NEURAL NETWORK QUANTUM STATES FOR THE NUCLEAR MANY-BODY PROBLEM

ALESSANDRO LOVATO

Celebrating 75 Years of the Nuclear Shell Model and Maria Goeppert-Mayer

Argonne
NATIONAL LABORATORY

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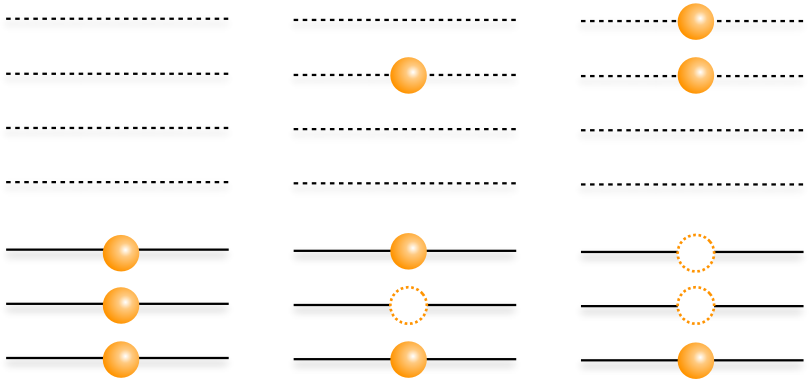
CURSE OF DIMENSIONALITY

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



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

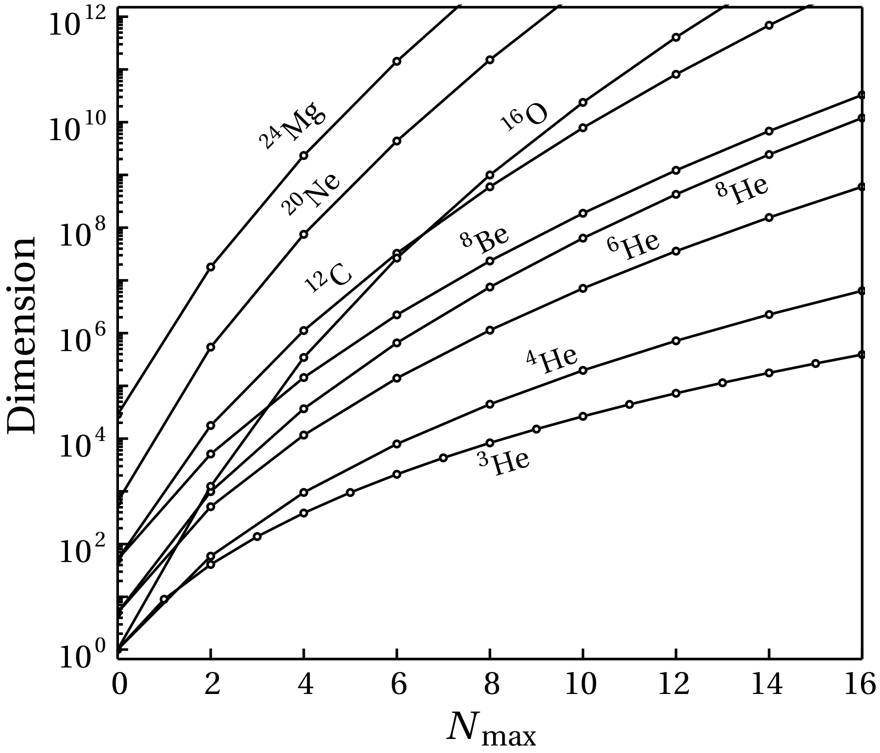
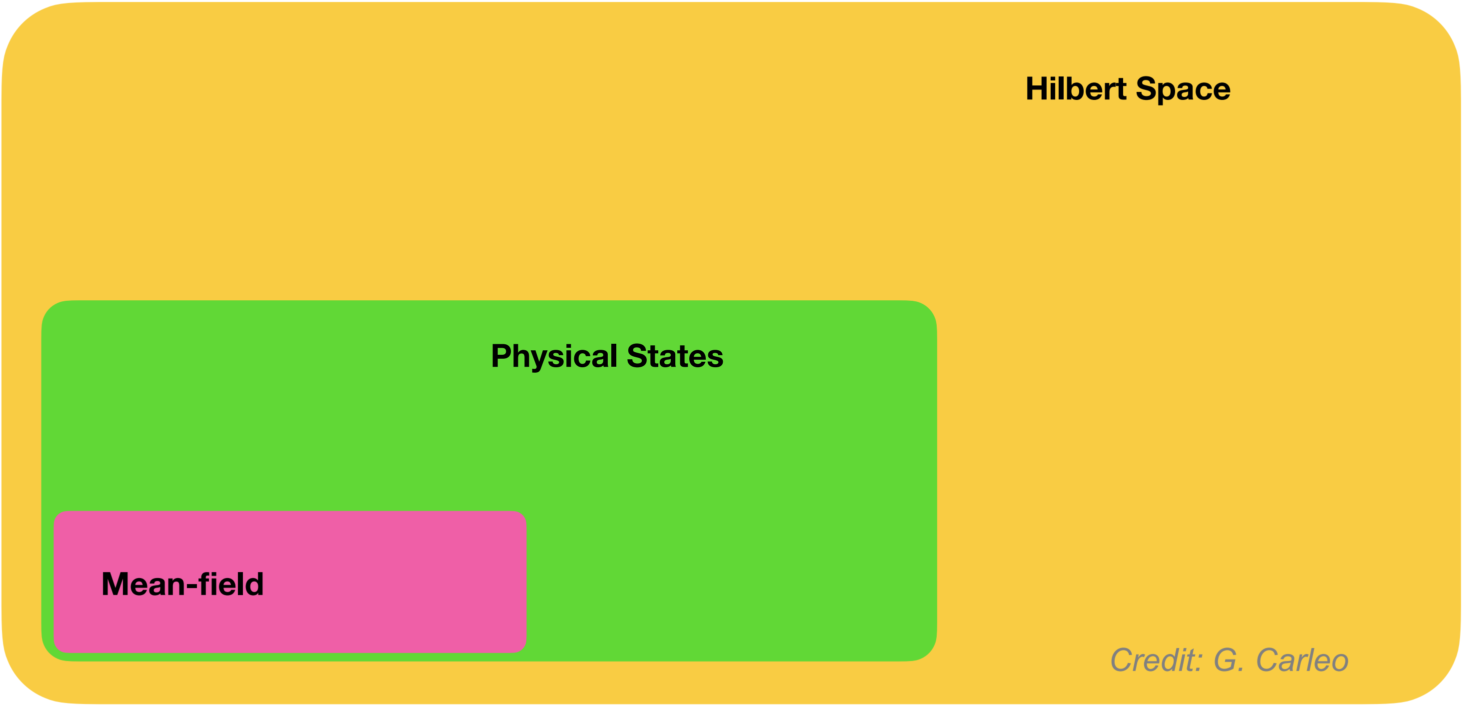


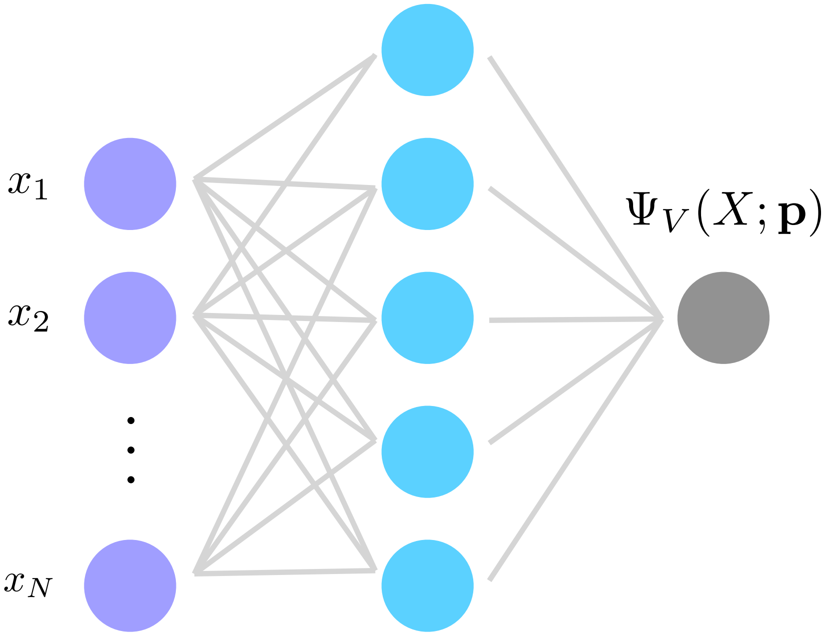
Image courtesy of Patrick Fasano

NEURAL-NETWORK QUANTUM STATES

Quantum states of physical interest have distinctive features and intrinsic structures



NEURAL-NETWORK QUANTUM STATES



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

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

ANTI-SYMMETRIC ANSATZ

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

ANTI-SYMMETRIC ANSATZ

Slater-Jastrow

$$\Phi_{SJ}(X) = e^{J(X)} \times \det \begin{bmatrix} \phi_1(x_1) & \phi_1(x_2) & \cdots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) & \cdots & \phi_2(x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(x_1) & \phi_N(x_2) & \cdots & \phi_N(x_N) \end{bmatrix}$$

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

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

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

ANTI-SYMMETRIC ANSATZ

Pfaffian-Jastrow

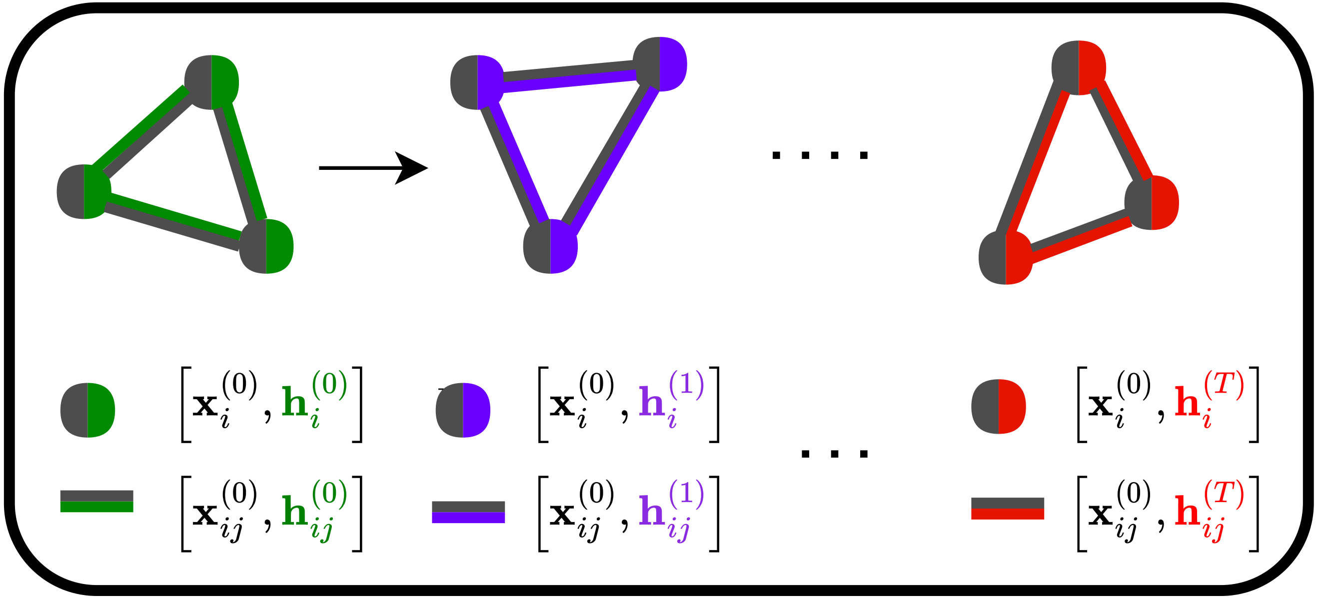
$$\Phi_{PJ}(X) = e^{J(X)} \times \text{pf} \begin{bmatrix} 0 & \phi(x_1, x_2) & \cdots & \phi(x_1, x_N) \\ \phi(x_2, x_1) & 0 & \cdots & \phi(x_2, x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(x_N, x_1) & \phi(x_N, x_2) & \cdots & 0 \end{bmatrix}$$

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

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

NEURAL BACKFLOW CORRELATIONS

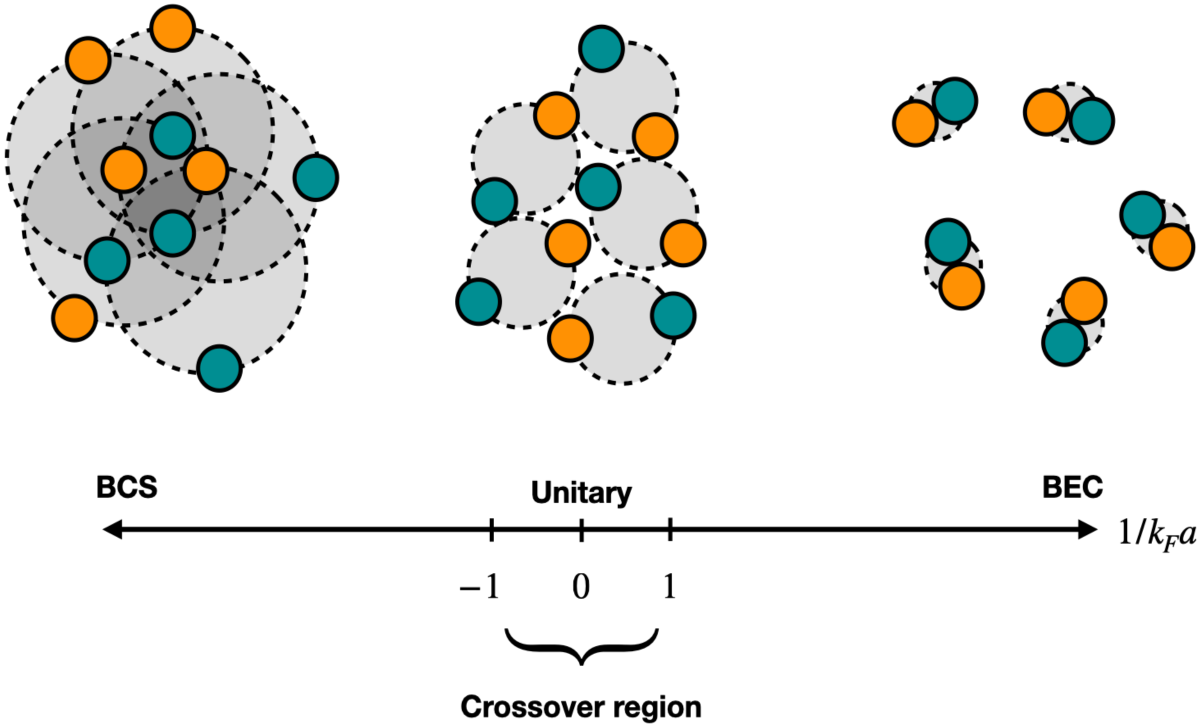
The nodal structure is improved with neural back-flow transformations $\mathbf{x}_i \rightarrow \mathbf{y}_i(\mathbf{x}_i; \mathbf{x}_{j \neq i})$



*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



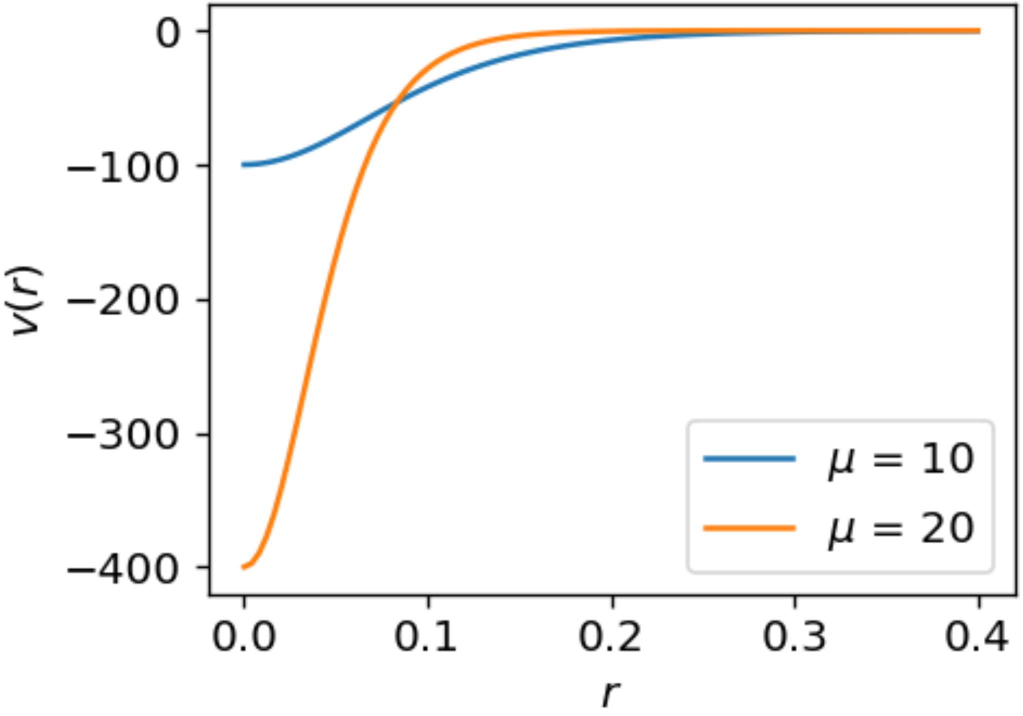
Credit: J. Kim

COLD FERMI GASES

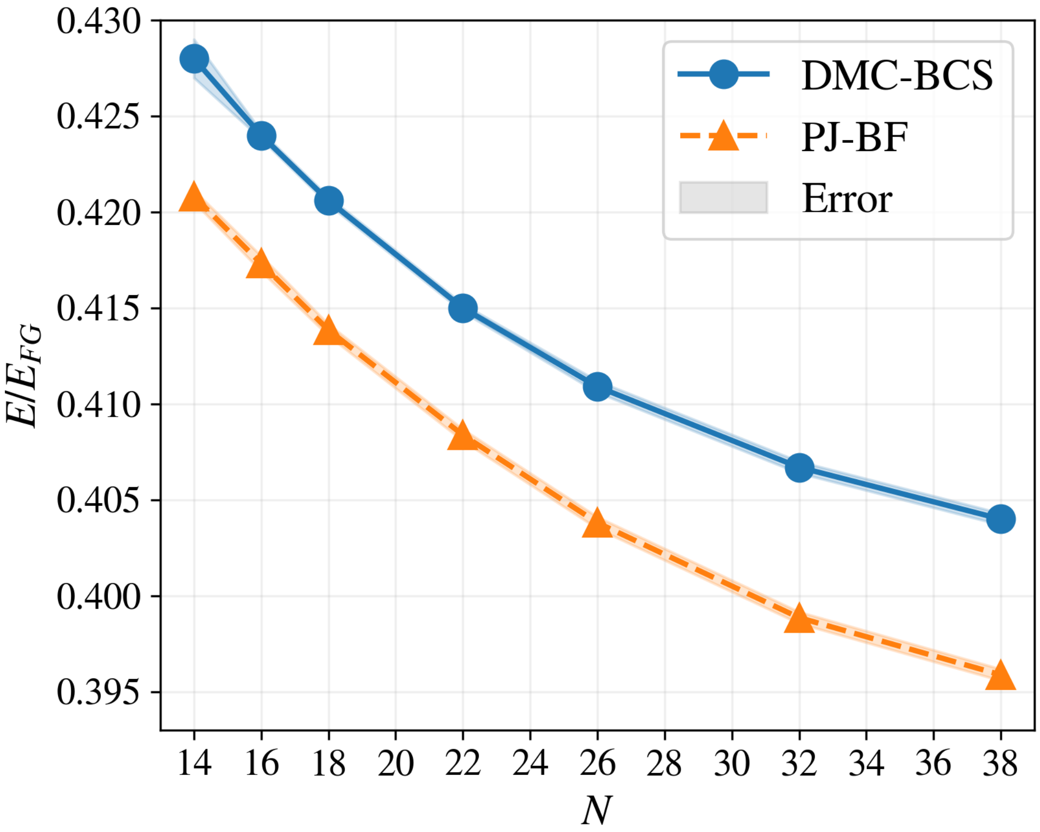
Interactions of mediated by a Pöschl-Teller potential

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

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



COLD FERMI GASES



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

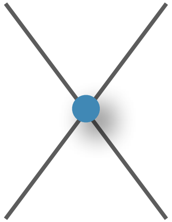
J. Kim, B. Fore, AL, et al. Commun.Phys. **7** (2024) 1, 148

“ESSENTIAL" HAMILTONIAN

Input: Hamiltonian inspired by a LO pionless-EFT expansion

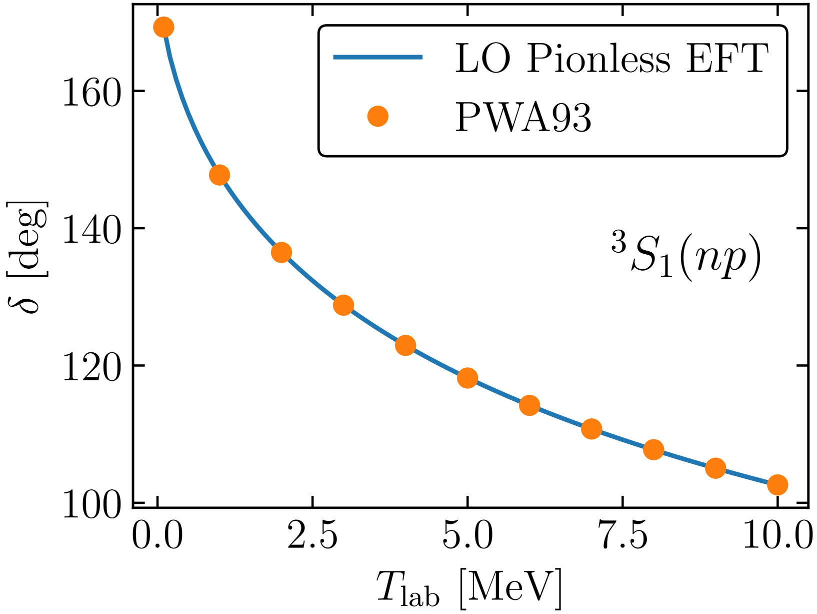
$$H_{LO} = -\sum_i \frac{\vec{\nabla}_i^2}{2m_N} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

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



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

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



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

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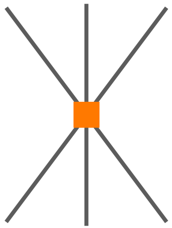
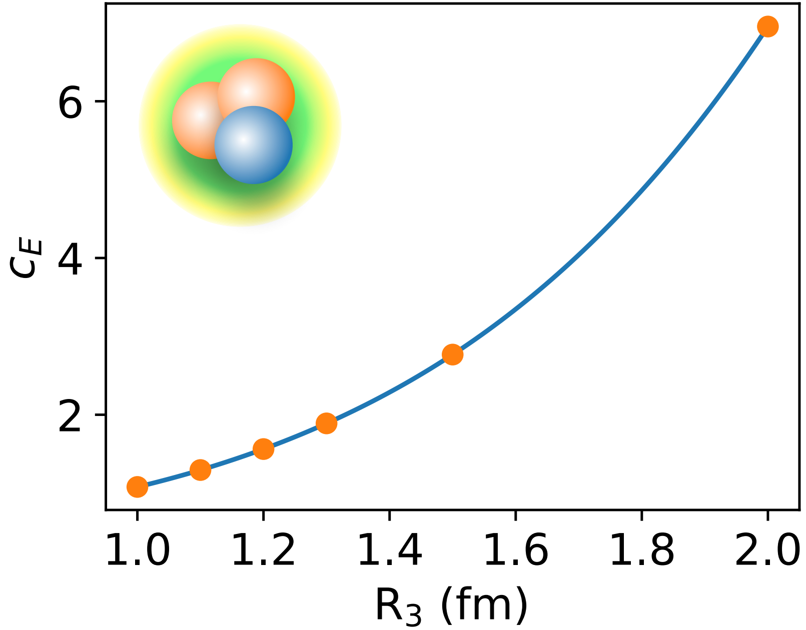
$$H_{LO} = -\sum_i \frac{\vec{\nabla}_i^2}{2m_N} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

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

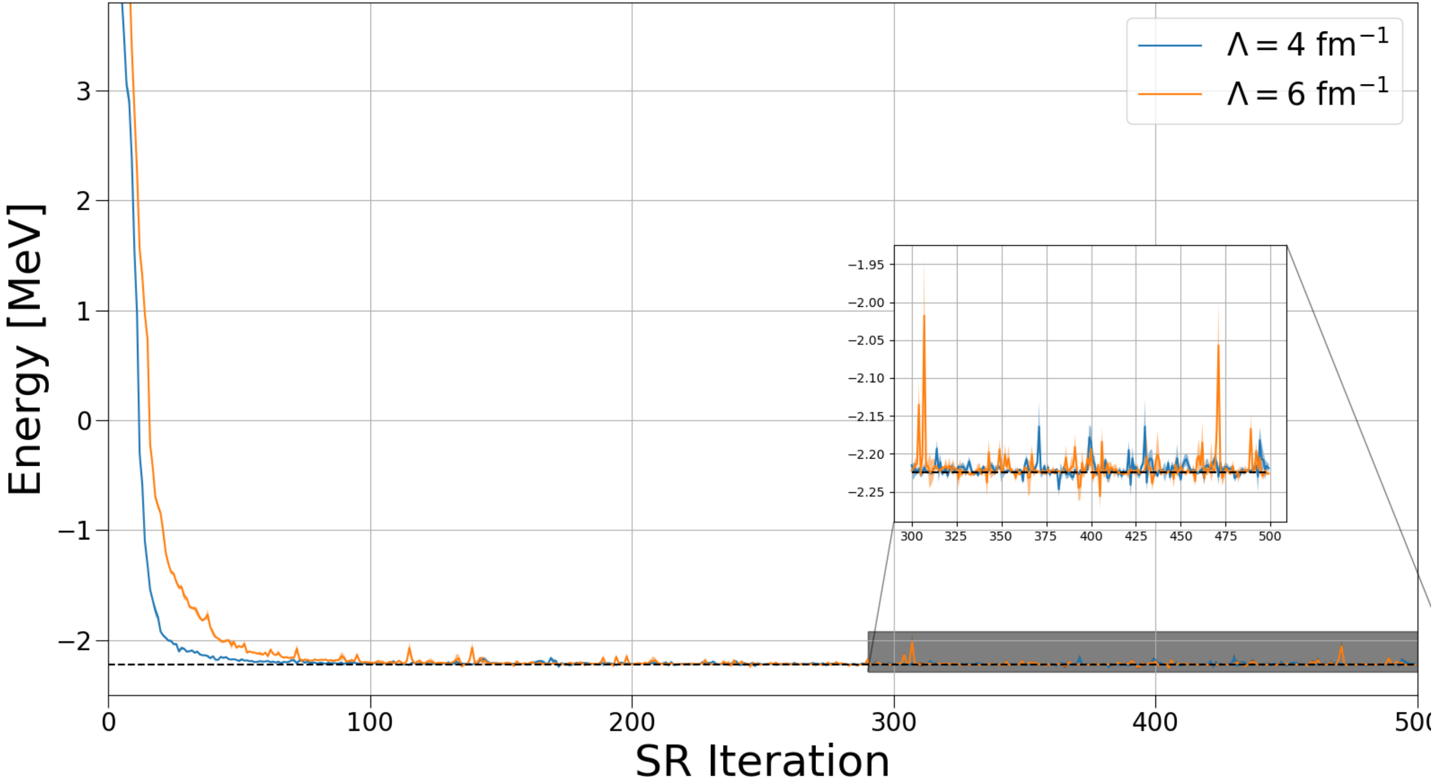


$$V_{ijk} \propto c_E \sum_{\mathrm{cyc}} e^{-(r_{ij}^2 + r_{jk}^2)/R_3^2}$$



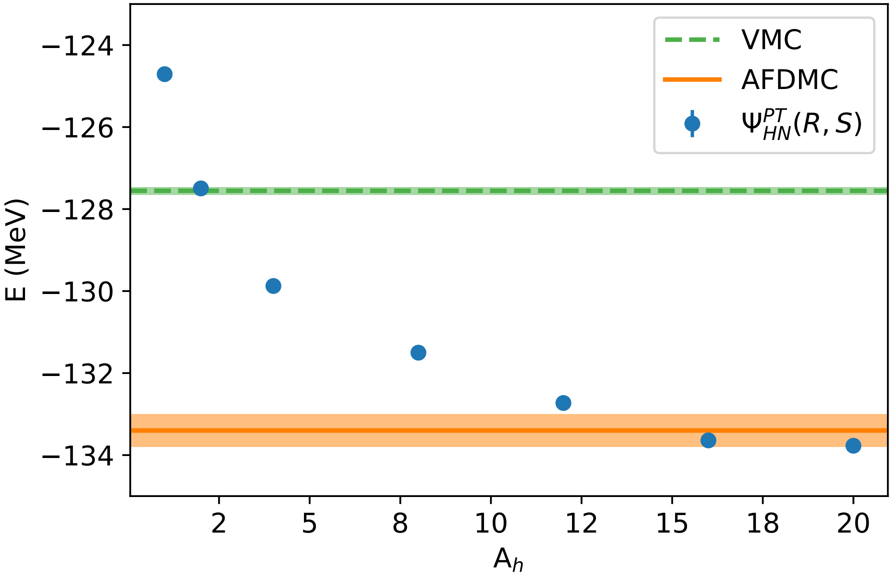
R. Schiavilla, AL, PRC **103**, 054003 (2021)

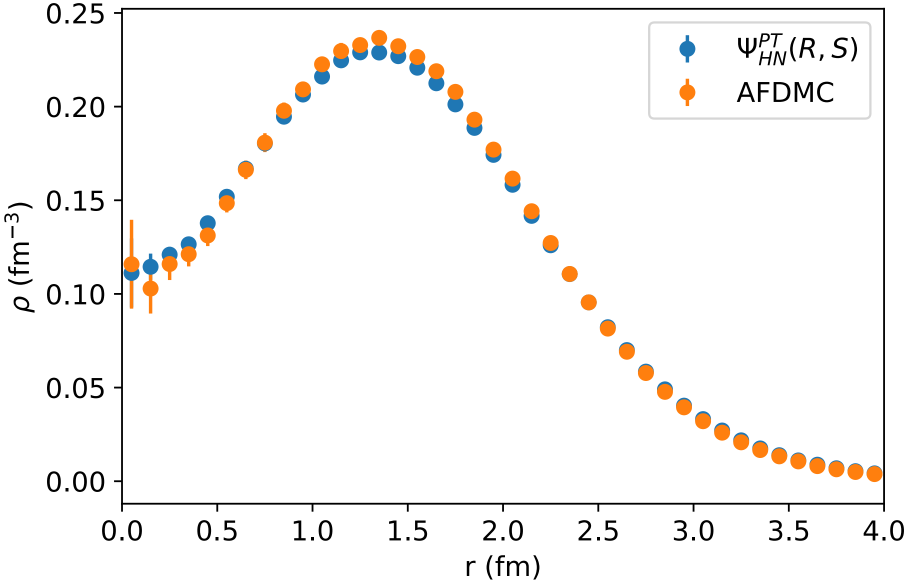
DEUTERON AGAIN



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

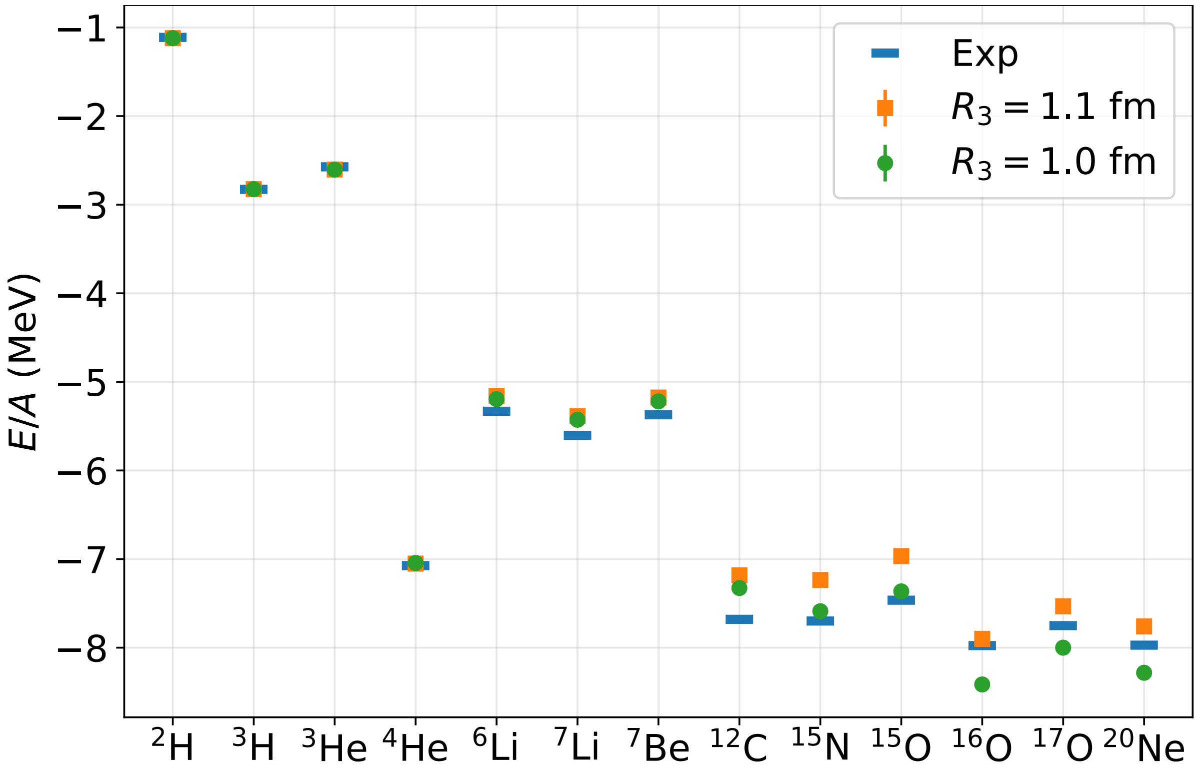
SELF-EMERGING SHELLS





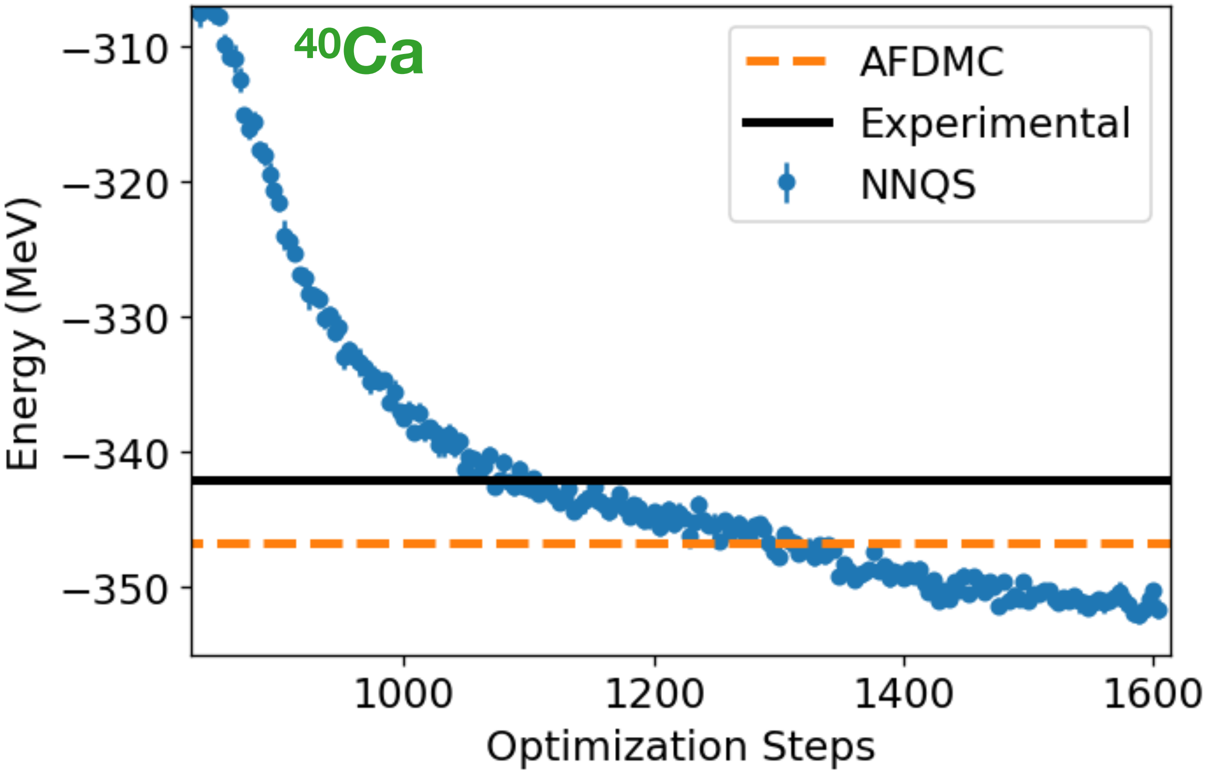
AL, et al., Phys. Rev. Res. **4** (2022) 4, 043178

REACHING NEON



A. Gnech, AL, et al., 2308.16266

AND BEYOND

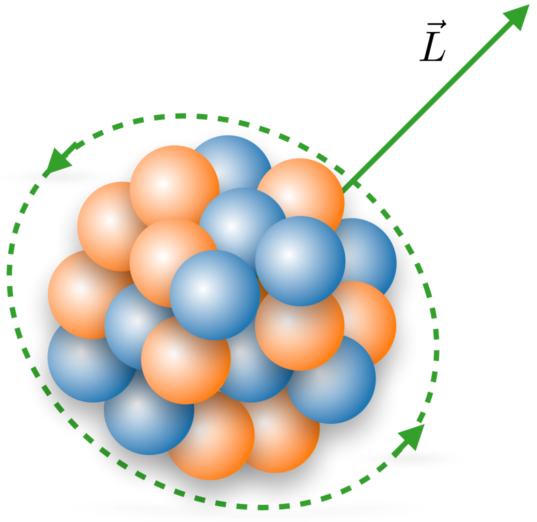


40Ca
AFDMC
Experimental
NNQS
−310
−320
−330
−340
−350
Energy (MeV)
1000
1200
1400
1600
Optimization Steps

MAGNETIC MOMENTS

The ground-state is generate in L_z

$$|\Psi_{HN}; L, S\rangle = \sum_{L_z S_z} c^{L,S}_{L_z S_z} |L, L_z; S, S_z\rangle.$$



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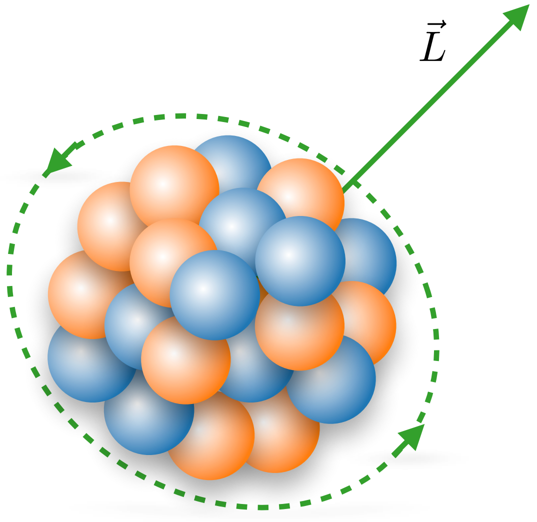
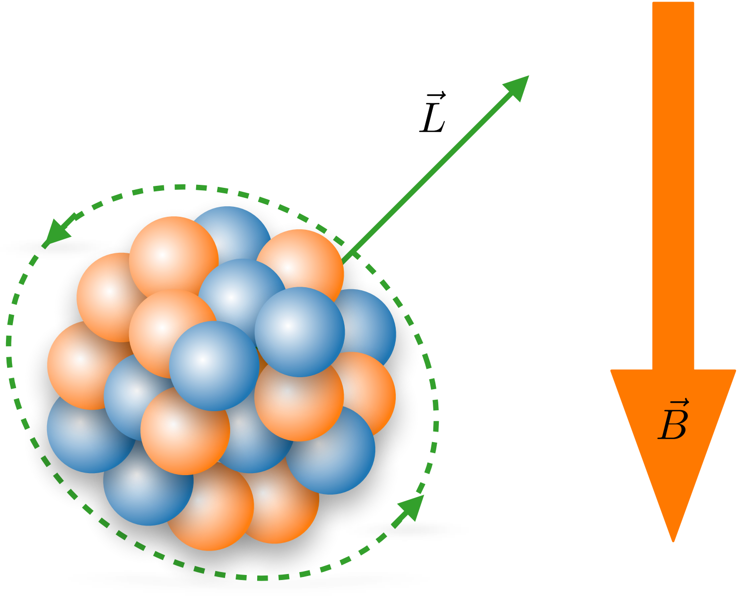


Remove this degeneracy by

$$H \to H - B_z L_z$$



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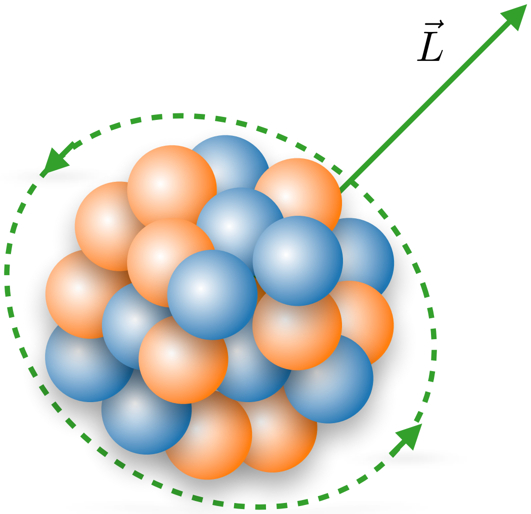
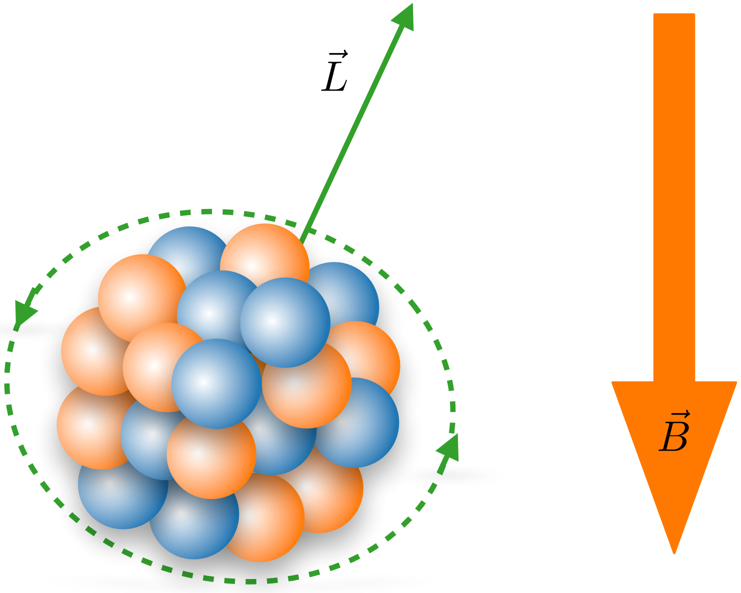


Remove this degeneracy by

$$H \rightarrow H - B_z L_z$$



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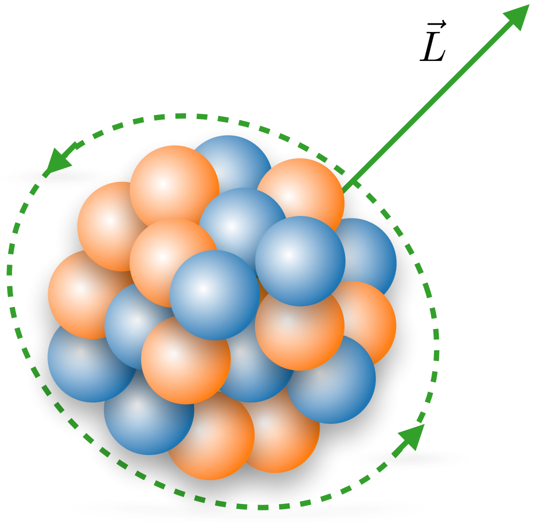

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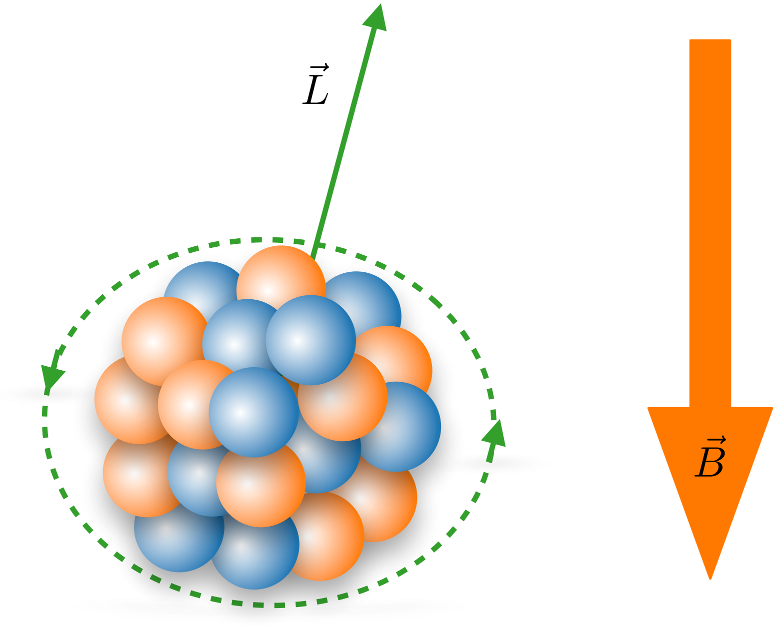

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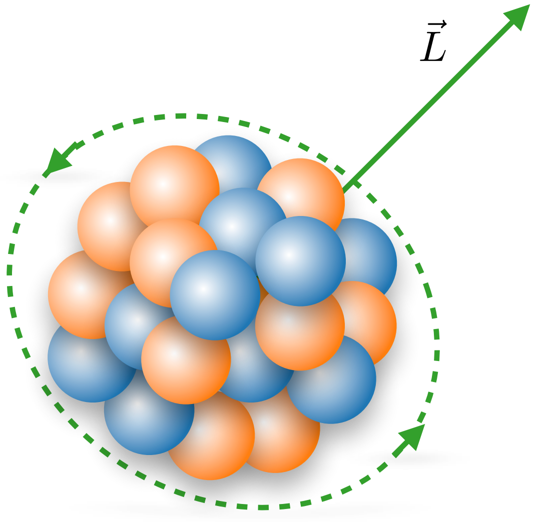

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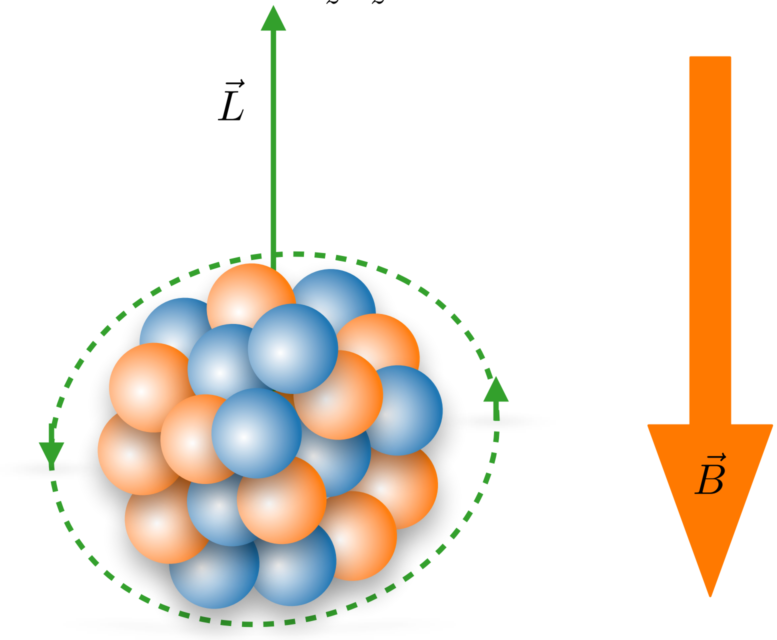
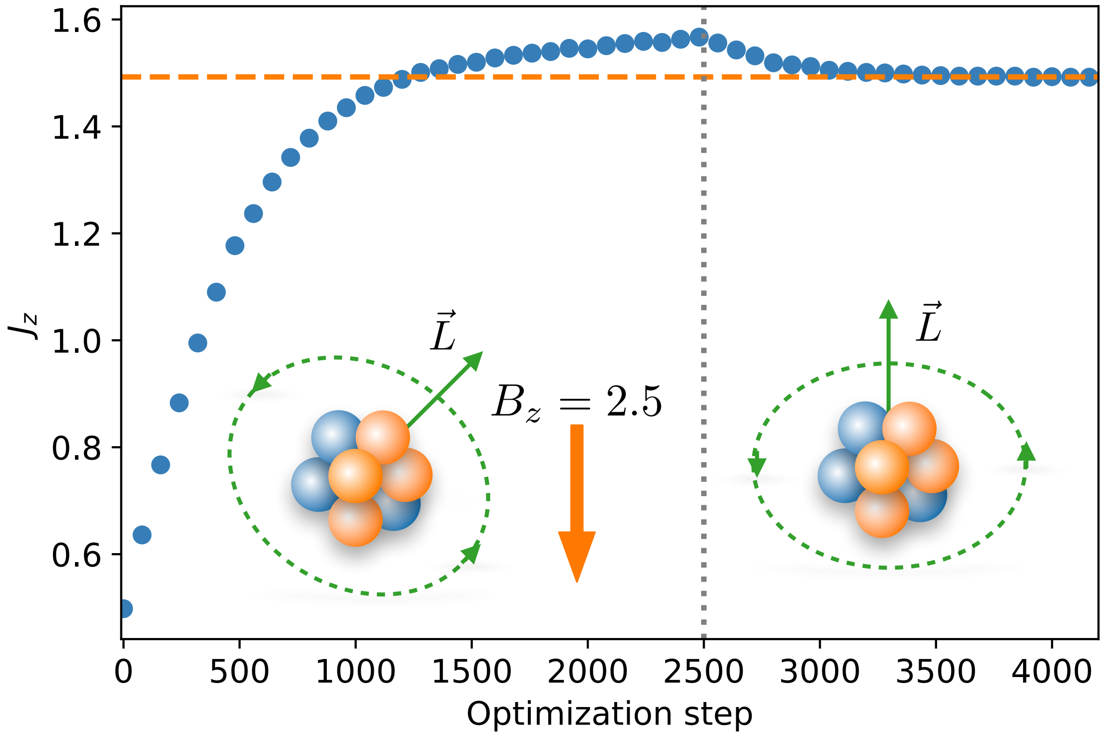
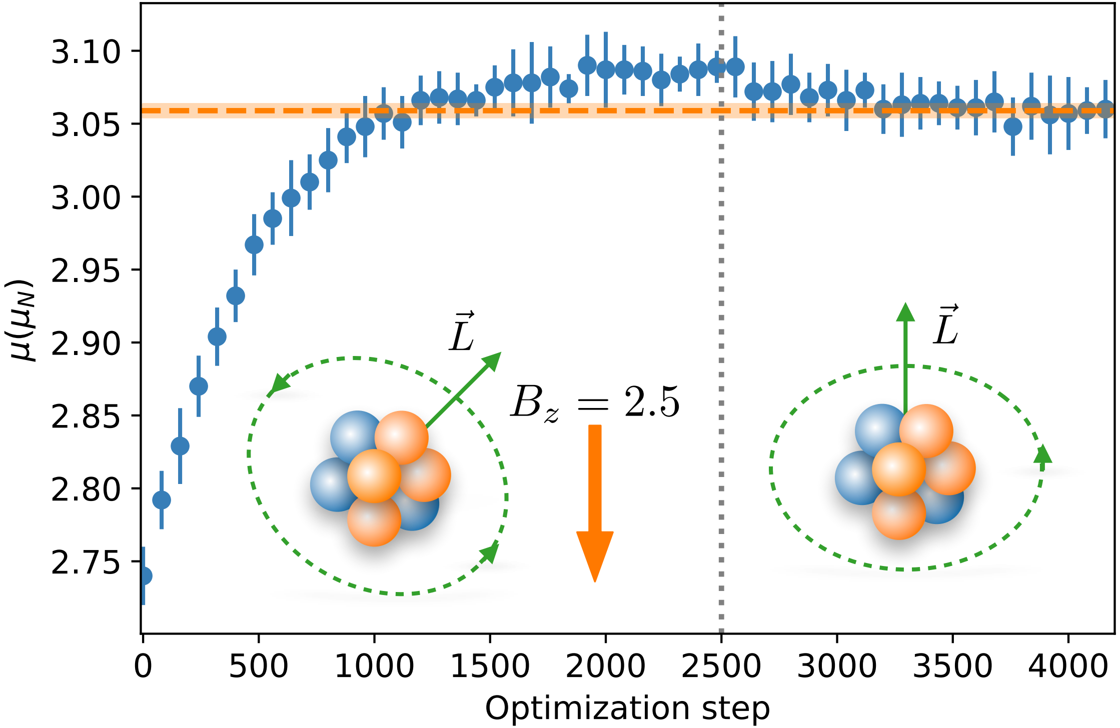


MAGNETIC MOMENTS

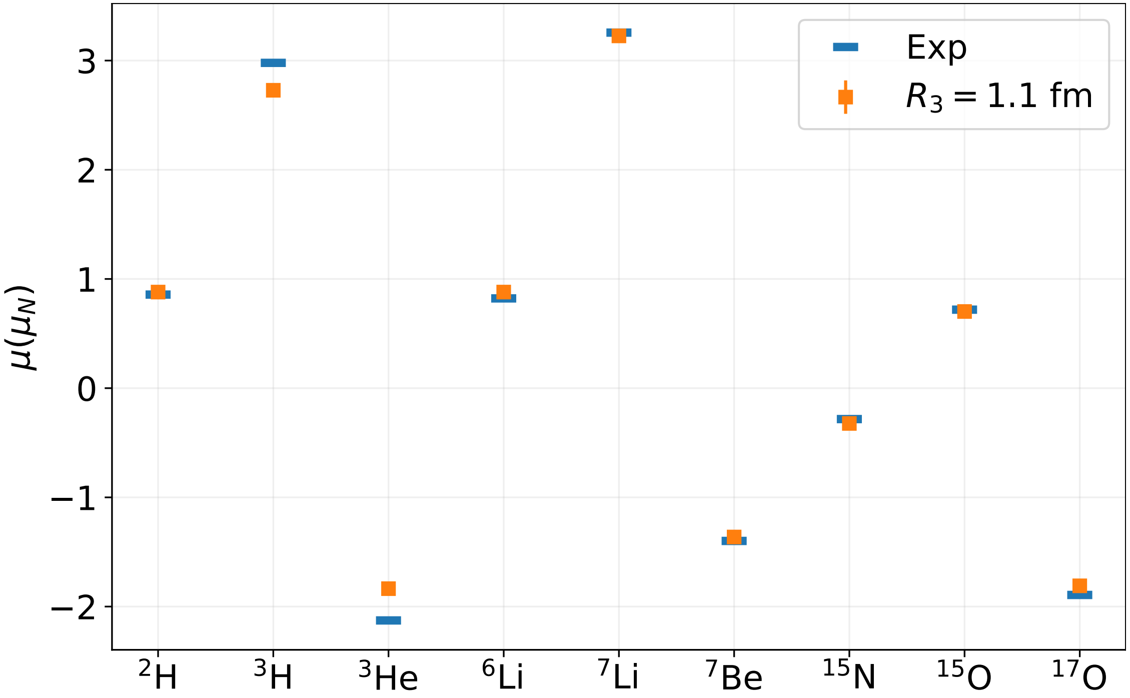


MAGNETIC MOMENTS



A. Gnech, AL, et al., 2308.16266

MAGNETIC MOMENTS



A. Gnech, AL, et al., 2308.16266

NEUTRON STARS

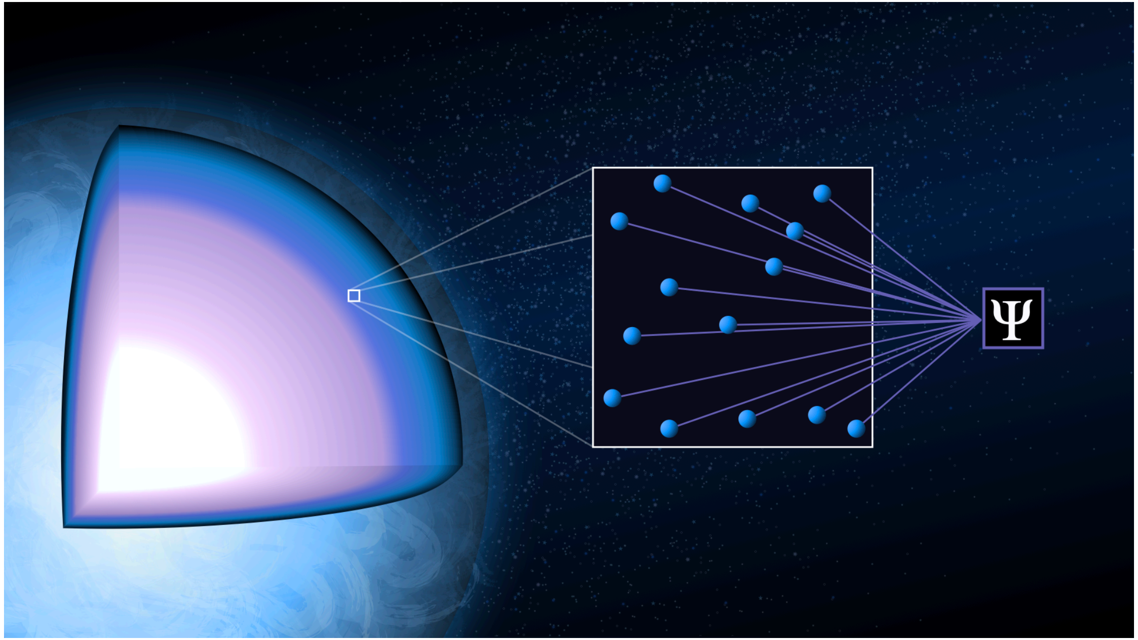
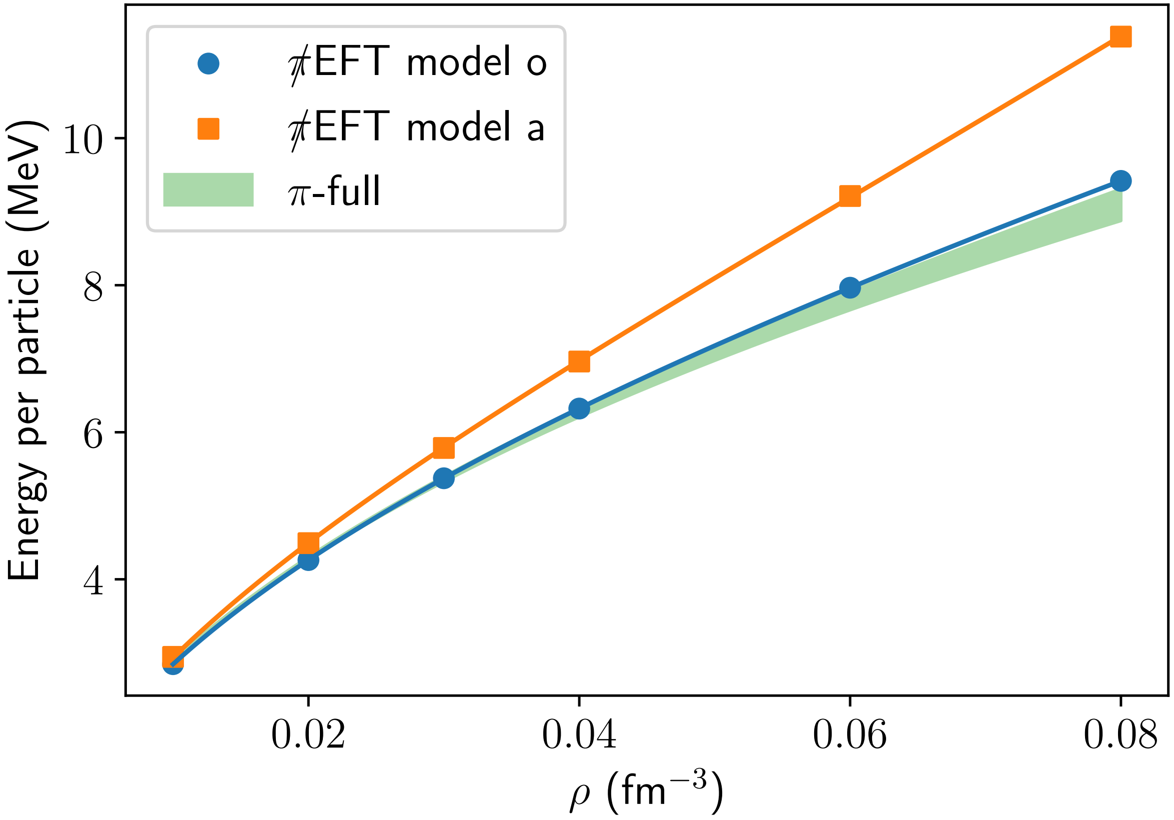


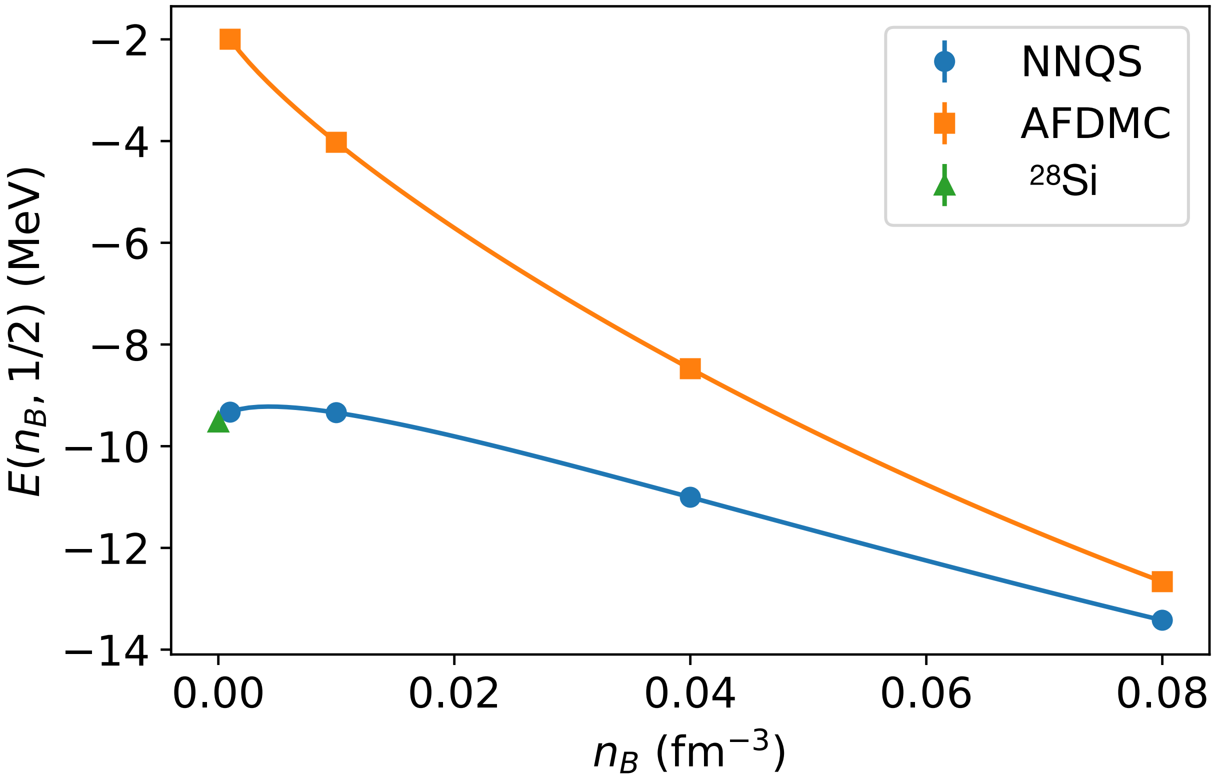
Image Credit: Jane Kim

DILUTE NEUTRON MATTER



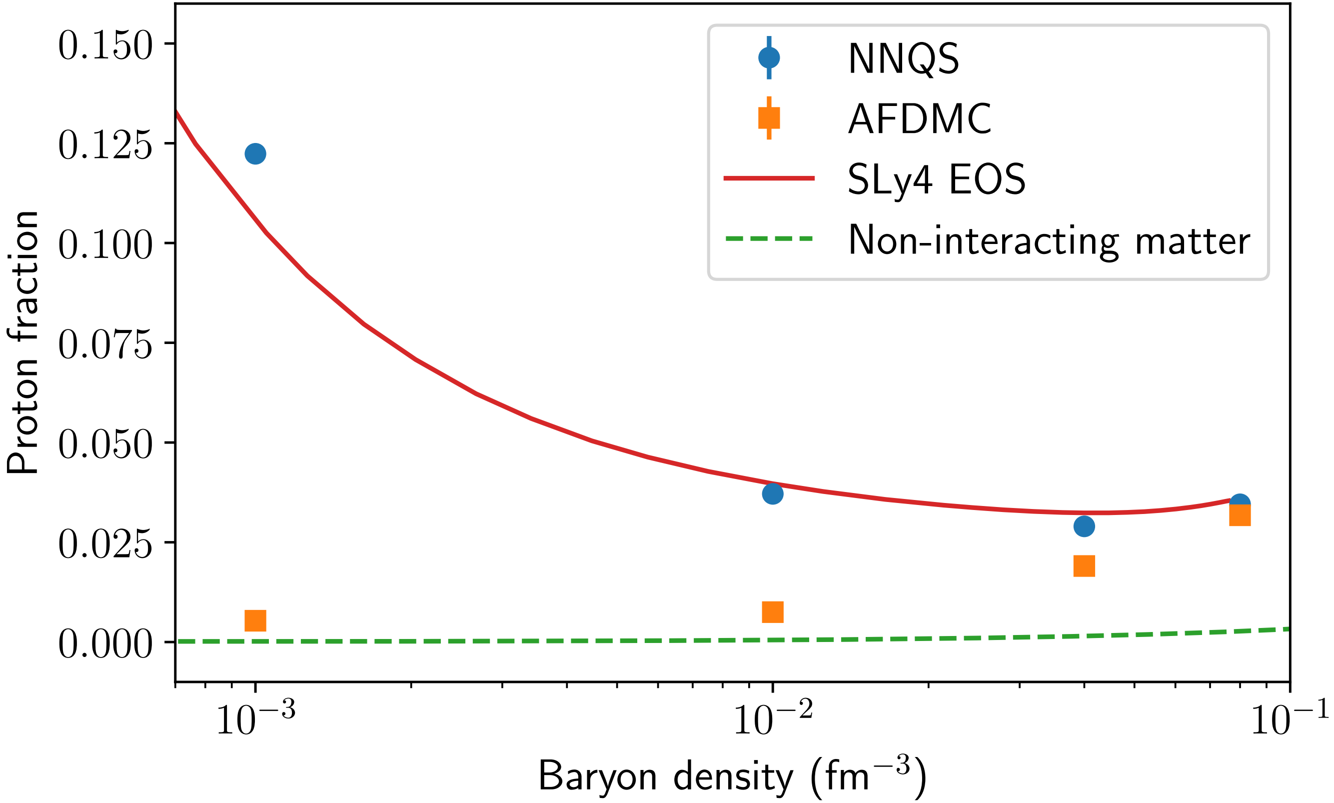
B. Fore, AL et al., Phys. Rev. Res. ***5****, 033062 (2023)*

DILUTE NUCLEONIC MATTER



B. Fore, AL, et al. in preparation

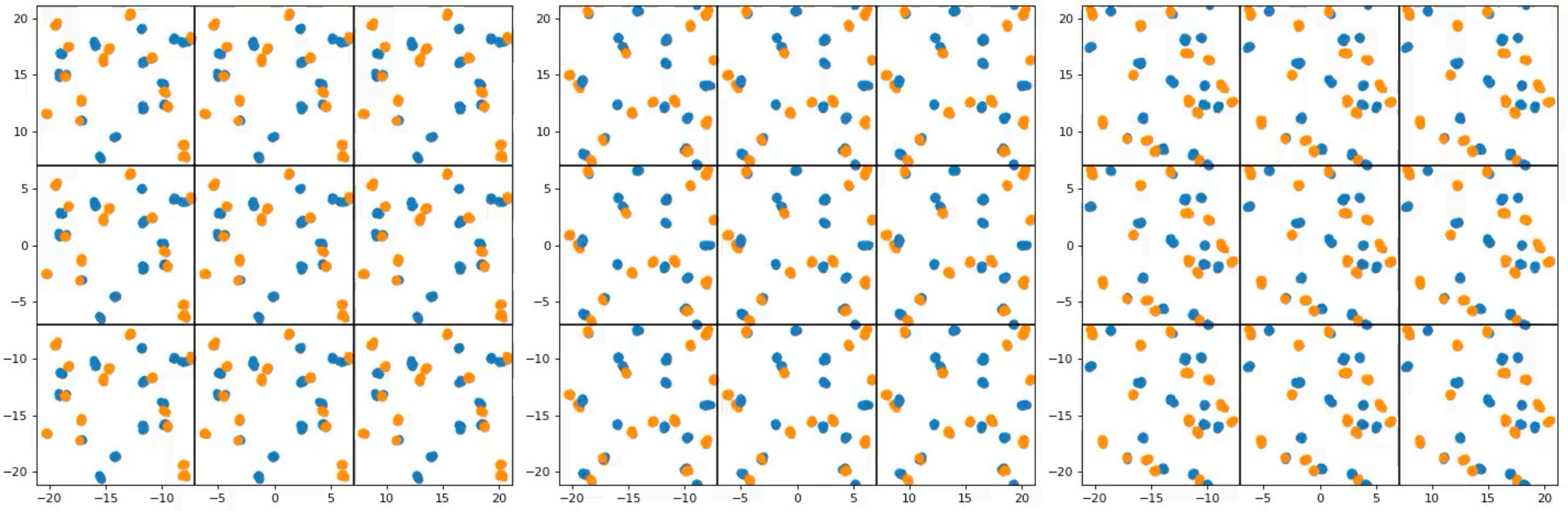
DILUTE NUCLEONIC MATTER



B. Fore, AL, et al. in preparation

DILUTE NUCLEONIC MATTER

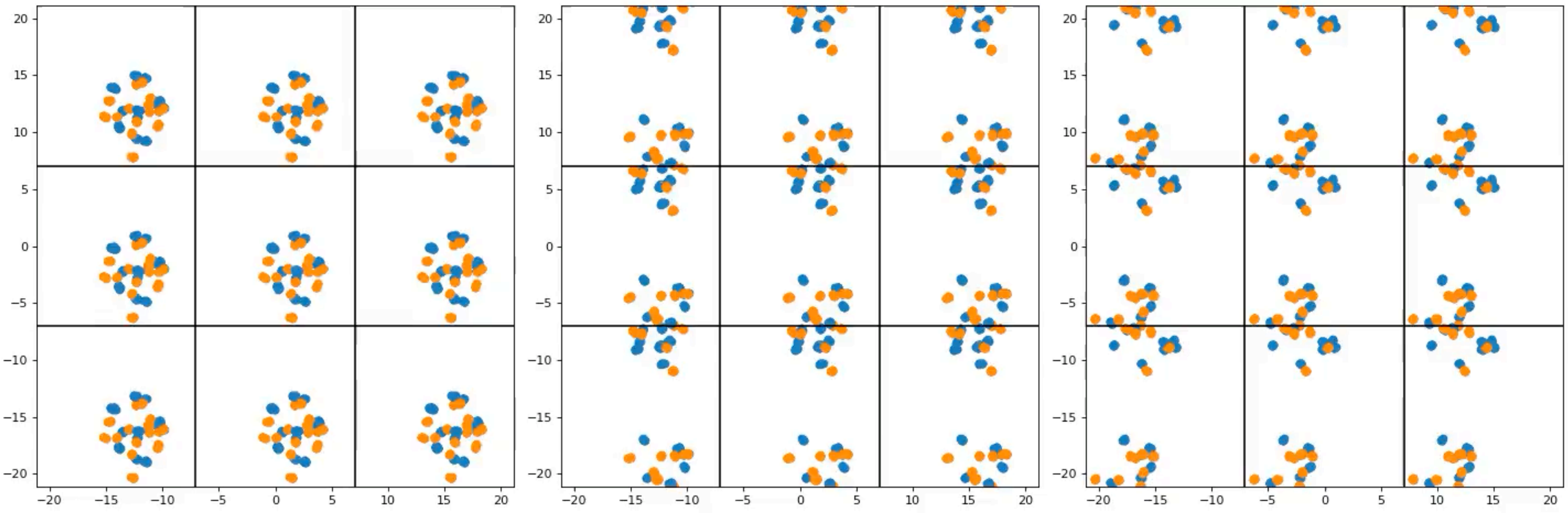
14 Neutrons, 14 Protons @ ρ=0.01 fm^{-3}



B. Fore, AL, et al. in preparation

DILUTE NUCLEONIC MATTER

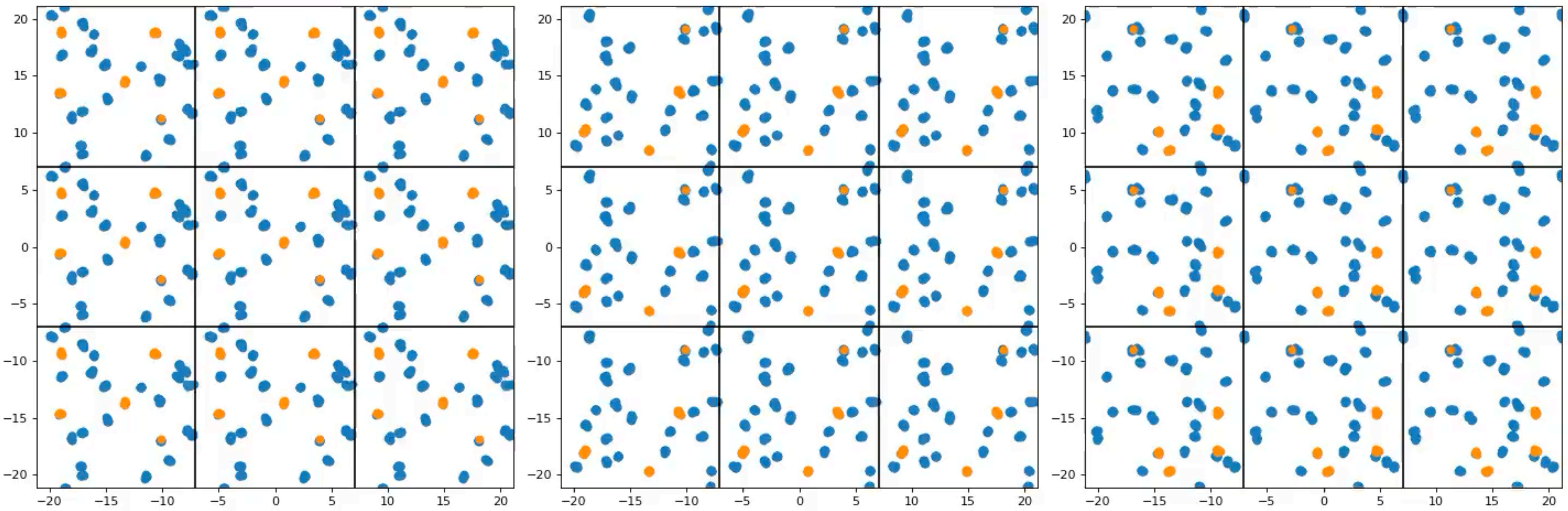
14 Neutrons, 14 Protons @ $\rho=0.01\ fm^{-3}$



B. Fore, AL, et al. in preparation

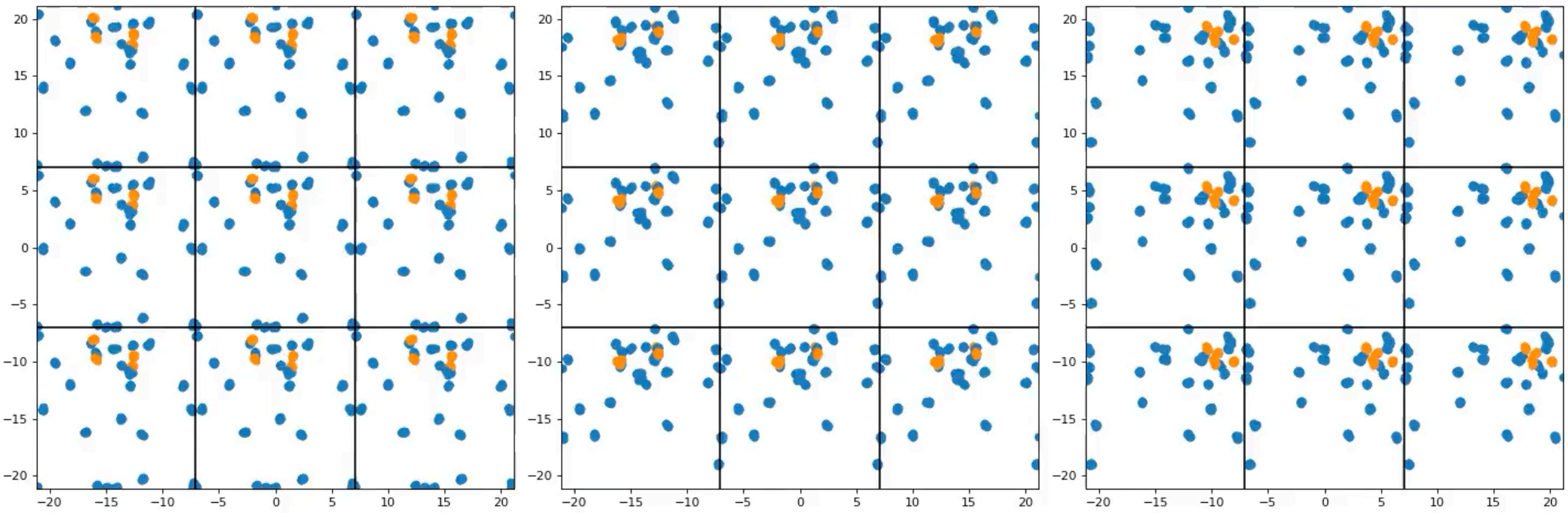
DILUTE NUCLEONIC MATTER

24 Neutrons, 4 Protons @ $\rho=0.01\ fm^{-3}$

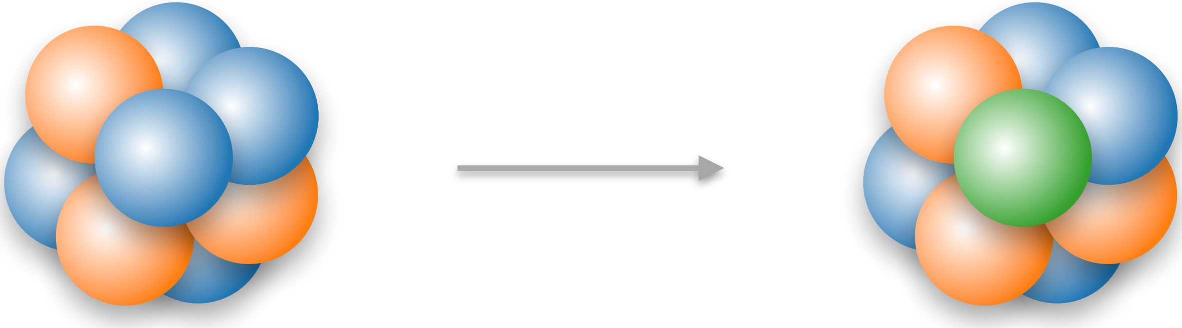


DILUTE NUCLEONIC MATTER

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



HYPERNUCLEI



$^{12}\mathrm{C}$

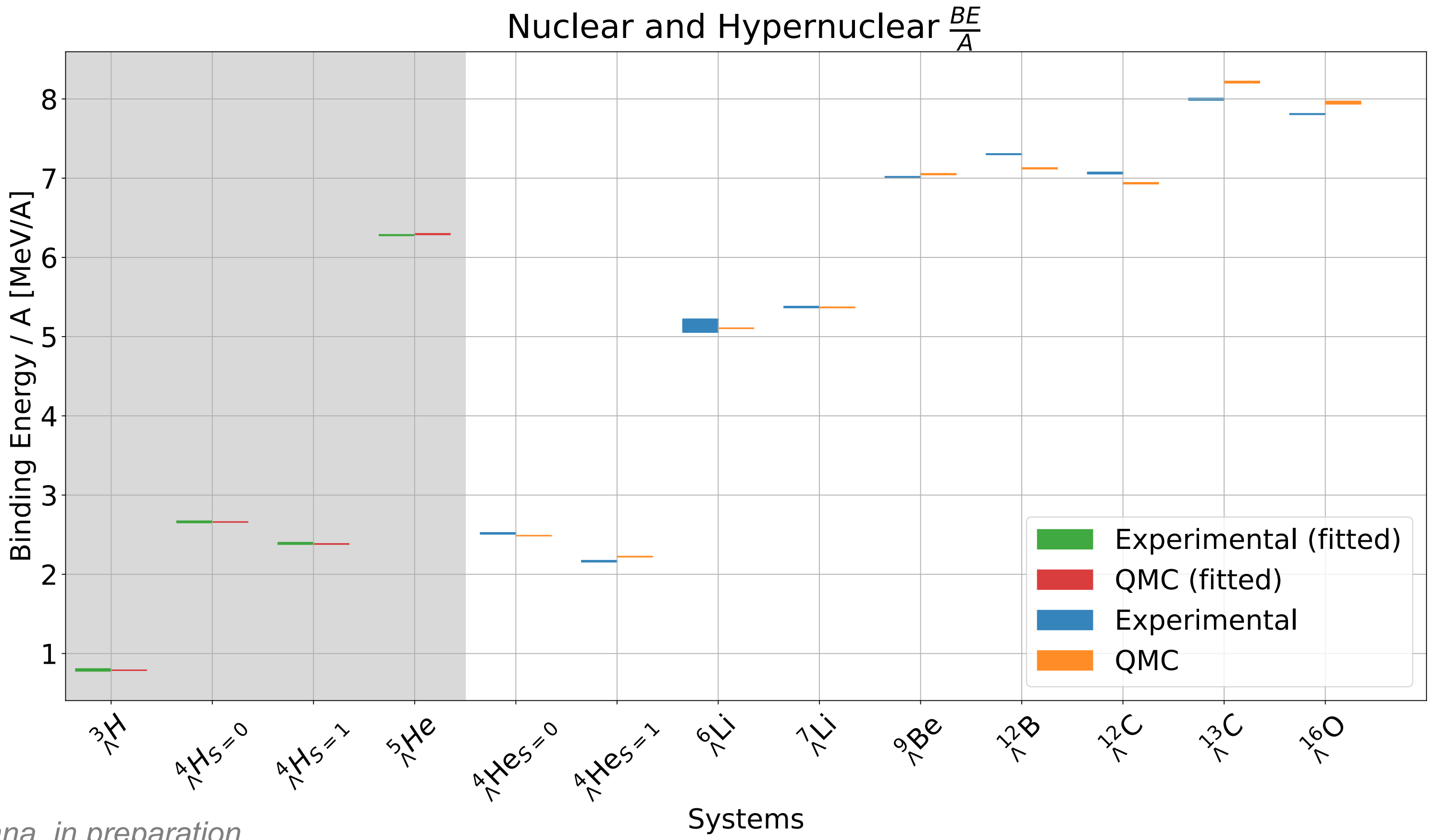
6 protons, 6 neutrons

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

6 protons, 5 neutrons, 1 lambda

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

HYPERNUCLEI



A. Di Donna, in preparation

CONCLUSIONS

NQS successfully applied to study:

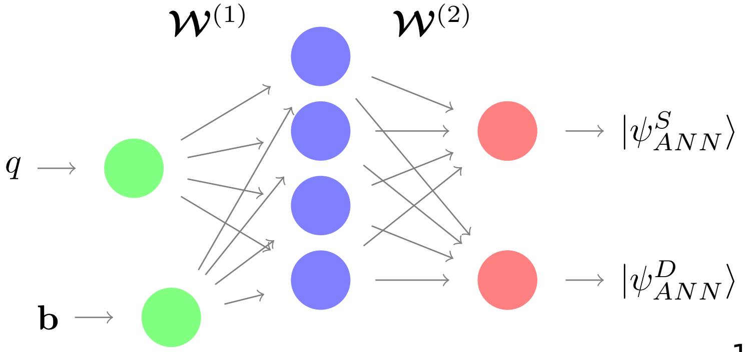
- ➡ Ultra-cold Fermi gases, outperforming state-of-the-art continuum DMC;
- ➡ Dilute nucleonic matter, including the self-emergence of nuclei;
- ➡ Essential Elements of nuclear binding

Ongoing efforts:

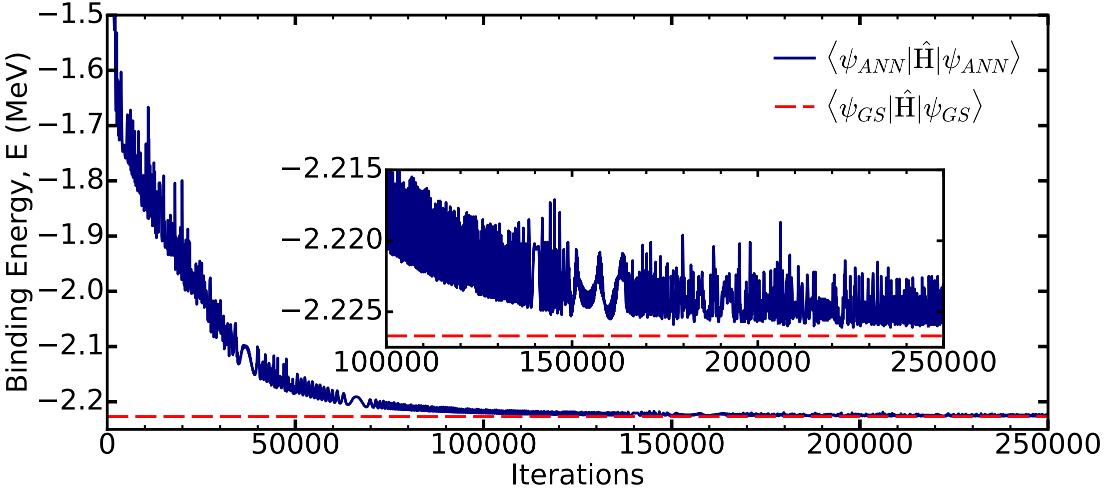
- ➡ Medium-mass nuclei
- ➡ Excited states
- ➡ Chiral-EFT potentials
- ➡ Real-time dynamics

THANK YOU

NEURAL-NETWORK QUANTUM STATES



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



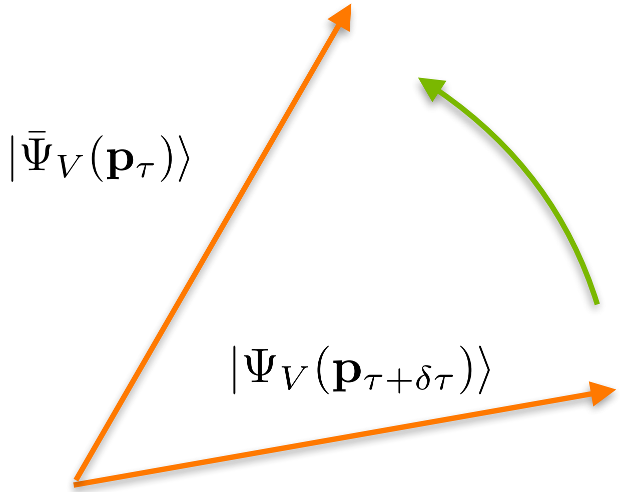
Keeble, Rios, PLB **809**, 135743 (2020)

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

WAVE FUNCTION OPTIMIZATION

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

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



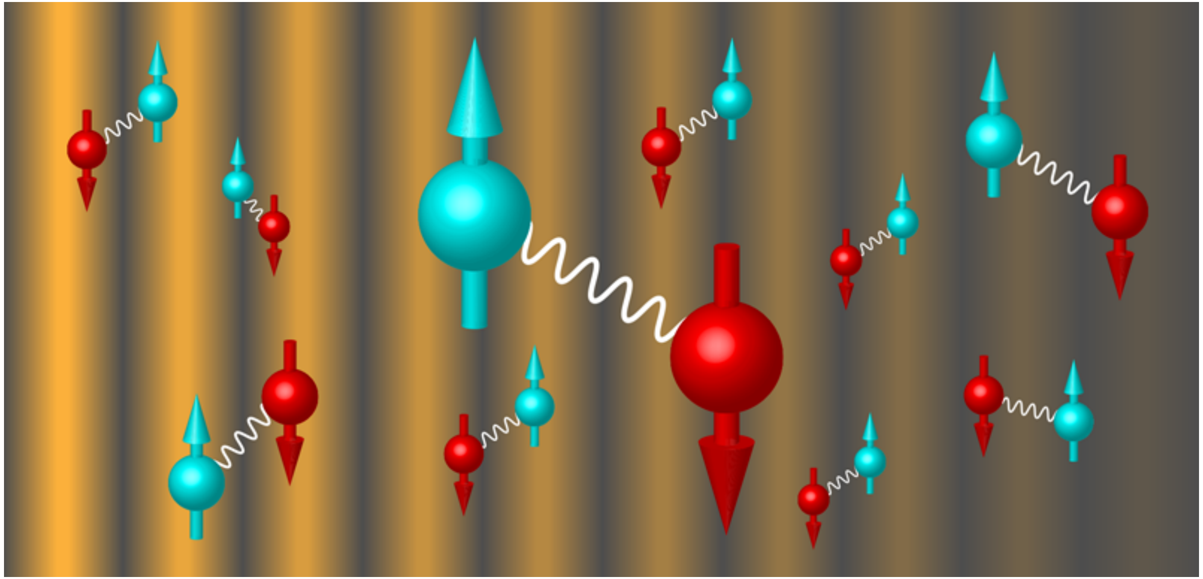
The parameters are updated as

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

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

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

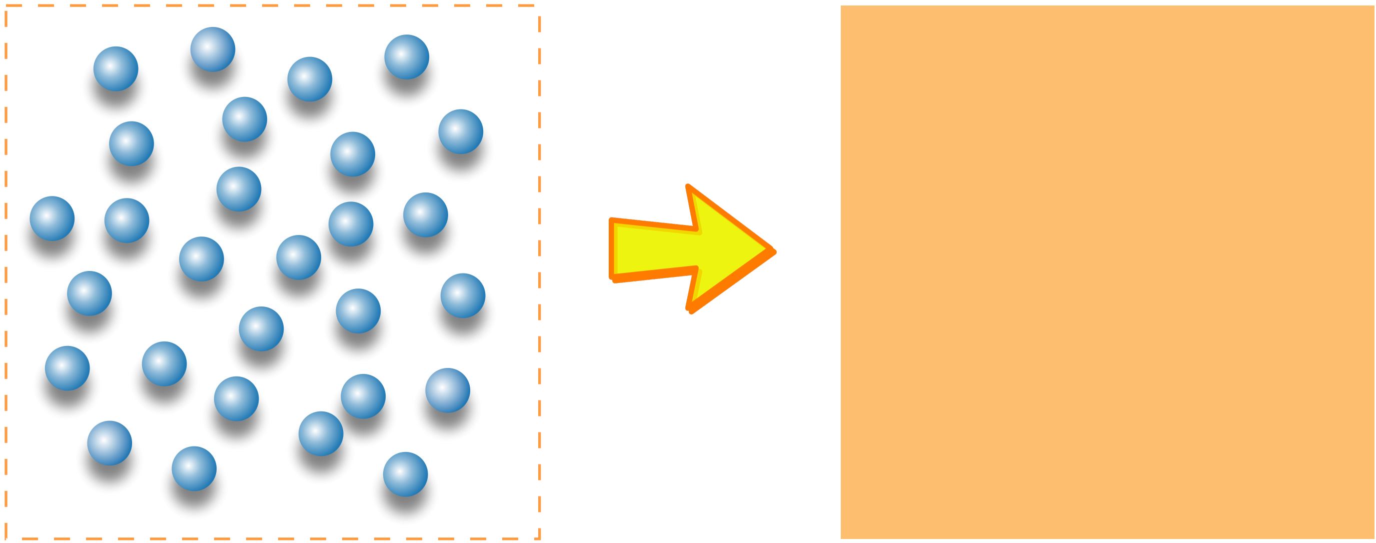
CONDENSED-MATTER DETOUR



HOMOGENOUS ELECTRON GAS

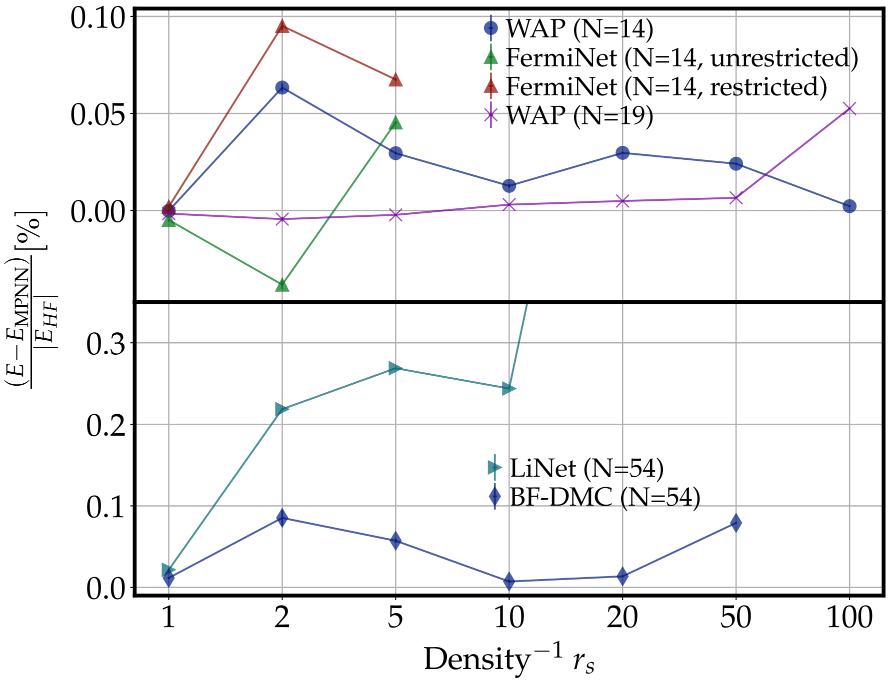
We develop translation invariant NQS to study the Homogeneous Electron Gas.

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

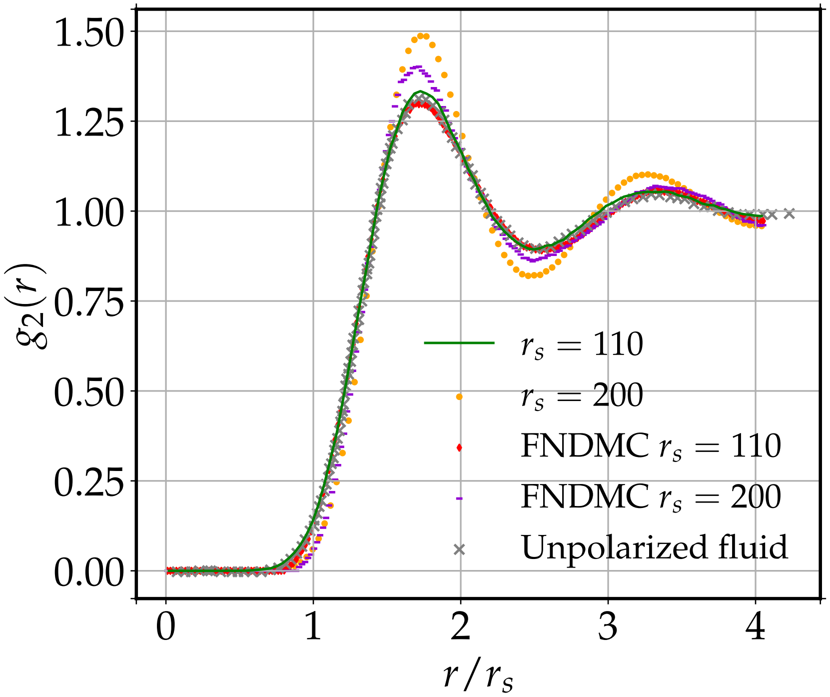


HOMOGENOUS ELECTRON GAS

Energies



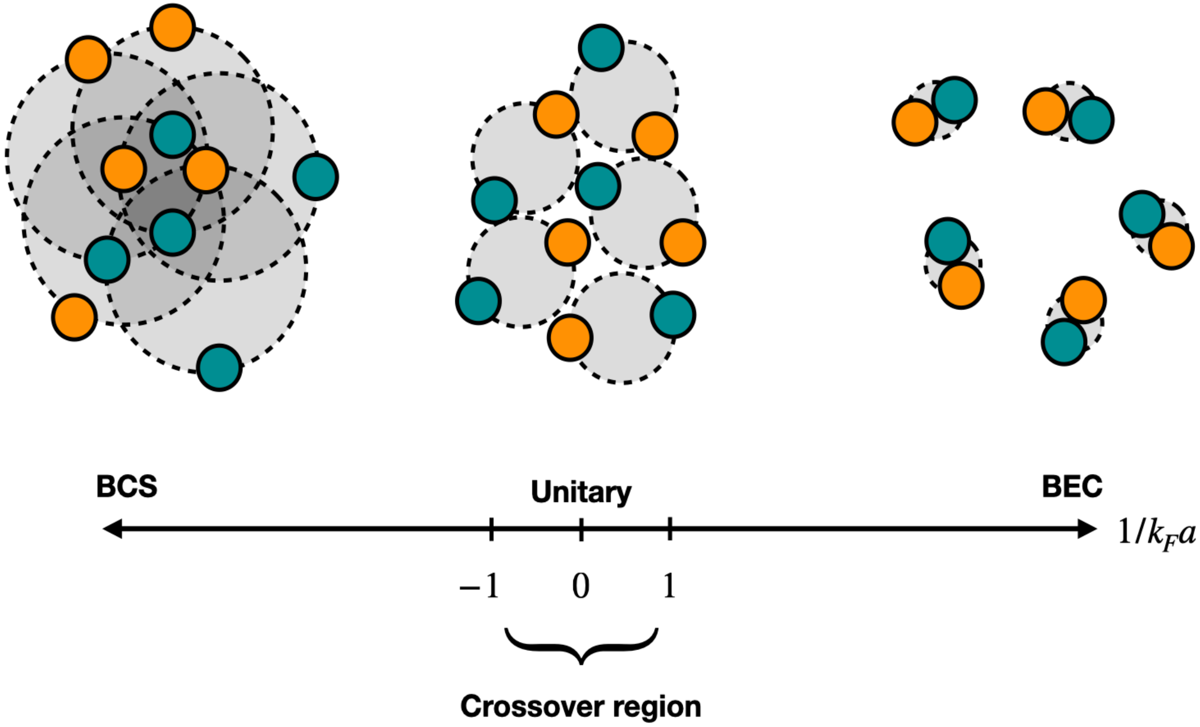
Correlation functions



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

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