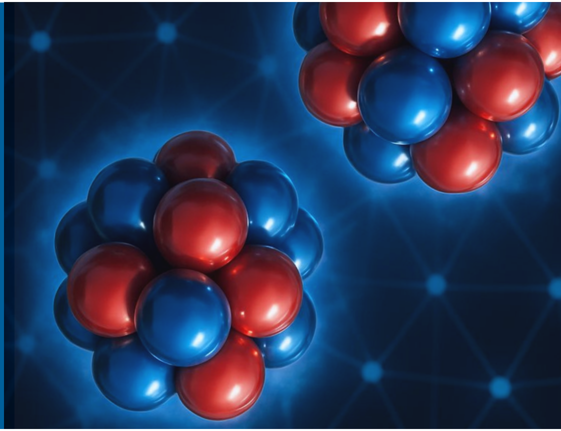
PIONLESS EFT WITH NEURAL QUANTUM STATES



JANE KIM

Argonne National Laboratory

INT Program 26-1: Nuclear Hamiltonians for Advancing Nuclear Physics and Beyond
Institute for Nuclear Theory, Seattle, WA
14 May 2026

VARIATIONAL MONTE CARLO

Based on the variational principle:

$$E(\theta) = \frac{\langle \Psi_\theta | \hat{H} | \Psi_\theta \rangle}{\langle \Psi_\theta | \Psi_\theta \rangle} \quad \Longrightarrow \quad \min_\theta E(\theta) \geq E_0$$

Use Monte Carlo integration to handle the high-dimensional integrals:

$$\frac{\langle \Psi_\theta | \hat{H} | \Psi_\theta \rangle}{\langle \Psi_\theta | \Psi_\theta \rangle} \approx \frac{1}{N_s} \sum_{i=1}^{N_s} \frac{1}{\Psi_\theta(X_i)} \hat{H} \Psi_\theta(X_i), \quad \text{where } X_i \sim |\Psi_\theta(X)|^2$$

Ψ_θ exact eigenstate $\quad \Longleftrightarrow \quad \sigma_E^2(\theta) = 0$

CONVENTIONAL VMC FOR NUCLEAR SYSTEMS

symmetric
short-range correlations

$$|\Psi\rangle = \hat{F}\,|\Phi\rangle$$

antisymmetric
long-range behavior, quantum numbers

e.g. $\hat{F} = \left(\hat{S}\sum_{i<j}\hat{F}_{ij}\right)\left(\hat{S}\sum_{i<j<k}(1+\hat{F}_{ijk})\right)$

$4^A \to \binom{A}{Z}\binom{A}{N_\uparrow} \sim \frac{4^A}{A}$ elements!

Coordinate-space, local Hamiltonians (strongly preferred)

Evaluating the wave function involves storing and manipulating a long vector of spin-isospin amplitudes

VMC can handle “hard” interactions, but difficult to design a good ansatz

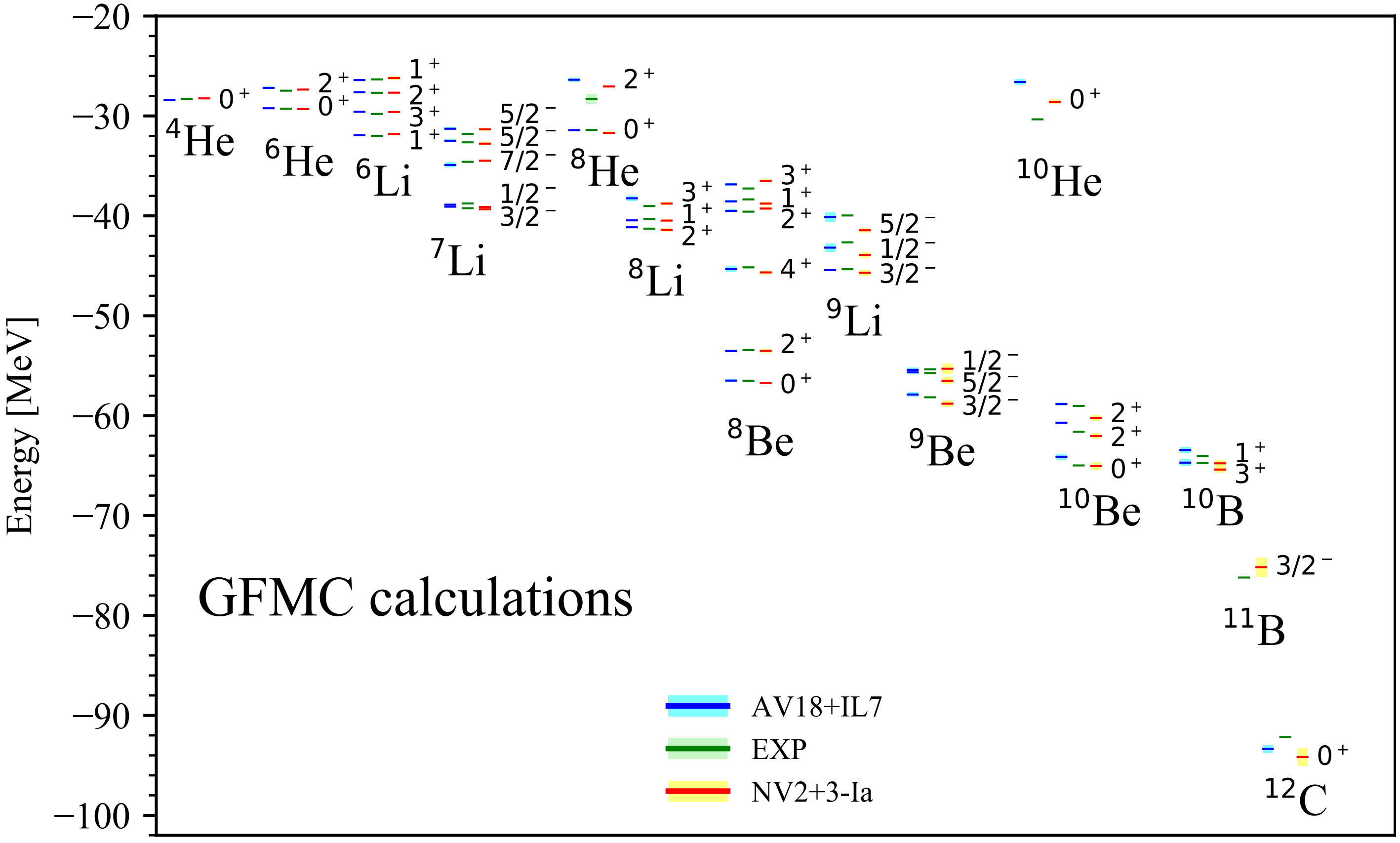
Always fine tuned with Green’s function Monte Carlo (GFMC)

ACCURACY OF VMC + GFMC

Percent-level accuracy for energies and radii

Local phenomenological and chiral interactions used here

Typically limited to $A \lesssim 13$ due to **exponential scaling**

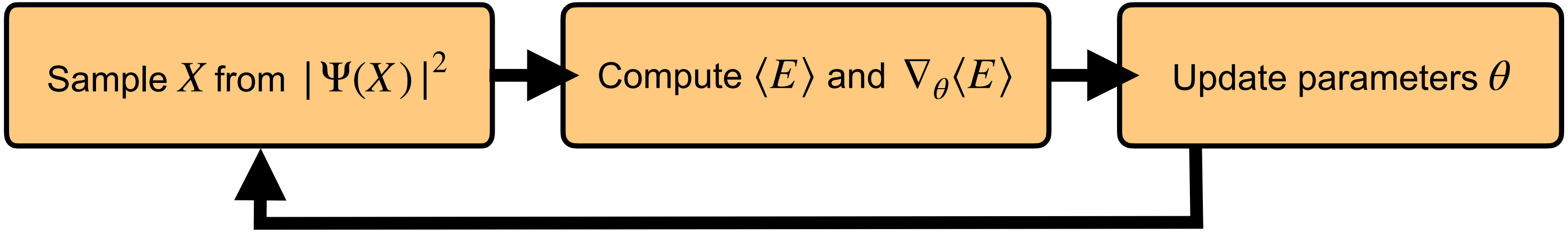


*M. Piarulli et al., PRL **120**, 052503 (2018)*

NEURAL QUANTUM STATES

Variational wave functions based on artificial neural networks

What is the input to the network?	Many-body configurations $X = \{\mathbf{x}_i\}_{i=1}^{A}$,	$\mathbf{x}_i = (\mathbf{r}_i, s_i^z, t_i^z)$
What is the output of the network?	The amplitude $\Psi(X)$	
How do you train the network?	Stochastic reconfiguration	



Sample X from $|\Psi(X)|^2$

Compute $\langle E \rangle$ and $\nabla_\theta \langle E \rangle$

Update parameters θ

G. Carleo and M. Troyer, Science 355, 6325 (2017).

WHY NEURAL QUANTUM STATES?

Traditional VMC relies on carefully engineered ansätze

Correlation structures are often Hamiltonian-dependent

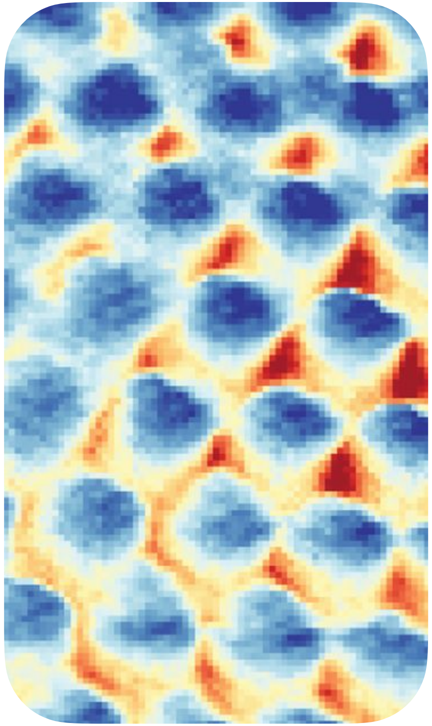
Important many-body correlations may not be obvious a priori

May accidentally bias the kinds of phases ansatz can find

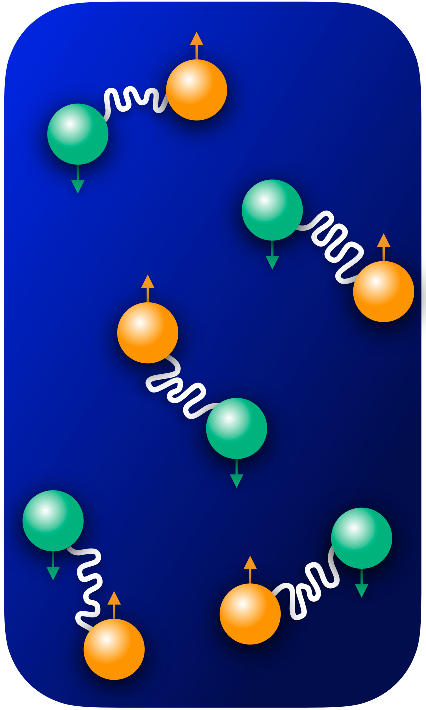
Goal: Design a single ansatz flexible enough to simultaneously describe many different systems and phases so emergent behavior is driven more directly by the Hamiltonian itself

Scaling: Exponential → polynomial

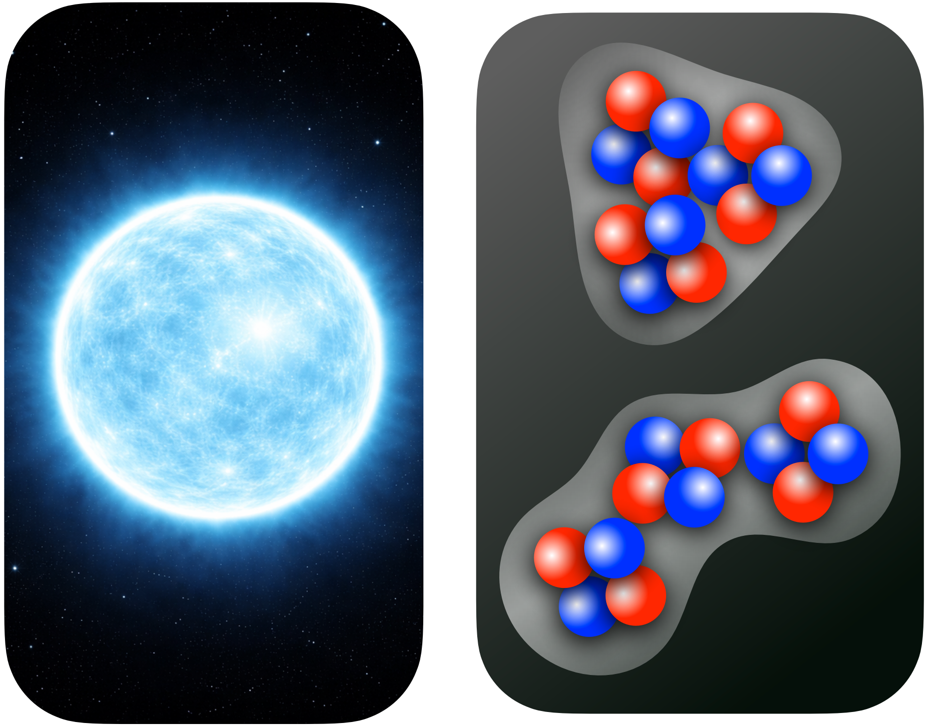
STRONGLY CORRELATED FERMIONS



Message-passing graph neural network to capture many-body correlations



Neural Pfaffian ansatz to capture superfluidity



Applications to nuclear systems

G. Carleo and M. Troyer, Science 355, 6325 (2017).

NEURAL QUANTUM STATES

$$\Psi(X) = F(X)\Phi(X)$$

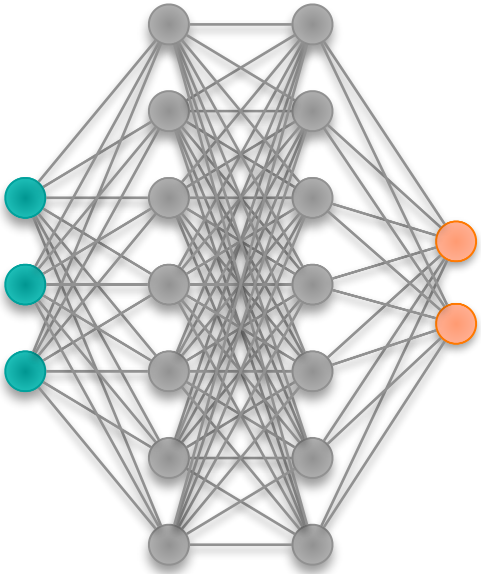
symmetric

antisymmetric

Similar idea as before, but parameterize by many feedforward neural networks…

very flexible mappings between two spaces
fast to evaluate
easy to differentiate

FEEDFORWARD NEURAL NETWORKS



Inspired by the structure of the brain

Nodes are organized into layers, connections between neighboring layers

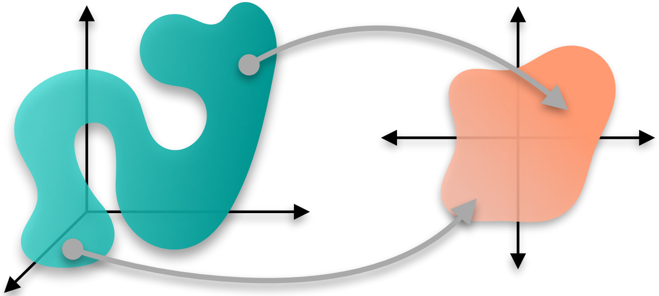
Compose affine transformations with nonlinear activation functions

highly optimized, trainable   simple, fast, fixed

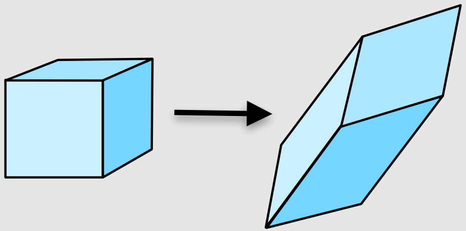
Universal approximation theorem: An FFNN with one hidden layer and enough hidden neurons can approximate any continuous function on a compact domain, to any desired accuracy.

BUT does not avoid curse of dimensionality!

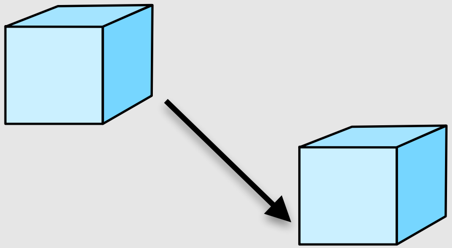
Backpropagation: Method for computing the gradient of an FFNN using the chain rule.



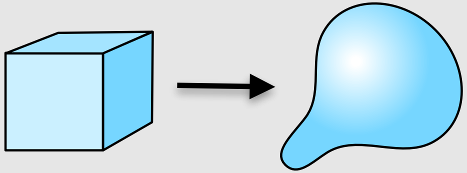
BUILDING BLOCKS*



Linear transformations

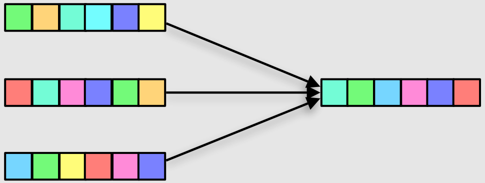


Translations

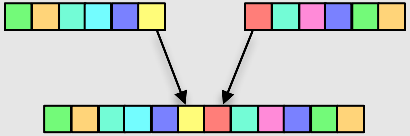


Activation functions

Applied element-wise, need to be fast and nonlinear



Pooling operations



Concatenation operations

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* for the neural networks in this talk…

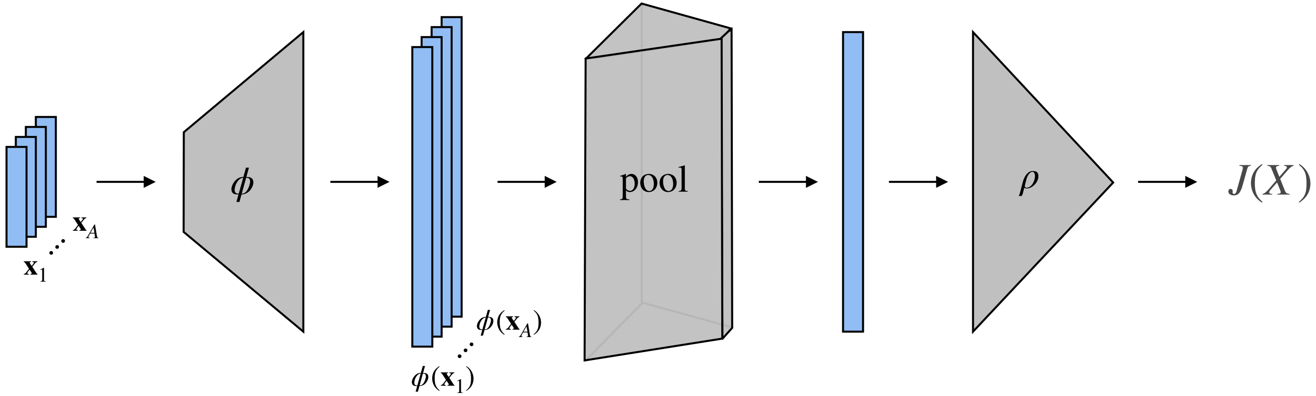
NEURAL QUANTUM STATES

$$\Psi(X) = F(X)\Phi(X)$$

symmetric

antisymmetric

Symmetric part: $F(X) = e^{J(X)}$ (positive definite)



Zaheer et al., arXiv:1703.06114 (2017)

NEURAL QUANTUM STATES

$$\Psi(X) = F(X)\Phi(X)$$

symmetric

antisymmetric

Antisymmetric part: often based on a Slater determinant

$$\Phi(X) = \det \begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_1(\mathbf{x}_2) & \cdots & \phi_1(\mathbf{x}_A) \\ \phi_2(\mathbf{x}_1) & \phi_2(\mathbf{x}_2) & \cdots & \phi_2(\mathbf{x}_A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_A(\mathbf{x}_1) & \phi_A(\mathbf{x}_2) & \cdots & \phi_A(\mathbf{x}_A) \end{bmatrix}$$

A independent neural networks
or one with A different outputs

NEURAL QUANTUM STATES

$$\Psi(X) = F(X)\Phi(X)$$

symmetric

antisymmetric

Antisymmetric part: we use one based on a Pfaffian

$$\Phi(X) = \det \begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_1(\mathbf{x}_2) & \cdots & \phi_1(\mathbf{x}_A) \\ \phi_2(\mathbf{x}_1) & \phi_2(\mathbf{x}_2) & \cdots & \phi_2(\mathbf{x}_A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_A(\mathbf{x}_1) & \phi_A(\mathbf{x}_2) & \cdots & \phi_A(\mathbf{x}_A) \end{bmatrix}$$

A independent neural networks
or one with A different outputs

$$\Phi(X) = \mathrm{pf} \begin{bmatrix} 0 & \phi(\mathbf{x}_1, \mathbf{x}_2) & \cdots & \phi(\mathbf{x}_1, \mathbf{x}_A) \\ -\phi(\mathbf{x}_1, \mathbf{x}_2) & 0 & \cdots & \phi(\mathbf{x}_2, \mathbf{x}_A) \\ \vdots & \vdots & \ddots & \vdots \\ -\phi(\mathbf{x}_1, \mathbf{x}_A) & -\phi(\mathbf{x}_2, \mathbf{x}_A) & \cdots & 0 \end{bmatrix}$$

One neural network parameterizing the pairing orbital

JK et al., Commun. Phys. ***7****, 148 (2024).*

NEURAL PFAFFIAN

Slater determinant is a special case of a Pfaffian → can capture different phases with one ansatz

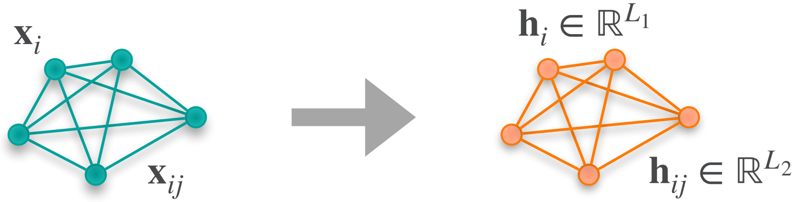
Number of trainable parameters is **independent of system size**

Odd and even systems share a pairing orbital

No reliance on shell closures or explicit many-body basis, works directly in continuous space

Scales the same as a determinant

Transferable to nuclear systems: spin-isospin dependent pairing orbitals without explicit coding



JK et al., Commun. Phys. ***7****, 148 (2024).*

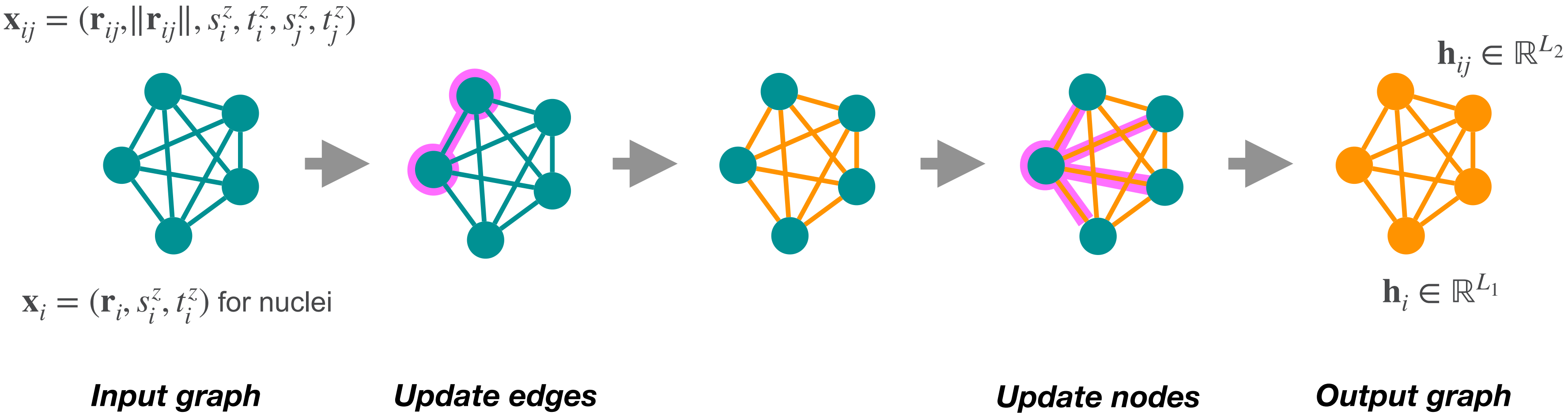
G. Pescia, JK, et al., PRB ***110****, 035108 (2024).*

GRAPH NEURAL NETWORKS

Iteratively builds local correlations by passing “messages” along edges

Used to find better representations of one- and two-body features of quantum system

New embeddings are used in place of the raw features



$\mathbf{x}_{ij} = (\mathbf{r}_{ij}, \|\mathbf{r}_{ij}\|, s_i^z, t_i^z, s_j^z, t_j^z)$

$\mathbf{x}_i = (\mathbf{r}_i, s_i^z, t_i^z)$ for nuclei

$\mathbf{h}_{ij} \in \mathbb{R}^{L_2}$

$\mathbf{h}_i \in \mathbb{R}^{L_1}$

Input graph

Update edges

Update nodes

Output graph

*G. Pescia, JK, et al., PRB **110**, 035108 (2024).*

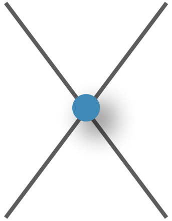
PIONLESS EFT HAMILTONIAN

A low-energy EFT of QCD with only nucleons as degrees of freedom

Appropriate when momenta are well below the pion mass, or for nuclear matter up to $\sim n_0/2$

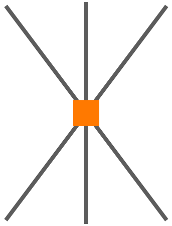
$$\hat{H}_{LO} = -\sum_i \frac{\nabla_i^2}{2m_i} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

- NN potential: fit to np scattering lengths and effective radii and the deuteron binding energy
- 3NF adjusted to reproduce the ^{3}H binding energy.



$$v_{ij}^{\mathrm{CI}} = \sum_{p=1}^{4} v^p(r_{ij}) O_{ij}^p \ ,$$

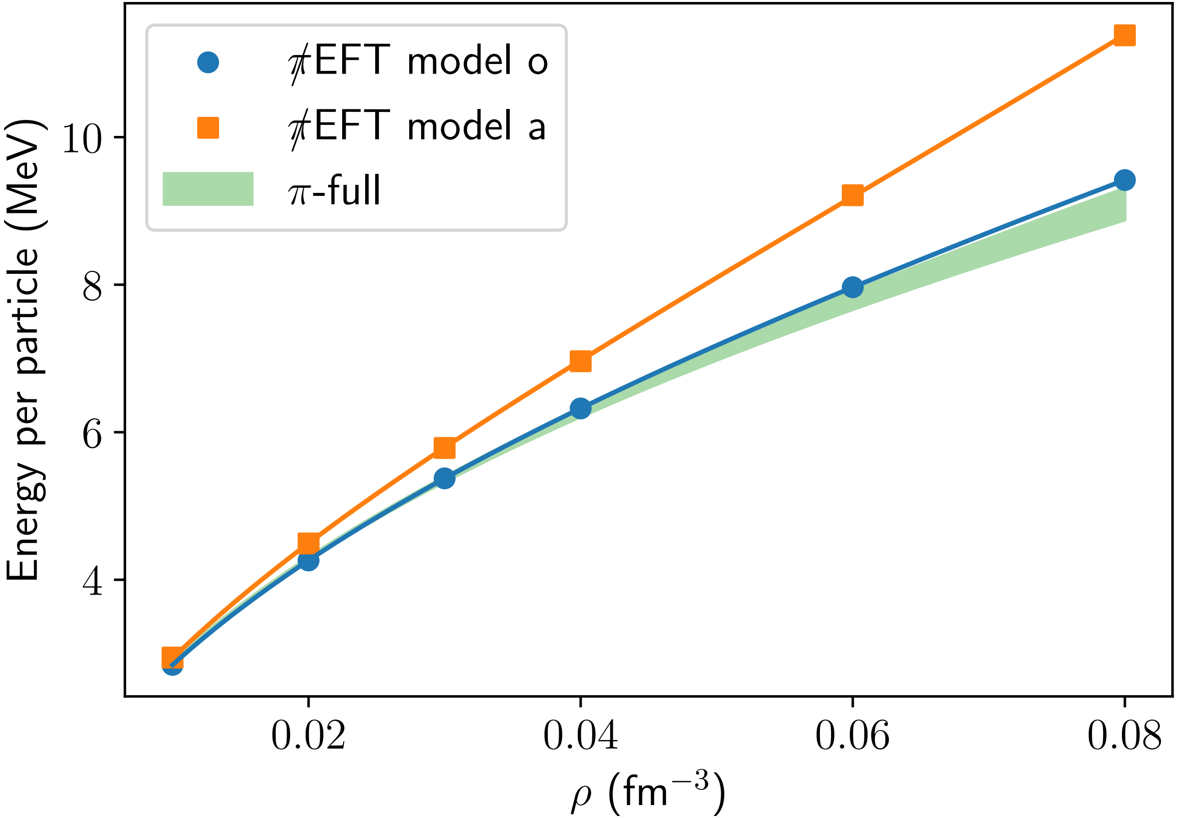
$$O_{ij}^{p=1,4} = (1, \tau_{ij}, \sigma_{ij}, \sigma_{ij}\tau_{ij})$$



$$V_{ijk} = \tilde{c}_E \sum_{\mathrm{cyc}} e^{-(r_{ij}^2 + r_{jk}^2)/R_3^2}$$

*R. Schiavilla, et al., PRC **103**, 054003(2021)*

PURE NEUTRON MATTER



This simple LO pionless EFT Hamiltonian compared to pionfull Hamiltonians at low densities

R. Schiavilla et al., PRC 103, 054003 (2021).

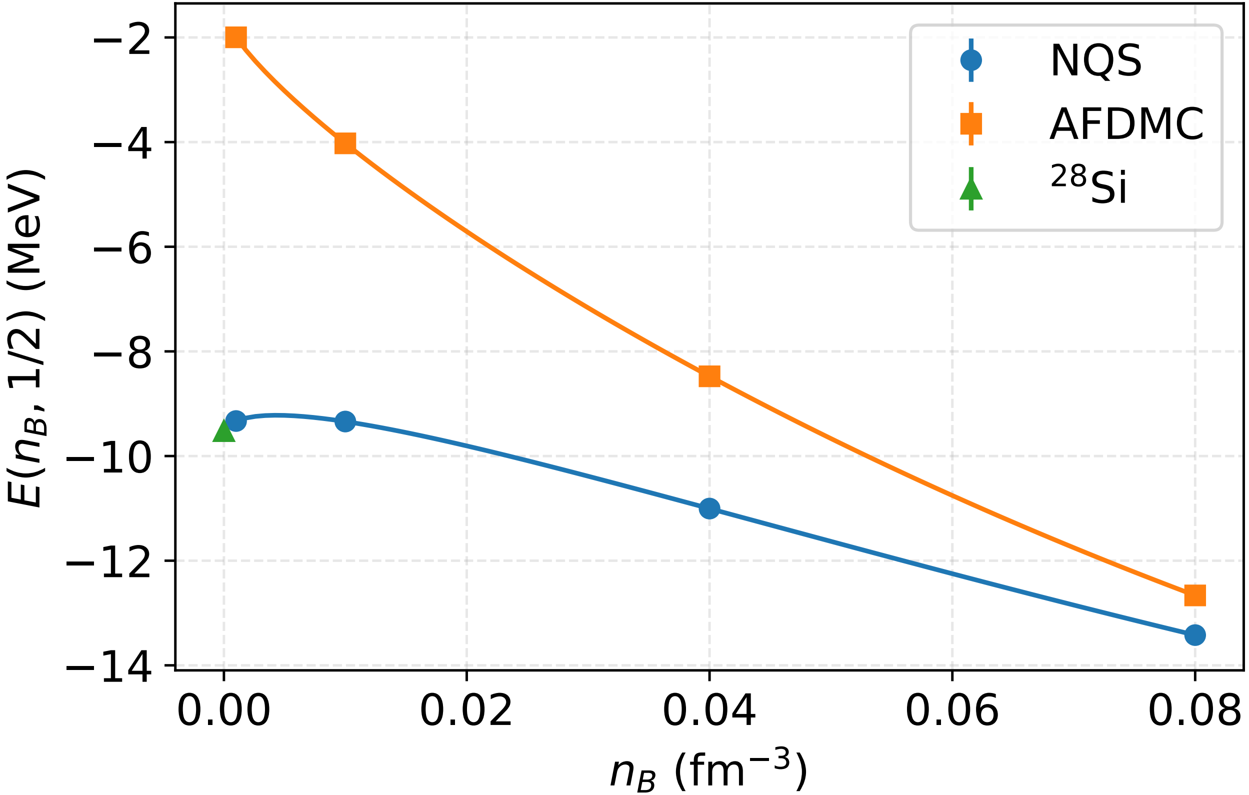
B. Fore, JK, et al., PRR 5, 033062 (2023).

SYMMETRIC NUCLEAR MATTER

Using the same pionless EFT Hamiltonian, except assume electromagnetic contribution is screened

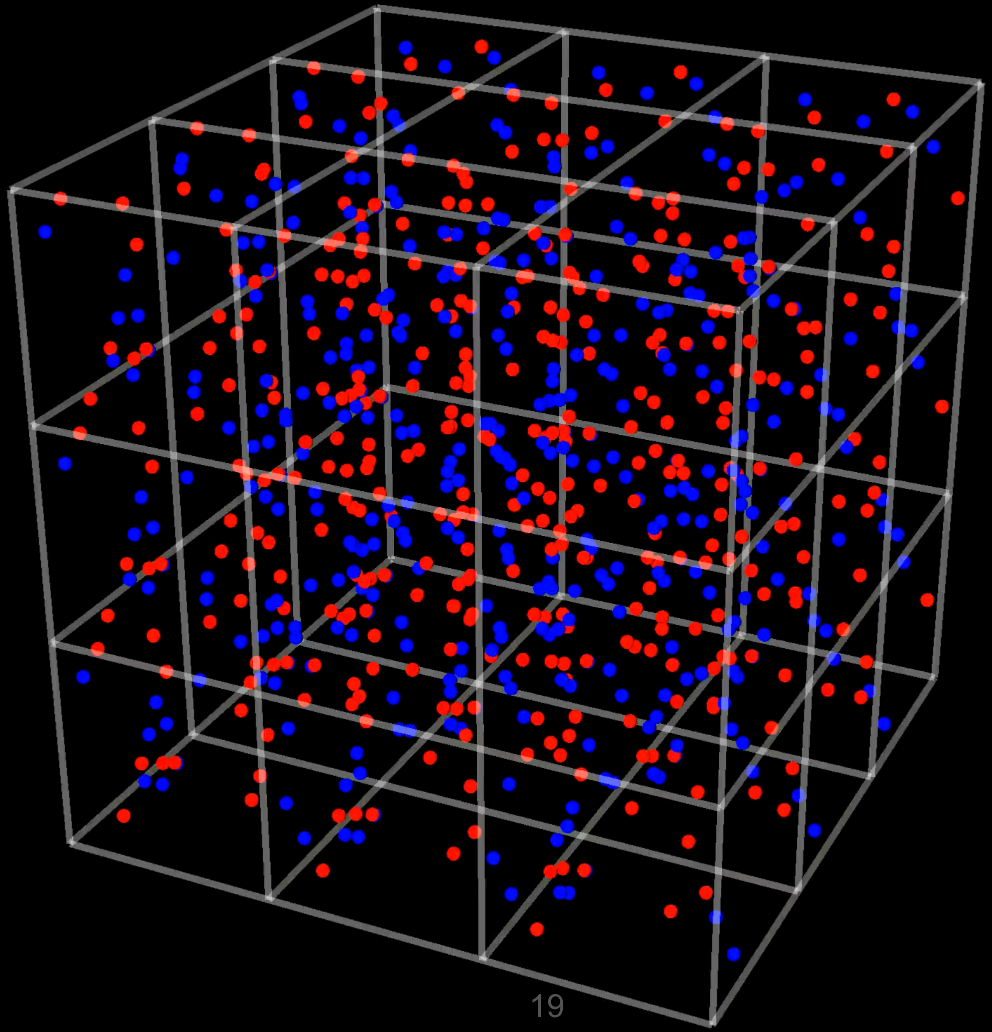
Compare with AFDMC for densities between $0.001\ \mathrm{fm}^{-3}$ and $0.08\ \mathrm{fm}^{-3}$

When $N = 28,$ Pfaffian NQS shows the formation of ^{28}Si at low densities



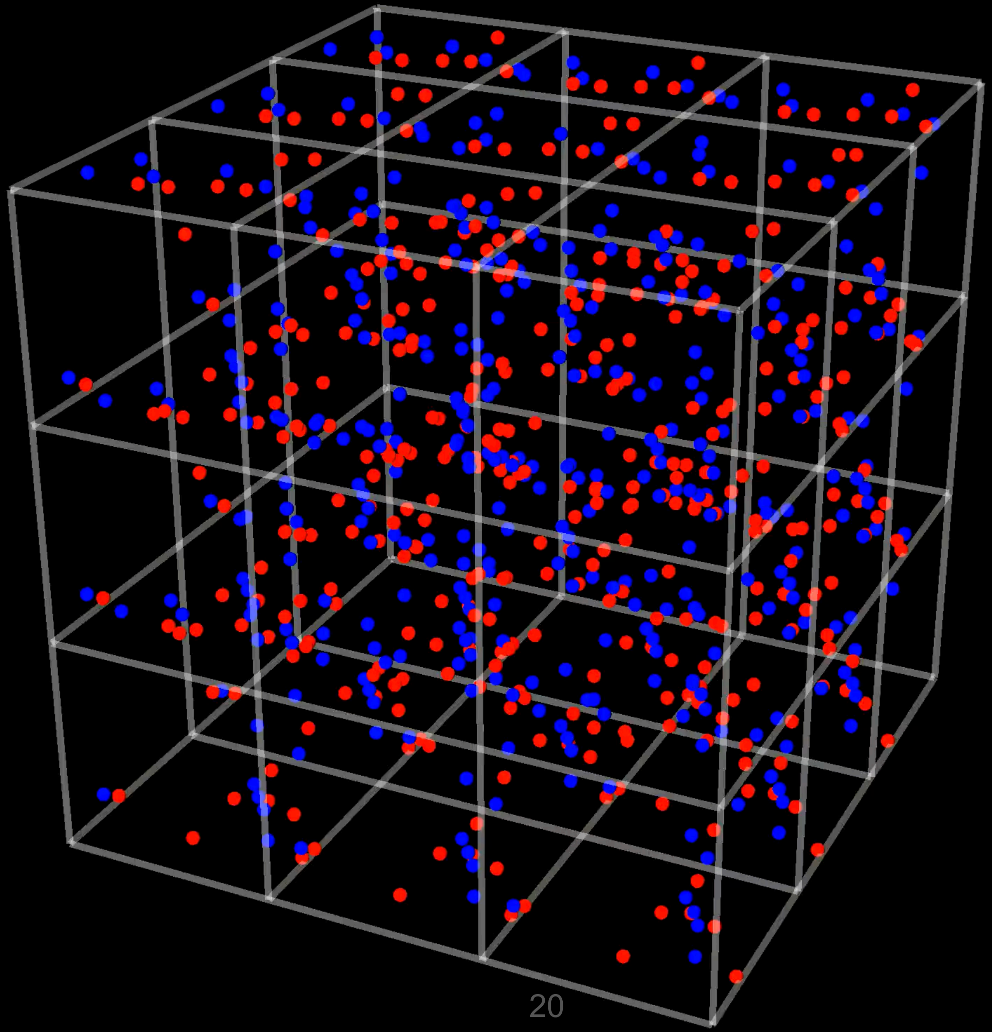
B. Fore, JK, et al., Commun. Phys. **8**, 108 (2025).

Symmetric Nuclear Matter



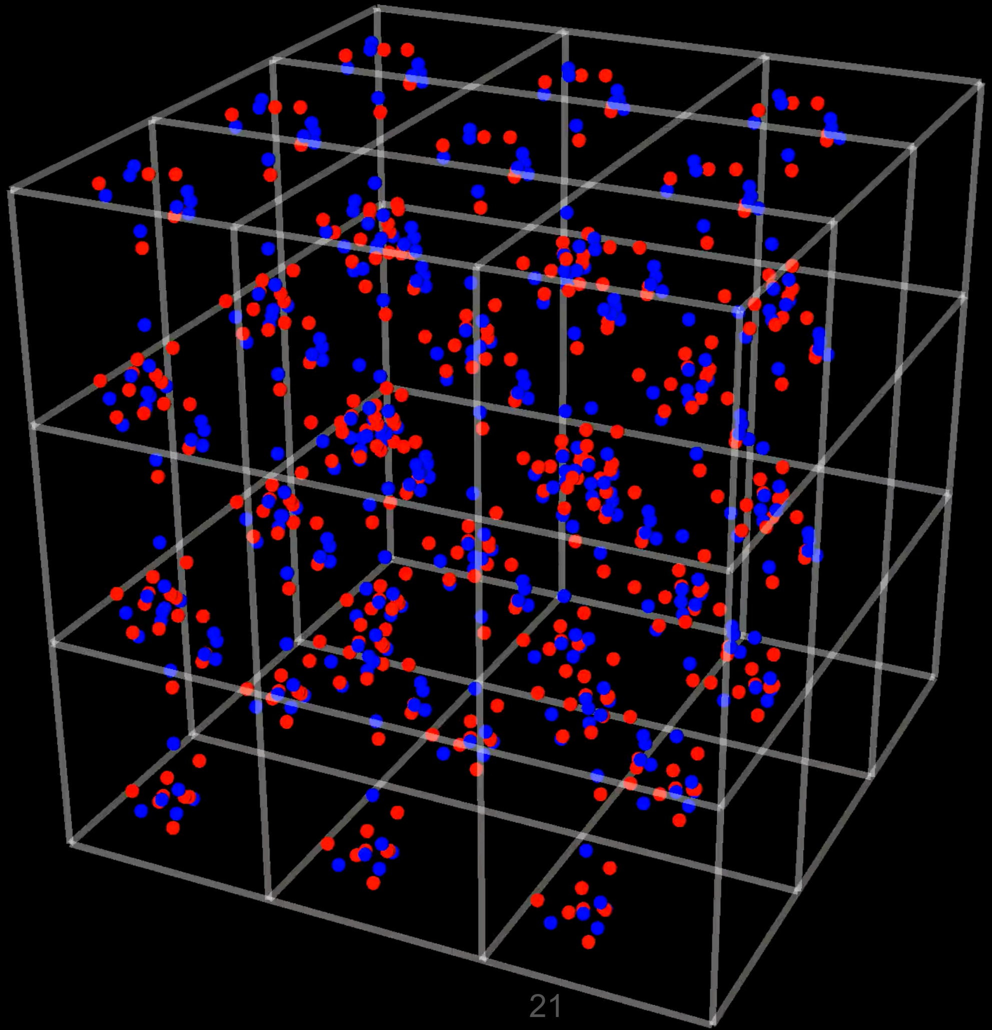
$n_B = 0.08\ \mathrm{fm}^{-3}$

Symmetric
Nuclear
Matter



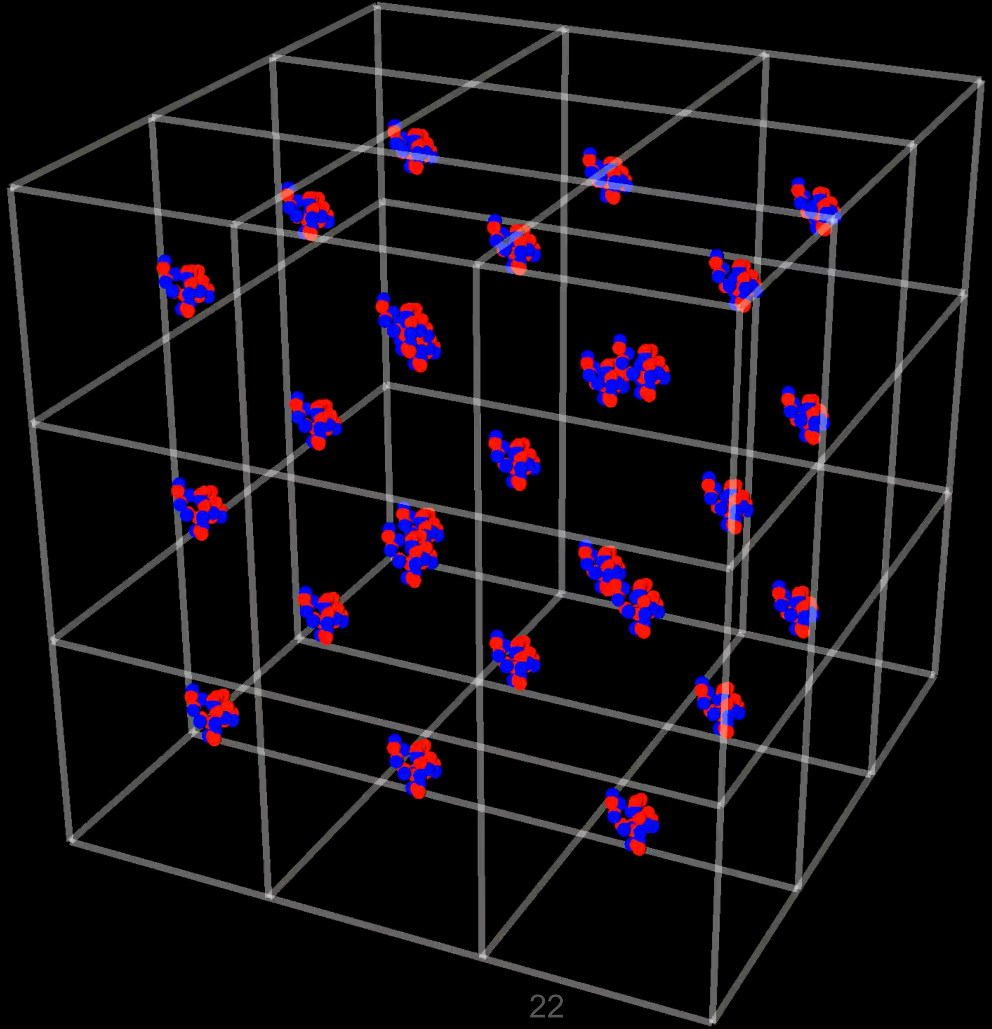
$n_B = 0.04 \ \mathrm{fm}^{-3}$

Symmetric Nuclear Matter



$n_B = 0.01\ \text{fm}^{-3}$

Symmetric
Nuclear
Matter



$n_B = 0.001\ \mathrm{fm}^{-3}$

LOW-DENSITY EQUATION OF STATE

Cluster expansion

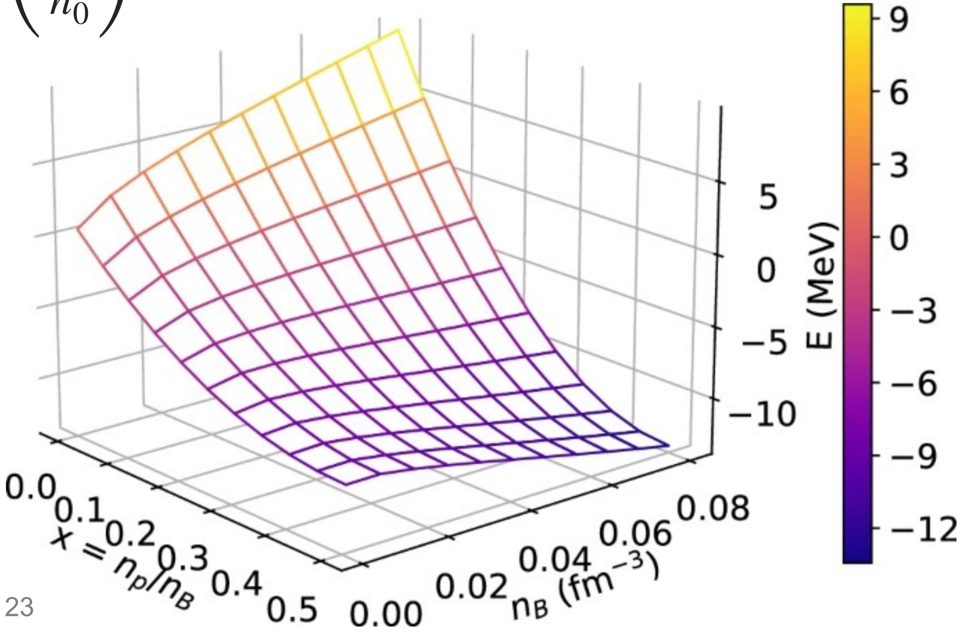
$$E(n_B, x) = a_0 + a_{2/3}\left(\frac{n_B}{n_0}\right)^{2/3} + a_1\left(\frac{n_B}{n_0}\right) + a_2\left(\frac{n_B}{n_0}\right)^2$$

Expansion in neutron richness

$$E(n_B, x) = E(n_B,\ 1/2) + (1-2x)^2 S(n_B)$$

$$S(n_B) = E(n_B,\ 0) - E(n_B,\ 1/2)$$

Finite-size effects are strong for small x



B. Fore, JK, et al., Commun. Phys. **8**, 108 (2025).

COMPOSITION OF NEUTRON STAR CRUSTS

Assume rates of beta decay and inverse beta decay are equal:

$$n \rightarrow p + e^- + \bar{\nu}_e$$

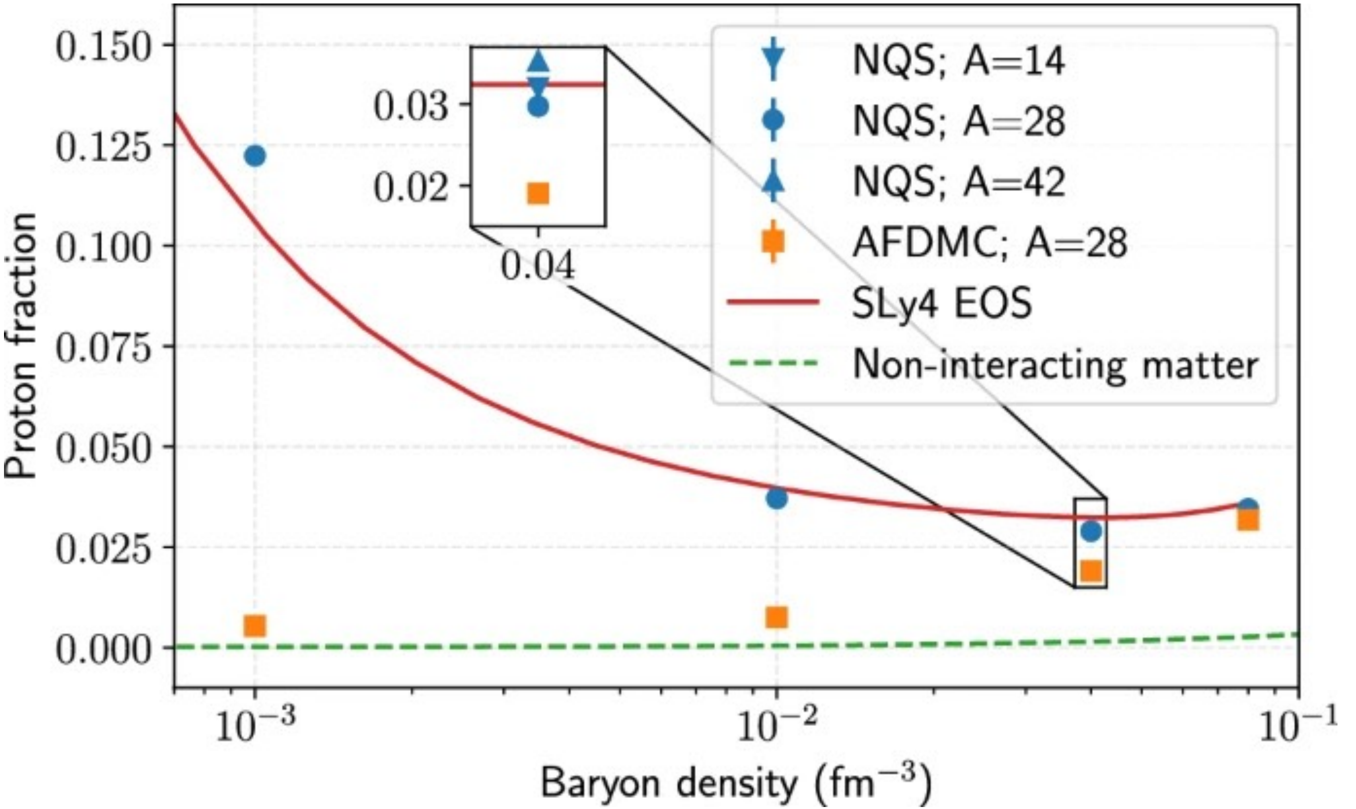
$$p + e^- \rightarrow n + \nu_e$$

$$\mu_n = \mu_p + \mu_e$$

Assume charge neutrality:

$$n_p = n_e$$

NQS agrees better with phenomenological Skryme models than AFDMC



B. Fore, JK, et al., Commun. Phys. **8**, 108 (2025).

TOWARDS MEDIUM-MASS NUCLEI

Key questions:

Which aspects of nuclear structure are governed by low-energy physics?

Which require resolving pion dynamics and short-distance details?

How sensitive are bulk observables to physics above the pion scale?

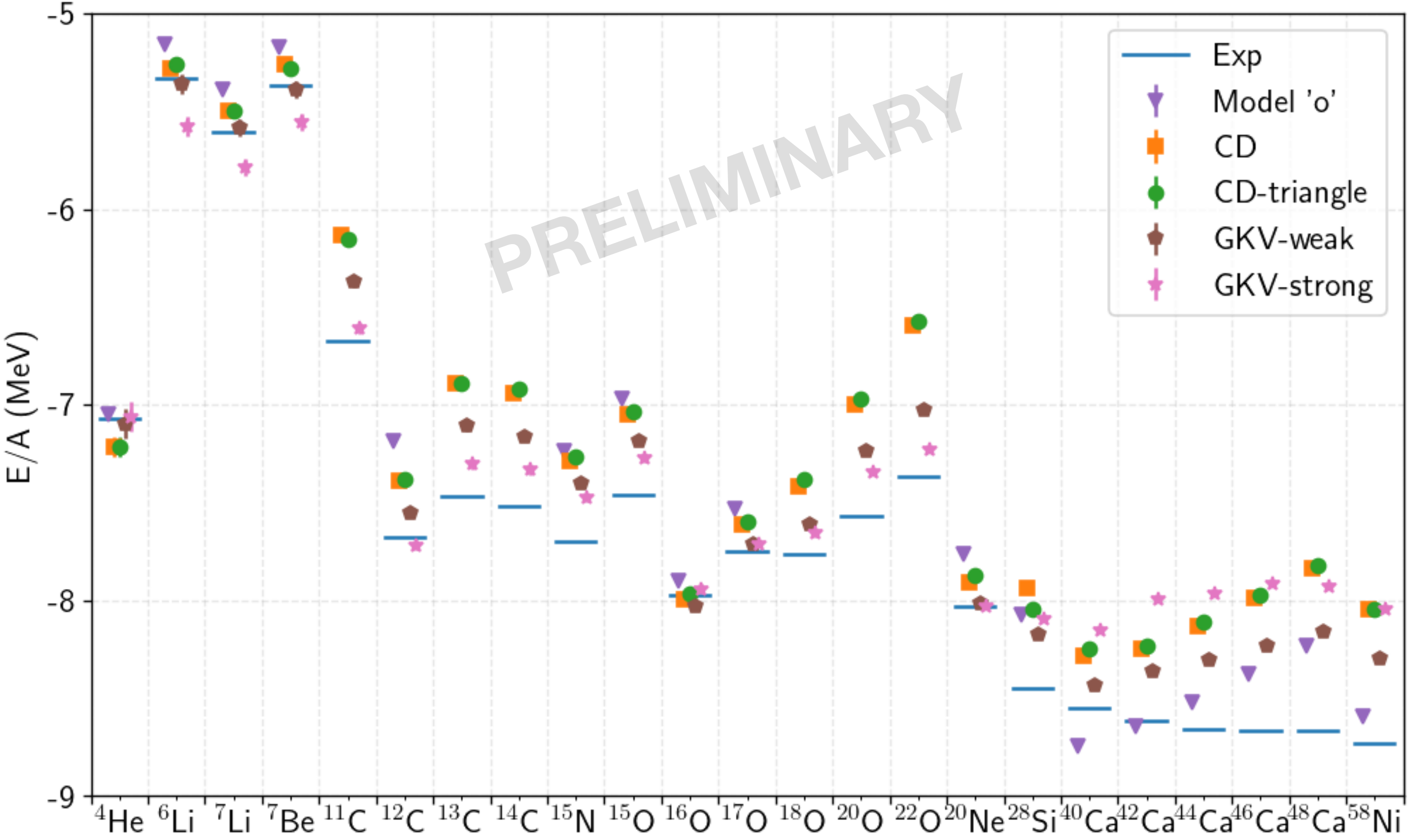
How much of nuclear binding is explained by near-unitary NN physics?

This work:

Use the **simplest LO pionless EFT Hamiltonians**

Treat them as a probe of universality, not a convergent microscopic theory

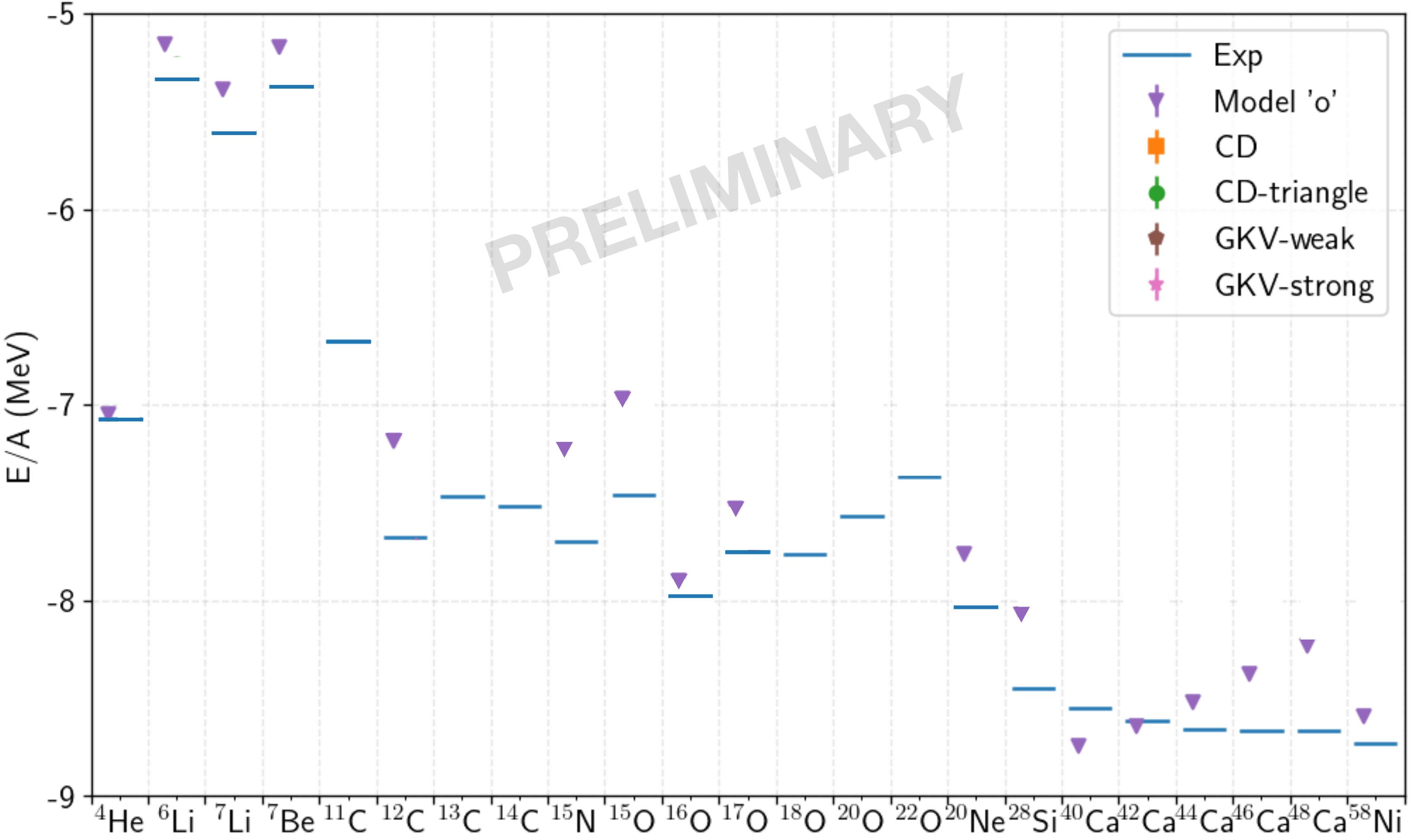
PRELIMINARY RESULTS: MEDIUM-MASS NUCLEI



B. Fore, JK, et al.,
in prep.

PRELIMINARY RESULTS: MEDIUM-MASS NUCLEI

B. Fore, JK, et al.,
in prep.



Our baseline (same interaction we used for dilute nuclear matter)

R. Schiavilla et al., PRC 103, 054003 (2021).

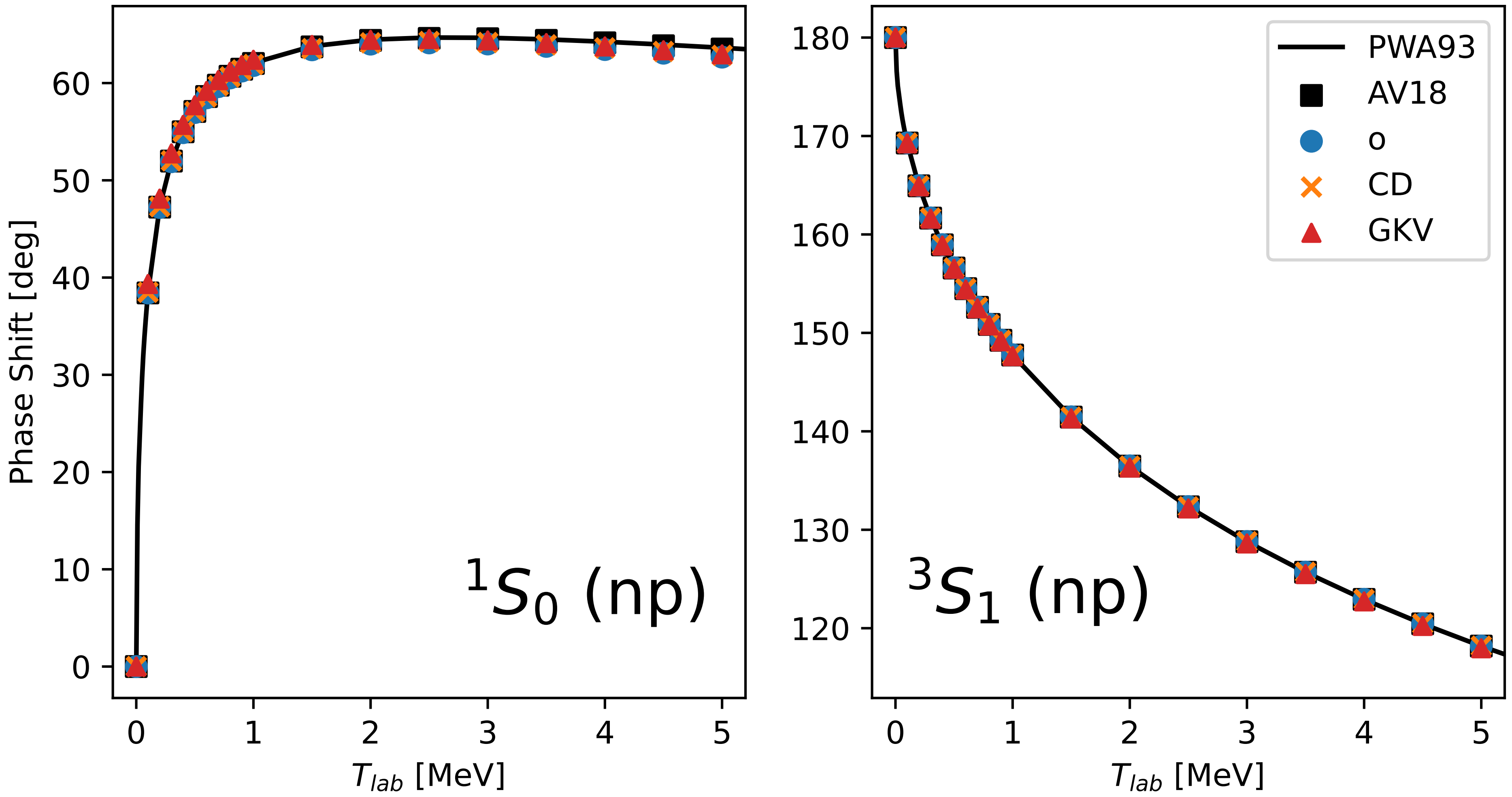
LECs: C_{01}, C_{10}, c_E

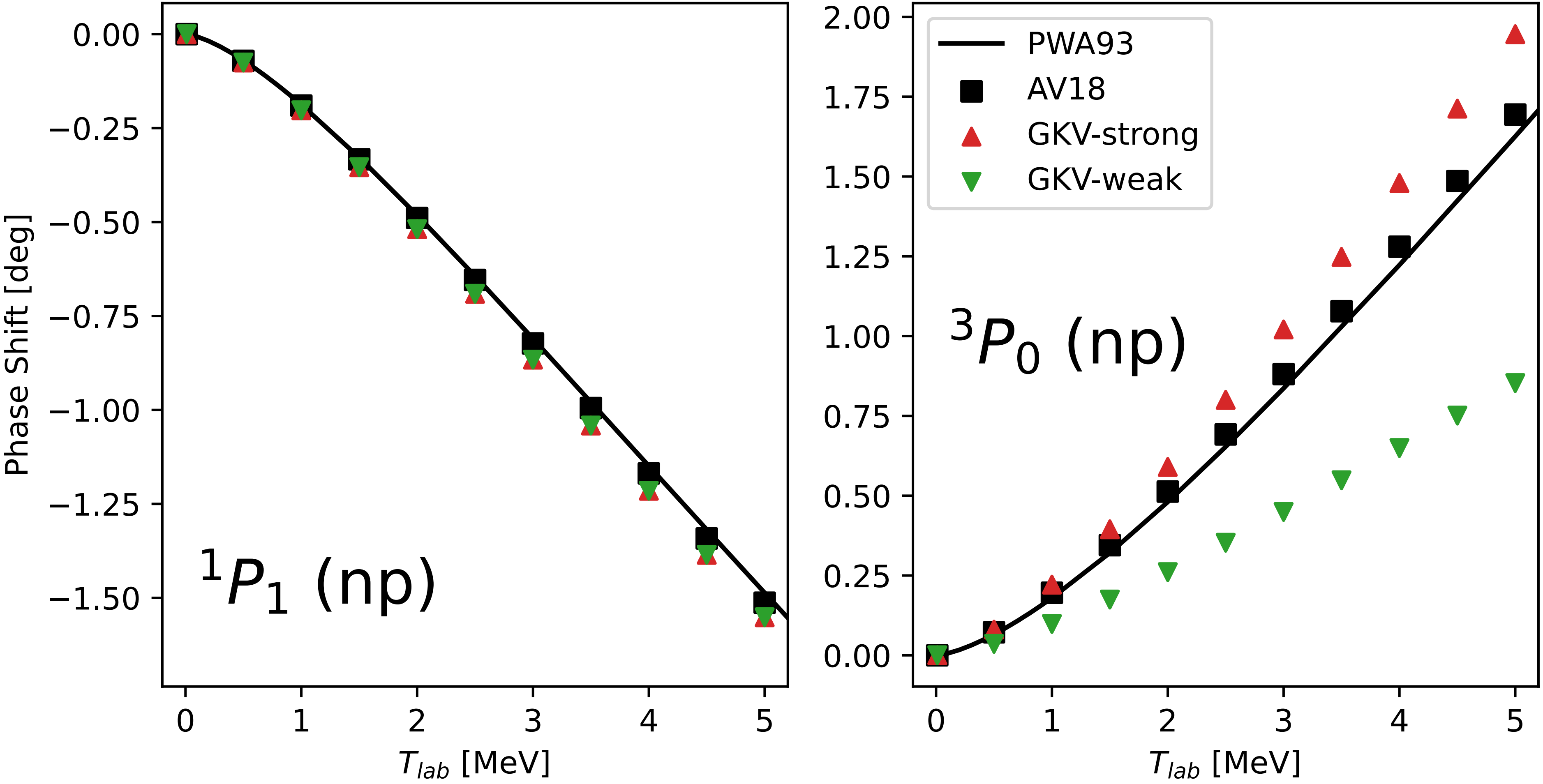
Gaussian regulators:

$R_0 \approx 1.55$ fm
$R_1 \approx 1.83$ fm
$R_3 = 1.1$ fm

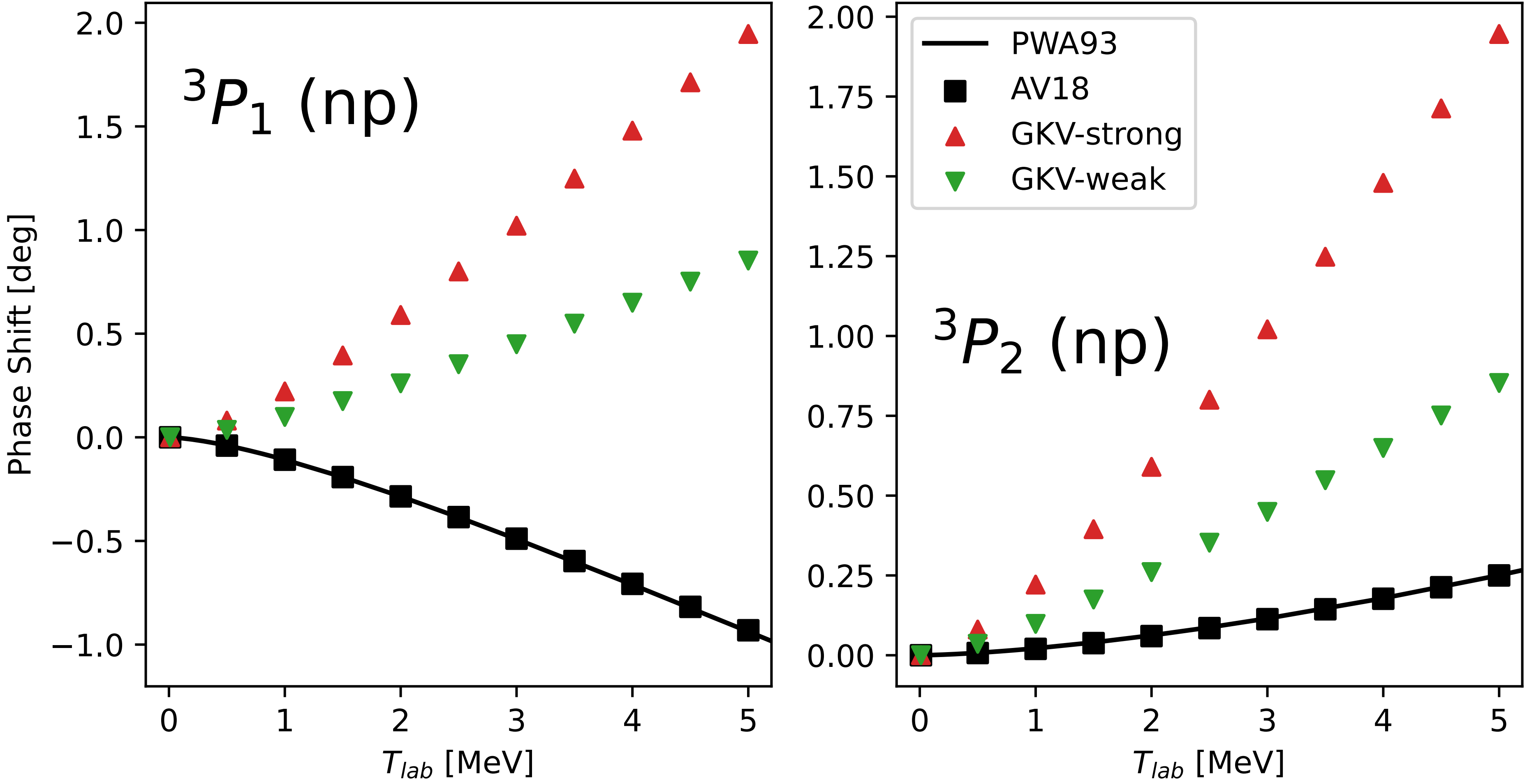
np scattering lengths and effective ranges in $S/T = 0/1,\ 1/0$

3NF fit to triton binding energy


Phase Shift [deg]
0
10
20
30
40
50
60
$^1S_0$ (np)
T_{lab} [MeV]
0
1
2
3
4
5
120
130
140
150
160
170
180
$^3S_1$ (np)
T_{lab} [MeV]
PWA93
AV18
o
CD
GKV



Phase Shift [deg]
0.00
−0.25
−0.50
−0.75
−1.00
−1.25
−1.50
$^1P_1$ (np)
0
1
2
3
4
5
T_{lab} [MeV]
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
$^3P_0$ (np)
PWA93
AV18
GKV-strong
GKV-weak
0
1
2
3
4
5
T_{lab} [MeV]


$^3P_1$ (np)
$^3P_2$ (np)
Phase Shift [deg]
T_{lab} [MeV]
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
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1
2
3
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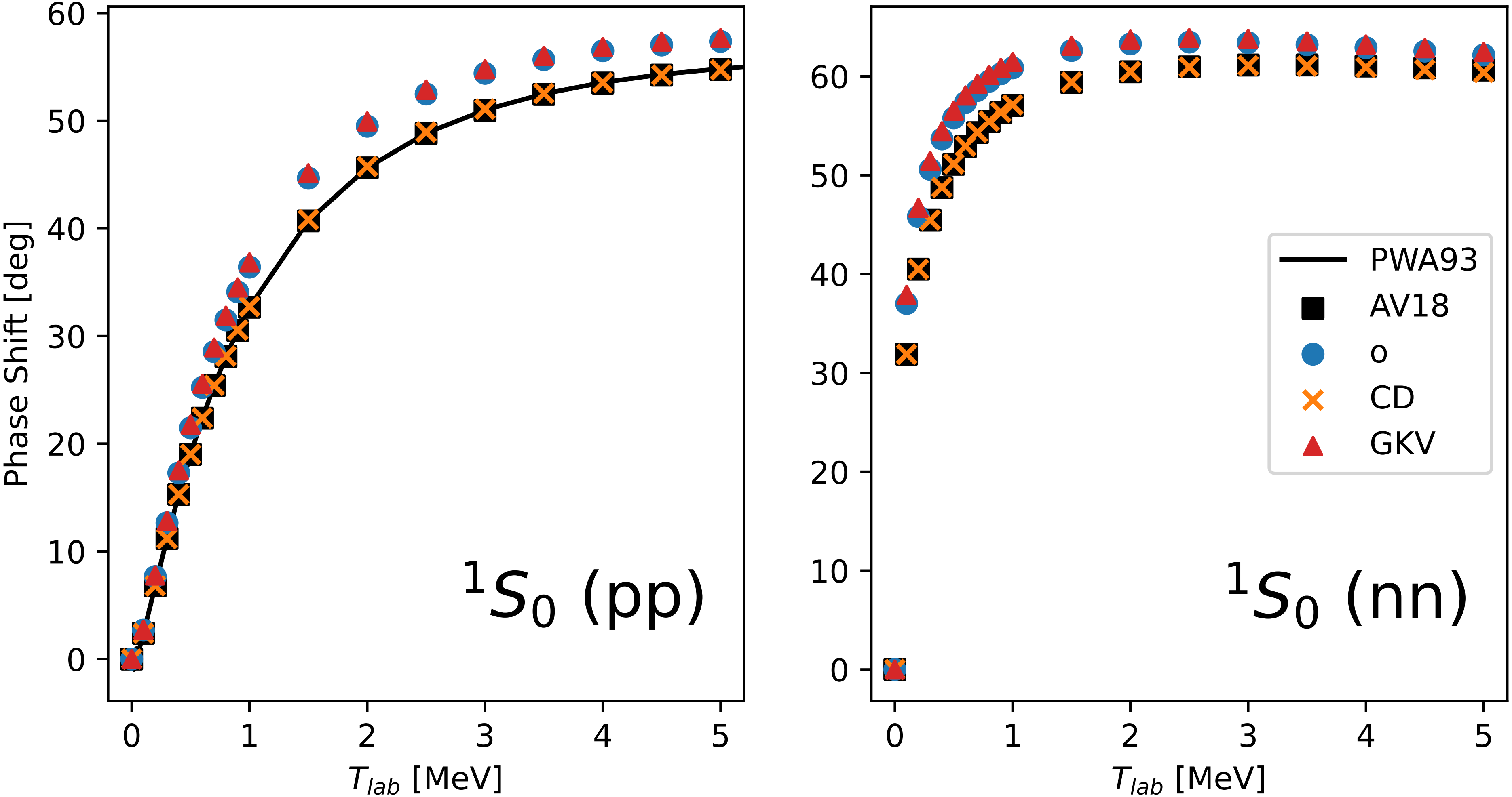
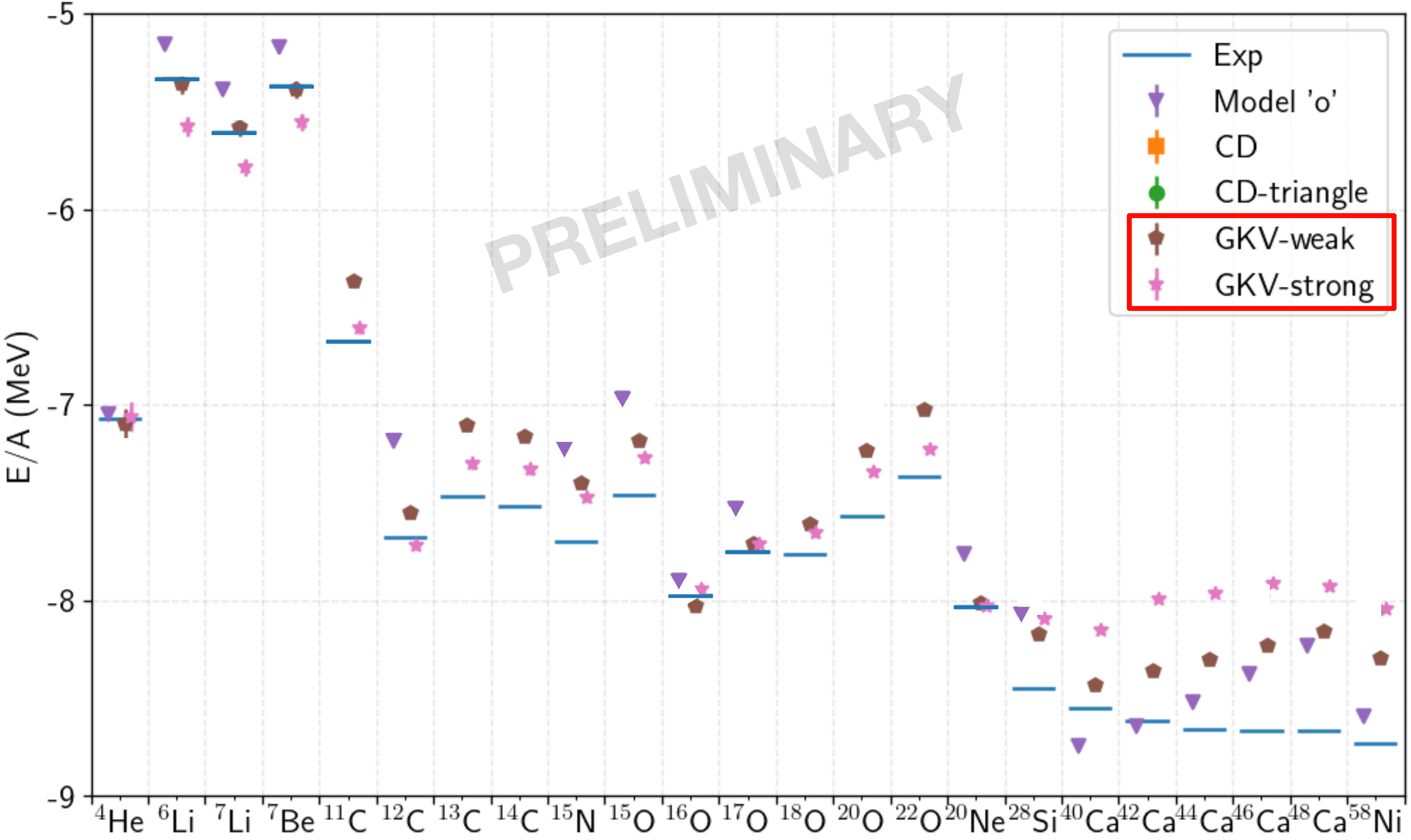
PWA93
AV18
GKV-strong
GKV-weak


Phase Shift [deg]
60
50
40
30
20
10
0
0
1
2
3
4
5
T_{lab} [MeV]
$^1S_0$ (pp)
60
50
40
30
20
10
0
T_{lab} [MeV]
$^1S_0$ (nn)
PWA93
AV18
o
CD
GKV

PRELIMINARY RESULTS: MEDIUM-MASS NUCLEI

B. Fore, JK, et al., in prep.



Add S/T = 0/0, 1/1

Fit different 3-body interactions by hand using NQS calculations of He-4 and O-16

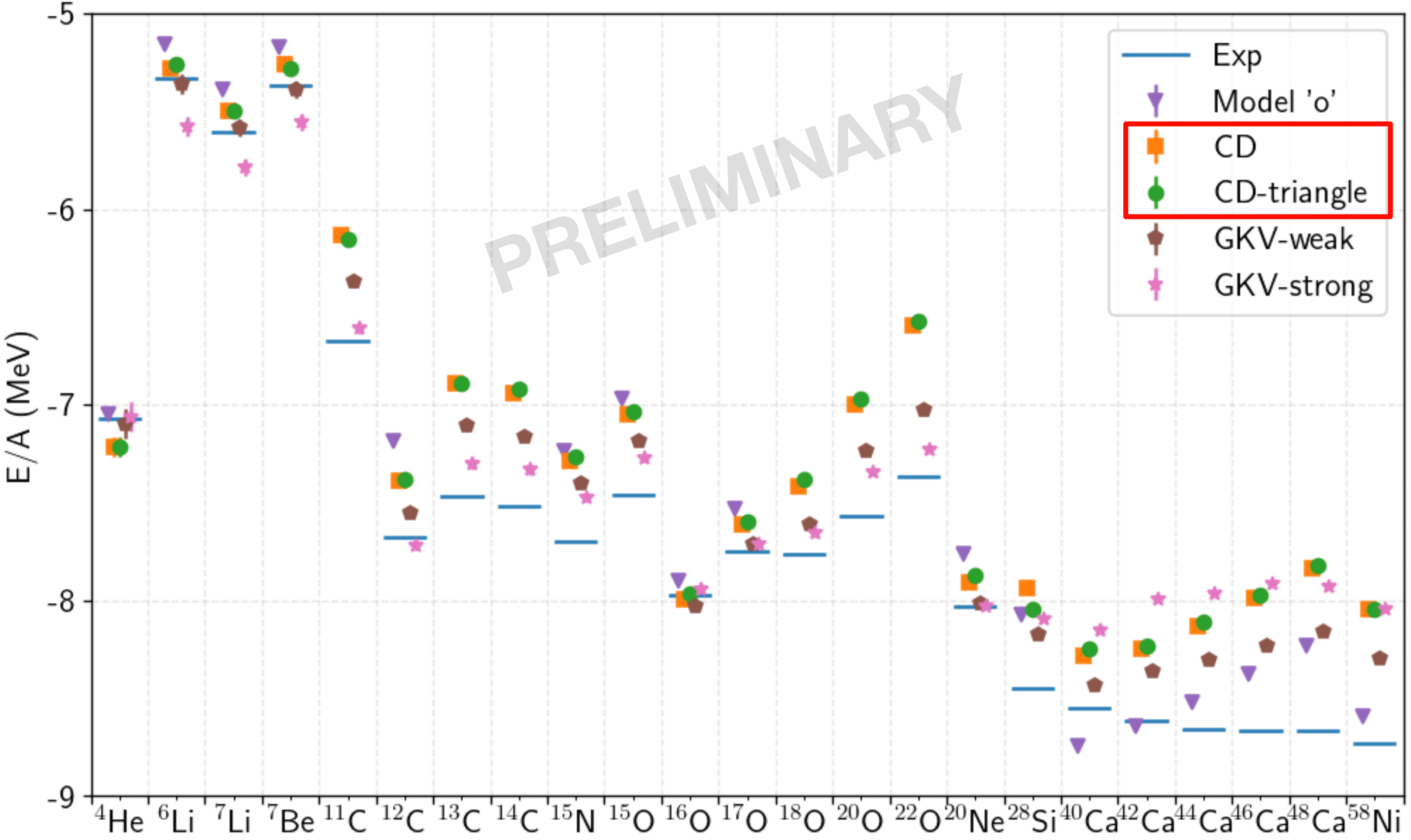
M. Gattobigio et al., PRC 100, 034004 (2019).

- s-wave scattering lengths and effective ranges
- triton binding energy
- C_{00} and C_{11} tuned to AV14 phase shifts for p-wave sector

C_{00} fixed, smaller C_{11} used for "weak" and larger for "strong"

B. Fore, JK, et al., in prep.

PRELIMINARY RESULTS: MEDIUM-MASS NUCLEI



Add CD and CA terms at LO to the 2-body interaction for $S/T = 0/1$

Fit different 3-body interactions by hand using NQS calculations of He-4 and O-16

Gaussian regulators:

$$R_0 = 1.537 \text{ fm}$$
$$R_1 = 1.813 \text{ fm}$$

Two additional LECs: C_{CD}, C_{CA}

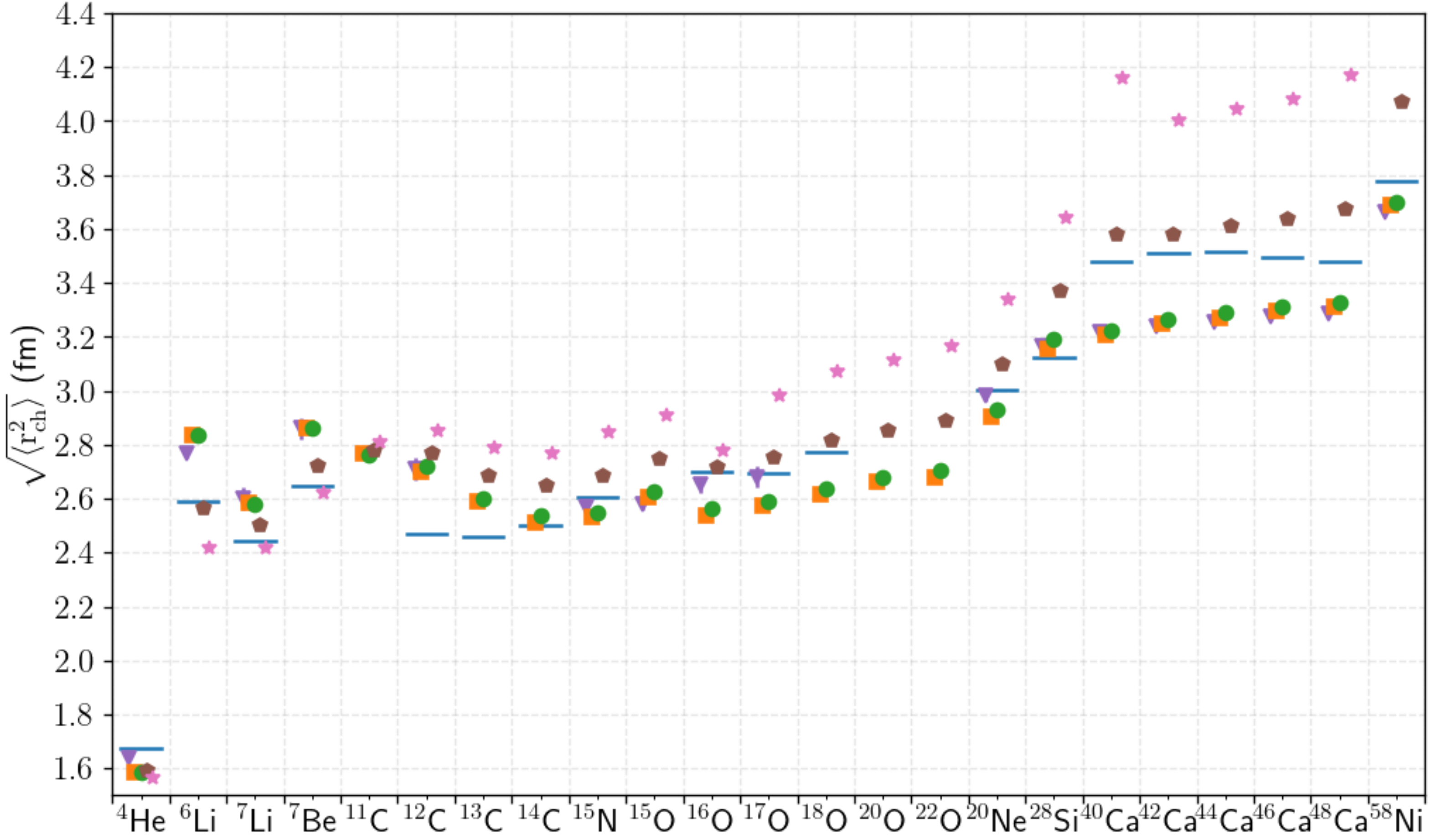
All two-body LECs fit to low-energy phase shifts up to 5 MeV

np, pp - Nijmegen

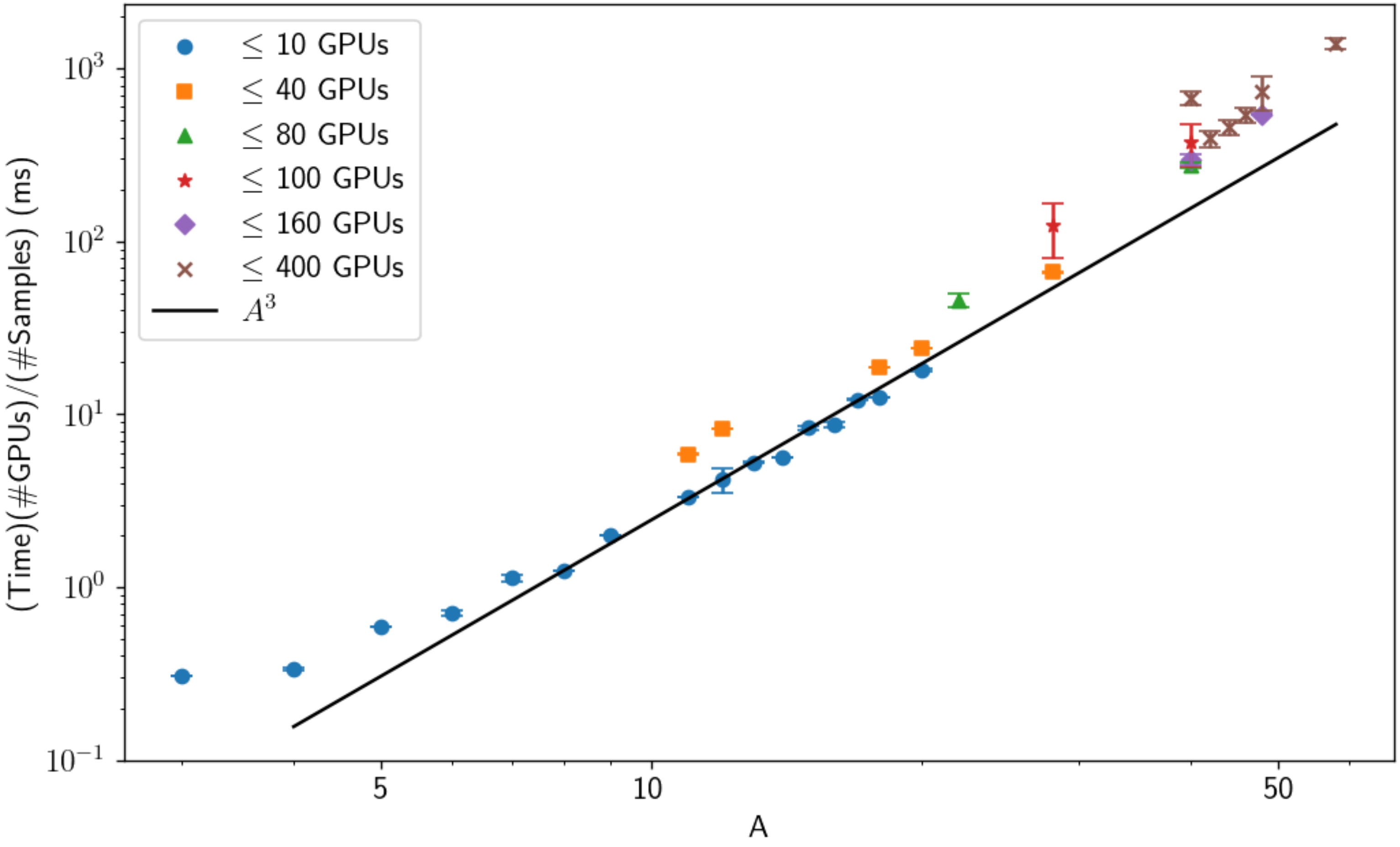
nn - Argonne $v18$

B. Fore, JK, et al., in prep.

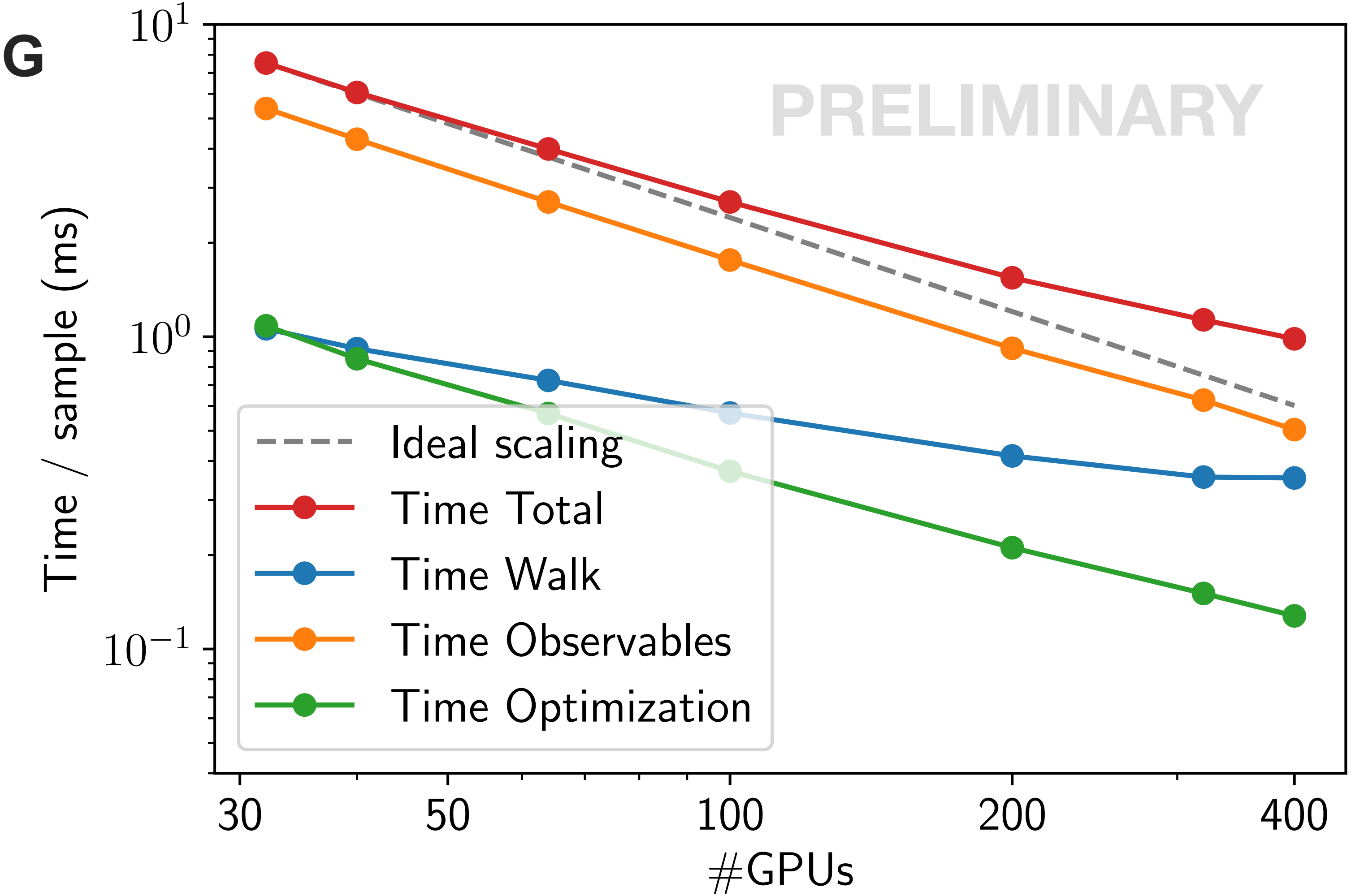
PRELIMINARY RESULTS: MEDIUM-MASS NUCLEI



SCALING


● ≤ 10 GPUs
■ ≤ 40 GPUs
▲ ≤ 80 GPUs
★ ≤ 100 GPUs
◆ ≤ 160 GPUs
× ≤ 400 GPUs
A^3
(Time)(#GPUs)/(#Samples) (ms)
10^3
10^2
10^1
10^0
10^{-1}
5
10
50
A

SCALING



PRELIMINARY
Time / sample (ms)
10^1
10^0
10^{-1}
30
50
100
200
400
#GPUs
Ideal scaling
Time Total
Time Walk
Time Observables
Time Optimization

OPEN QUESTIONS

Where should the complexity live: Hamiltonian or wave function?

What does “systematic improvability” mean for NQS?

Why do these simple interactions work better than they should for medium-mass nuclei?

What physical structures will force us to invent new NQS architectures?

Thank you!

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