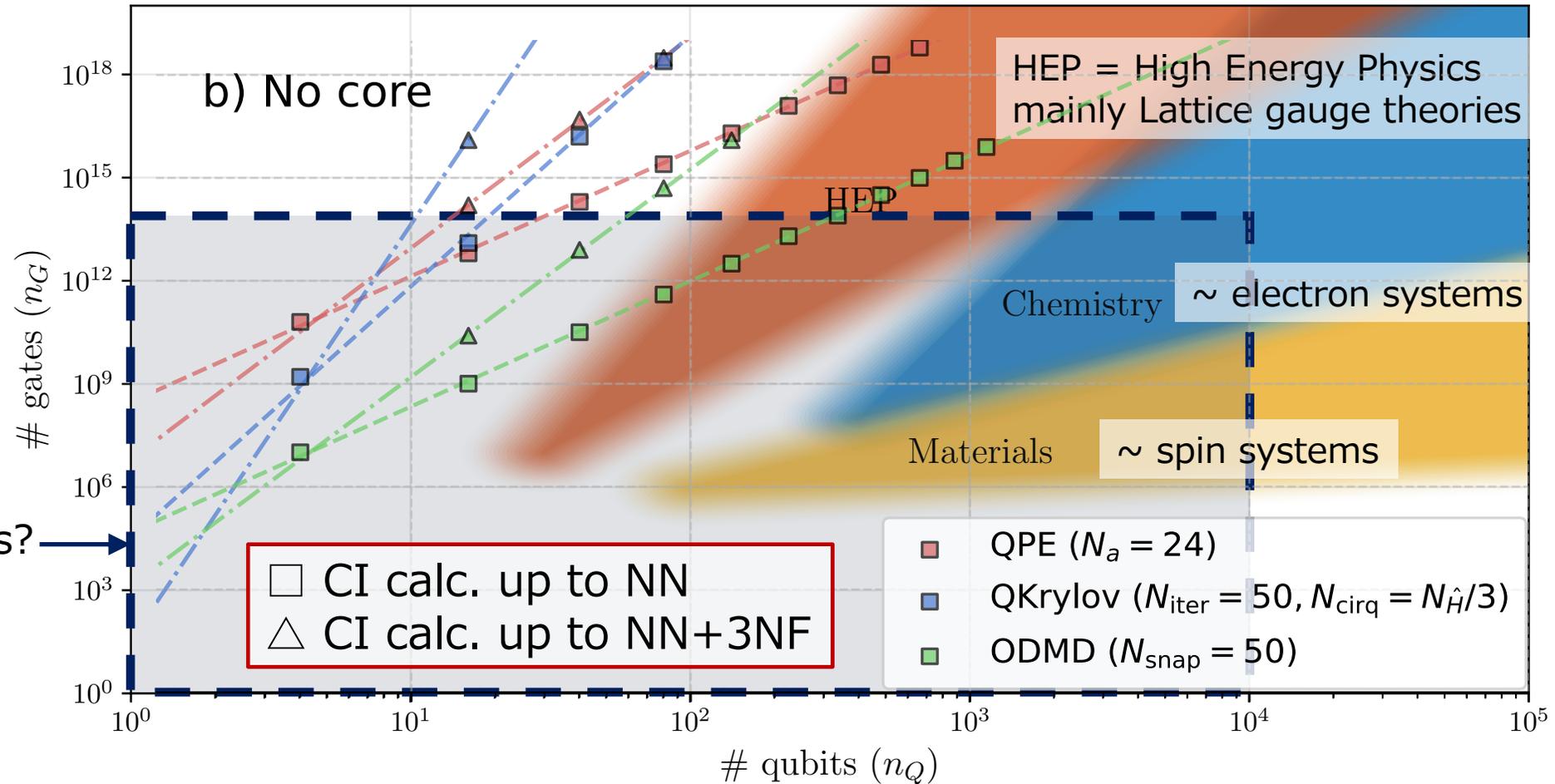
p	12 qubits	psd	36 qubits
sd	24 qubits	sdpf	64 qubits
pf	40 qubits	psfdg	100 qubits

- emax up to 10 (11 major shells)
- e3max = 3 × emax, up to e=4

N_a : ancilla qubits, N_{iter}/N_{snap} : 繰り返し回数, QKrylovはPauli stringのgroupingを考慮 (~1/3 reduction)

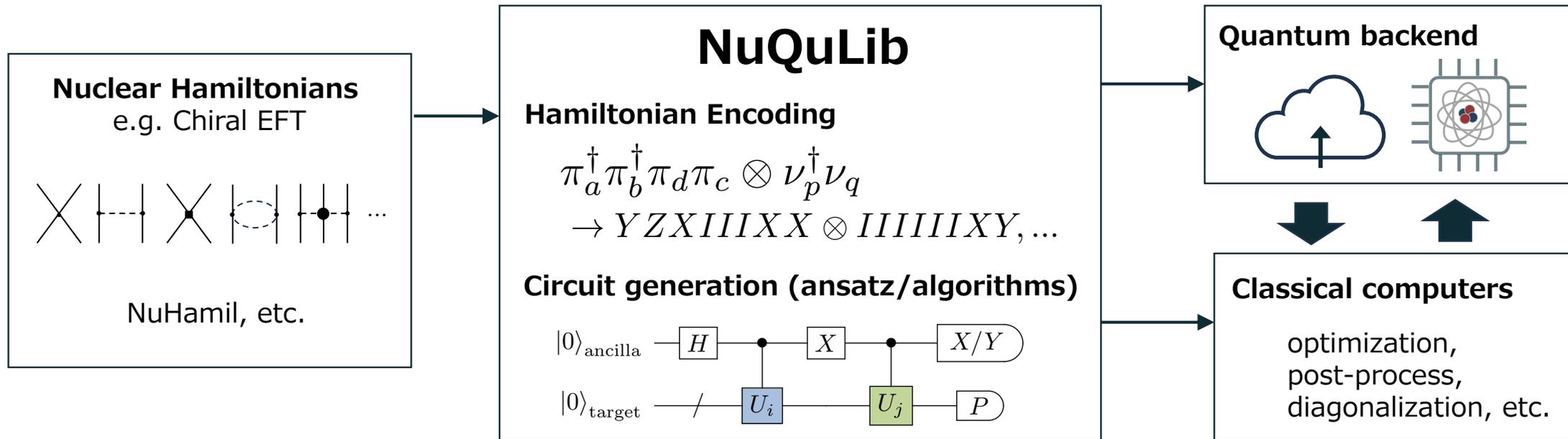
Resource estimation for Nuclear Structure Calc.

overlay on Figure in [arXiv: 2509.09882](https://arxiv.org/abs/2509.09882) NERSC@LBNL roadmap



異種フェルミオンの自由度/non-localityからくるリソース増大が顕著
ただし上の図は、conservative estimates (改善あるのみ)

SY, E.Rrapaj@LBNL, T.Miyagi@Tsukuba, A.Baroni@ORNL



- Hamiltonian encoding e.g. Chiral EFT NN/3NF
- Resource estimation for NISQ/E-FTQC/FTQC algorithms
- Circuits for VQE, QPE, QKrylov, ODMD, QSCI/SQD, etc.

まとめ

- 核力に依拠した構造・反応計算の到達領域の拡大・進展が進んでいる。
特に実験が難しい領域 (例: p/n-dripline, 超重) で、信頼に足る予言のため
不定性評価が不可欠だがpost-HF/CI計算などが律速 (c.f. emulators)
 - 量子計算機に寄せられる期待も大きい...要求リソースは極めて高い
 - ⇒ 核子系の強相関を手懐ける状態作成法 (古典計算の効率化にも)
 - ⇒ 原子核-tailoredな量子アルゴリズム
- NISQ/FTQCの両方の観点から、これらの探求が不可欠

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NuQuLib and resource estimation:

Ermal Rrapaj(LBNL), Takayuki Miyagi(Tsukuba), Alessandro Baroni(ORNL)

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MLPhyS 学術変革領域研究(A) 学習物理学の創成
Foundation of "Machine Learning Physics"

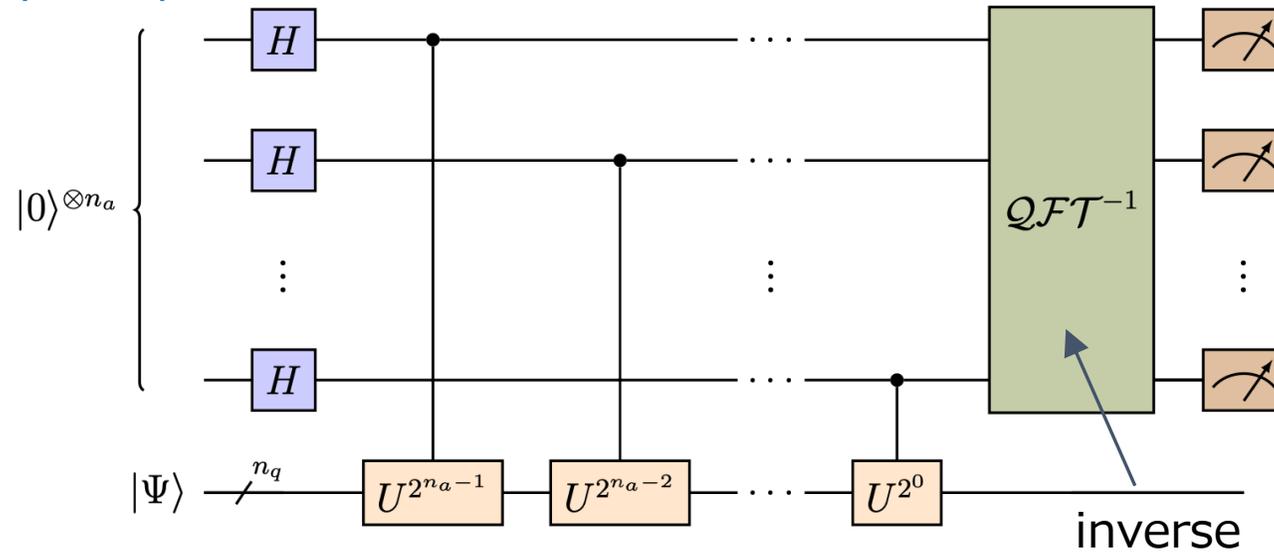


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Quantum Phase Estimation (QPE)/量子位相推定

AY Kitaev [arXiv:quant-ph/9511026](https://arxiv.org/abs/quant-ph/9511026)



inverse
Quantum Fourier Transform

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

系のHamiltonianで実時間発展。補助量子ビット(ancilla)に位相の情報をQFT⁺で埋め込んでEnergyを推定。精度は $\sim 2\pi/2^{n_a}$

Krylov subspace method

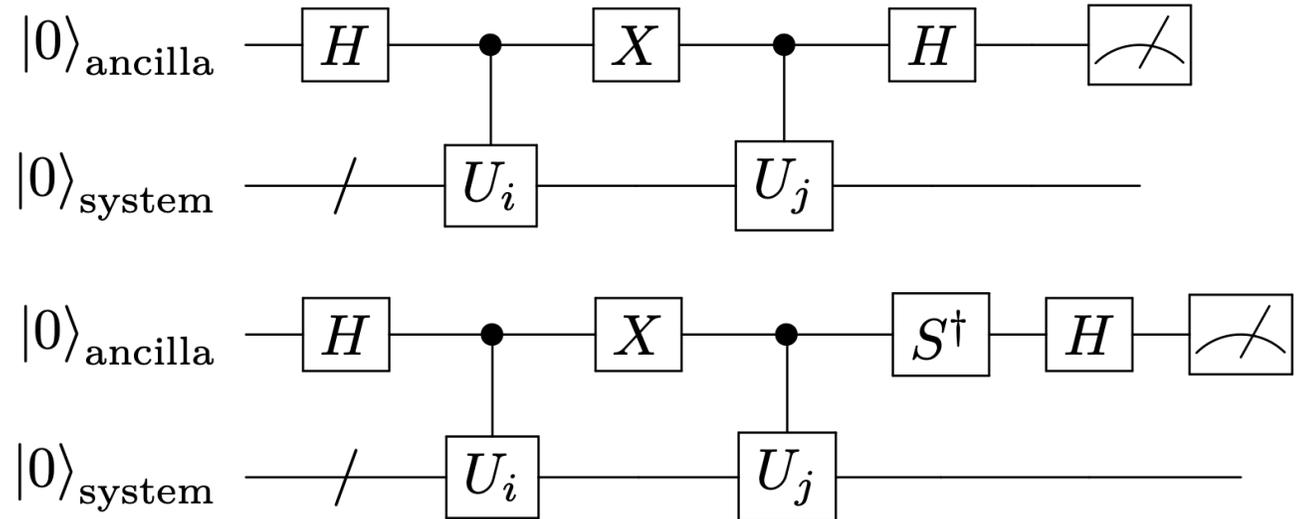
$$\mathcal{K}_m(H, |\psi\rangle) = \text{span}\{|\psi\rangle, H|\psi\rangle, H^2|\psi\rangle, \dots, H^{m-1}|\psi\rangle\}$$

$$|\Phi\rangle_0, e^{-iHt_1}|\Phi\rangle_0, \dots, e^{-iHt_M}|\Phi\rangle_0$$

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

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

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



Circuits for conventional QKrylov

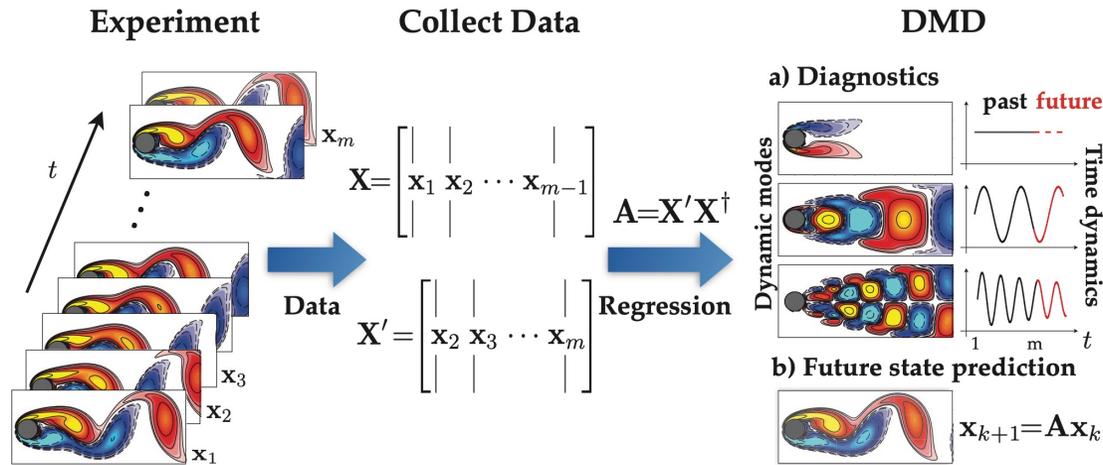
[Phys. Rev. A 105, 022417 \(2022\)](#)

PROS: Access to “wavefunctions” → many observables

CONS: cost to measure each H term is huge... especially in Nucl. Phys.

some variants (with less quantum resources) are available

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



To replace the time evolution by a linear map

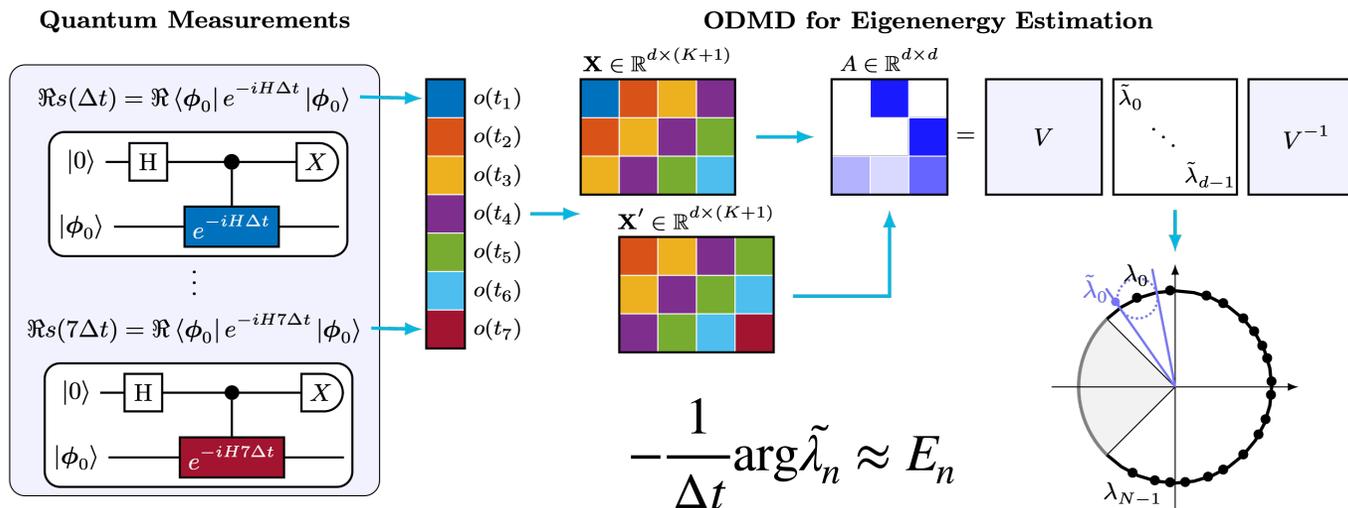
$$X \equiv \begin{pmatrix} | & & | \\ \mathbf{x}_1 & \cdots & \mathbf{x}_N \\ | & & | \end{pmatrix}, Y \equiv \begin{pmatrix} | & & | \\ \mathbf{x}_2 & \cdots & \mathbf{x}_{N+1} \\ | & & | \end{pmatrix}$$

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

$$A \approx YX^+ = Y(V_r \Sigma_r^{-1} U_r^\dagger)$$

$$\tilde{A} = U_r^\dagger A U_r \approx U_r^\dagger Y V_r \Sigma_r^{-1}$$

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 need only overlaps

c.f. Quantum Krylov

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

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