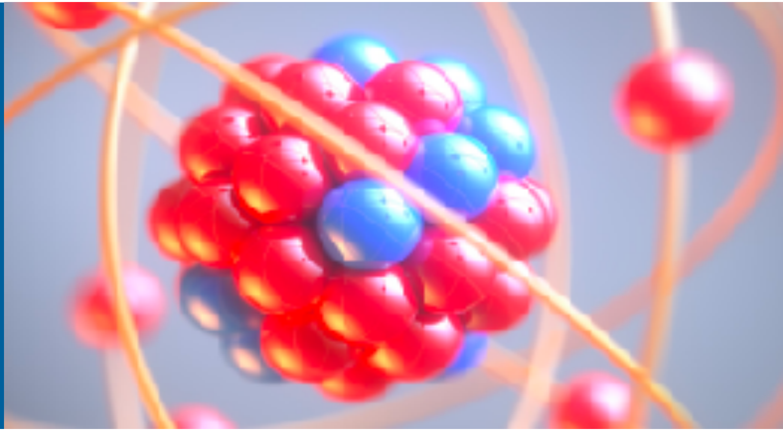
VARIATIONAL LEARNING QUANTUM WAVE FUNCTIONS



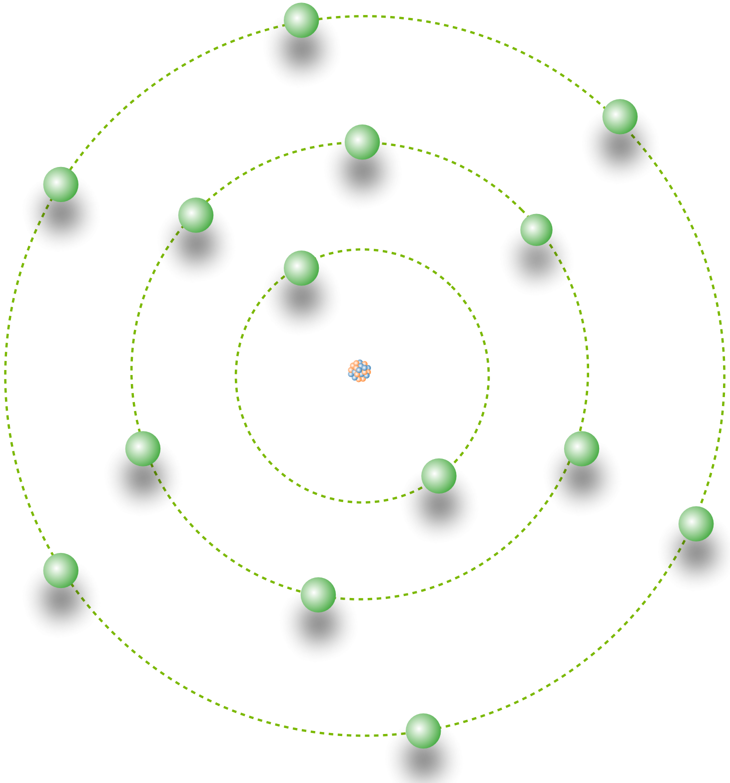
ALESSANDRO LOVATO

Intro to AI-driven Science on Supercomputers:
A Student Training Series

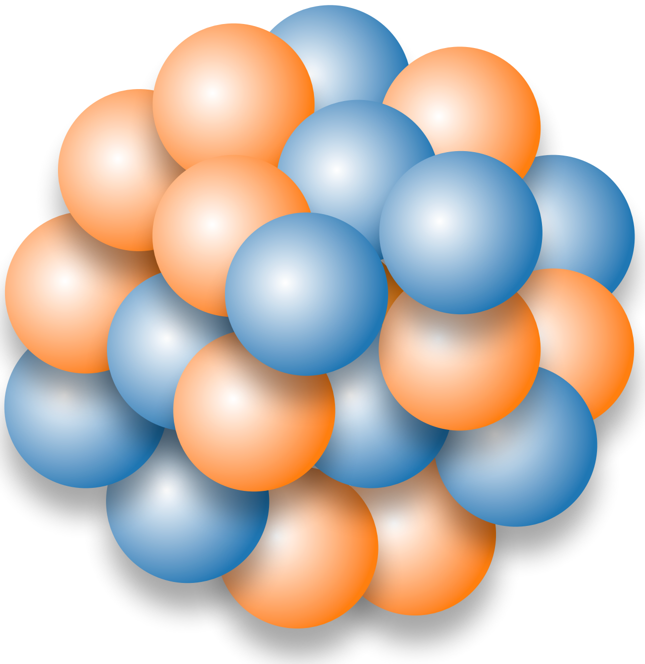
March 12, 2024

Argonne NATIONAL LABORATORY

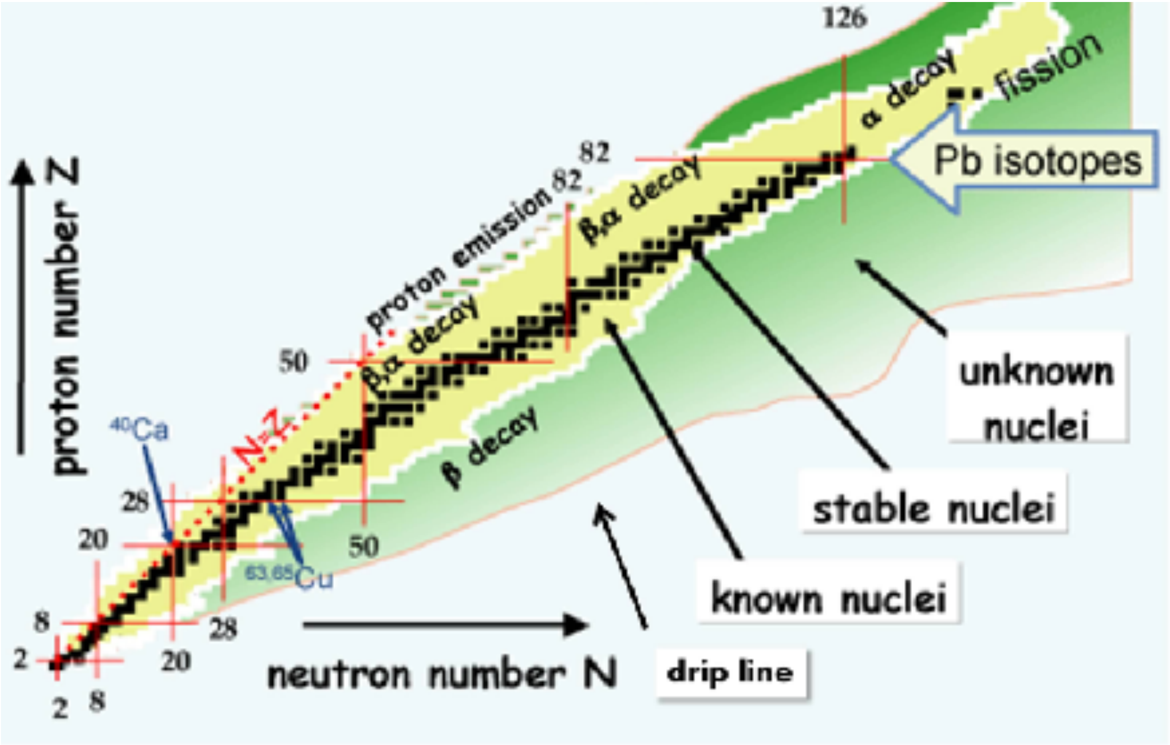
ATOMIC NUCLEI



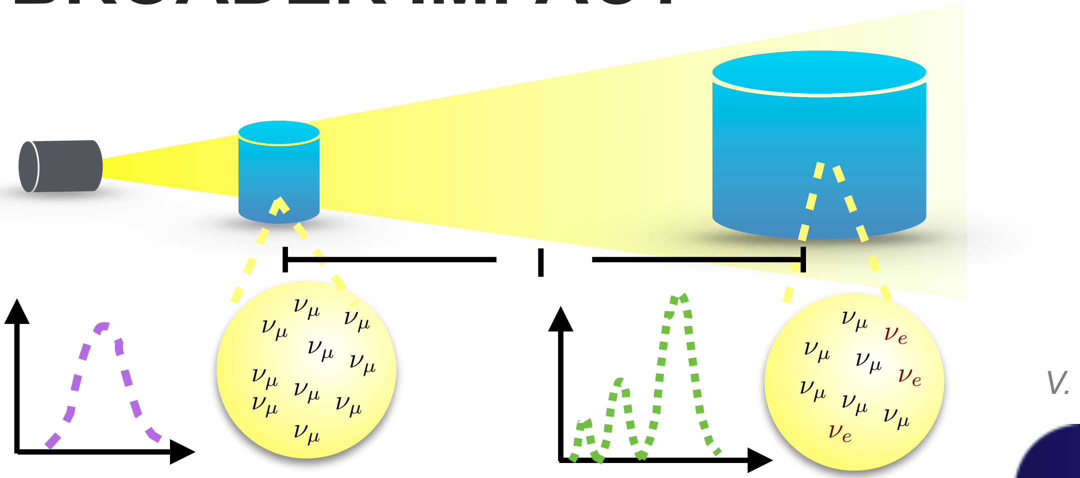
ATOMIC NUCLEI



ATOMIC NUCLEI

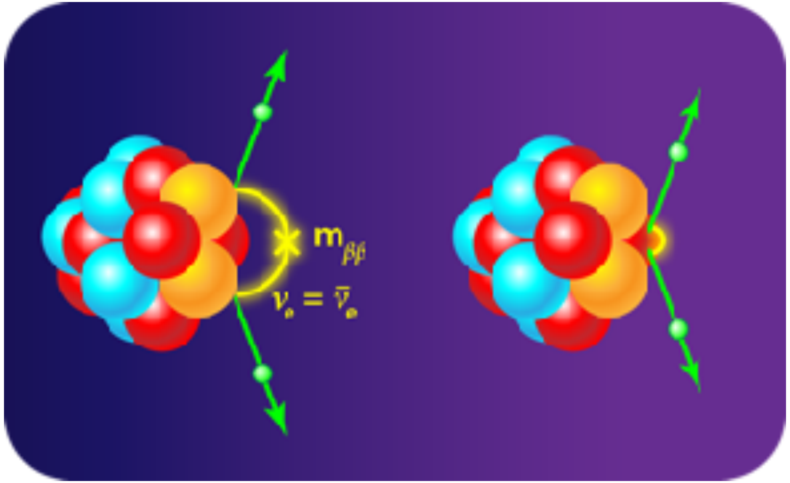


BROADER IMPACT

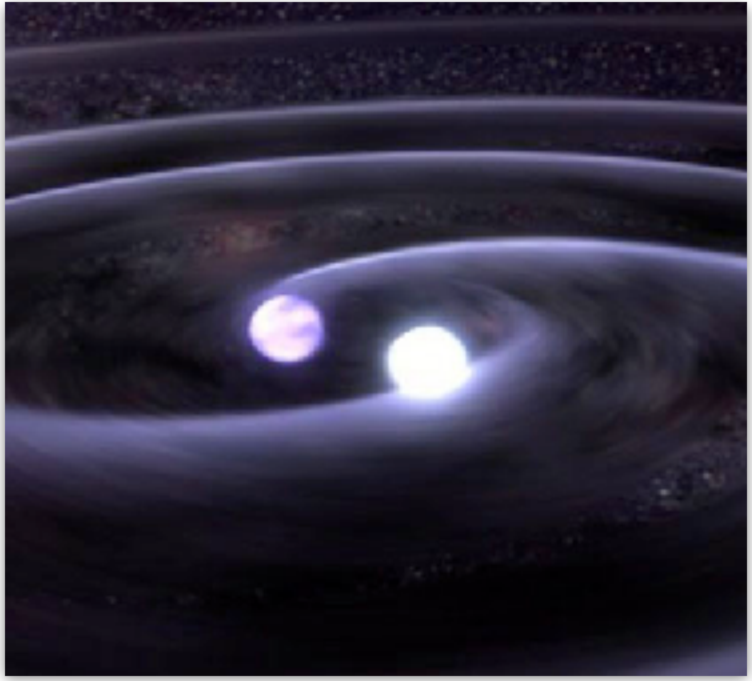


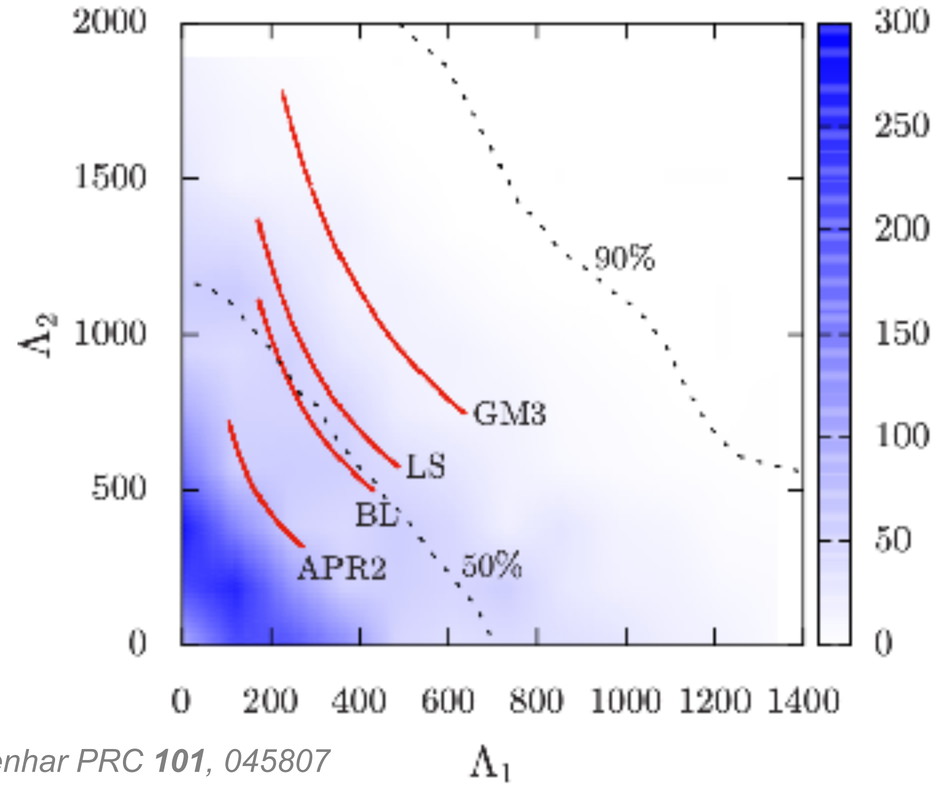
Credit: N. Rocco

V. Cirigliano, et al., J.Phys.G 49 (2022) 12, 120502



BROADER IMPACT

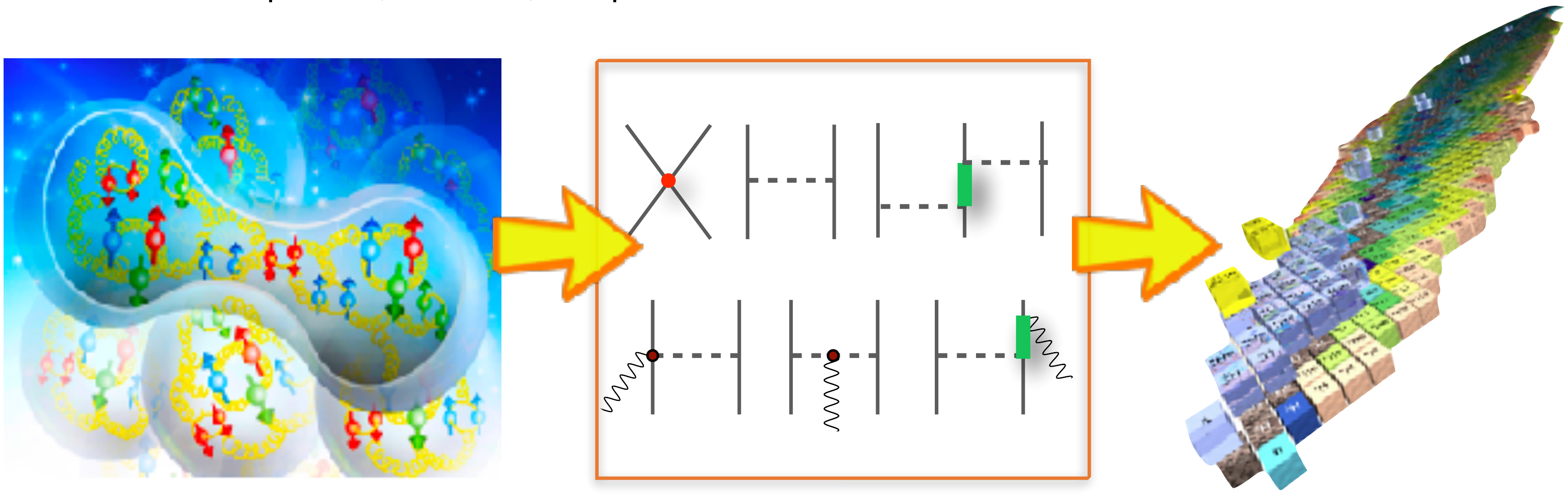




*A. Sabatucci, O. Benhar PRC **101**, 045807*

“AB-INITIO” NUCLEAR PHYSICS

In the low-energy regime, quark and gluons are confined within hadrons and the relevant degrees of freedoms are protons, neutrons, and pions

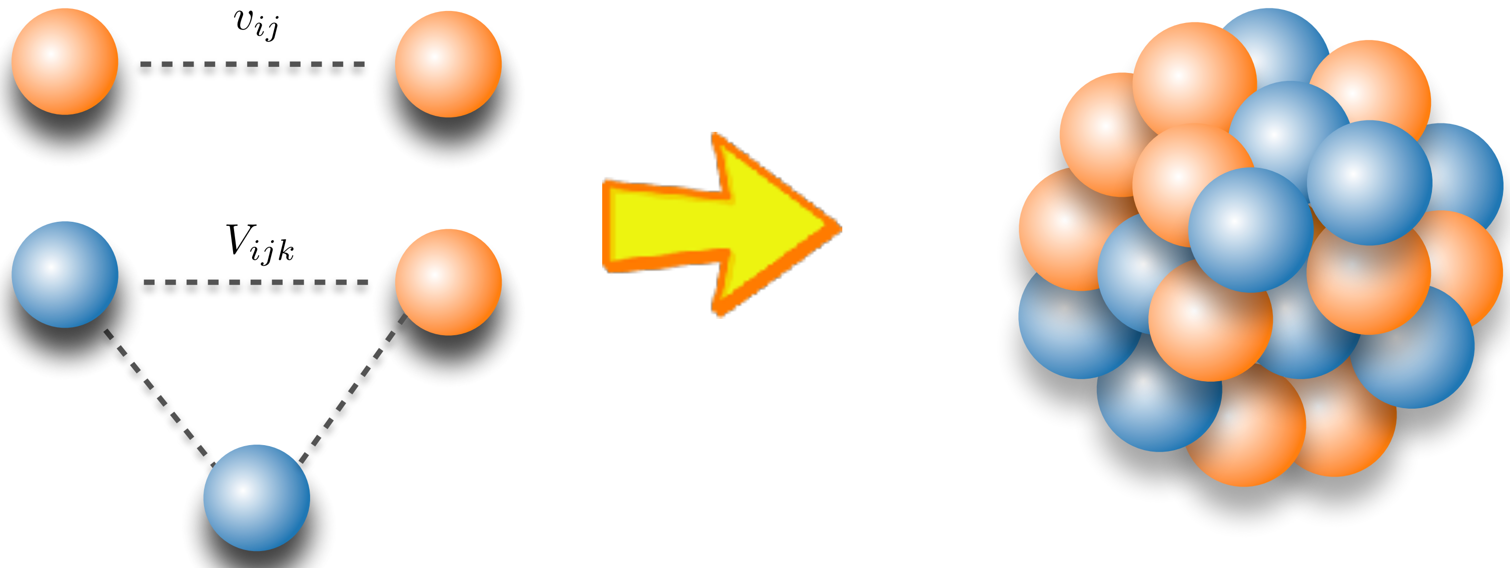


Effective field theories are the link between QCD and nuclear observables.

THE QUANTUM MANY-BODY PROBLEM

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

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$



THE QUANTUM MANY-BODY PROBLEM

- Nuclear forces are spin (and isospin) dependent

- Non relativistic many body theory aims at solving the many-body Schrödinger equation

$$H\Psi_n(x_1,\dots,x_A) = E_n\Psi_n(x_1,\dots,x_A) \quad \longleftrightarrow \quad x_i \equiv \{\mathbf{r}_i, s_i^z, t_i^z\}$$

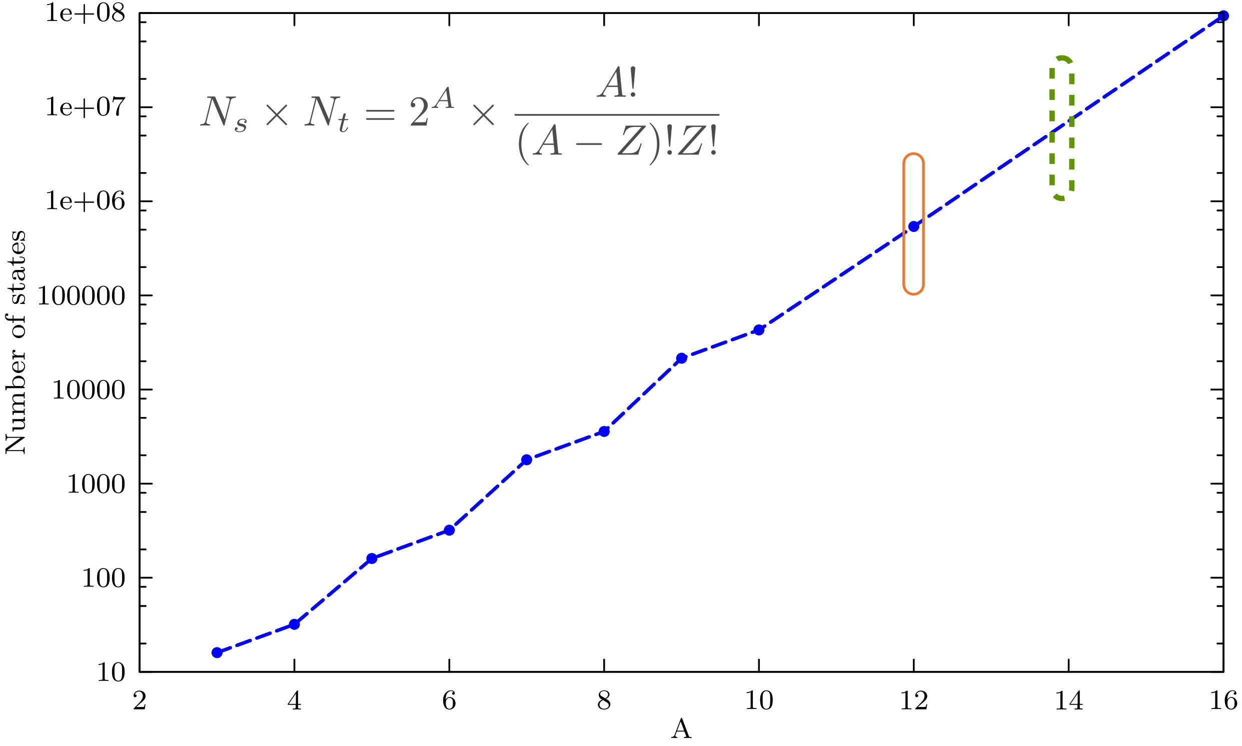
- Nucleons are fermions, so the wave function must be anti-symmetric

$$\Psi_n(x_1,\dots,x_i,\dots,x_j,x_A) = -\Psi_n(x_1,\dots,x_j,\dots,x_i,x_A)$$

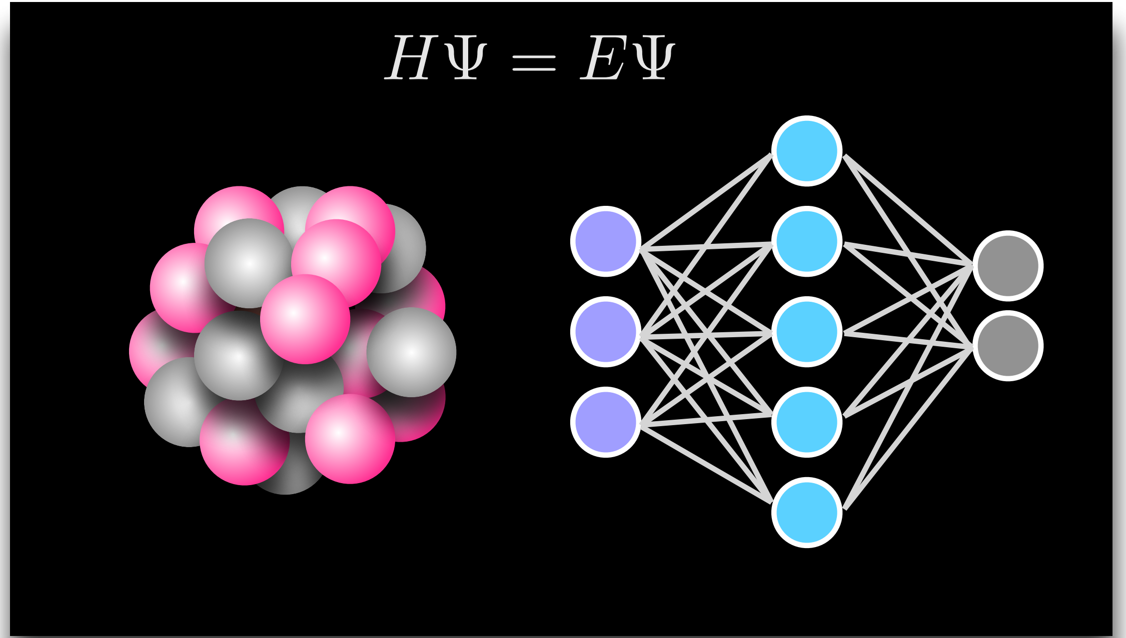
GREEN'S FUNCTION MONTE CARLO

The GFMC uses a many-body representation of the spin-isospin degrees of freedom

$$\langle \mathbf{R}|\Psi(\tau)\rangle = \begin{pmatrix} a_{\uparrow\uparrow\uparrow}(\mathbf{R}) \\ a_{\downarrow\uparrow\uparrow}(\mathbf{R}) \\ a_{\uparrow\downarrow\uparrow}(\mathbf{R}) \\ a_{\downarrow\downarrow\uparrow}(\mathbf{R}) \\ a_{\uparrow\uparrow\downarrow}(\mathbf{R}) \\ a_{\downarrow\uparrow\downarrow}(\mathbf{R}) \\ a_{\uparrow\downarrow\downarrow}(\mathbf{R}) \\ a_{\downarrow\downarrow\downarrow}(\mathbf{R}) \end{pmatrix}$$



NEURAL NETWORK QUANTUM STATES



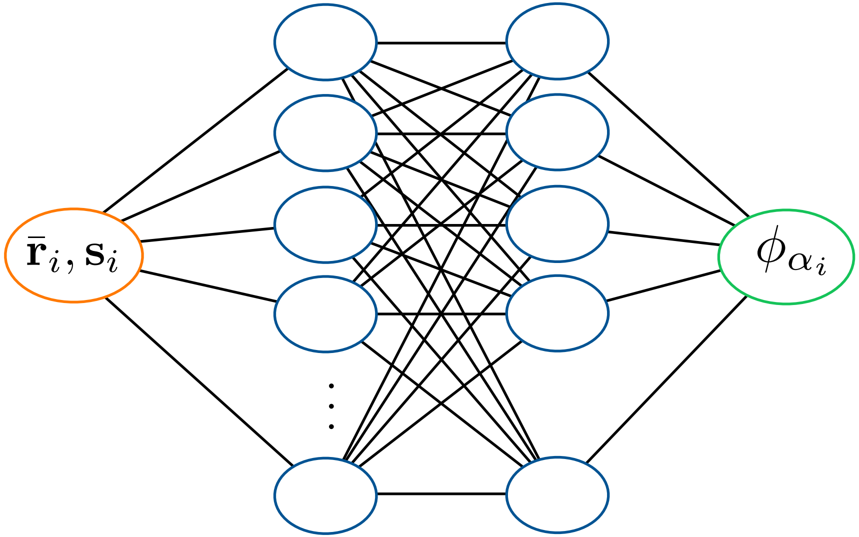
NEURAL SLATER-JASTROW ANSATZ

Product of mean-field state modulated by a flexible correlator factor

$$\Psi_{SJ}(X) = e^{J(X)}\Phi(X)$$

Mean-field: Slater determinant of single-particle orbitals

$$\det \begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_1(\mathbf{x}_2) & \cdots & \phi_1(\mathbf{x}_N) \\ \phi_2(\mathbf{x}_1) & \phi_2(\mathbf{x}_2) & \cdots & \phi_2(\mathbf{x}_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(\mathbf{x}_1) & \phi_N(\mathbf{x}_2) & \cdots & \phi_N(\mathbf{x}_N) \end{bmatrix}$$



Each orbital is a FFNN that takes as input

$$\bar{\mathbf{r}}_i = \mathbf{r}_i - \mathbf{R}_{CM}$$

NEURAL SLATER-JASTROW ANSATZ

“Manually” imposing permutation-invariance scales factorially with A

$$J(X) = j(x_1, x_2, x_3) + j(x_1, x_3, x_2) + j(x_2, x_1, x_3) + j(x_2, x_3, x_1) + j(x_3, x_1, x_2) + j(x_3, x_2, x_1)$$

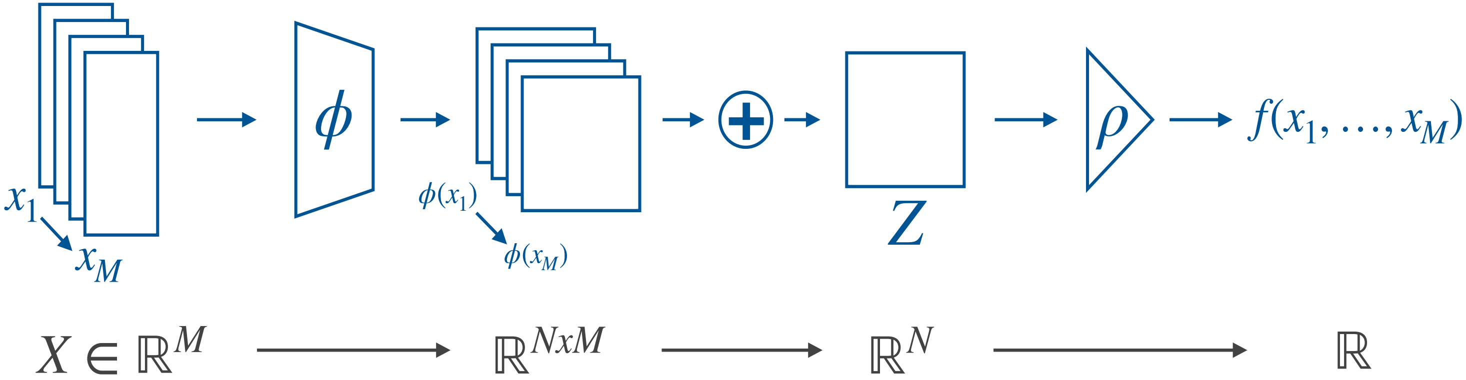
NEURAL SLATER-JASTROW ANSATZ

"Manually" imposing permutation-invariance scales factorially with A

$$J(X) = j(x_1, x_2, x_3) + j(x_1, x_3, x_2) + j(x_2, x_1, x_3) + j(x_2, x_3, x_1) + j(x_3, x_1, x_2) + j(x_3, x_2, x_1)$$

Solution: "deep-sets" →

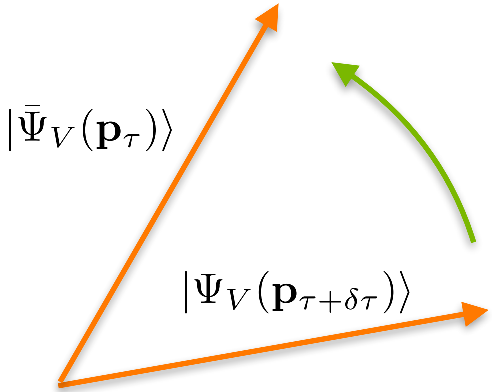
$$J(X) = \rho_F\Big[\sum_i \vec{\phi}_{\mathcal{F}}(\bar{\mathbf{r}}_i, \mathbf{s}_i)\Big]$$



WAVE FUNCTION OPTIMIZATION

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

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



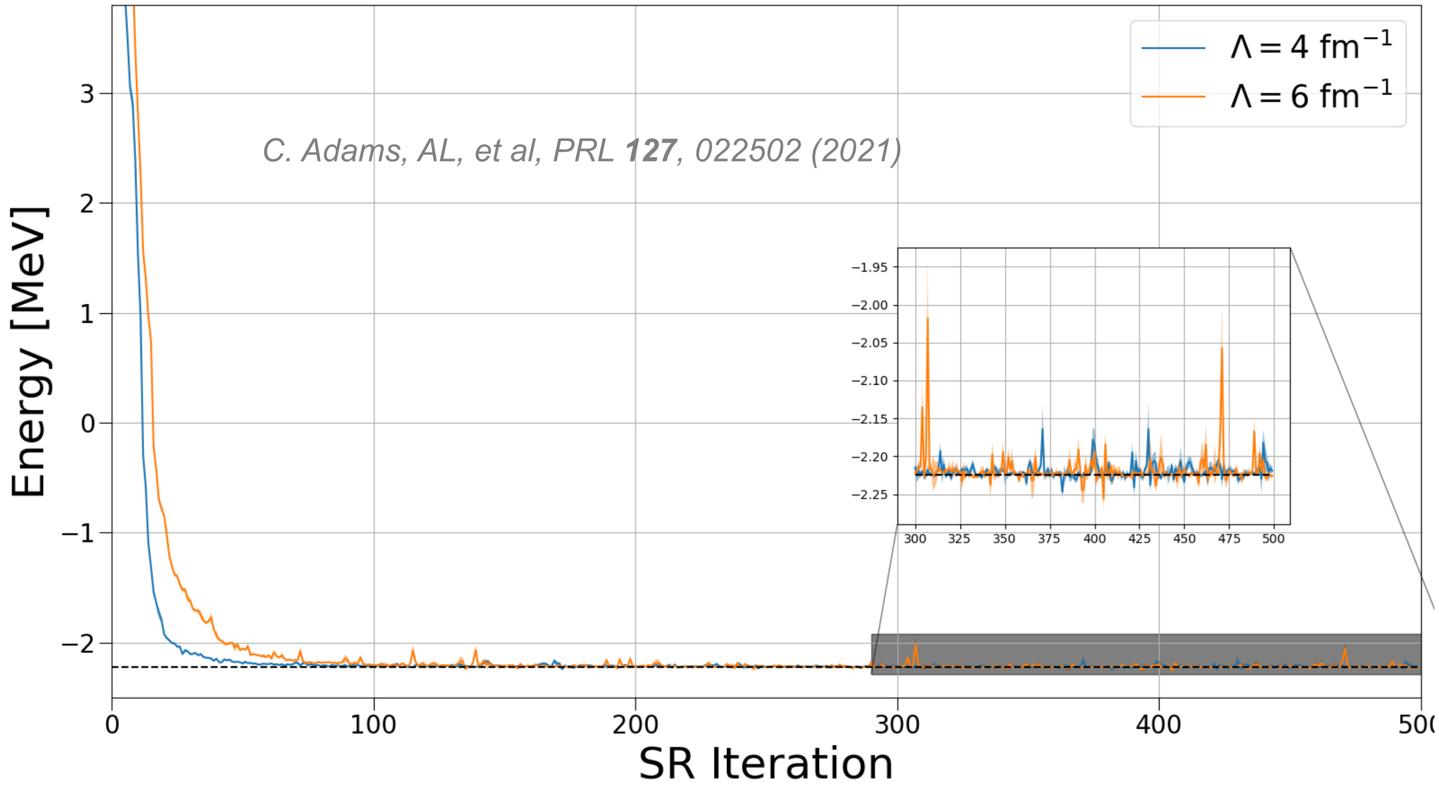
The parameters are updated as

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

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

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

STOCHASTIC RECONFIGURATION



COMPARISON WITH GFMC

- The ANN Slater Jastrow ansatz outperforms conventional Jastrow correlations

	Λ	VMC-ANN	VMC-JS	GFMC	GFMC$_c$
^{2}H	4 fm^{-1}	−2.224(1)	−2.223(1)	−2.224(1)	-
	6 fm^{-1}	−2.224(4)	−2.220(1)	−2.225(1)	-
^{3}H	4 fm^{-1}	−8.26(1)	−7.80(1)	−8.38(2)	−7.82(1)
	6 fm^{-1}	−8.27(1)	−7.74(1)	−8.38(2)	−7.81(1)
^{4}He	4 fm^{-1}	−23.30(2)	−22.54(1)	−23.62(3)	−22.77(2)
	6 fm^{-1}	−24.47(3)	−23.44(2)	−25.06(3)	−24.10(2)

- Differences with the GFMC due to deficiencies in the Slater-Jastrow ansatz

$$\Psi_{SJ}(X) = e^{J(X)}\Phi(X)$$

C. Adams, AL, et al, PRL **127**, 022502 (2021)

HIDDEN NUCLEONS ANSATZ

$$\Phi(X) = \det \begin{bmatrix} \phi_1(x_1) & \phi_1(x_2) & \phi_1(x_3) & \phi_1(x_4) \\ \phi_2(x_1) & \phi_2(x_2) & \phi_2(x_3) & \phi_2(x_4) \\ \phi_3(x_1) & \phi_3(x_2) & \phi_3(x_3) & \phi_3(x_4) \\ \phi_4(x_1) & \phi_4(x_2) & \phi_4(x_3) & \phi_4(x_4) \end{bmatrix}$$

HIDDEN NUCLEONS ANSATZ

$$\Psi_{\mathrm{HN}}(X) = \det \begin{bmatrix} \phi_1(x_1) & \phi_1(x_2) & \phi_1(x_3) & \phi_1(x_4) & \phi_1(y_1) & \phi_1(y_2) \\ \phi_2(x_1) & \phi_2(x_2) & \phi_2(x_3) & \phi_2(x_4) & \phi_2(y_1) & \phi_1(y_2) \\ \phi_3(x_1) & \phi_3(x_2) & \phi_3(x_3) & \phi_3(x_4) & \phi_3(y_1) & \phi_1(y_2) \\ \phi_4(x_1) & \phi_4(x_2) & \phi_4(x_3) & \phi_4(x_4) & \phi_4(y_1) & \phi_1(y_2) \\ \chi_1(x_1) & \chi_1(x_2) & \chi_1(x_3) & \chi_1(x_4) & \chi_1(y_1) & \chi_2(y_2) \\ \chi_2(x_1) & \chi_2(x_2) & \chi_2(x_3) & \chi_2(x_4) & \chi_2(y_1) & \chi_2(y_2) \end{bmatrix}$$

Visible orbitals on visible coordinates

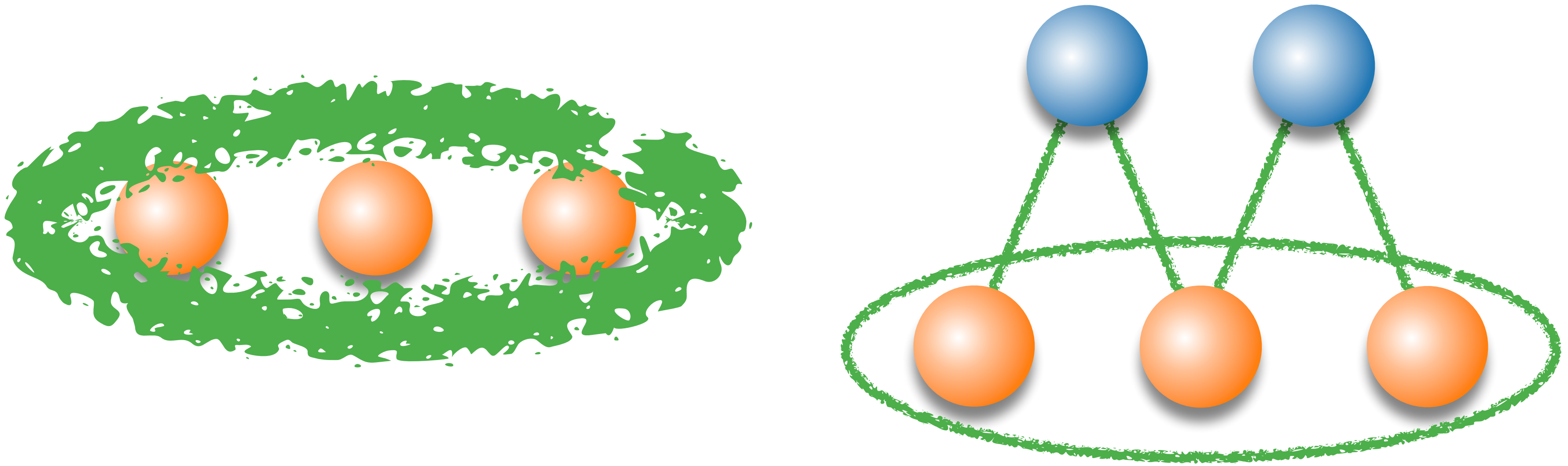
Visible orbitals on hidden coordinates

Hidden orbitals on visible coordinates

Hidden orbitals on hidden coordinates

*J. R. Moreno, et al., PNAS **119,** 2122059119(2022)*

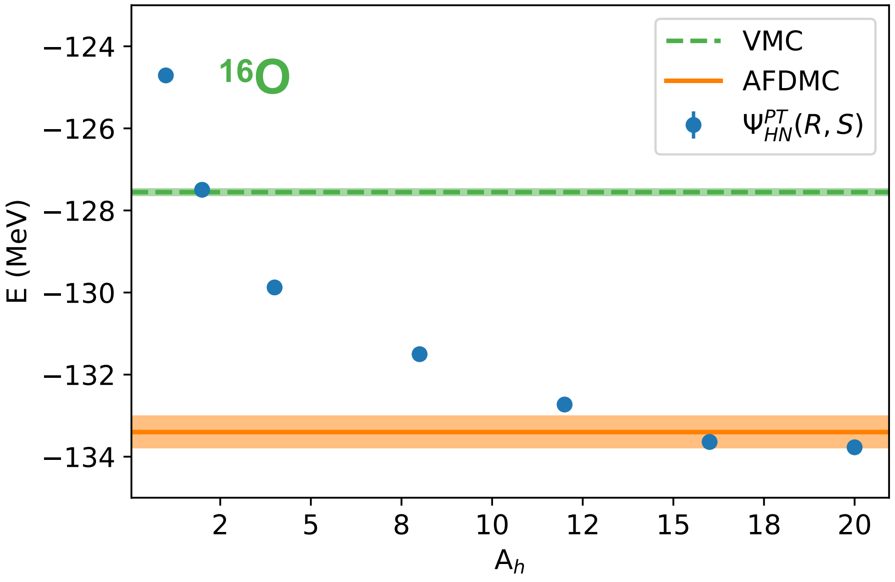
HIDDEN NUCLEONS ANSATZ

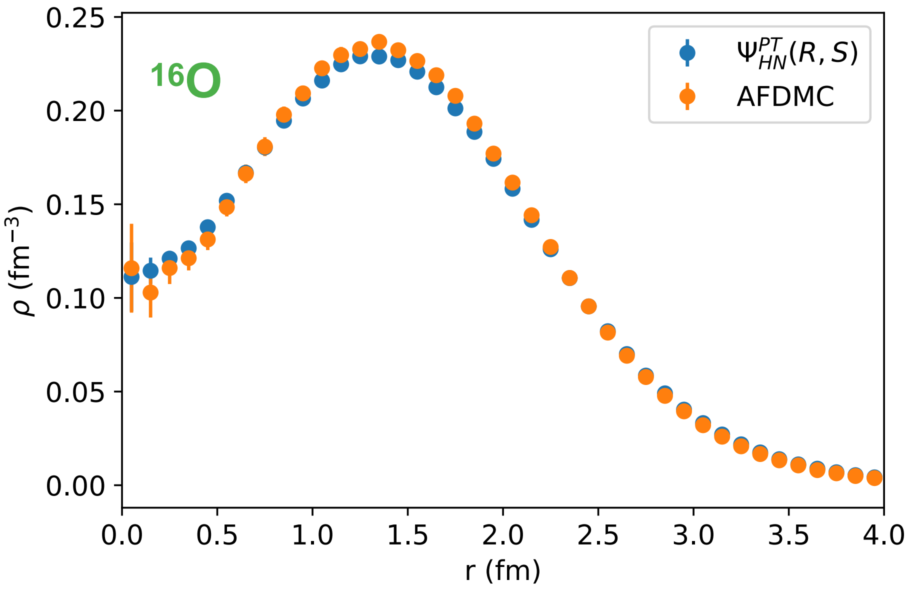


HIDDEN NUCLEONS ANSATZ

We extend the reach of neural quantum states to ^{16}O

In addition to its ground-state energy, we evaluate the point-nucleon density of ^{16}O with A_h=16



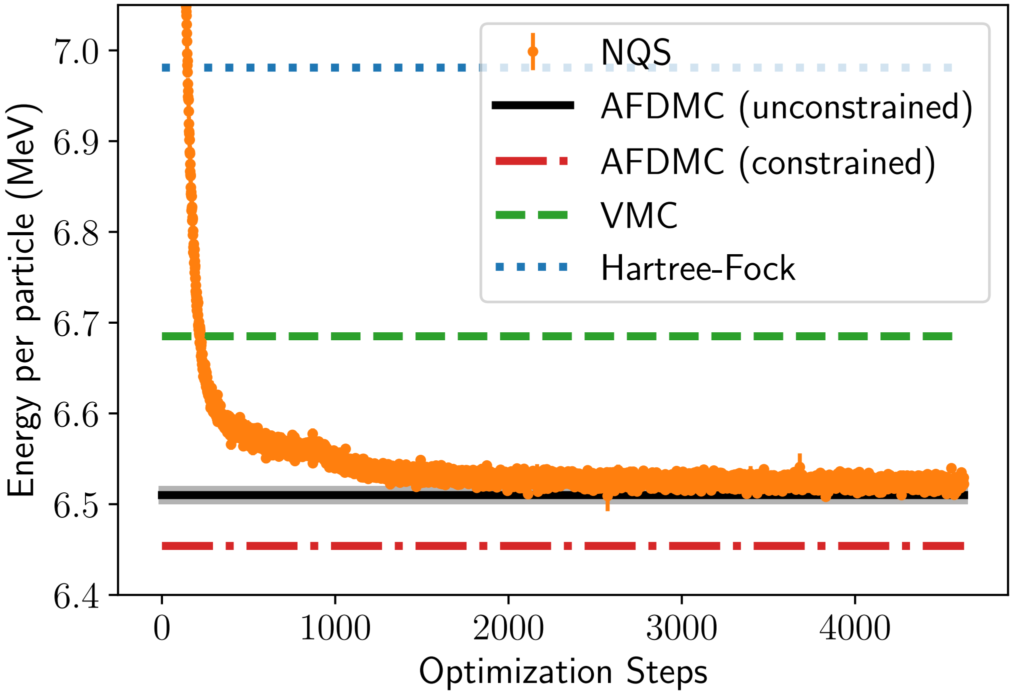


AL, et al., Phys. Rev. Res. ***4*** *(2022) 4, 043178*

DILUTE NEUTRON MATTER

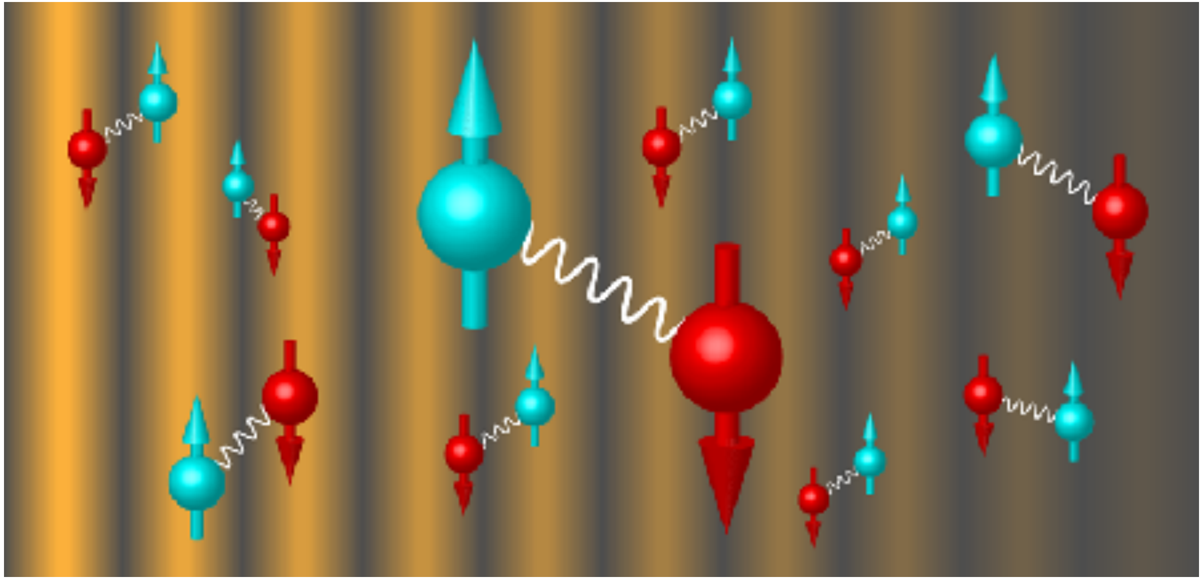
- ➡ **NQS**: 100 hours on NVIDIA-A100
- ➡ **AFDMC**: 1.2 million Intel-KNL hours

14 Neutrons @ ρ=0.04 fm^{-3}



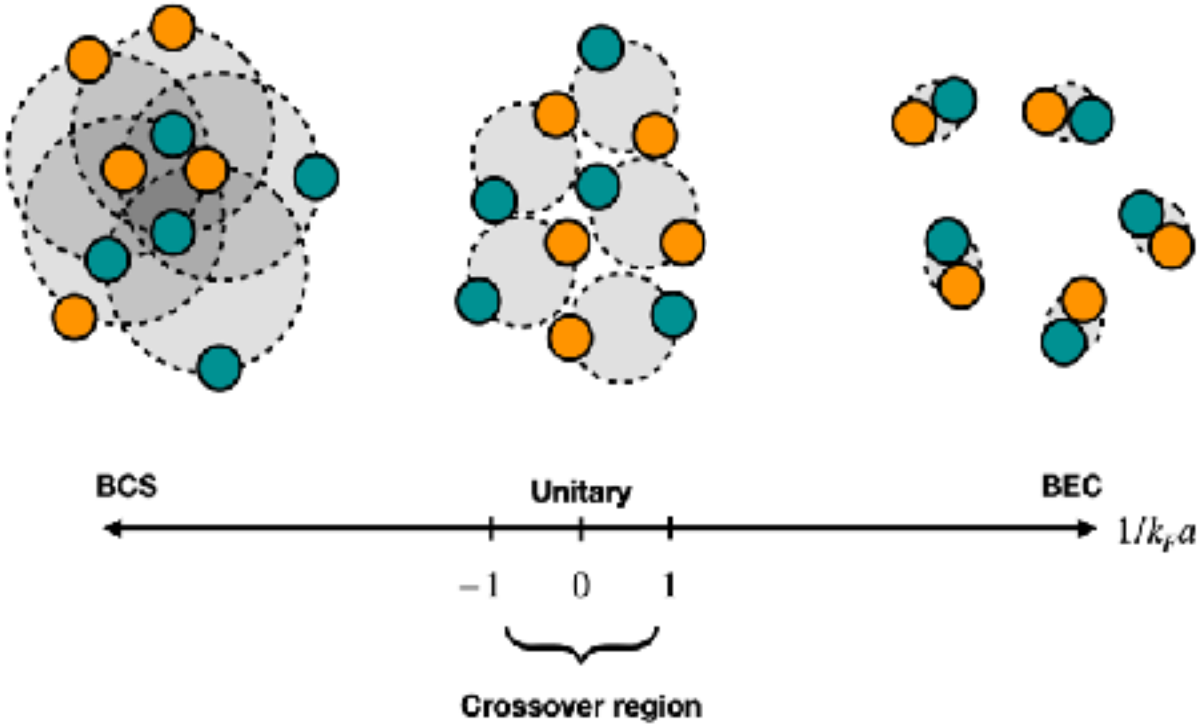
B. Fore, AL et al., *Phys. Rev. Res.* **5**, 033062 (2023)

CONDENSED-MATTER DETOUR



COLD FERMI GASES

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



COLD FERMI GASES

We introduce a Pfaffian-Jastrow ansatz

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

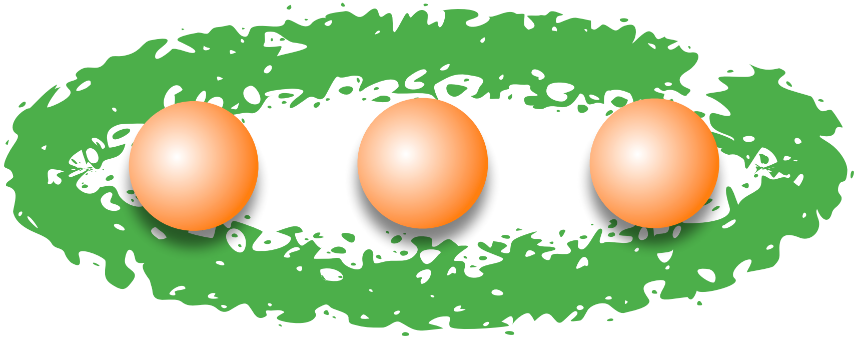
In order for the above matrix to be skew-symmetric, the neural pairing orbitals are taken to be

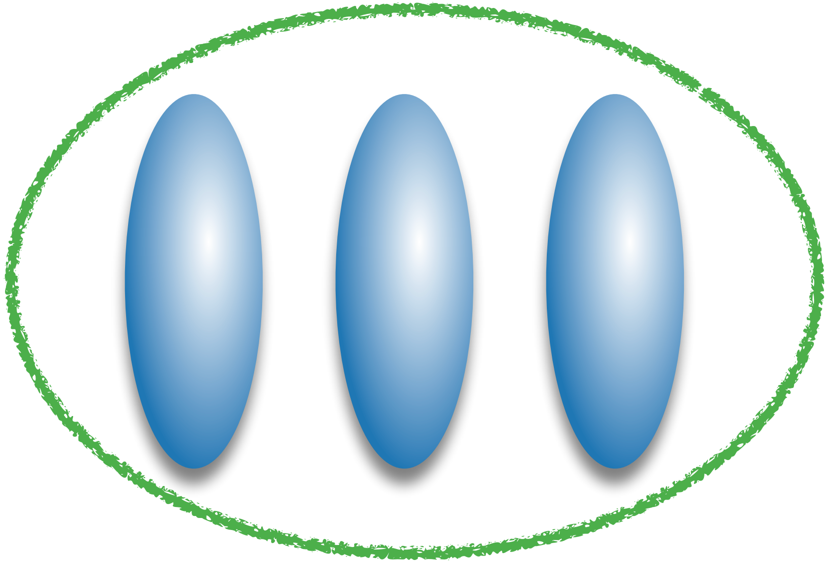
$$\phi(x_i,x_j) = \eta(x_i,x_j) - \eta(x_j,x_i)$$

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

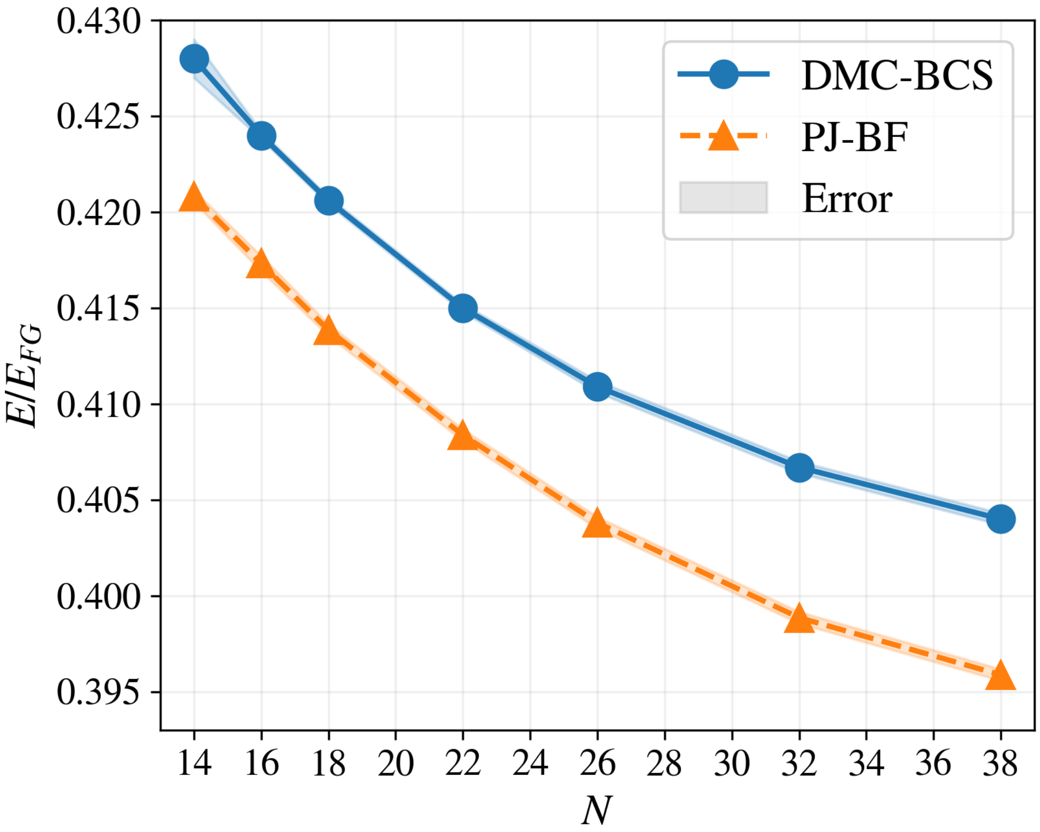
HOMOGENOUS ELECTRON GAS

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





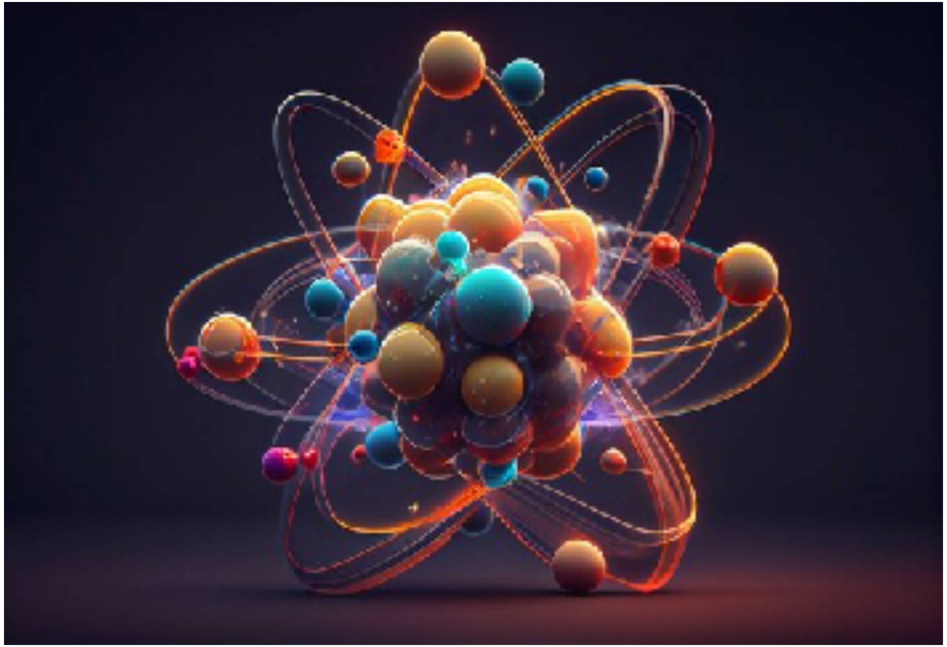
COLD FERMI GASES



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

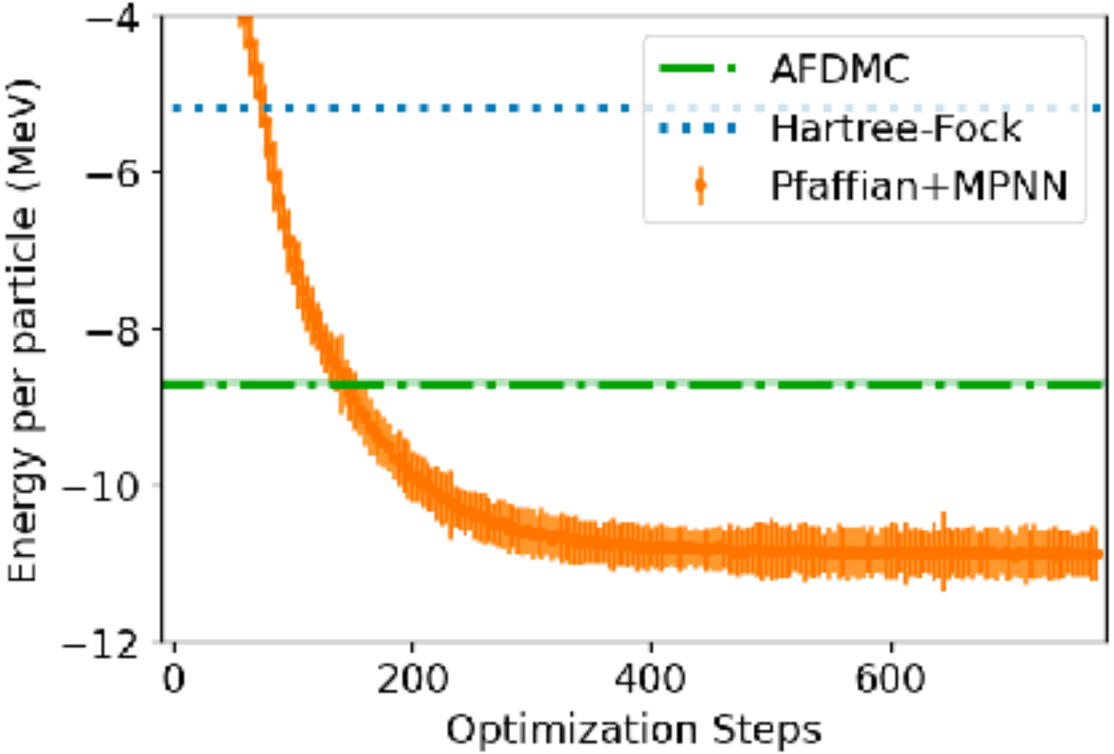
J. Kim, B. Fore, AL, et al. arXiv:2305.08831

BACK TO NUCLEAR PHYSICS



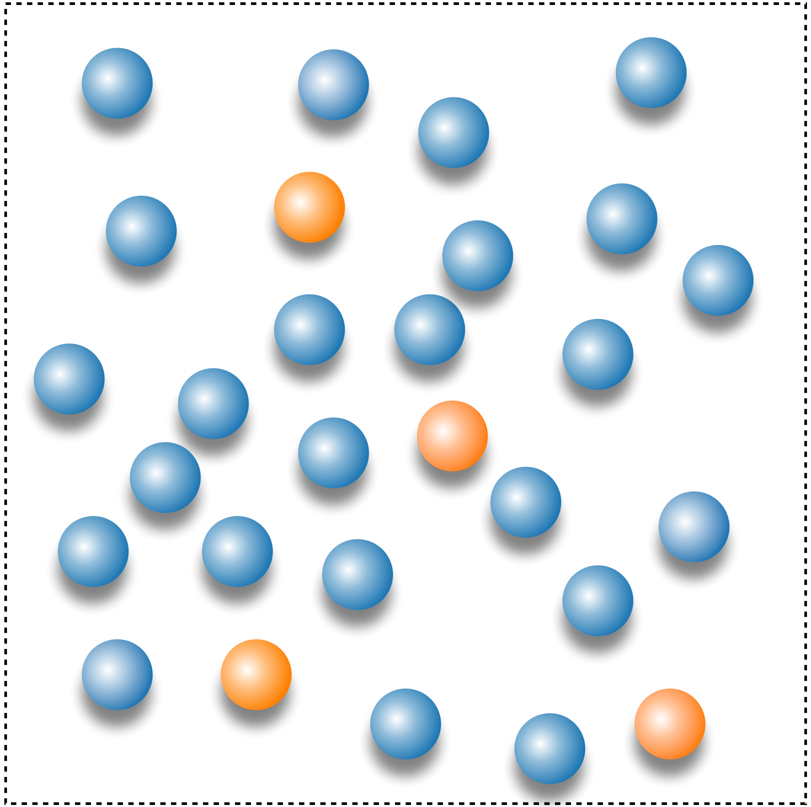
DILUTE NUCLEONIC MATTER WITH MPNN

14 Neutrons, 14 Protons @ ρ=0.04 fm^{-3}



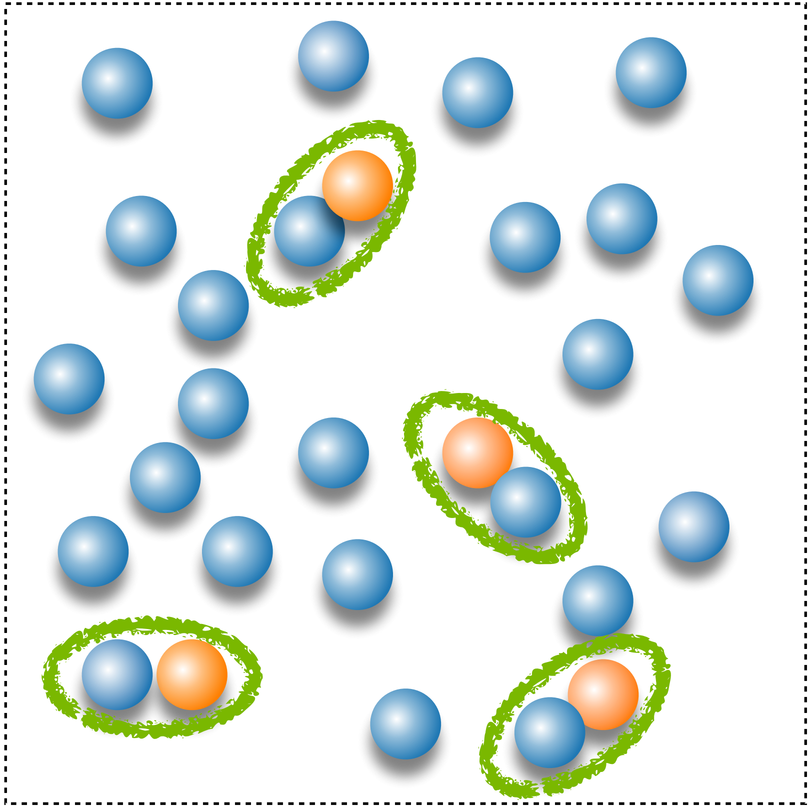
DILUTE NUCLEONIC MATTER WITH MPNN

Liquid phase



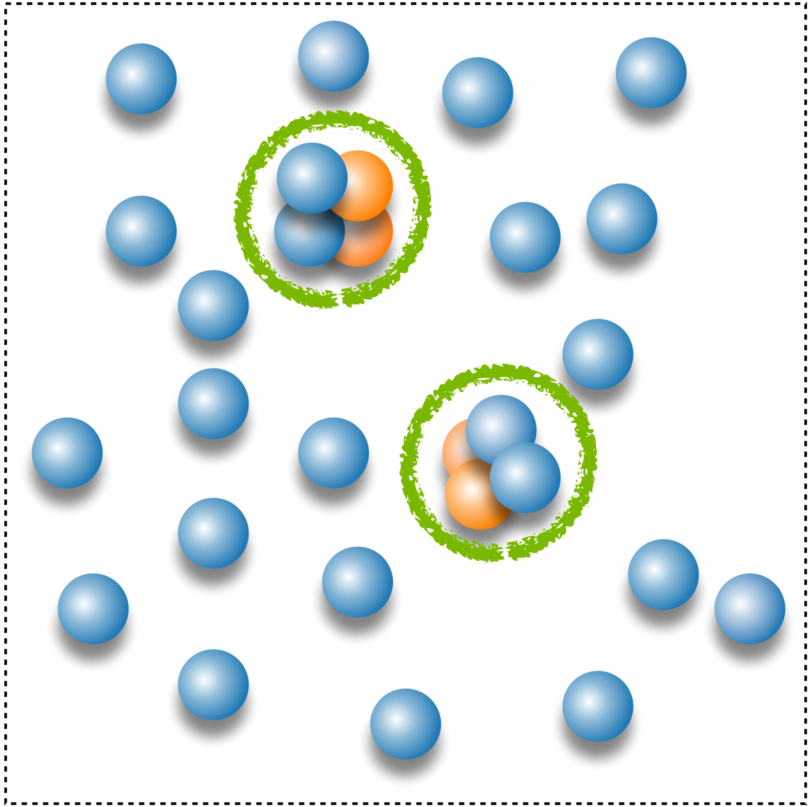
DILUTE NUCLEONIC MATTER WITH MPNN

^2H clusters



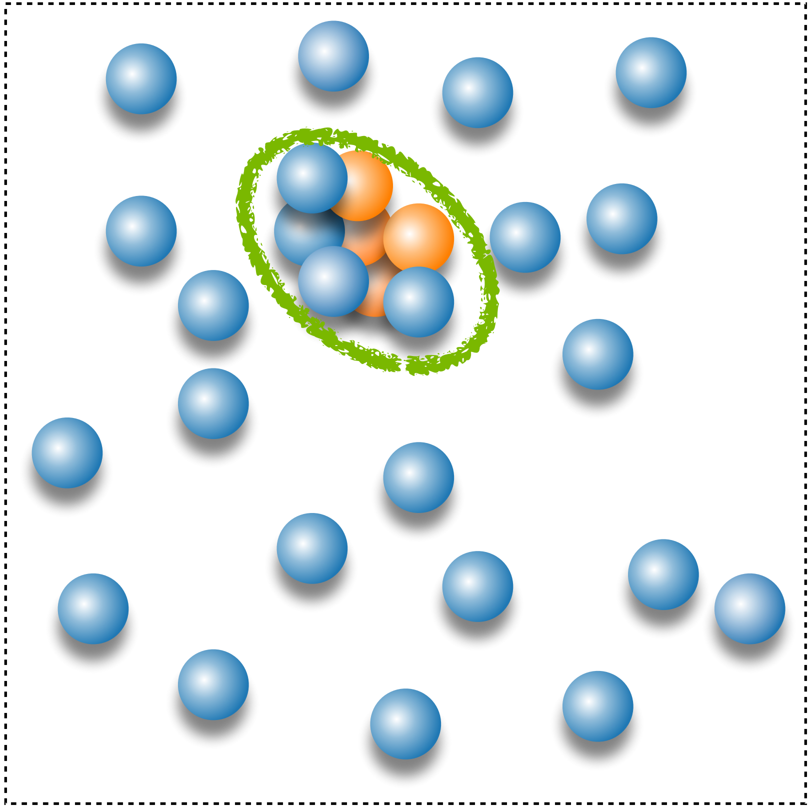
DILUTE NUCLEONIC MATTER WITH MPNN

^{4}He clusters



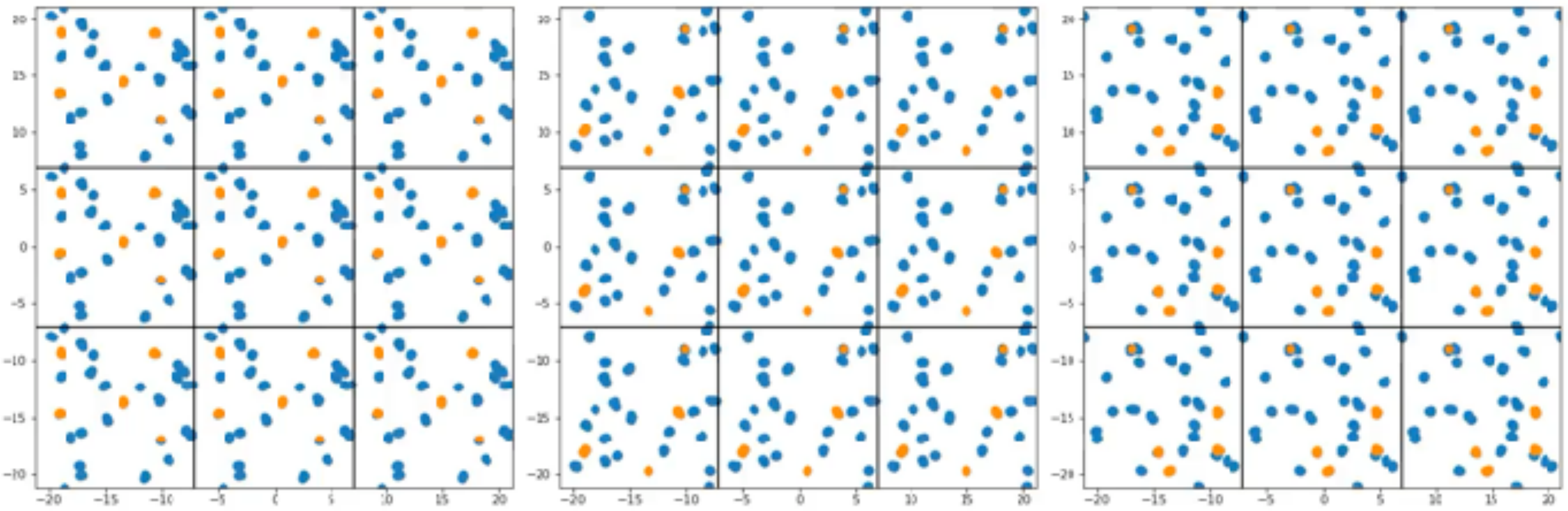
DILUTE NUCLEONIC MATTER WITH MPNN

^{8}Be clusters



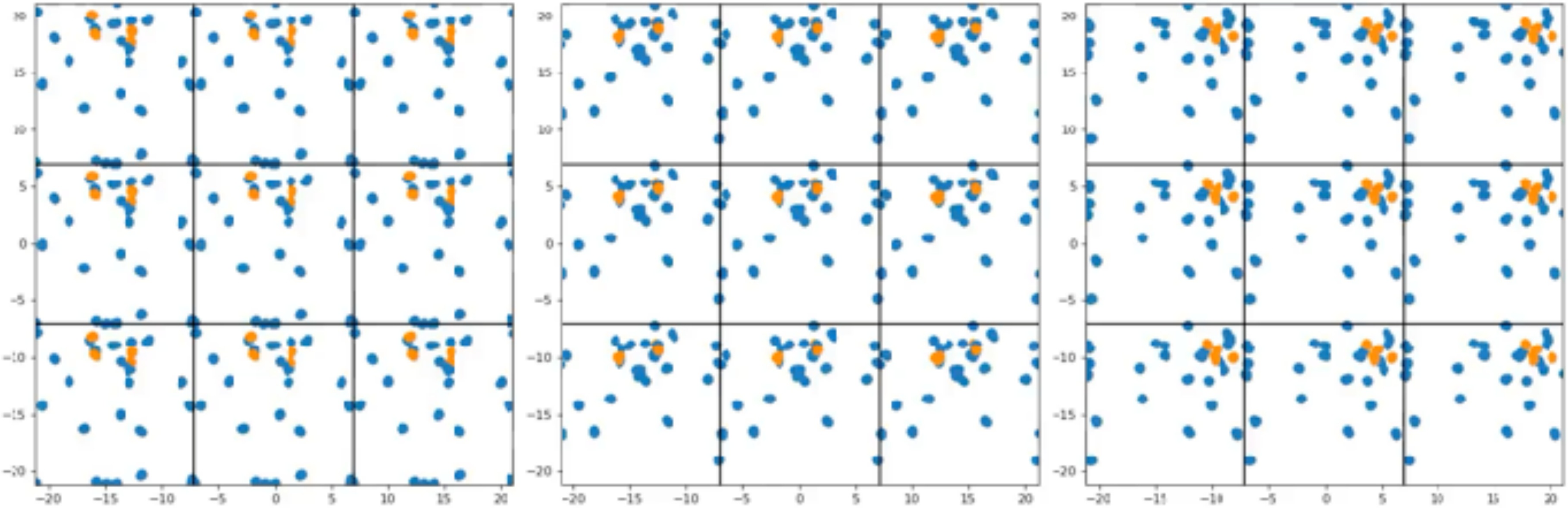
DILUTE NUCLEONIC MATTER WITH MPNN

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



DILUTE NUCLEONIC MATTER WITH MPNN

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



OUTLOOK AND PERSPECTIVES

- **Neural network quantum states** can efficiently approximate quantum-many body wave functions across different energy scales

  ➡ Atoms and molecules;

  ➡ Cold atoms;

  ➡ Atomic nuclei and neutron-star matter;

- Perspectives in **real-time dynamics**, relevant for fission, fusion and neutrino-oscillation experiments

THANK YOU