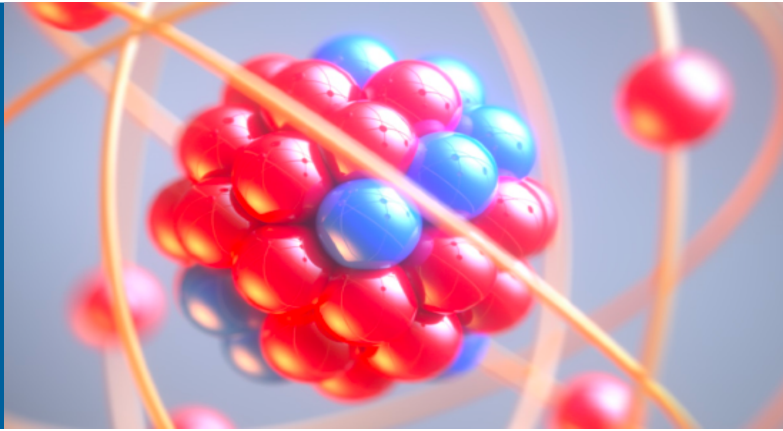
VARIATIONAL LEARNING QUANTUM WAVE FUNCTIONS



ALESSANDRO LOVATO

Argonne NATIONAL LABORATORY

QNP2024 - The 10th International Conference on Quarks and Nuclear Physics

July 10, 2024

COLLABORATORS

Argonne National Laboratory: C. Adams, **P. Fasano, B. Fore, J.Fox, A. Tropiano**, R. B. Wiringa

EPFL: G. Carleo, **J. Nys, G. Pescia**

Fermilab: N. Rocco

Los Alamos National Laboratory: S. Gandolfi

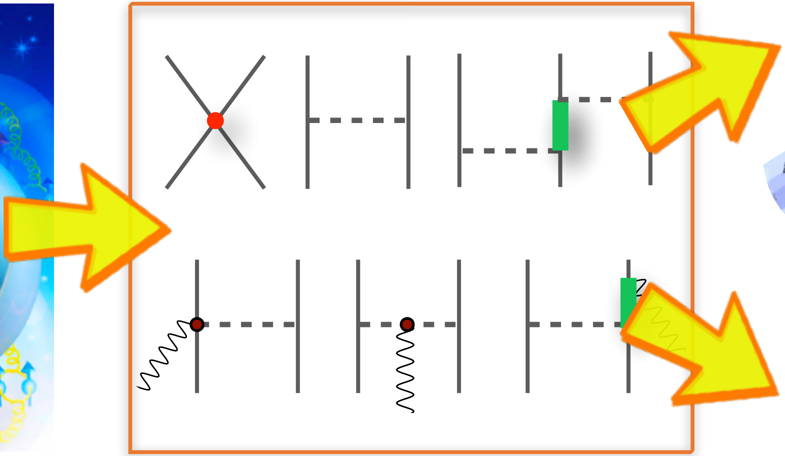
Michigan State University: M. Hjorth-Jensen

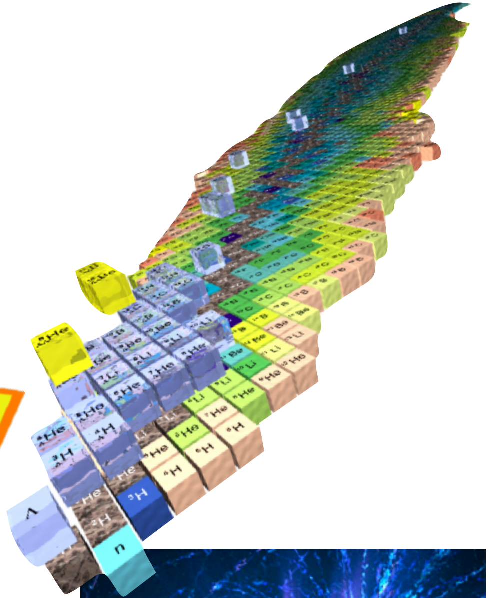
Ohio University: **J. Kim**

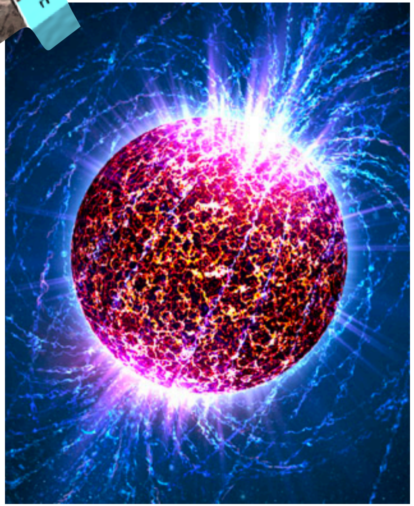
SISSA: M. Rigo

University of Trento: **A. Di Donna,** F. Pederiva

"AB-INITIO" NUCLEAR THEORY

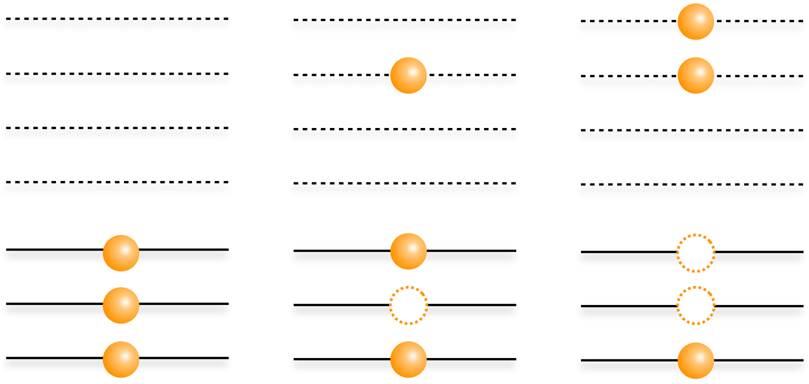






CONFIGURATION-INTERACTION METHODS

$$\Psi_0(x_1, \ldots, x_A) = \sum_n c_n \Phi_n(x_1, \ldots, x_A)$$



$|\Phi_0\rangle$ $|\Phi_{h_2}^{p_3}\rangle$ $|\Phi_{h_2 h_3}^{p_3 p_4}\rangle$

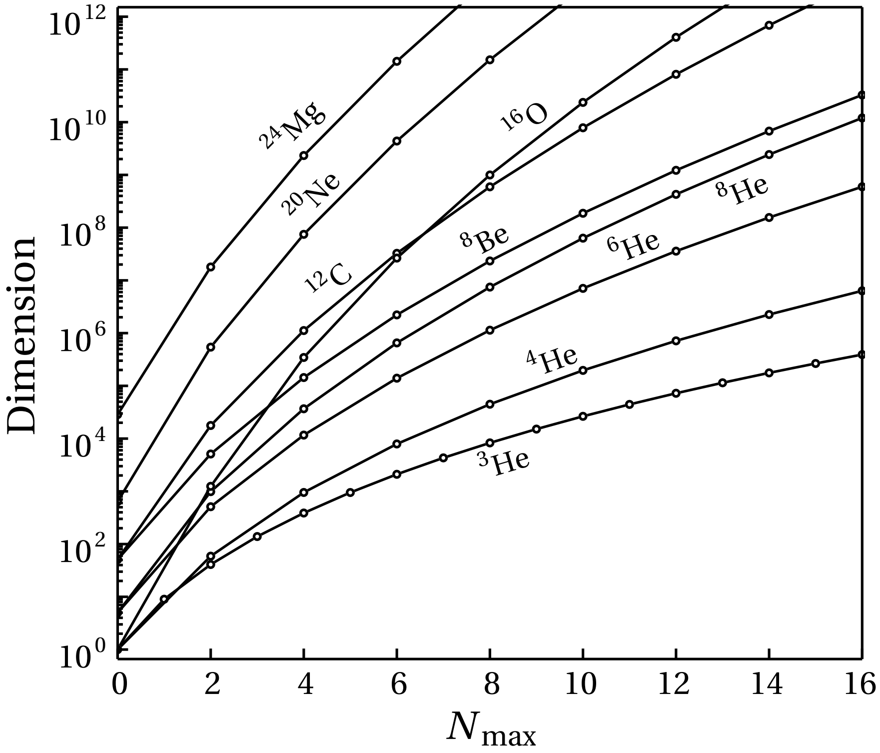
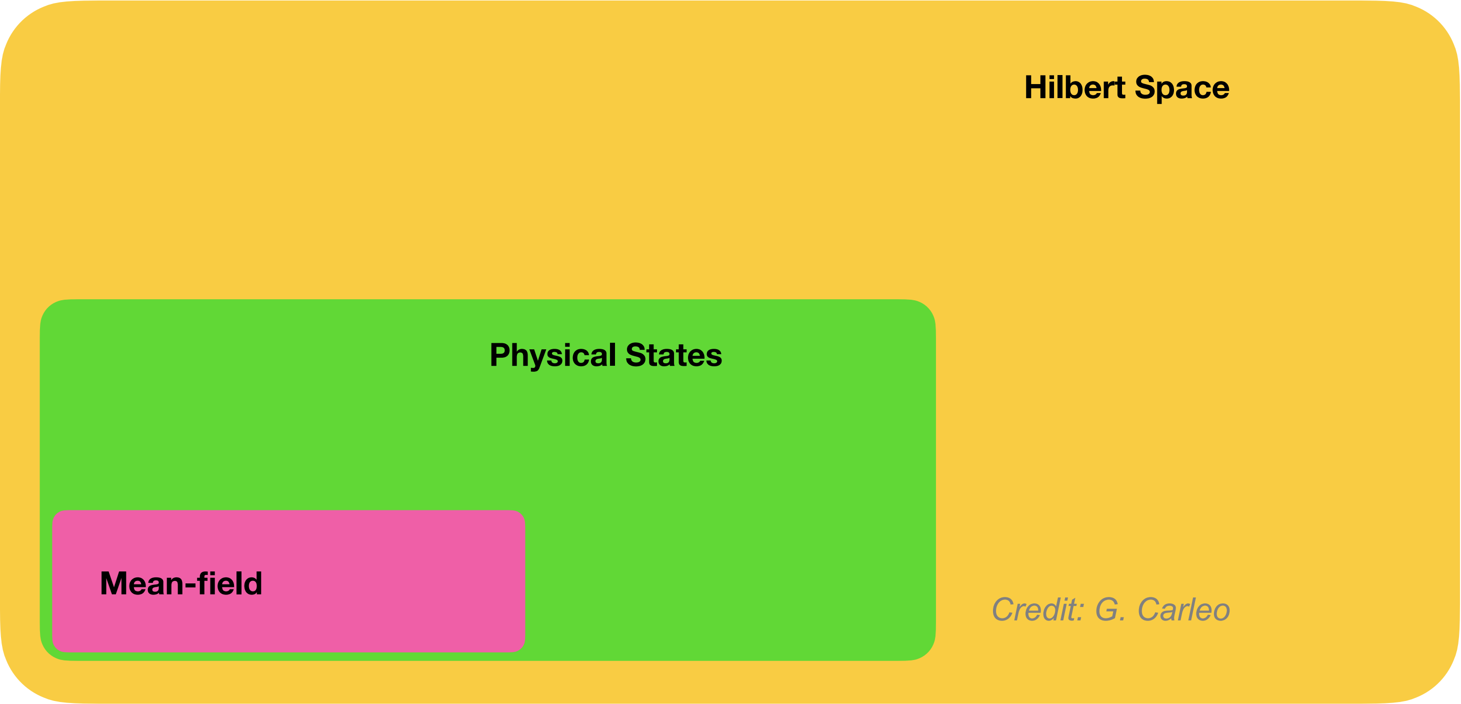


Image courtesy of Patrick Fasano

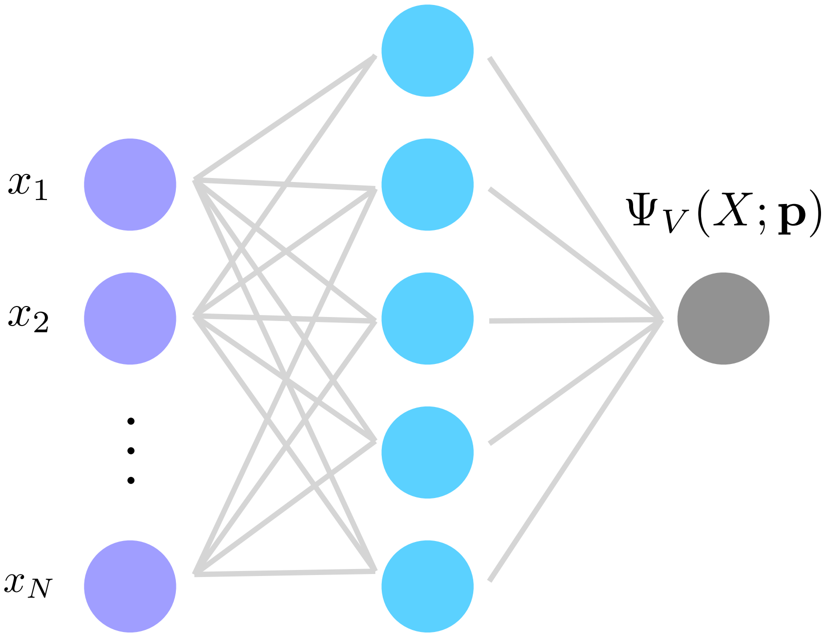
NEURAL-NETWORK QUANTUM STATES

Quantum states of physical interest have distinctive features and intrinsic structures



NEURAL-NETWORK QUANTUM STATES

NQS are now widely and successfully applied to study condensed-matter systems



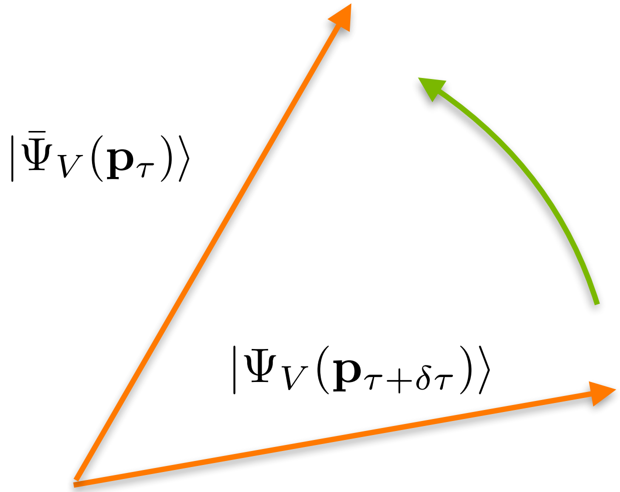
$$E_V \equiv \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} > E_0$$

$$E_V \simeq \frac{1}{N} \sum_{X \in |\Psi_V(X)|^2} \frac{\langle X | H | \Psi_V \rangle}{\langle X | \Psi_V \rangle}$$

WAVE FUNCTION OPTIMIZATION

ANN trained by performing an imaginary-time evolution in the variational manifold

$$
\begin{cases}
|\bar{\Psi}_V(\mathbf{p}_\tau\rangle \equiv (1 - H\delta\tau)|\Psi_V(\mathbf{p}_\tau)\rangle \\
\mathbf{p}_{\tau+\delta\tau} = \underset{\mathbf{p}\in R^d}{\arg\max}\left(\left|\langle\bar{\Psi}_V(\mathbf{p}_\tau)|\Psi_V(\mathbf{p}_{\tau+\delta\tau})\rangle\right|^2\right)
\end{cases}
$$



The parameters are updated as

$$
\mathbf{p}_{\tau+\delta\tau} = \mathbf{p}_\tau - \delta\tau S^{-1}\mathbf{g}_\tau
$$

J. Stokes, at al., Quantum 4, 269 (2020).

S. Sorella, Phys. Rev. B 64, 024512 (2001)

NEURAL-NETWORK QUANTUM STATES

Nucleons are fermions

$$\Psi_V(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_A) = -\Psi_V(x_1, \ldots, x_j, \ldots, x_i, \ldots, x_A)$$

Slater-Jastrow ansatz

$$\Psi_V(X) = e^{J(X)}\Phi(X) \quad ; \quad \Phi(X) = \det \begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_1(\mathbf{x}_2) & \cdots & \phi_1(\mathbf{x}_N) \\ \phi_2(\mathbf{x}_1) & \phi_2(\mathbf{x}_2) & \cdots & \phi_2(\mathbf{x}_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(\mathbf{x}_1) & \phi_N(\mathbf{x}_2) & \cdots & \phi_N(\mathbf{x}_N) \end{bmatrix}$$

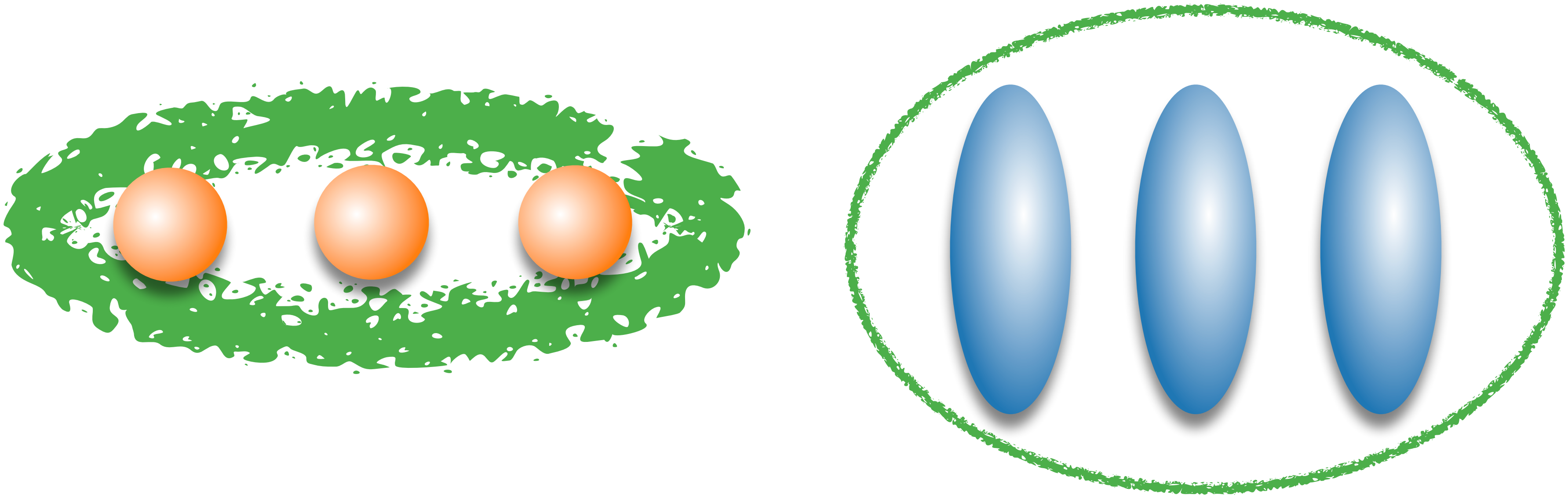
*J. Stokes et al., PLB, **102**, 205122 (2020)*

*Pfau et al., PRR **2**, 033429 (2020)*

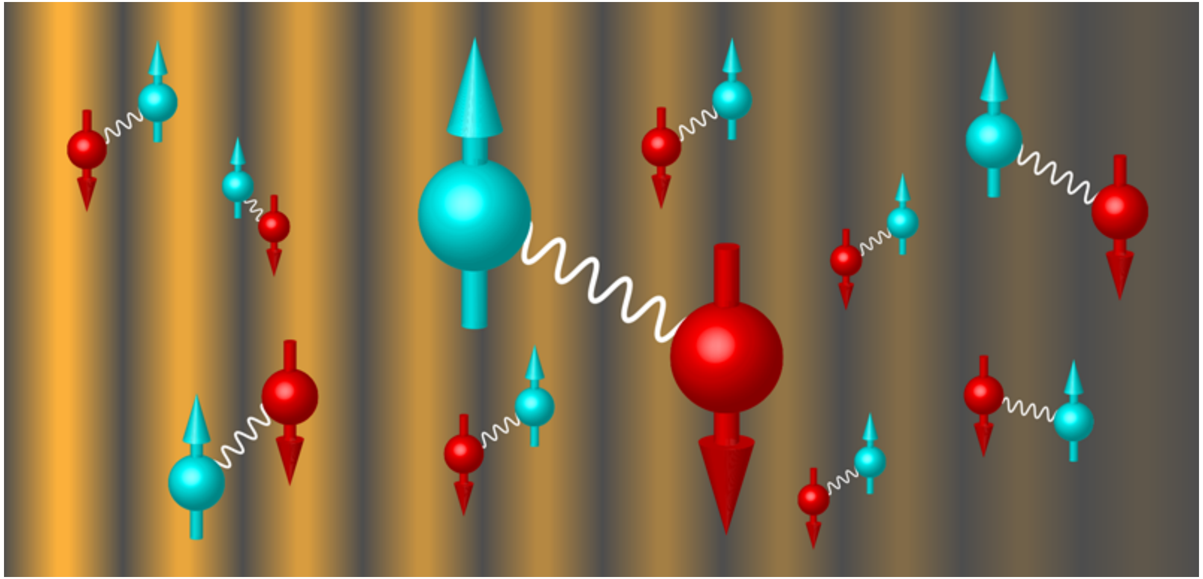
*Hermann et al., Nature Chemistry, **12**, 891 (2020)*

NEURAL BACKFLOW CORRELATIONS

The nodal structure is improved with neural back-flow transformations $\mathbf{x}_i \rightarrow \phi(\mathbf{x}_i; \mathbf{x}_{j\neq i})$



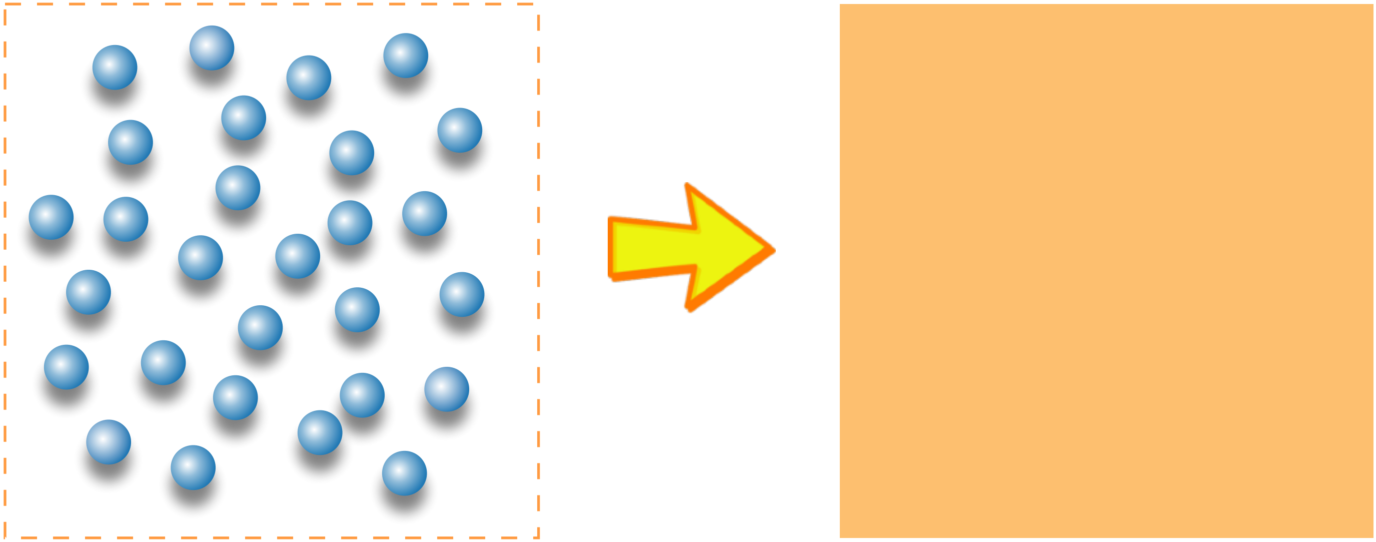
CONDENSED-MATTER DETOUR



HOMOGENOUS ELECTRON GAS

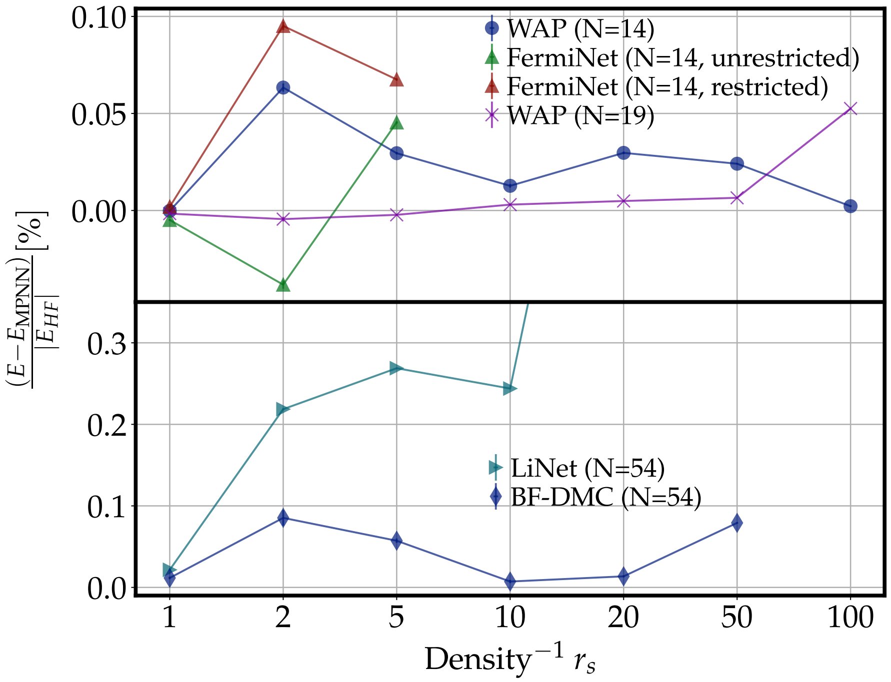
We develop translation invariant NQS to study the Homogeneous Electron Gas.

$$H = -\frac{1}{2r_s^2}\sum_{i}^{N}\nabla_{\vec{r}_i}^2 + \frac{1}{r_s}\sum_{i<j}^{N}\frac{1}{||\vec{r}_i - \vec{r}_j||} + \text{const.}$$

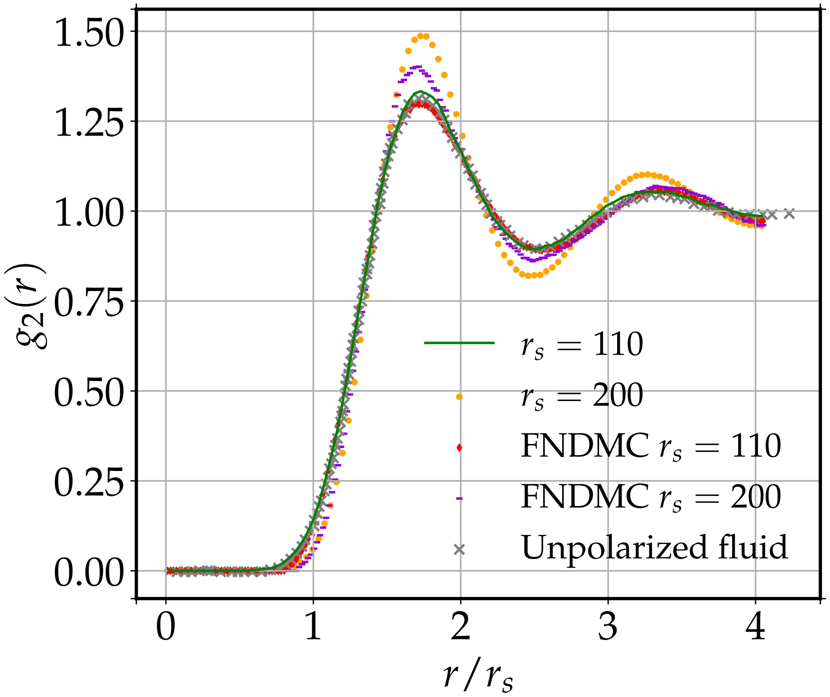


HOMOGENOUS ELECTRON GAS

Energies



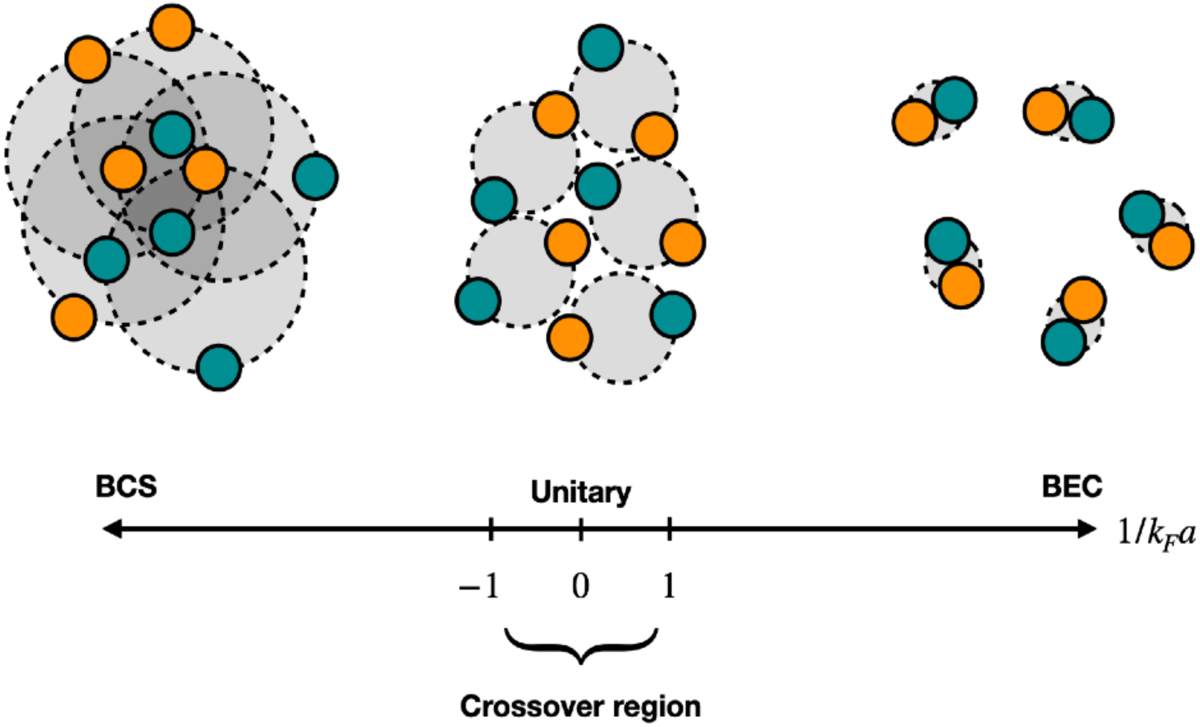
Correlation functions



G. Pescia, et al., Phys. Rev. B **110** (2024) 3, 035108

COLD FERMI GASES

Periodic-NQS to solve the two-components Fermi gas in the BCS- BEC crossover region



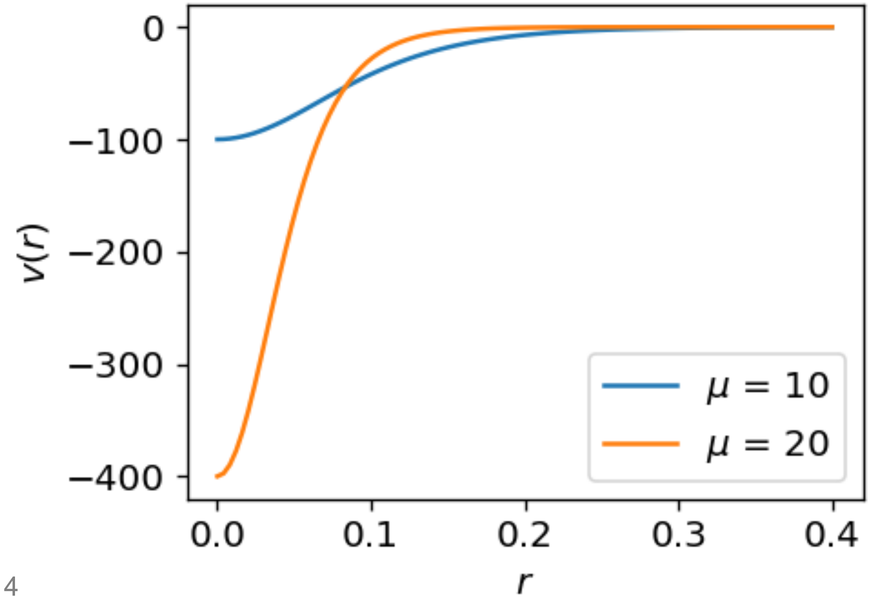
COLD FERMI GASES

We model the 3D unpolarized gas of fermions with the Hamiltonian

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} v_{ij}$$

- Modified Pöschl-Teller potential between opposite-spin particles

$$v_{ij} = (\delta_{s_i,s_j} - 1) v_0 \frac{2\hbar^2}{m} \frac{\mu^2}{\cosh^2(\mu r_{ij})}$$



COLD FERMI GASES

We introduce a Pfaffian-Jastrow ansatz

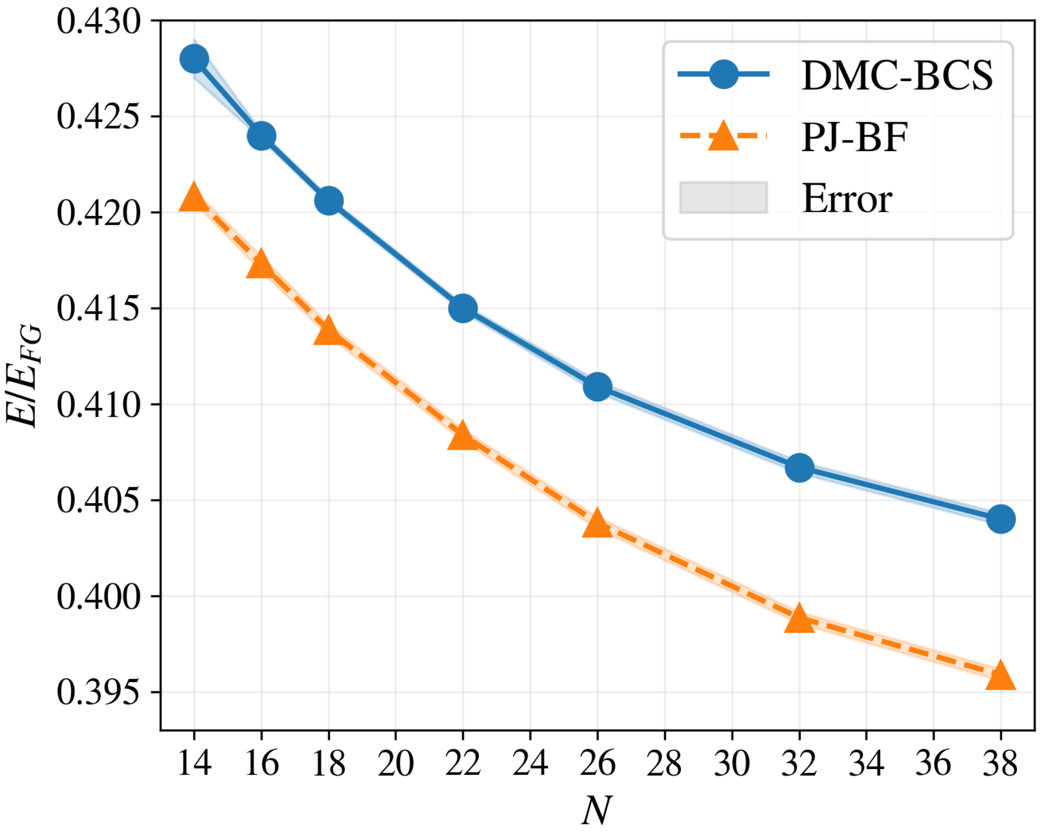
$$\Phi_{PJ}(X) = \text{pf}\begin{bmatrix} 0 & \phi(x_1, x_2) & \cdots & \phi(x_1, x_N) \\ \phi(x_2, x_1) & 0 & \cdots & \phi(x_2, x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(x_N, x_1) & \phi(x_N, x_2) & \cdots & 0 \end{bmatrix}$$

In order for the above matrix to be skew-symmetric, the neural pairing orbitals are taken to be

$$\phi(x_i, x_j) = \eta(x_i, x_j) - \eta(x_j, x_i)$$

Example: $$\text{pf}\begin{bmatrix} 0 & \phi_{12} & \phi_{13} & \phi_{14} \\ -\phi_{12} & 0 & \phi_{23} & \phi_{24} \\ -\phi_{13} & -\phi_{23} & 0 & \phi_{34} \\ -\phi_{14} & -\phi_{24} & -\phi_{34} & 0 \end{bmatrix} = \phi_{12}\phi_{34} - \phi_{13}\phi_{24} + \phi_{14}\phi_{23}$$

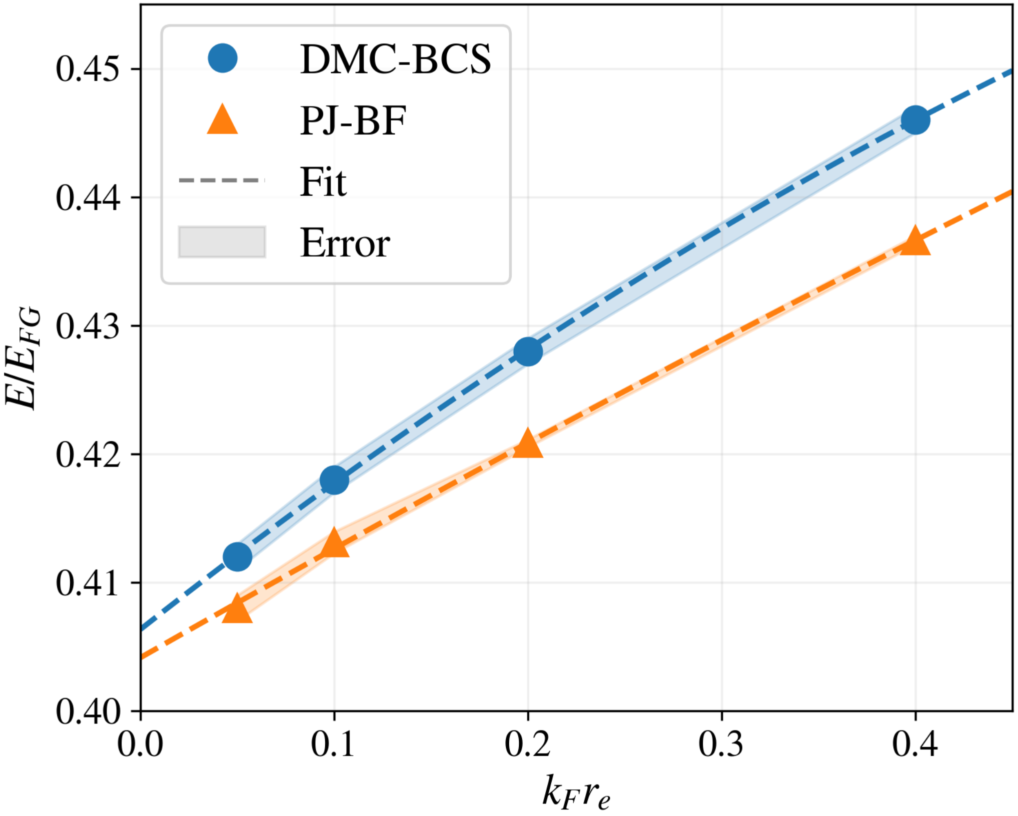
COLD FERMI GASES



$$\left(\frac{E}{E_{FG}}\right)_{\mathrm{exp}} = \xi = 0.376(5)$$

J. Kim, B. Fore, AL, et al. *Commun.Phys.* **7** (2024) 1, 148

COLD FERMI GASES



$$\left(\frac{E}{E_{FG}}\right)_{\mathrm{exp}} = \xi = 0.376(5)$$

J. Kim, B. Fore, AL, et al. Commun.Phys. **7** (2024) 1, 148

BACK TO NUCLEAR PHYSICS

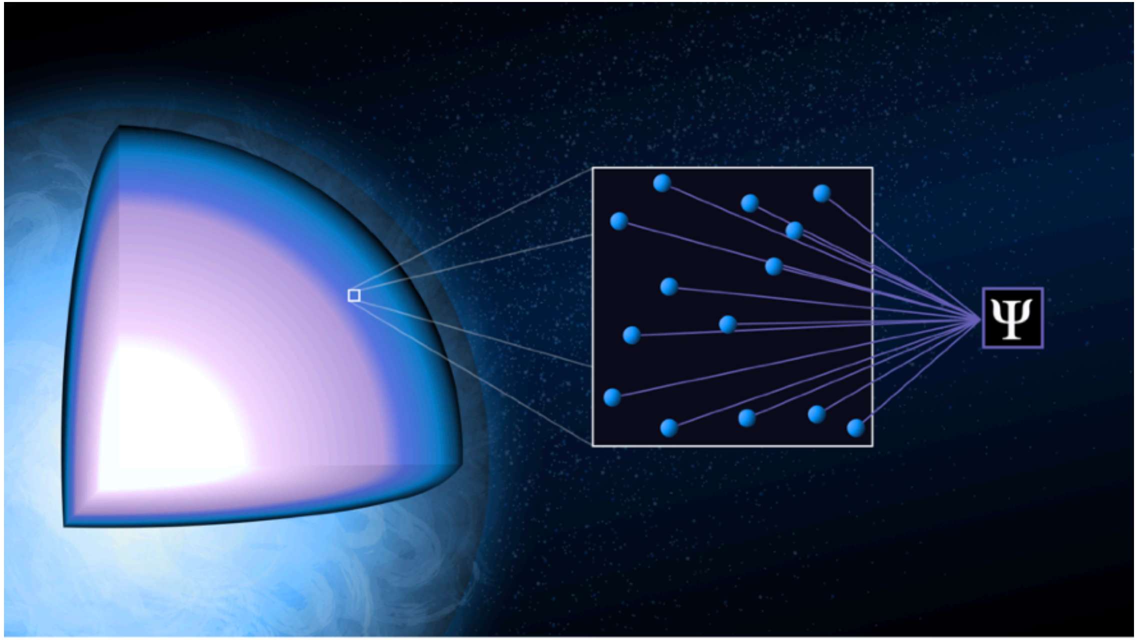
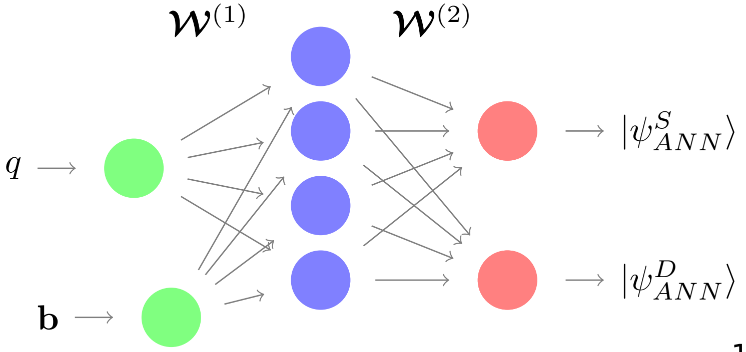
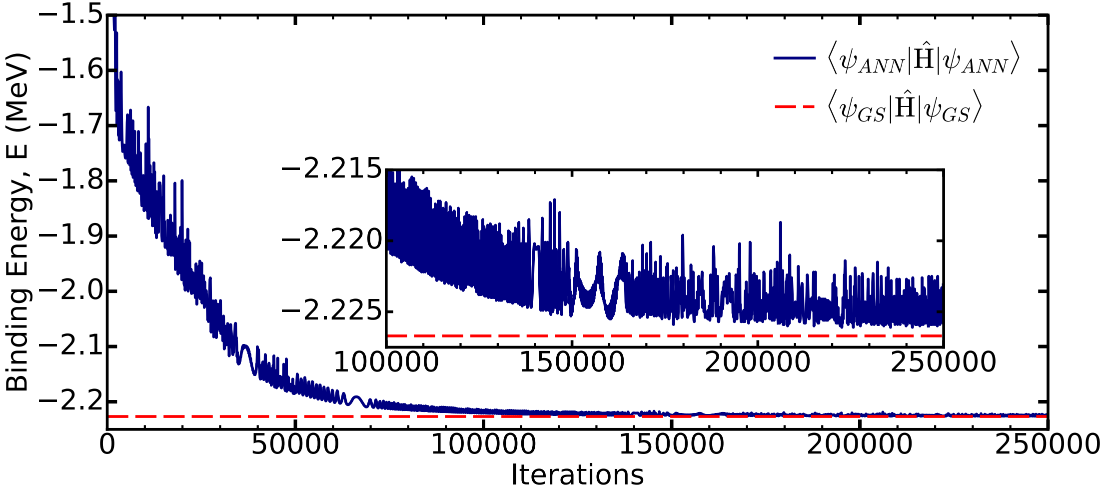


Image Credit: Jane Kim

NEURAL-NETWORK QUANTUM STATES



$$E^{\mathcal{W}} = \frac{\left\langle \Psi^{\mathcal{W}}_{\text{ANN}} \right| \hat{H} \left| \Psi^{\mathcal{W}}_{\text{ANN}} \right\rangle}{\left\langle \Psi^{\mathcal{W}}_{\text{ANN}} \middle| \Psi^{\mathcal{W}}_{\text{ANN}} \right\rangle}$$



*Keeble, Rios, PLB **809**, 135743 (2020)*

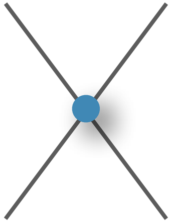
*Sarmiento, et al., EPJ **139** (2024) 2, 189*

“ESSENTIAL" HAMILTONIAN

Input: Hamiltonian inspired by a LO pionless-EFT expansion

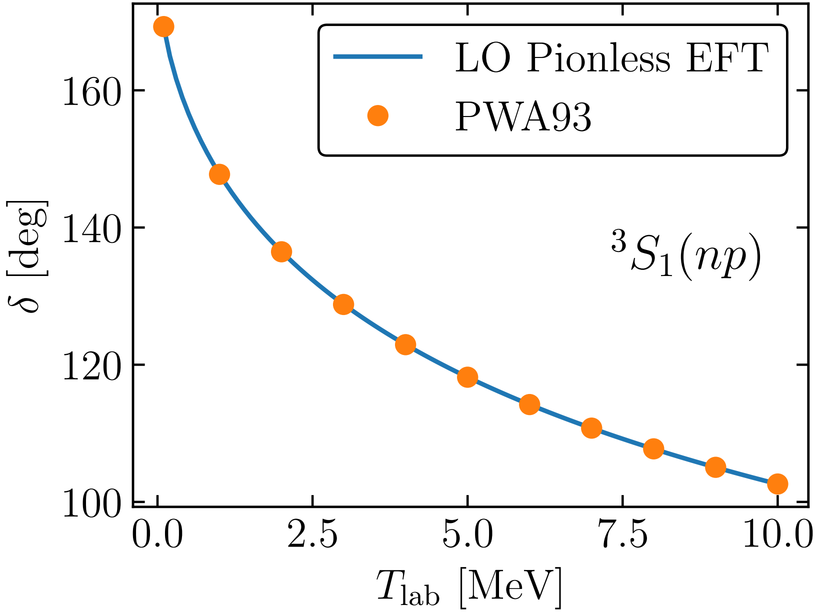
$$H_{LO} = -\sum_i \frac{\vec{\nabla}_i^2}{2m_N} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

- NN potential fit to s-wave np scattering lengths and effective ranges



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

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



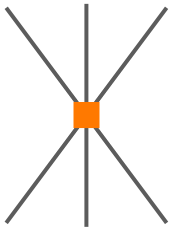
R. Schiavilla, AL, PRC **103**, 054003 (2021)

"ESSENTIAL" HAMILTONIAN

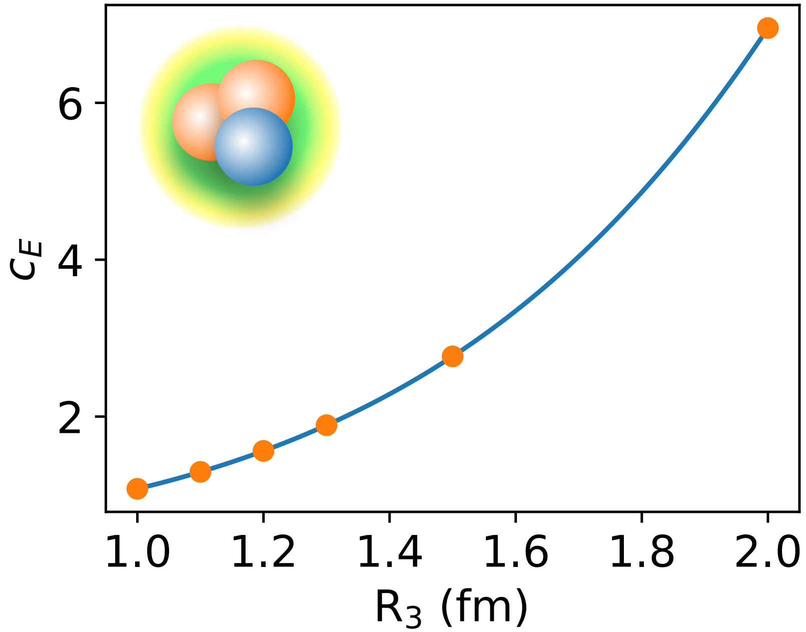
Input: Hamiltonian inspired by a LO pionless-EFT expansion

$$H_{LO} = -\sum_i \frac{\vec{\nabla}_i^2}{2m_N} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

- 3NF adjusted to reproduce the energy of ^{3}H.



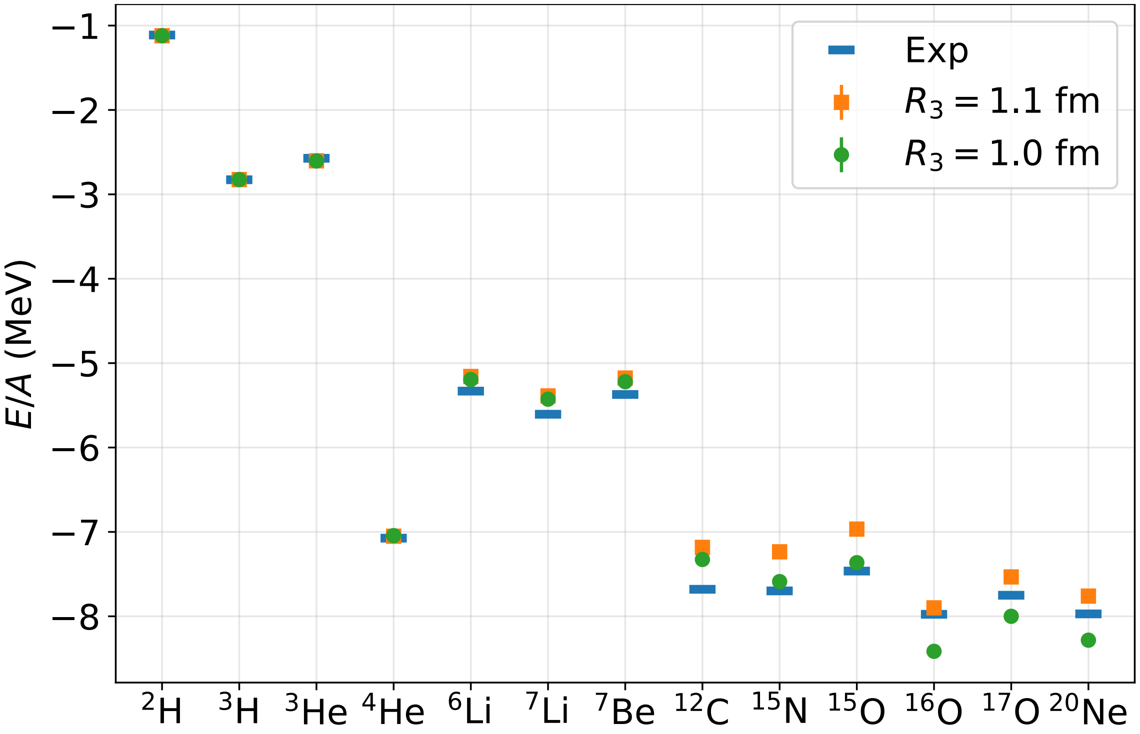
$$V_{ijk} \propto c_E \sum_{\text{cyc}} e^{-(r_{ij}^2 + r_{jk}^2)/R_3^2}$$



R. Schiavilla, AL, PRC **103**, 054003 (2021)

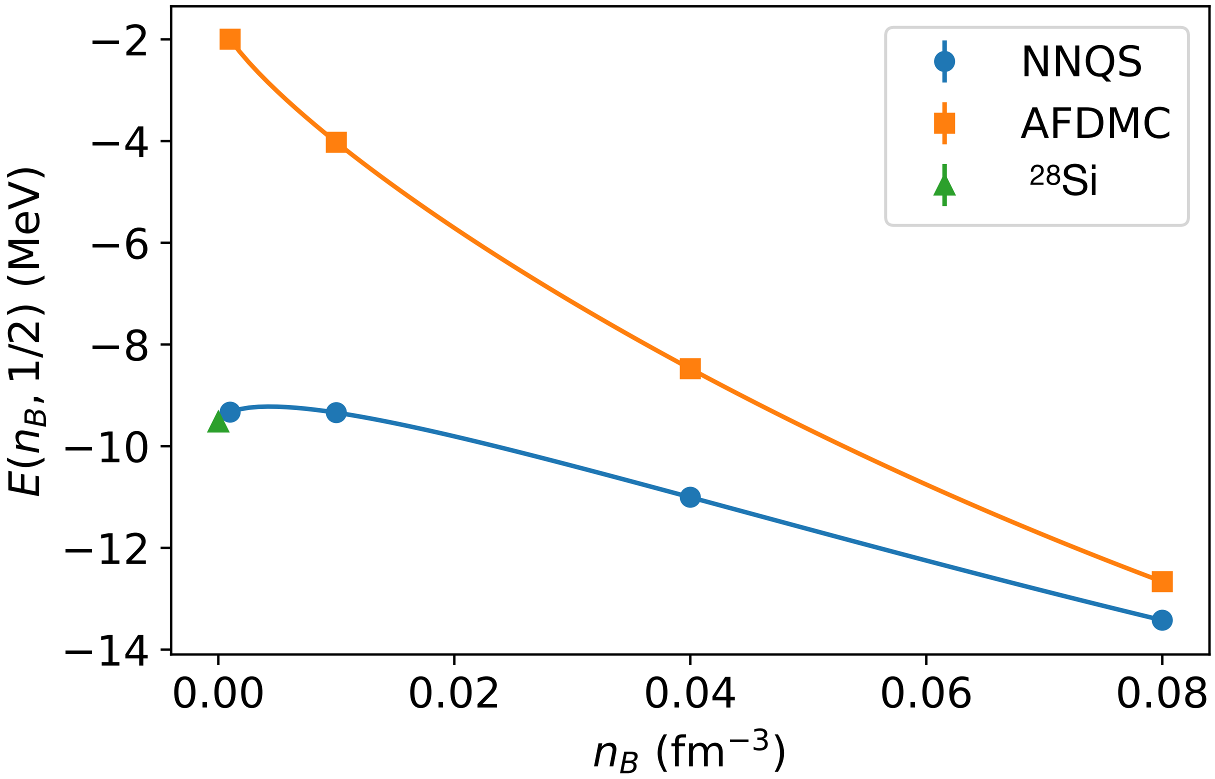
“ESSENTIAL" HAMILTONIAN

Our “essential” Hamiltonian reproduces well the spectrum of different nuclei



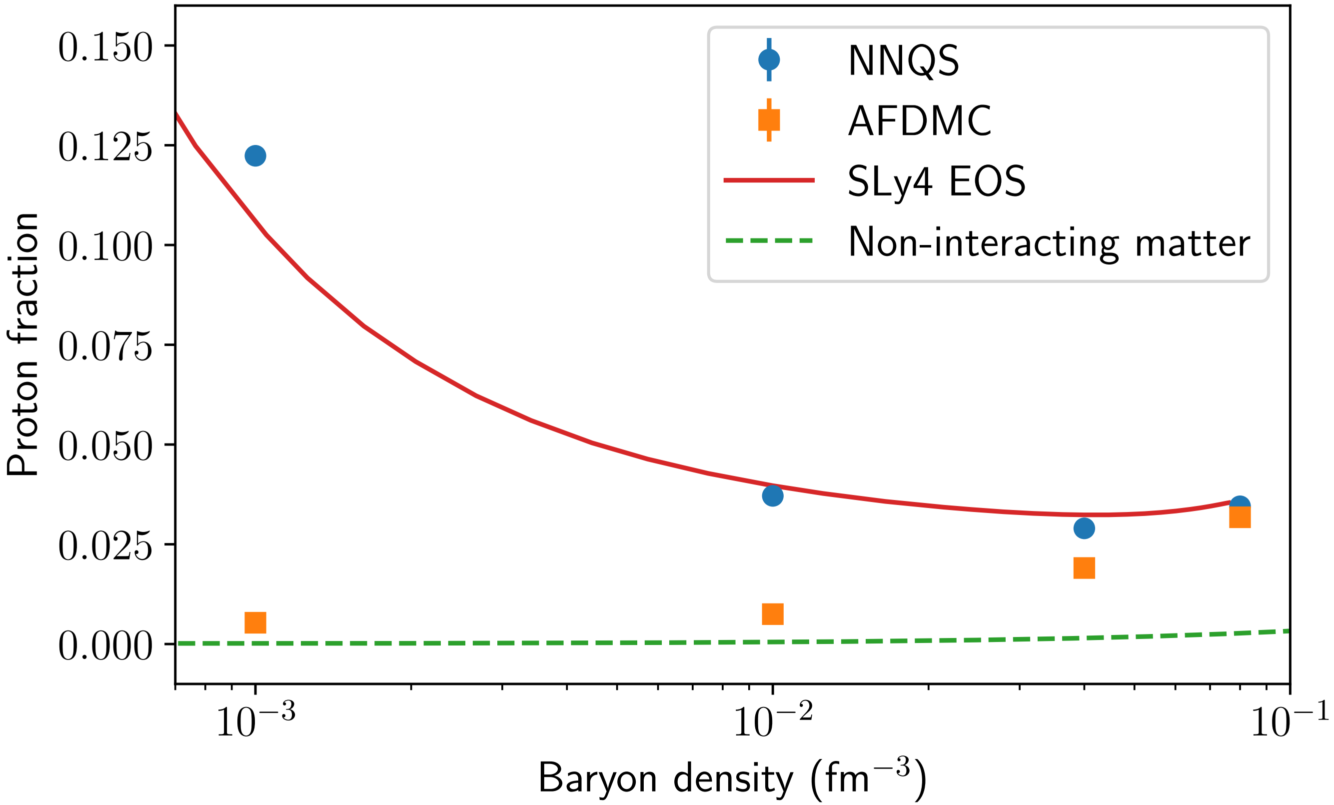
A. Gnech, AL, et al., 2308.16266

DILUTE NUCLEONIC MATTER



B. Fore, AL, et al. in preparation

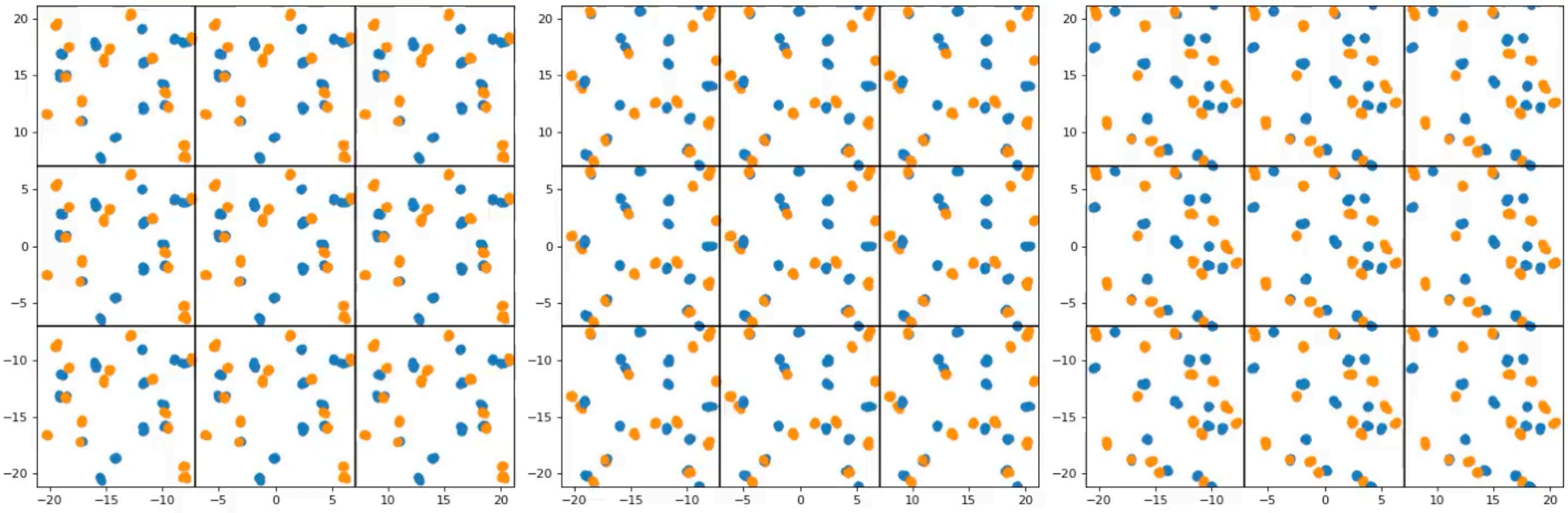
DILUTE NUCLEONIC MATTER



B. Fore, AL, et al. in preparation

DILUTE NUCLEONIC MATTER

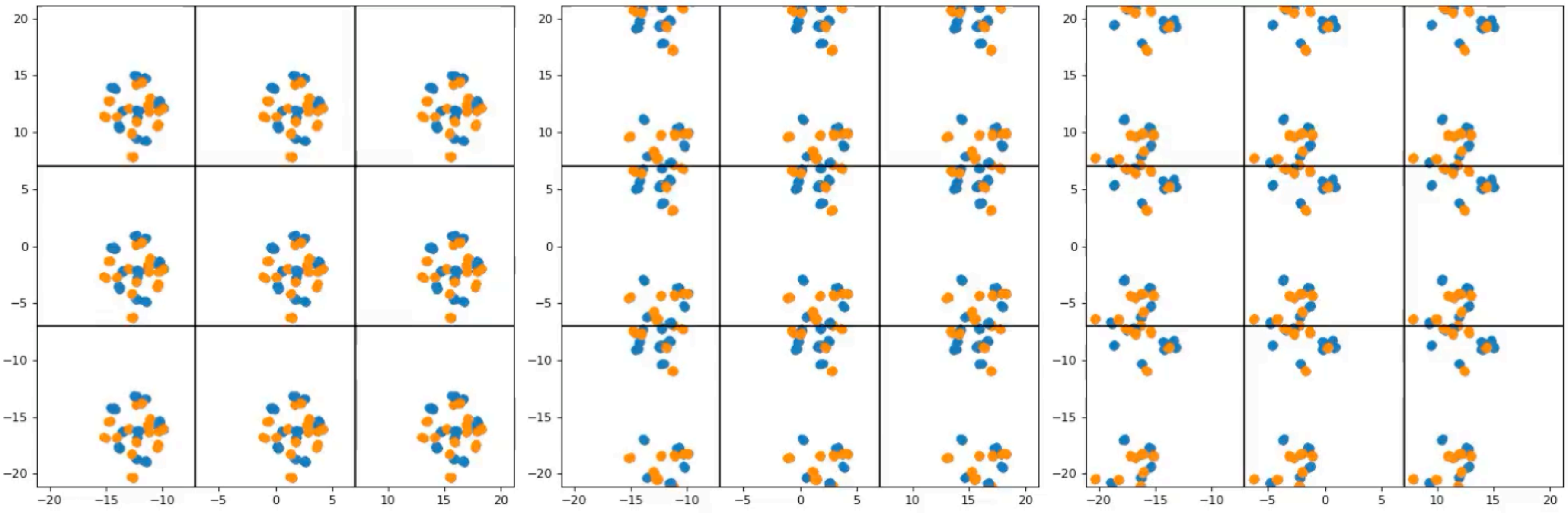
14 Neutrons, 14 Protons @ ρ=0.01 fm^{-3}



B. Fore, AL, et al. in preparation

DILUTE NUCLEONIC MATTER

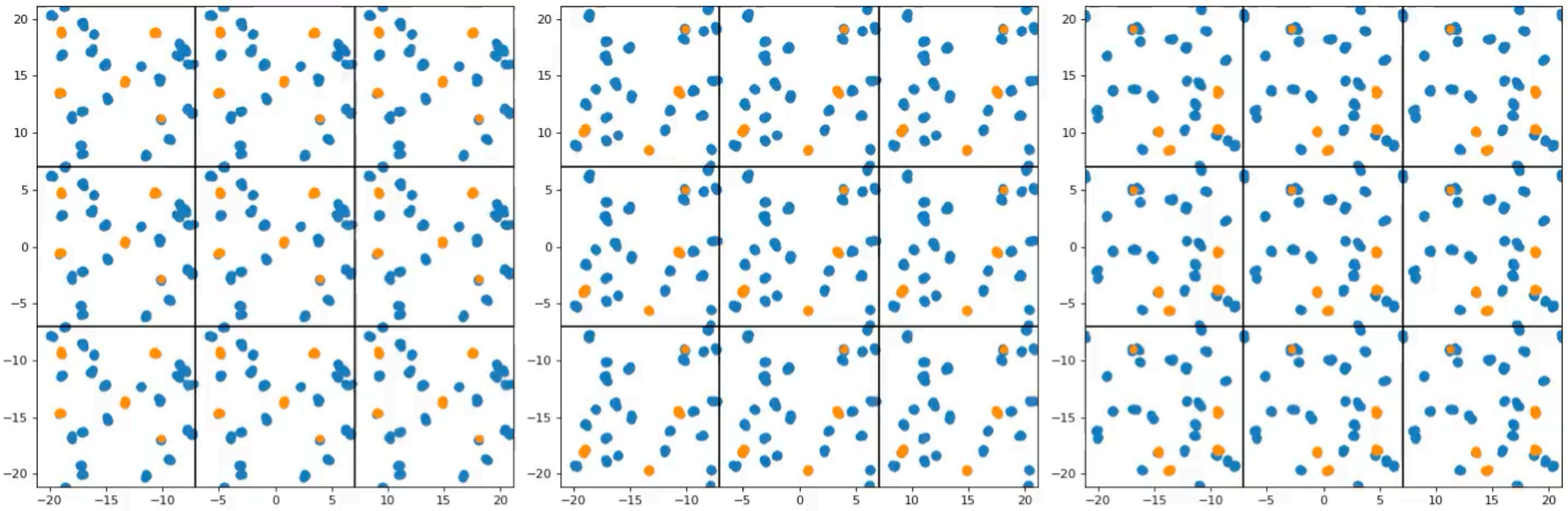
14 Neutrons, 14 Protons @ ρ=0.01 fm^{-3}



B. Fore, AL, et al. in preparation

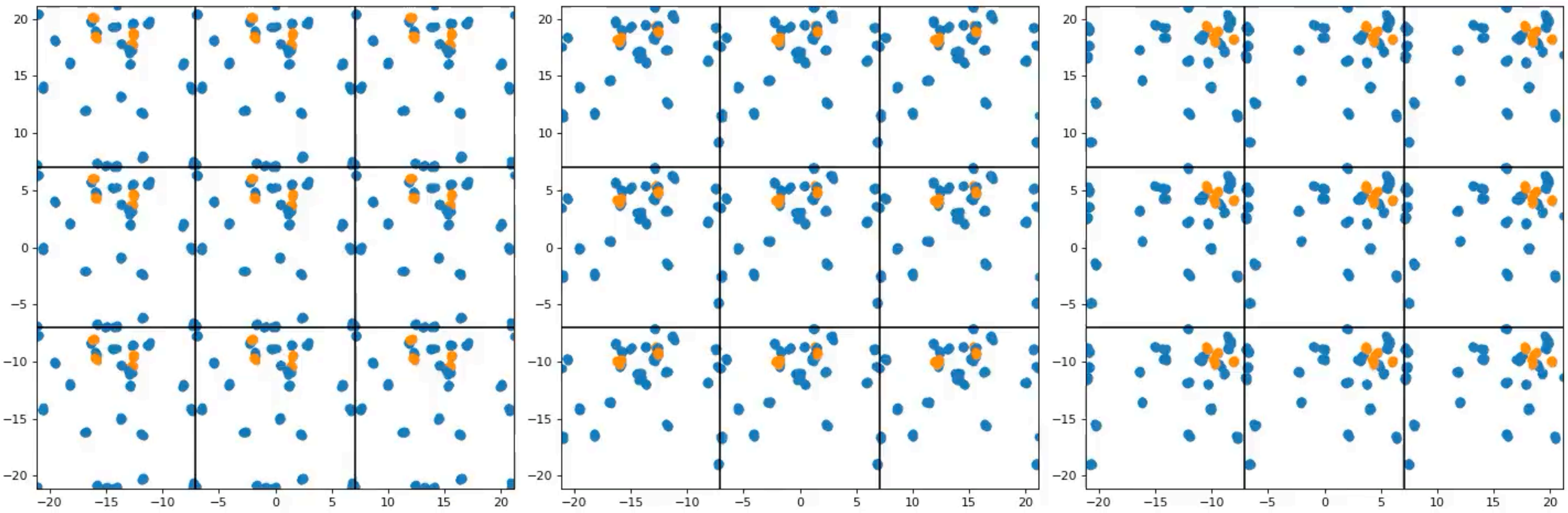
DILUTE NUCLEONIC MATTER

24 Neutrons, 4 Protons @ ρ=0.01 fm^{-3}

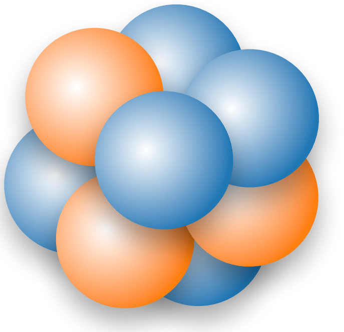


DILUTE NUCLEONIC MATTER

24 Neutrons, 4 Protons @ ρ=0.01 fm^{-3}

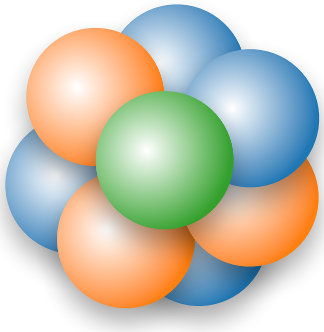


HYPERNUCLEI



$^{12}\mathrm{C}$

6 protons, 6 neutrons

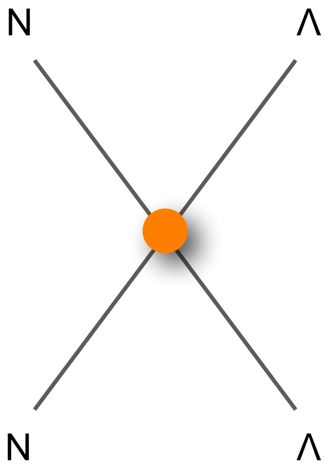


$^{12}_{\Lambda}\mathrm{C}$

6 protons, 5 neutrons, 1 lambda

HYPERNUCLEI

Input: Hamiltonian inspired by a LO pionless-EFT expansion



$$V_{\Lambda N} = \sum_{S,T} v_{ST}(r_{ij})\hat{P}_{ST}$$

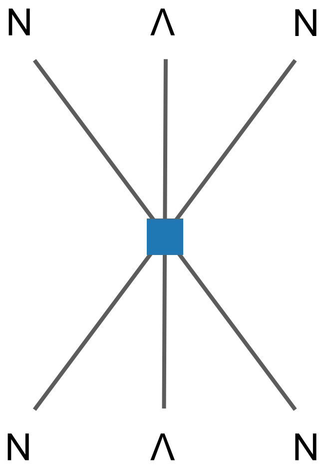
➡ T=1/2, S=1

➡ T=1/2, S=0

Parameters are determined by fitting proton-Λ scattering length and effective range

HYPERNUCLEI

Input: Hamiltonian inspired by a LO pionless-EFT expansion



$$V_{\Lambda NN} = \sum_{S,T} D_{S,T} v_{ST}(r_{i\Lambda}) v_{ST}(r_{j\Lambda}) \hat{Q}_{ST}$$

- T=0, S=1/2
- T=0, S=3/2
- T=1, S=1/2

Parameters are determined by fitting ${}^{3}_{\Lambda}\mathrm{H}$, ${}^{4}_{\Lambda}\mathrm{H}(S=0)$, ${}^{4}_{\Lambda}\mathrm{H}(S=1)$, and ${}^{5}_{\Lambda}\mathrm{He}$.

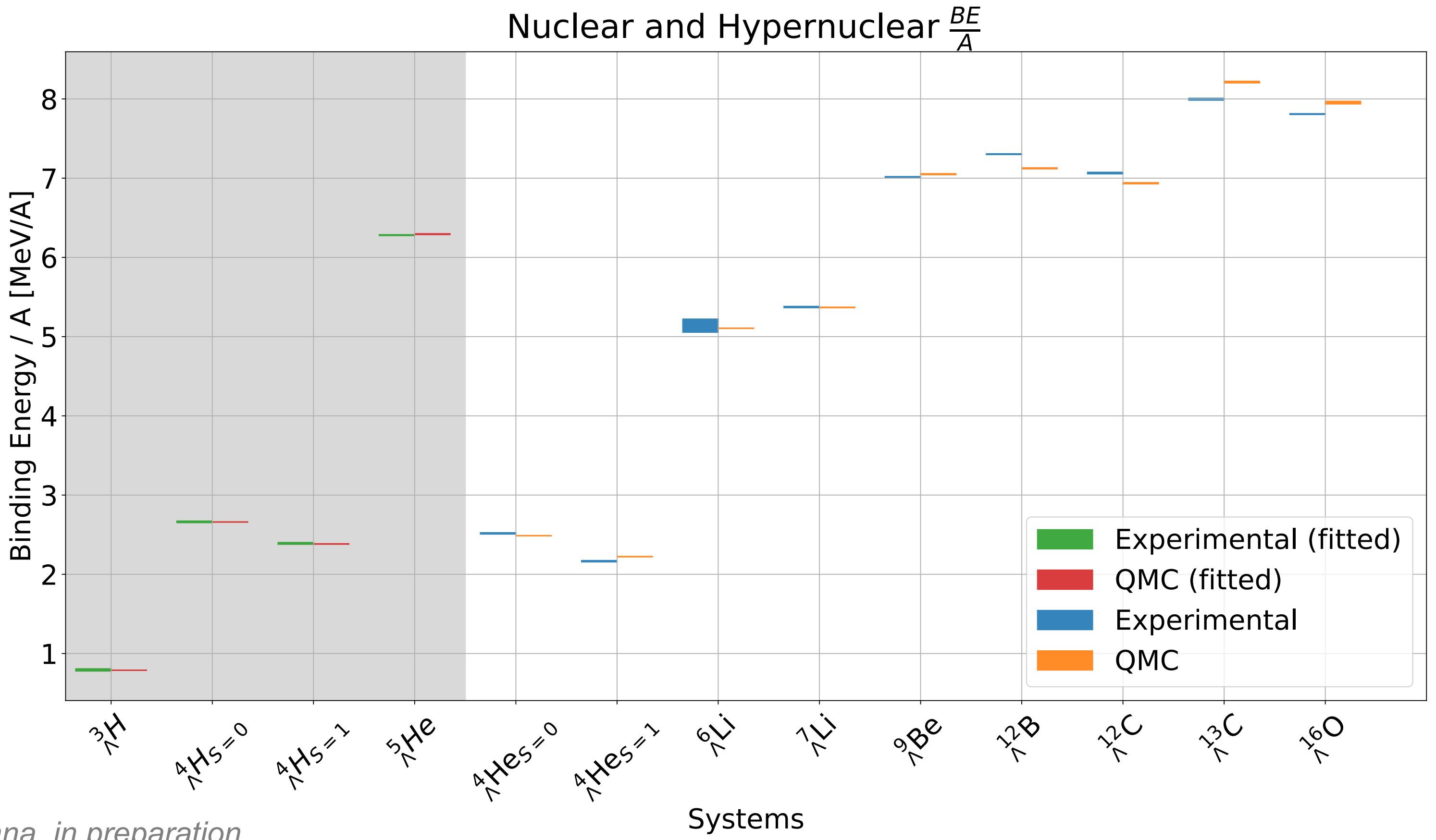
HYPERNUCLEI

No terms in the Hamiltonian mix lambda and nucleons: **distinguishable**

Andrea Di Donna proposed the following ansatz

$$\Psi(x_\Lambda, x_1, \ldots, x_A) = \mathcal{U}(x_\Lambda; x_1, \ldots, x_A) \times \Psi_{HN}(x_1, \ldots, x_A)$$

HYPERNUCLEI



A. Di Donna, in preparation

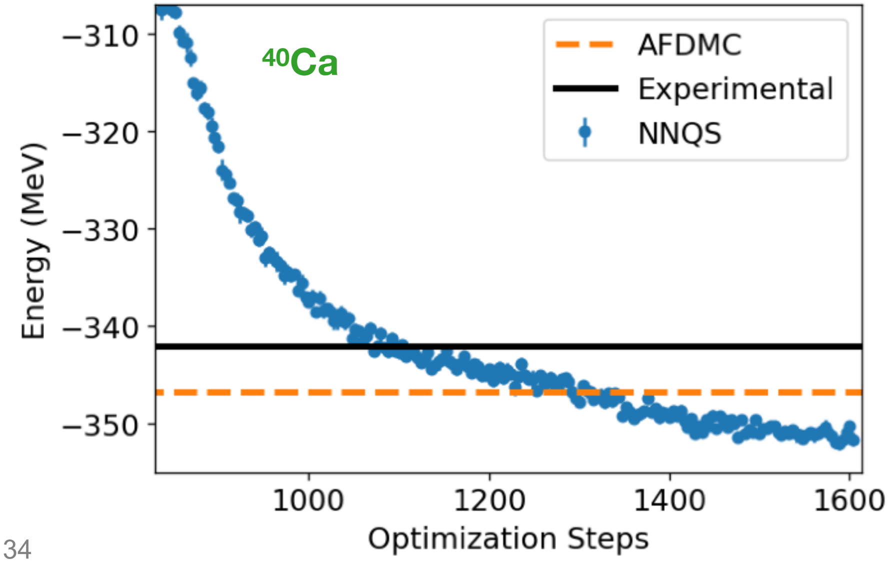
CONCLUSIONS

NQS successfully applied to study:

- ➡ Ultra-cold Fermi gases, outperforming state-of-the-art continuum DMC;
- ➡ Dilute nucleonic matter, including the self-emergence of nuclei;
- ➡ Essential Elements of nuclear binding

Ongoing efforts:

- ➡ Medium-mass nuclei
- ➡ Excited states
- ➡ Chiral-EFT potentials
- ➡ Real-time dynamics



THANK YOU