INPC-2025, Daejeon, 2025.5.30

Recent Progress in Machine Learning and Quantum Computing for Nuclear Physics Problems

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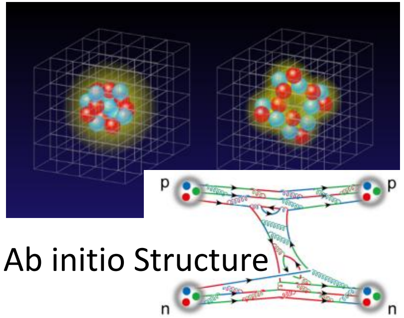
CONTENTS

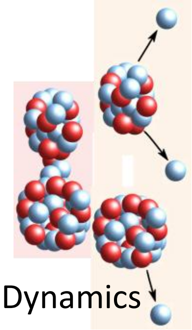
Computation and theoretical nuclear physics

- Close relationship between computational capabilities and nuclear physics



Ab initio Structure

Nuclear Astrophysics

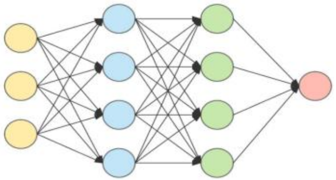


Nuclear Dynamics

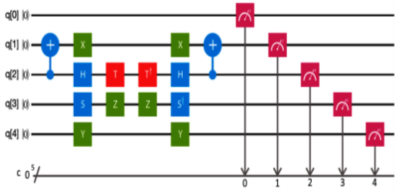
Support by advanced computing methodology

Supercomputing

Machine Learning

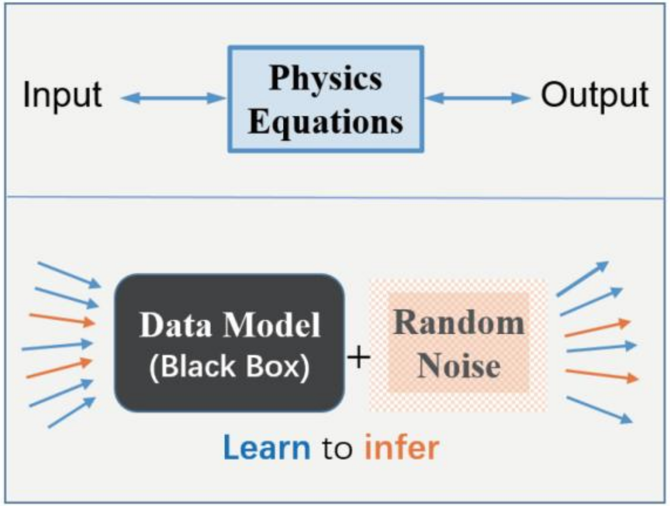


Quantum computing



Machine Learning: A new paradigm for science

- Data correlations vs. Physics equations
- Huge data, high-dimensional, imperfect, noisy, heterogenous data, sparse but rare data
- Inference of information and new physics from data



RMP

Colloquium: Machine learning in nuclear physics

Amber Boehnlein, Markus Diefenthaler, Nobuo Sato, Malachi Schram, Veronique Ziegler, Cristiano Fanelli, Morten Hjorth-Jensen, Tanja Horn, Michelle P. Kuchera, Dean Lee, Witold Nazarewicz, Peter Ostroumov, Kostas Orginos, Alan Poon, Xin-Nian Wang, Alexander Scheinker, Michael S. Smith, and Long-Gang Pang

Rev. Mod. Phys. **94**, 031003 (2022) - Published 8 September 2022

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• Invited Review •

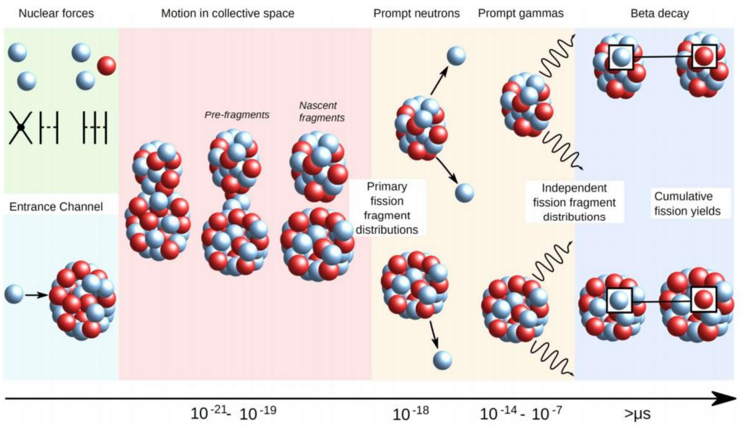
August 2023 Vol. 66 No. 8: 282001
https://doi.org/10.1007/s11433-023-2116-0

Machine learning in nuclear physics at low and intermediate energies

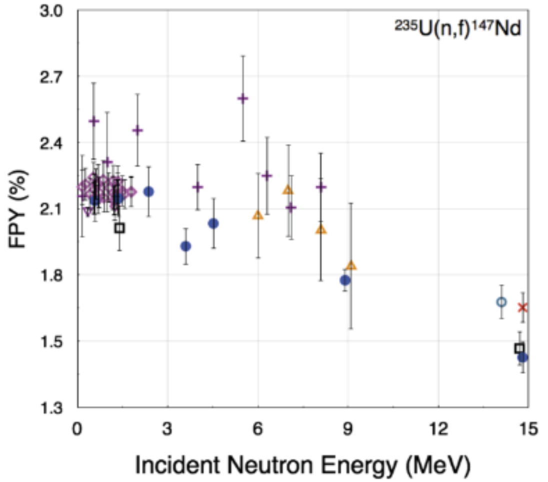
Wanbing He[1,2*], Qingfeng Li[3,4*], Yugang Ma[1,2*], Zhongming Niu[5*], Junchen Pei[6,7*], and Yingxun Zhang[8,9*]

Infer from imperfect nuclear data

- Fission yields are key nuclear data for applications
- Measured fission yields are usually noisy, discrepant, incomplete



M. Bender et al, J. Phys. G. 47 113002(2020)



M.E. Gooden et al., Nucl. Data Sheets 131, 319(2016)

Major evaluated nuclear data libs (ENDF, JENDL, JEFF, CENDL), only 3 energy points: thermal, 0.5 MeV and 14 MeV

Key issues： energy dependence； uncertainty propagation

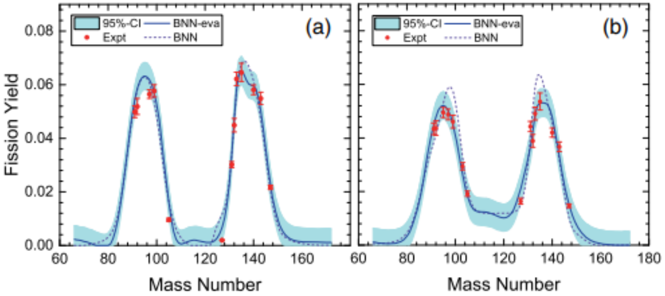
Bayesian Evaluation of fission yields

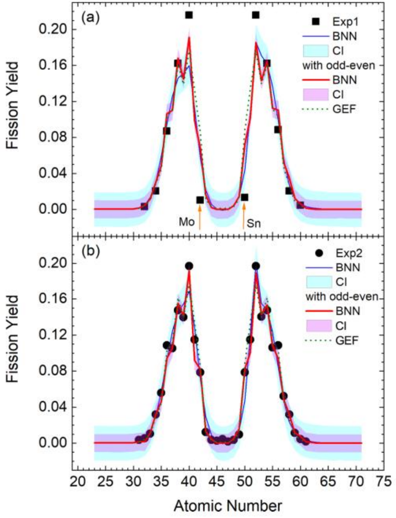
- Incomplete fission yields

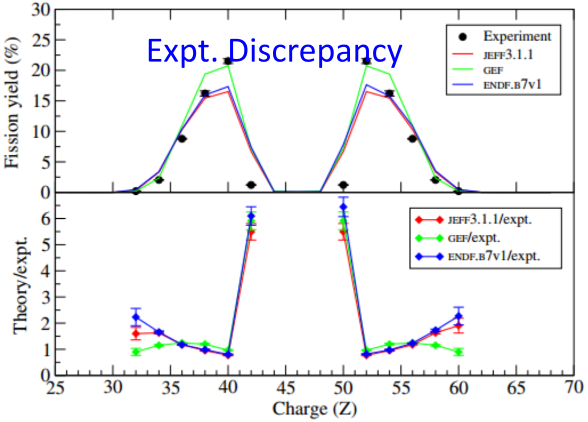
Z.A. Wang, J.C. Pei, Y. Liu, Y. Qiang
PRL **123**, 122501 (2019)

- Discrepant charge yields

C. Y. Qiao, J.C.Pei, et al., PRC 103, 034621 (2021)





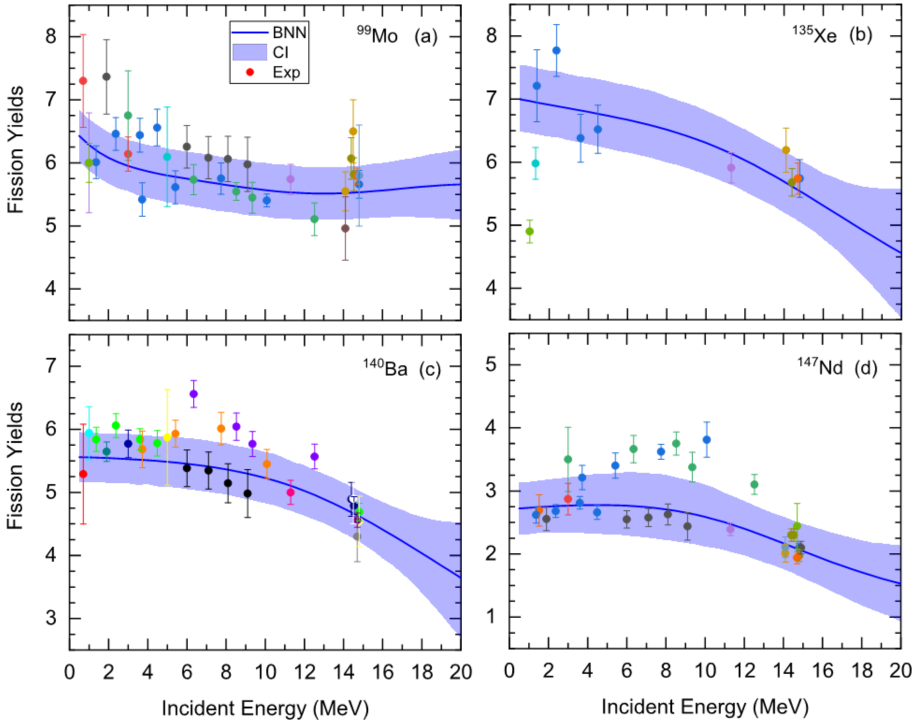


J. N. Wilson et al., Phys. Rev. Lett. 118, 222501(2017)
D. Ramos et al., Phys. Rev. Lett. 123, 092503(2019)

Bayesian Data Fusion

- Data fusion can obtain more comprehensive, useful and reliable information than separated data

Data Fusion of different experiments, evaluate yield-energy relations



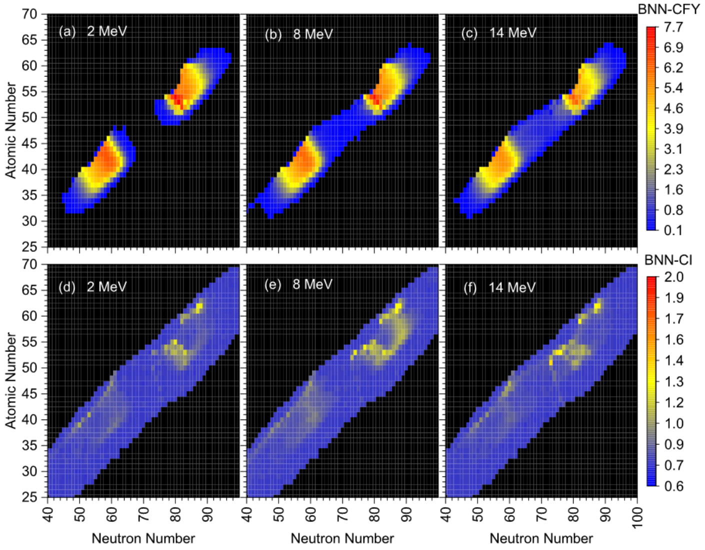
Z. A. Wang, J. C. Pei, Y. J. Chen, C. Y. Qiao, F. R. Xu, Z. G. Ge, and N. C. Shu， Phys. Rev. C 106, L021304 (2022)

- Uncertainties include global model uncertainties and local data uncertainties
- Exploit maximum values of raw and expensive nuclear data

Bayesian Data Fusion

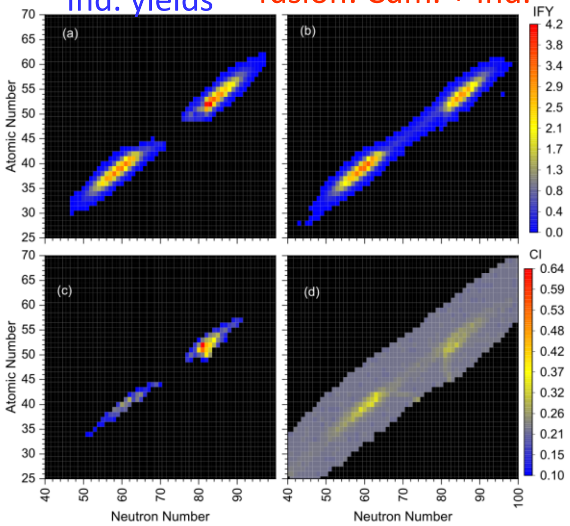
- Energy dependence of all fission fragments, for practical applications
- Cumulative yields have more data, independent yields have very few data

Cum. yields



Ind. yields

heterogeneous data fusion: Cum. + Ind.

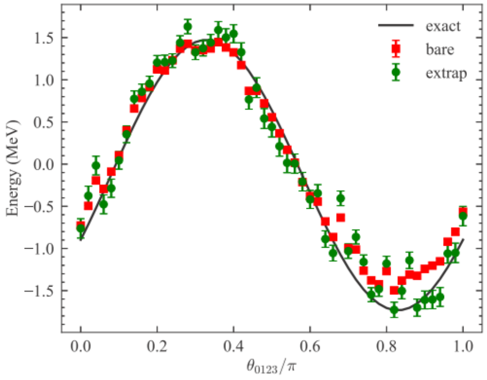


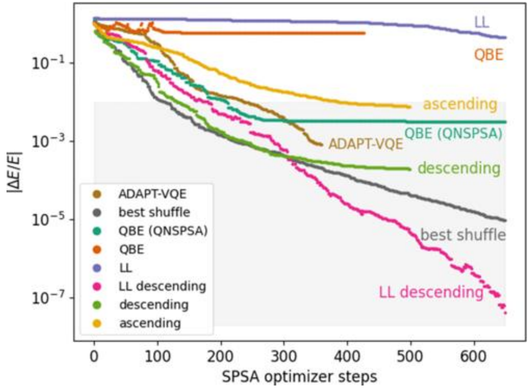
*Heterogeneous data fusion (HDF): when one kind data is sparse at some energies, it can benefit from energy dependence of other data via HDF

Quantum computing in nuclear physics

- Current status of quantum computing in nuclear physics

2018: Cloud Quantum Computing of an Atomic Nucleus, PRL 120, 210501
  VQE, unitary coupled-cluster, deuteron
2020: PRC 102, 064624 ---$n(p, d)\gamma$, time dependent evolution operator, error mitigation
2020: PRL 125, 230502---quantum-phase-estimate + symmetry projection
2021: PRA 104, 012611---Coulomb excitation of deuteron
2021: Phys. Rev. C 104, 024305---Lipkin model, VQE, error mitigation
2022: Phys. Rev. C 106, 024319 (2022).---Lipkin model, quantum EoM,
2022: Phys. Rev. C 106, 034325(2022)----^{6}Li, UCC, VQE
2022: I. Stetcu, A. Baroni, J. Carlson, Phys. Rev. C 105, 064308 (2022), UCC
2023: P. Lv, S. Wei, H.-N. Xie, G. Long, SCPMA 66, 240311 (2023).
2023: C.J.Jiang, J.Pei, finite-temperature pairing Hamiltonian, PRC 2023
2023. Shell model calculations, Sci. Rep. 13, 12291(2023)
2024: Scattering phase shifts, PRC 109, L061001(2024)
2025: Complex Scaling of Resonances, PLB 860(2025)139187



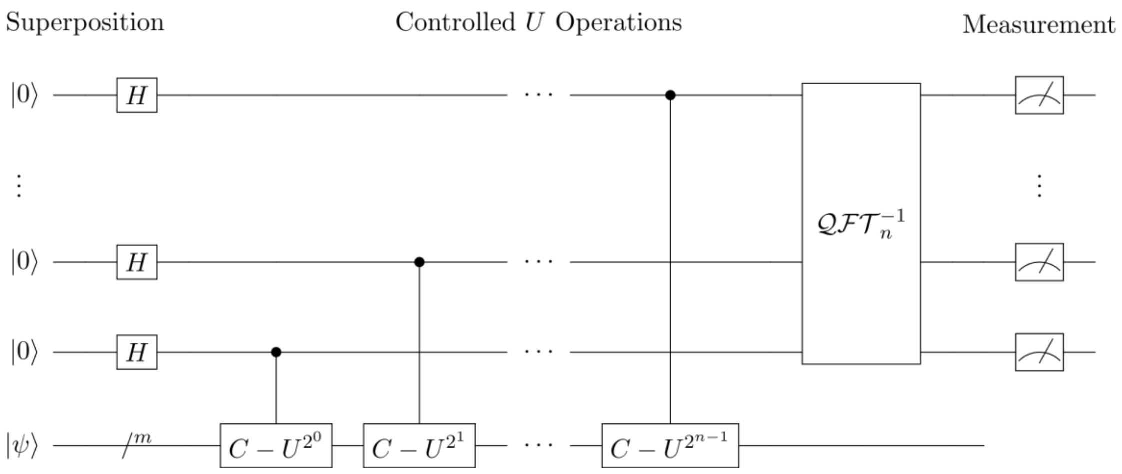


Quantum Computing for many-body systems

- **Quantum many-body problem**: exponential speedup (without noise)
- quantum fast Fourier transform to find eigenvalues and eigenvectors： Quantum Phase Estimate,

Phys. Rev. Lett. 83, 5162 （1999）

$$\hat{U}(t) = e^{-iHt} = (e^{-iH_1(t/m)}e^{-iH_2(t/m)}\cdots e^{-iH_k(t/m)})^m$$

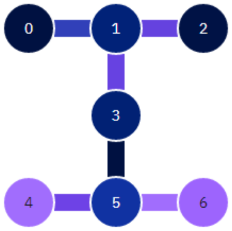


$$U = e^{iH\Delta t} \Rightarrow U|\Psi\rangle = e^{iE\Delta t}|\Psi\rangle = e^{i2\pi\phi}|\Psi\rangle; E = \frac{2\pi\phi}{\Delta t}$$

Quantum computing in real devices

ibm_oslo OpenQASM 3

7 Qubits	Status:	Online	Median CNOT Error:	8.556e-3
32 QV	Total pending jobs:	21 jobs	Median SX Error:	2.668e-4
2.6K CLOPS	Processor type ⓘ:	Falcon r5.11H	Median Readout Error:	2.080e-2
	Version:	1.0.21	Median T1:	184.43 us
	Basis gates:	CX, ID, RZ, SX, X	Median T2:	41.99 us

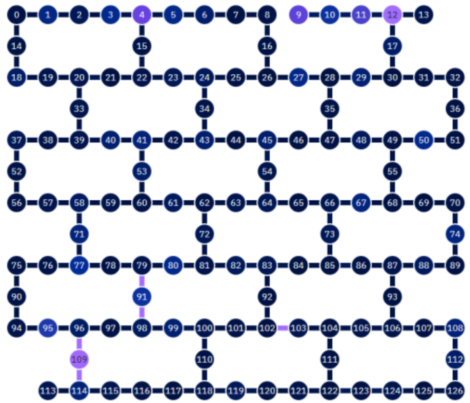


Not fully connected

ibm_washington OpenQASM 3

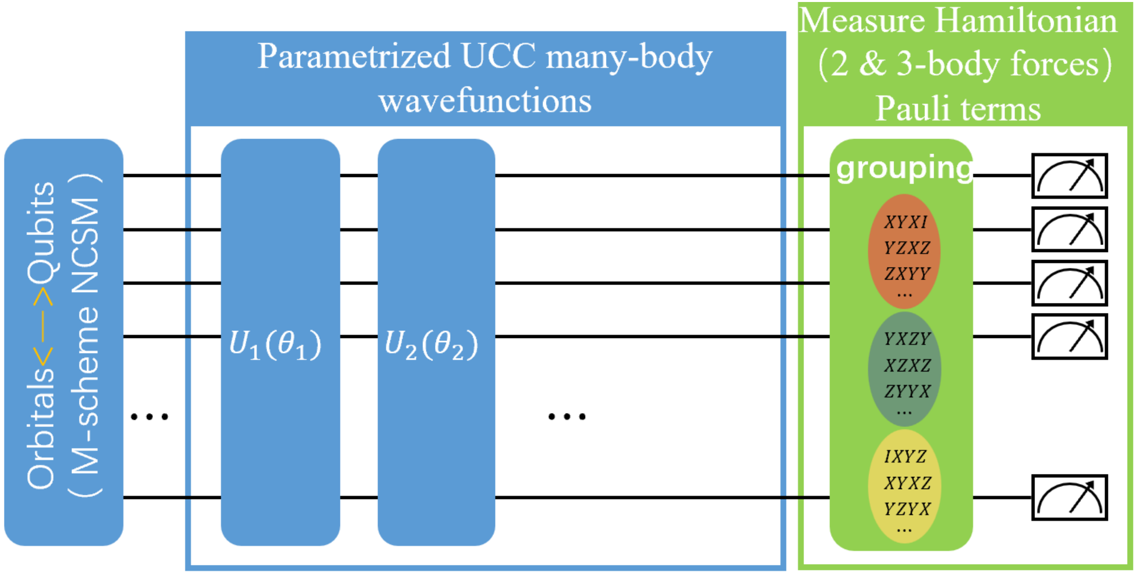
Details

127 Qubits	Status:	Online	Median CNOT Error:	1.187e-2
64 QV	Total pending jobs:	34 jobs	Median SX Error:	2.892e-4
850 CLOPS	Processor type ⓘ:	Eagle r1	Median Readout Error:	1.520e-2
	Version:	1.6.17	Median T1:	100.85 us
	Basis gates:	CX, ID, RZ, SX, X	Median T2:	86.04 us



Source of noise： CNOT gates， readout, decoherence

Variational Quantum Eigensolver (VQE)



- Pros
  - Least request of resources
  - Noise resistance
  - Error mitigation
- Cons
  - Too complex for complex problems
  - Costly measurement

hybrid quantum-classical algorithm, wide applications in NISQ devices

Low-Noise Variational circuit

- The pairing Hamiltonian: direct seniority model mapping

$$\hat{H} = -G \sum_{m,m'>0} a^{+}_{m'} a^{+}_{-m'} a_{-m} a_{m} = -G \sum_{m,m'>0} s_{+}^{(m')} s_{-}^{(m)}$$

Chongji Jiang and Junchen Pei, Phys. Rev. C 107, 044308 (2023)

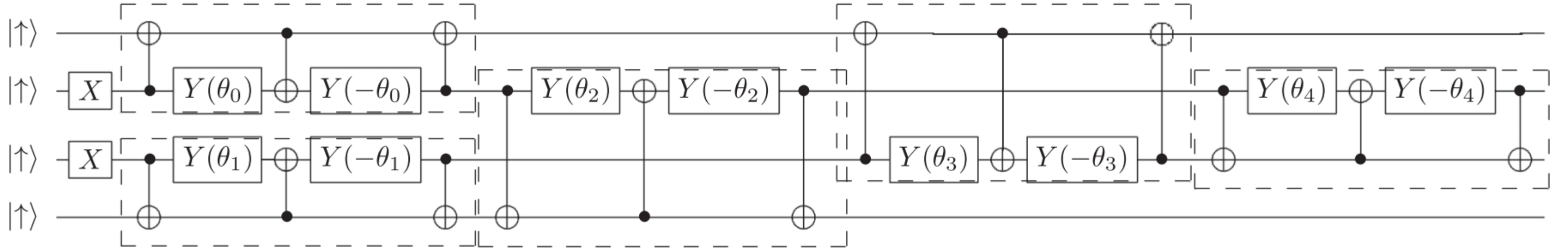
For Ω=4, the circuit is much more complex, has serious noise problems

$$|\psi(\vec{\theta})\rangle = \prod_i U_i(\theta_i)\,|\psi_0\rangle$$

$$U_i(\theta_i) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \sin\theta & \cos\theta & 0 \\ 0 & \cos\theta & -\sin\theta & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- Particle-number preserving building blocks

  Significantly reduce the noise



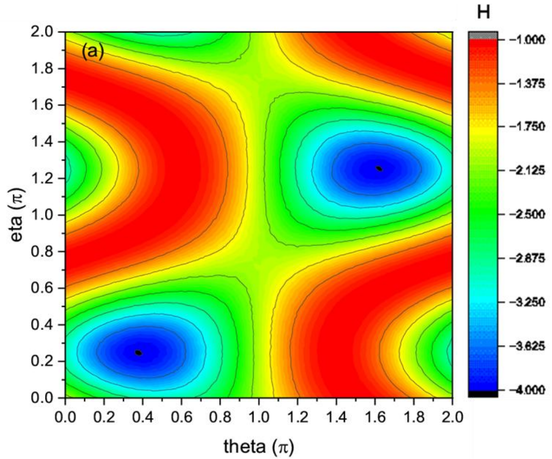
Efficient computation for excited states

- VQD: variational quantum deflation
- Solve an effective Hamiltonian

O. Higgott, D. Wang, S. Brierley, Quantum 3, 156 (2019).

$$E(\lambda_k) \equiv \langle\psi(\lambda_k)|\hat{H}|\psi(\lambda_k)\rangle + \sum_{j=0}^{k-1} \beta_j |\langle\psi(\lambda_k)|\psi(\lambda_j)\rangle|^2$$

$$\hat{H}(k) \equiv \hat{H} + \sum_{j=0}^{k-1} \lambda_j |j\rangle\langle j|$$



Crucial to calculate overlap: $\boxed{|\langle 0|U^\dagger(j)U(k)|0\rangle|^2}$

Need at most twice the circuit depth

Advantages:

- VQD works for general Hamiltonian problems and requires least resources to compute excited states compared to other methods
- Can obtain degenerate states, first application in nuclear physics

Chongji Jiang and Junchen Pei, Phys. Rev. C 107, 044308 (2023)

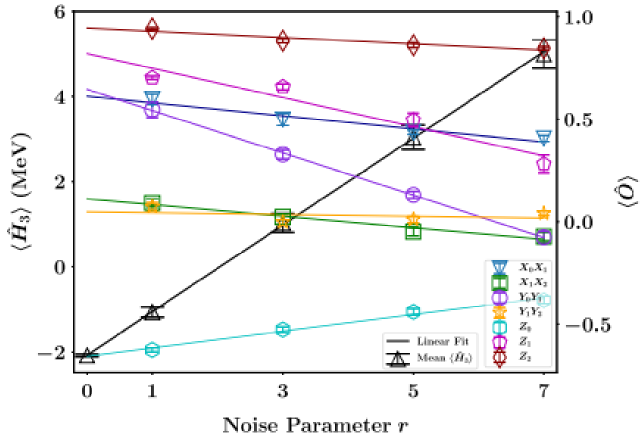
Error mitigation

- readout error $P(0|1), P(1|0)$ $\rightarrow$ inverse matrix

$$S_k = \begin{pmatrix} P_{0,0}^k & P_{0,1}^k \\ P_{1,0}^k & P_{1,1}^k \end{pmatrix}$$

- zero-noise extrapolation

$$\mathrm{CNOT} \cdot \mathrm{CNOT} = I$$

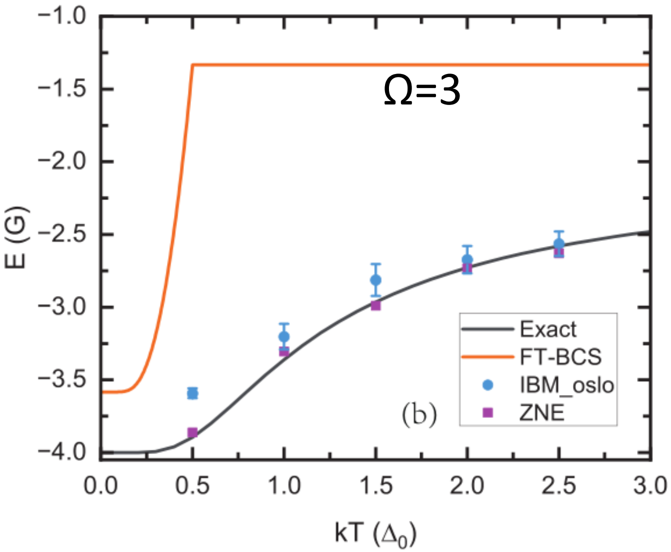


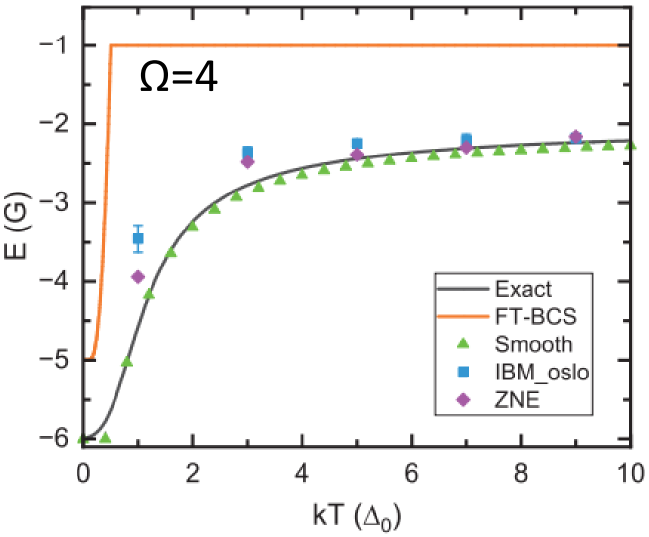
Eigenstate	$\lvert\psi\rangle$	E(Qiskit)	E(IBM_oslo)	E(R-Miti)	E(ZNE)	E(R-Miti+ZNE)
g.s.	$0.588\lvert\uparrow\uparrow\downarrow\rangle + 0.554\lvert\uparrow\downarrow\uparrow\rangle + 0.590\lvert\downarrow\uparrow\uparrow\rangle$	-4.013	-3.751	-3.871	-3.919	-4.123
1st es	$0.309\lvert\uparrow\uparrow\downarrow\rangle + 0.651\lvert\uparrow\downarrow\uparrow\rangle - 0.693\lvert\downarrow\uparrow\uparrow\rangle$	-1.024	-1.126	-1.107	-1.093	-1.064
	$0.809\lvert\uparrow\uparrow\downarrow\rangle - 0.569\lvert\uparrow\downarrow\uparrow\rangle - 0.146\lvert\downarrow\uparrow\uparrow\rangle$	-1.004	-1.109	-1.086	-1.006	-0.978

E.F. Dumitrescu, et al, Phys. Rev. Lett. 120, 210501 (2018)
Chongji Jiang and Junchen Pei, Phys. Rev. C 107, 044308 (2023)

Pairing at finite temperature

- We expect a smooth transition of superfliudity in finite systems
- Finite-temperature BCS theory break down, strong many-body correlations are important





Variational circuit is same as zero temperature

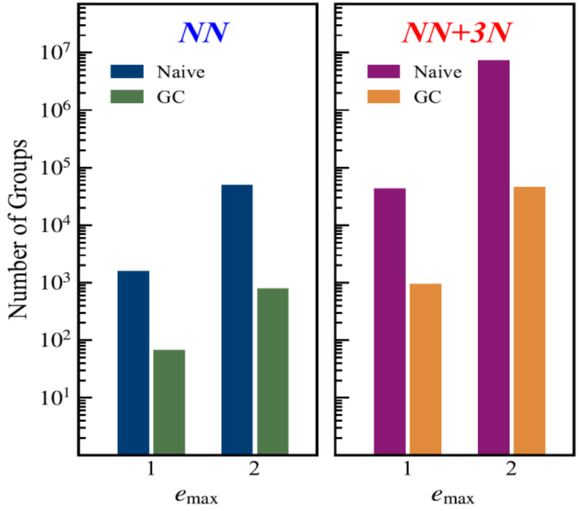
Error mitigated results are close to exact results, in particular at high temperatures

C.J.Jiang, J.C.Pei, Phys.Rev.C 107, 044308 (2023)

Towards Ab initio calculations

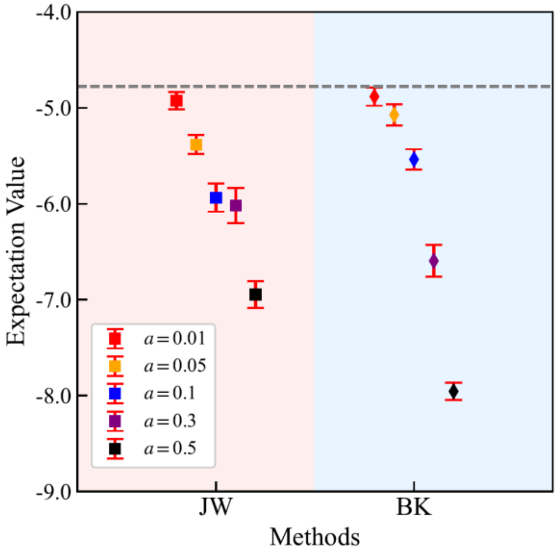
Chongji Jiang, J.Pei, in preparation

- Quantum computing of 3H, 3He
- With chiral nuclear force, 16 qubits, *sp*-shell, m-scheme,~3000 gates



Huge number of Pauli terms due to three-body force, measurements are too costly

Simultaneous grouping measurement



Different mapping performance with varying noise scale

Summary & Outlook

- Bayesian machine learning has advantageous in evaluating imperfect data, which is a salient feature for nuclear physics
- Data fusion and physics informed machine learning will be useful for nuclear physics
- Noisy Quantum computing is a new challenging and new algorithms are needed
- We implement low-noisy circuit, error mitigation, efficient method for excited states, for a finite-temperature pairing Hamiltonian
- Ab initio calculations of light nuclei with simultaneous measurements and different mapping

Thank you for your attention!