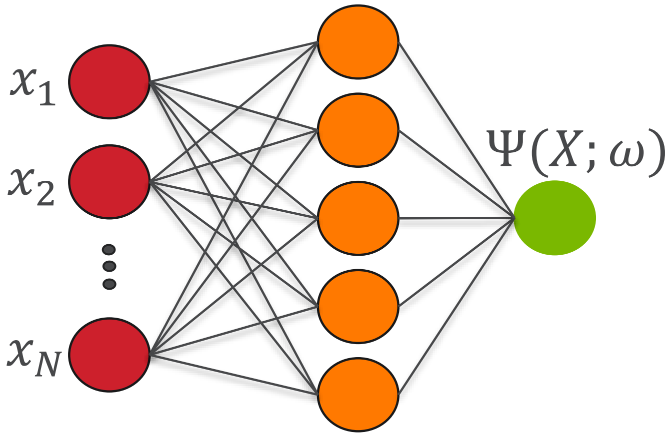
MODELING LOW-DENSITY NUCLEAR MATTER WITH NEURAL QUANTUM STATES



BRYCE FORE

Fifth Gogny Conference
Paris, France
December 12th 2024

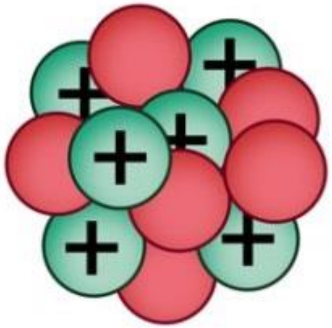
QUANTUM MANY-BODY METHODS

THE NUCLEAR MANY-BODY PROBLEM

Many-body Schrödinger equation

$$\left(-\sum_i \frac{\nabla_i^2}{2m_N} + V\right)|\Psi_0\rangle = E_0|\Psi_0\rangle$$

Nuclei



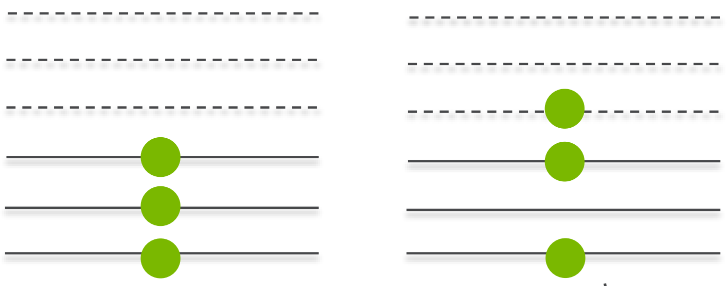
Neutron stars

THE NUCLEAR MANY BODY METHODS

Configuration-interaction

$$|\Psi_0\rangle = \sum_{h_1,\dots,p_1,\dots} c_{h_1\dots}^{p_1\dots} \left|\Phi_{h_1\dots}^{p_1\dots}\right\rangle$$

$$\left|\Phi_{h_1\dots}^{p_1\dots}\right\rangle = a_{p_1}^{\dagger} \dots a_{h_1} \dots |\Phi_0\rangle$$



$$|\Phi_0\rangle \qquad \left|\Phi_{h_2}^{p_1}\right\rangle$$

Quantum Monte Carlo

$$|\Psi_V\rangle = \sum_n c_n |\Psi_n\rangle$$

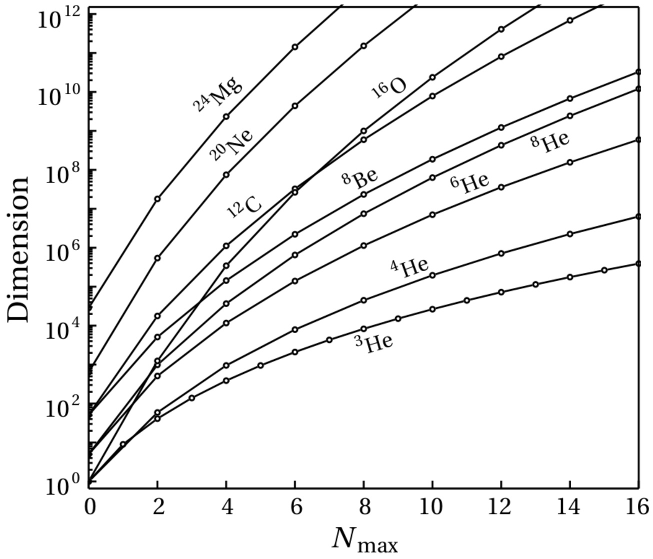
$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

$$\lim_{\tau\to\infty} e^{-(H-E_0)\tau}\,|\Psi_V\rangle = c_o|\Psi_0\rangle$$

CURSE OF DIMENSIONALITY

Configuration-interaction

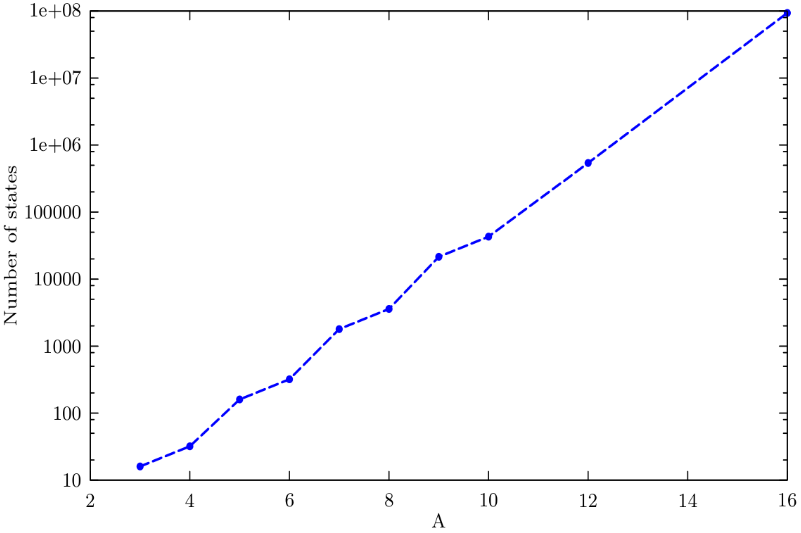
$$\binom{N}{A} = \frac{N!}{(N-A)!\,A!}$$



Credit: Patrick Fasano

Green's function Monte Carlo

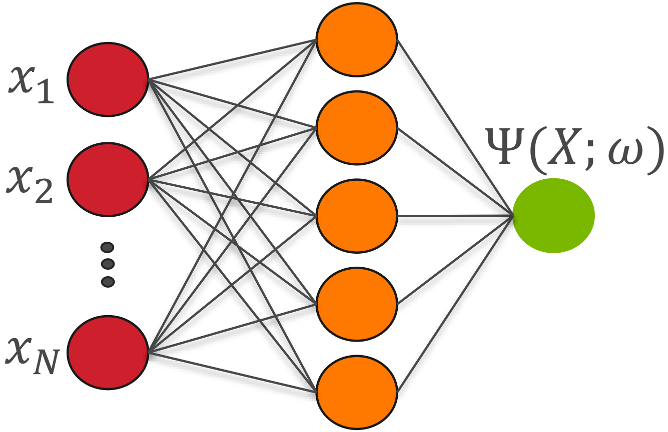
$$\lim_{\tau\to\infty} e^{-(H-E_0)\tau}\left|\Psi_V\right\rangle = c_o\left|\Psi_0\right\rangle$$

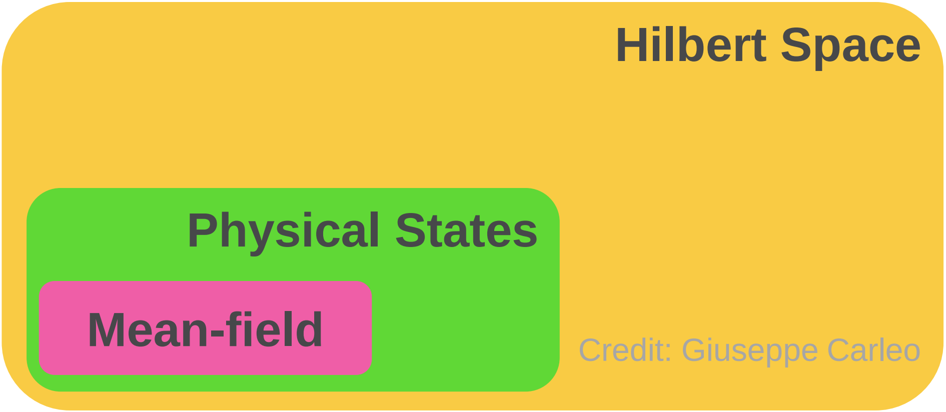


Credit: Alessandro Lovato

NEURAL NETWORK QUANTUM STATES

- Artificial neural networks compactly represent complex high-dimensional functions
- Most quantum states of interest have distinctive features and intrinsic structures





SCALING AND COMPUTATIONAL PERFORMANCE

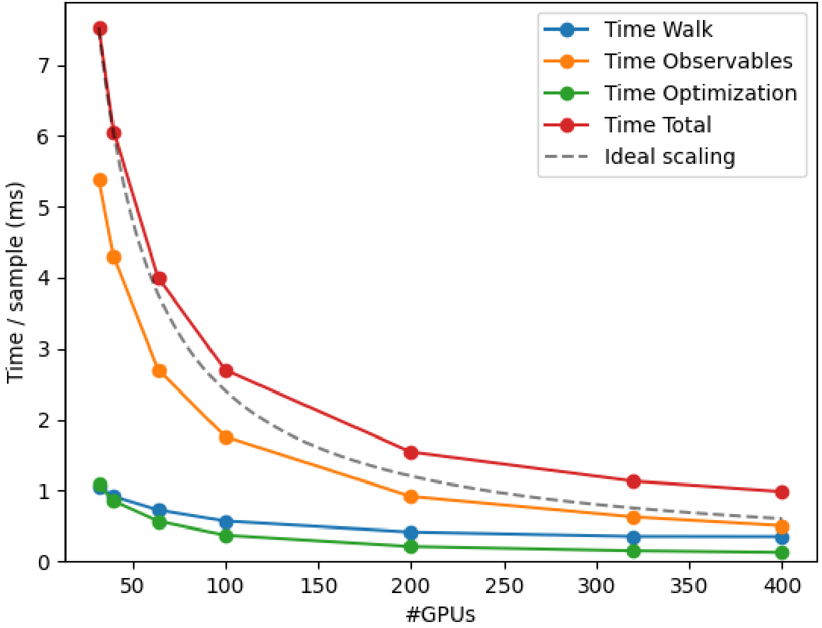
Scaling with system size

Conventional QMC: $O(2^A)$

Neural quantum states: $O(A^5)$

A = Number of particles in system

Scaling with resources



VARIATIONAL MONTE CARLO WITH NQS

1. Create the NQS wavefunction

$$\Psi_V(R,S;\omega) = e^{U(R,S;\omega)}\Phi(R,S;\omega)$$

2. Compute its energy (Metropolis-Hastings algorithm)

$$\frac{\langle \Psi_V | O | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} \approx \frac{1}{N_{conf}} \sum_{\{R,S\}} O_L(R,S)$$

3. Minimize the energy w.r.t parameters, ω, to reach the ground state

$$E_0 \leq E_V = \frac{\langle \Psi_V | \hat{H} | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle}$$

FERMIONIC WAVEFUNCTIONS

$$\Psi_V(X) = e^{U(X)}\Phi(X)$$

$$\Psi(\dots, x_i, \dots x_j \dots) = -\Psi(\dots, x_j, \dots x_i \dots)$$

$$U(\dots, x_i, \dots x_j \dots) = \quad U(\dots, x_j, \dots x_i \dots)$$

$$\Phi(\dots, x_i, \dots x_j \dots) = -\Phi(\dots, x_j, \dots x_i \dots)$$

- Build in fermion antisymmetry for network compactness
- Permutation-invariant Jastrow function improves ansatz flexibility
- Build U and Φ functions from fully connected, deep neural networks

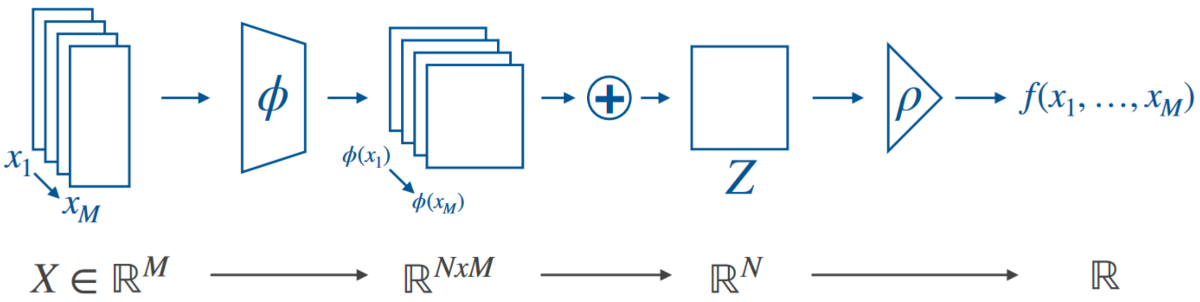
DEEP SET ARCHITECTURE

- Generic permutation invariant function

$$U(X) = \rho\left(\sum_i \vec{\phi}\,(x_i)\right)$$

$$\vec{\phi}: \mathbb{R}^5 \to \mathbb{R}^N$$

$$\rho: \mathbb{R}^N \to \mathbb{R}$$



Wagstaff et al., arXiv:1901.09006 (2019)

Zaheer et al., arXiv:1703.06114 (2017)

NEURAL SLATER-JASTROW ANSATZ

- Slater determinants used in other methods to represent many-body states
- Slater determinant to enforce antisymmetry
- Single particle wavefunctions represented by neural networks

$$\Psi_V(X) = e^{U(X)}\Phi(X)$$

$$\Phi(X) = \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \cdots & \phi_1(x_N) \\ \phi_2(x_1) & & & \vdots \\ \vdots & & & \\ \phi_n(x_1) & \cdots & & \phi_n(x_N) \end{vmatrix}$$

NEURAL PFAFFIAN ANSATZ

- Slater determinant → Pfaffian
- Build in antisymmetry through a single pairing network rather than determinant of single-particle states

$$det(M) = pf(M)^2$$

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

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

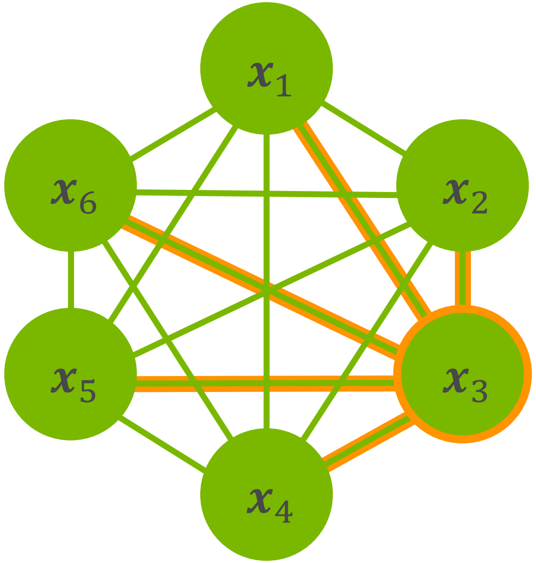
J. Kim, *Commun Phys* **7**, 148 (2024)

MESSAGE PASSING NEURAL NETWORK

Backflow transformation representable by updates to fully connected graph

$$\boldsymbol{x}_i \rightarrow f(\boldsymbol{x}_i; \{\boldsymbol{x}_j\}_{j \neq i})$$

- Update edge values based on vertices
- Update vertex values based on connected edges
- Retains ordering information for antisymmetry operation



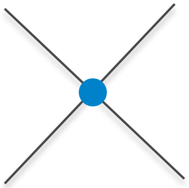
NQS RESULTS

PIONLESS EFT HAMILTONIAN

- Pionless-EFT Hamiltonian

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

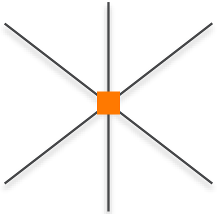
- NN potential fit to
  - np scattering lengths
  - effective radii
  - deuteron binding energy



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

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

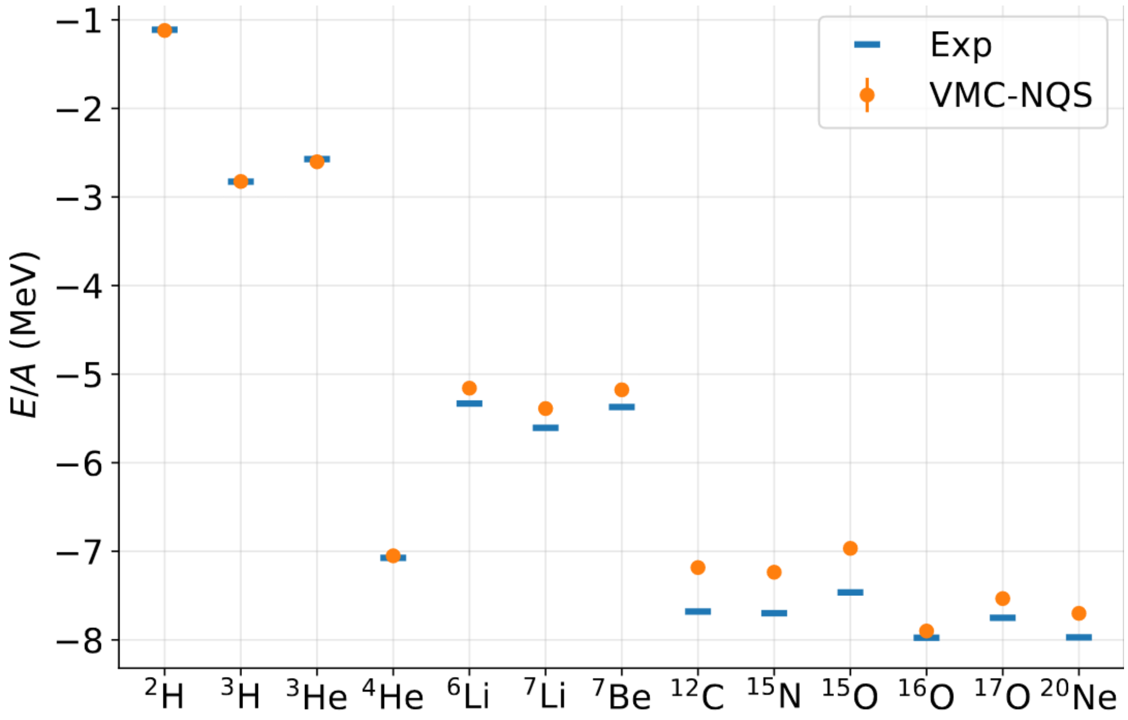
- Three body potential adjusted to reproduce ^{3}H binding



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

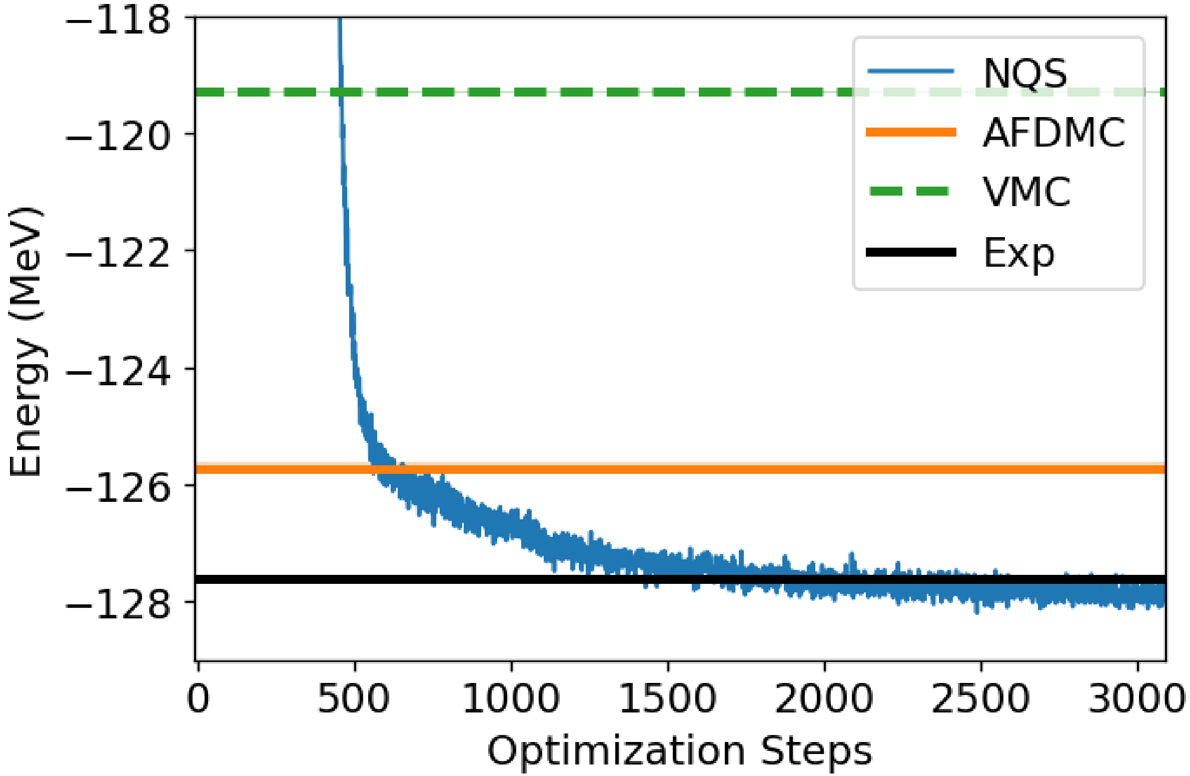
R. Schiavilla, PRC 103, 054003(2021)

NEURAL QUANTUM STATE RESULTS IN NUCLEI

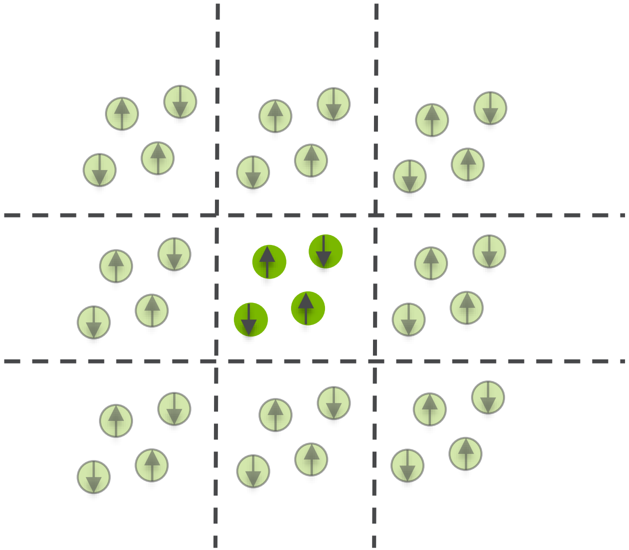


A. Gnech, Phys. Rev. Lett. 133, 142501

RESULTS IN 16O



BULK NUCLEAR MATTER SETUP

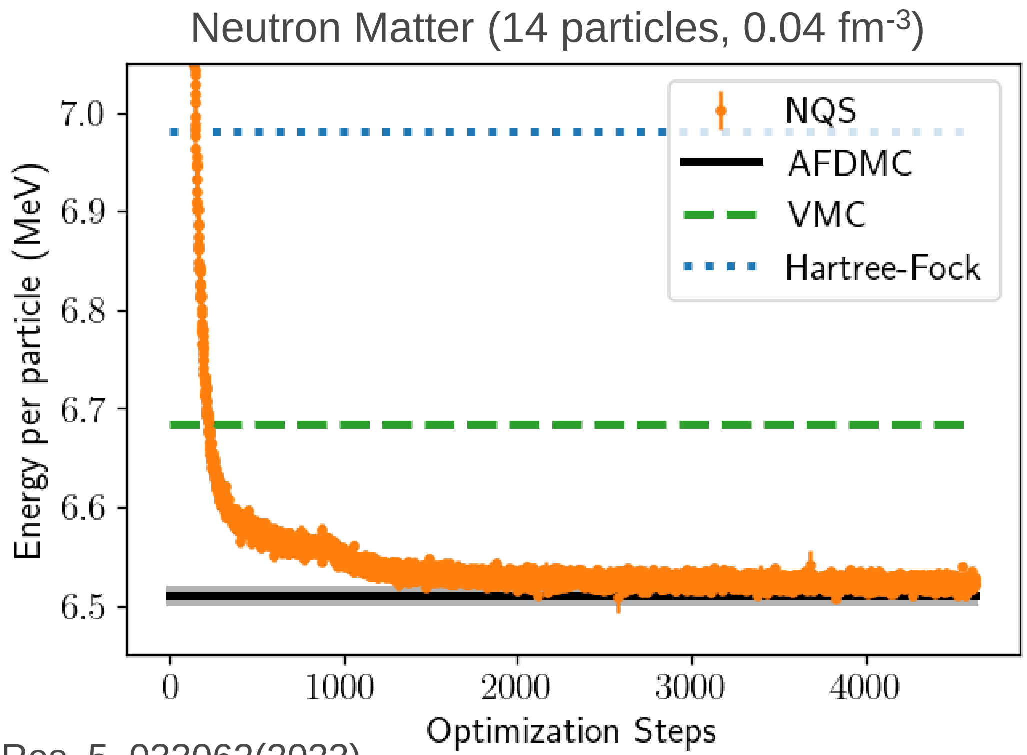


- Periodic boundary conditions and coordinate system

$$\mathbf{r}_i \longrightarrow \tilde{\mathbf{r}}_i = \left\{ \sin\left(\frac{2\pi}{L}\mathbf{r}_i\right), \cos\left(\frac{2\pi}{L}\mathbf{r}_i\right) \right\}$$

- Potential energy contribution from particle images
- Remove Coulomb potential

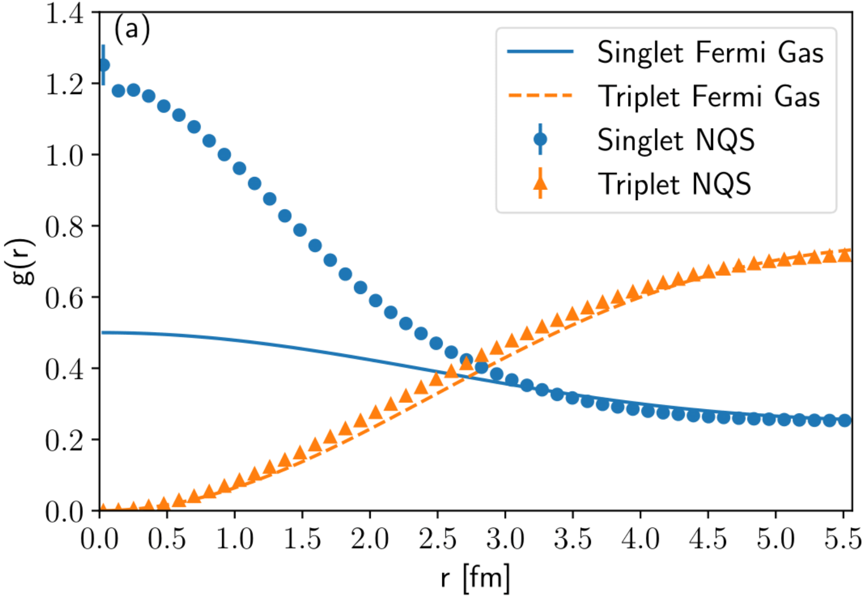
PURE NEUTRON MATTER



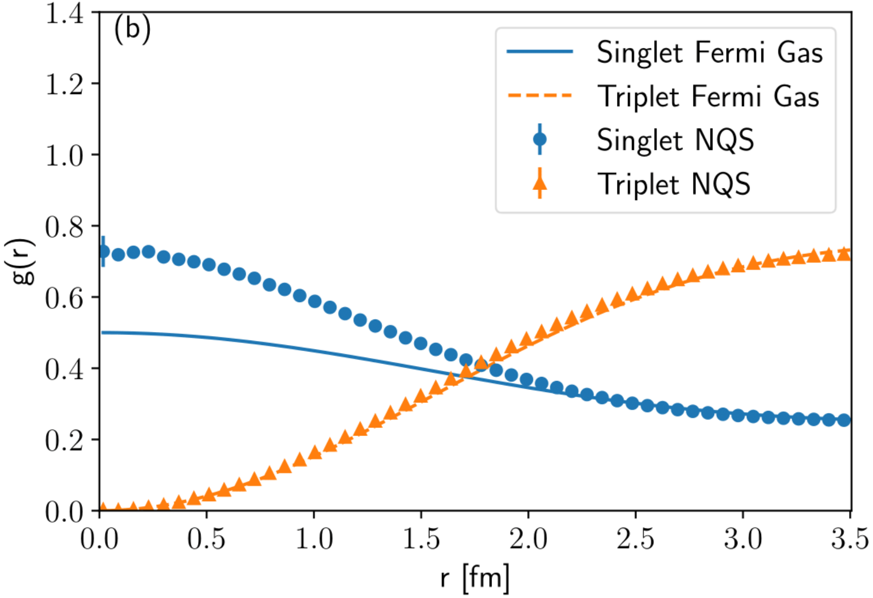
B. Fore, Phys. Rev. Res. 5, 033062(2023)

TWO-BODY PAIR DISTRIBUTIONS

0.01 fm^{-3}

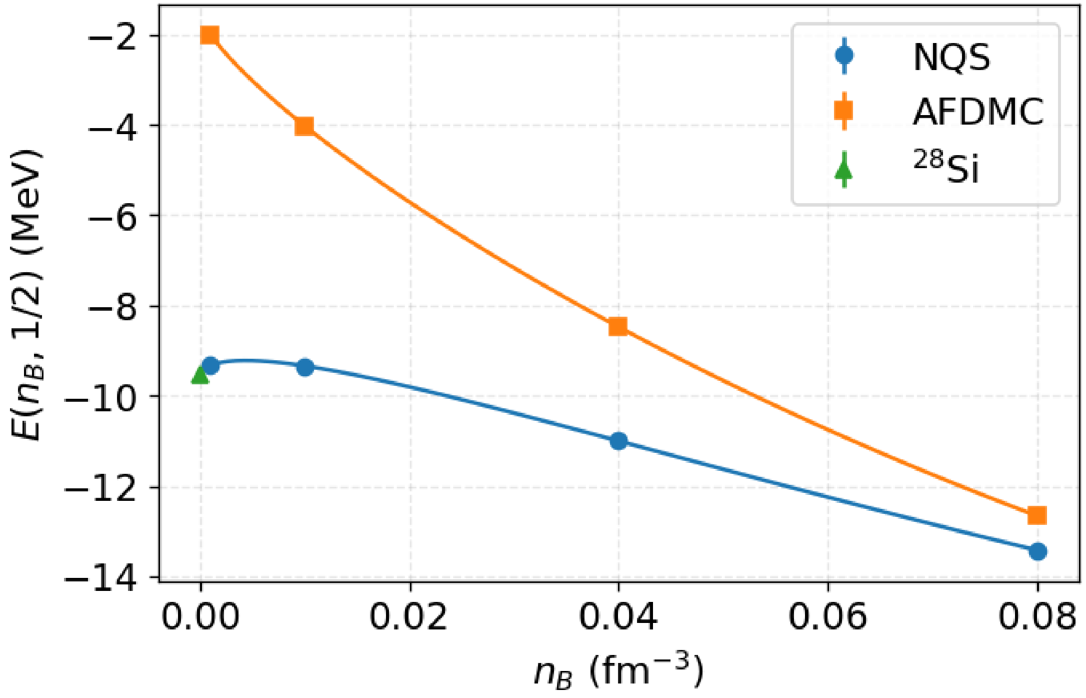


0.04 fm^{-3}



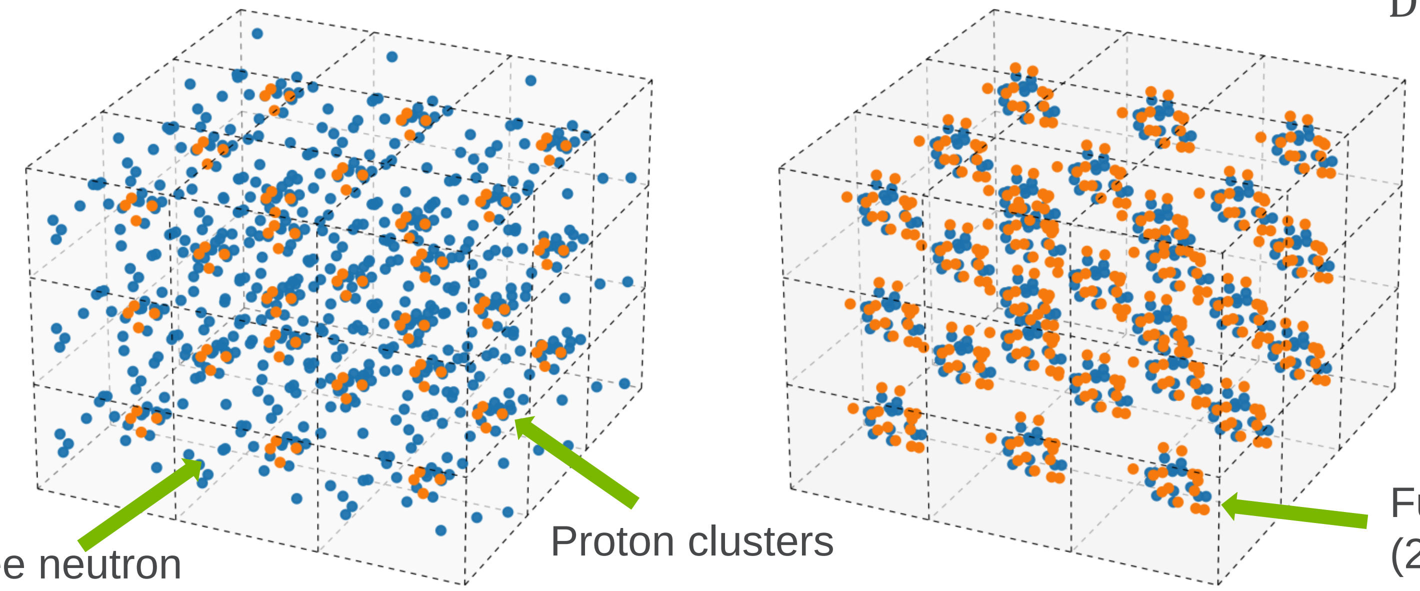
B. Fore, Phys. Rev. Res. 5, 033062(2023)

SYMMETRIC NUCLEAR MATTER



B. Fore, arXiv:2407.21207

SELF EMERGING CLUSTERING

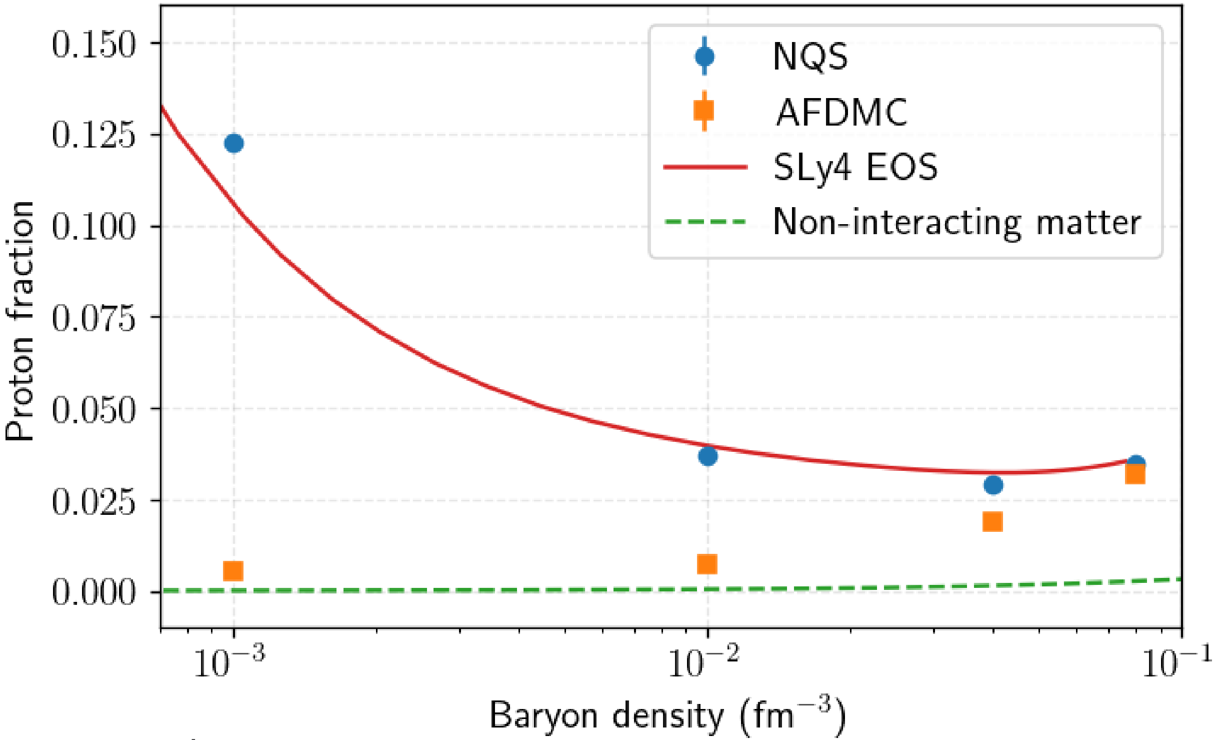


4 protons; 24 neutrons

14 protons; 14 neutrons

B. Fore, arXiv:2407.21207

NUCLEAR MATTER PROTON FRACTION



B. Fore, arXiv:2407.21207

Assumptions:

- Charge neutrality

$$n_p = n_e$$

- Beta equilibrium

$$\mu_e = \mu_n - \mu_p$$

CONCLUSIONS AND NEXT STEPS

- Conclusions:
  - Favorable scaling with number of fermions
  - Universal and accurate approximations for fermion wavefunctions
  - Scaling to leadership-class computers
  - NQS can model a variety of phases of nuclear matter material

- Next steps:
  - Improved nuclear potential including tensor term
  - Expanding to larger nuclei and larger periodic systems to avoid finite size effects
  - Excited state calculations

COLLABORATORS

Argonne National Laboratory — A. Lovato, A. Tropiano

Ohio University — J. Kim

Michigan State University — M. Hjorth-Jensen

THANK YOU

METROPOLIS-HASTINGS SAMPLING

Sampling algorithm:

- Randomly sample coordinates, R', and spins, S'

$$P_R = \frac{|\Psi_V(R',S)|^2}{|\Psi_V(R,S)|^2} \qquad P_S = \frac{|\Psi_V(R,S')|^2}{|\Psi_V(R,S)|^2}$$

- If P is greater than uniform random variable from 0 to 1, accept new values
- Observables are estimated by taking averages over sampled configurations

$$\frac{\langle \Psi_V | O | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} = \frac{\sum_S \int dR \, |\Psi_V(R,S)|^2 \, O_L(R,S)}{\sum_S \int dR \, |\Psi_V(R,S)|^2} \approx \frac{1}{N_{conf}} \sum_{\{R,S\}} O_L(R,S)$$

$$O_L = \frac{\langle RS | O | \Psi_V \rangle}{\langle RS | \Psi_V \rangle}$$

NQS OPTIMIZATION

Improve wavefunction by minimizing energy expectation value

$$E_0 \leq E_V = \frac{\left\langle \Psi_V \middle| \hat{H} \middle| \Psi_V \right\rangle}{\langle \Psi_V | \Psi_V \rangle}$$

Gradient of energy ($G_i = \frac{dE_V}{d\omega_i}$)

$$G_i = 2\left(\frac{\left\langle \partial_i \Psi_V \middle| \hat{H} \middle| \Psi_V \right\rangle}{\langle \Psi_V | \Psi_V \rangle} - E_V \frac{\langle \partial_i \Psi_V | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} \right)$$

Parameters at step s are updated as

$$\omega^{s+1} = \omega^s - \eta G$$

STOCHASTIC RECONFIGURATION

Improve wavefunction by minimizing energy expectation value

$$E_0 \leq E_V = \frac{\left\langle \Psi_V \middle| \hat{H} \middle| \Psi_V \right\rangle}{\langle \Psi_V | \Psi_V \rangle}$$

Gradient of energy ($G_i = \frac{dE_V}{d\omega_i}$), supplemented by Quantum Fisher Information S_{ij}

$$G_i = 2\left(\frac{\left\langle \partial_i \Psi_V \middle| \hat{H} \middle| \Psi_V \right\rangle}{\langle \Psi_V | \Psi_V \rangle} - E_V \frac{\langle \partial_i \Psi_V | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle}\right); \quad S_{ij} = \frac{\left\langle \partial_i \Psi_V \middle| \partial_j \Psi_V \right\rangle}{\langle \Psi_V | \Psi_V \rangle} - \frac{\langle \partial_i \Psi_V | \Psi_V \rangle \left\langle \Psi_V \middle| \partial_j \Psi_V \right\rangle}{\langle \Psi_V | \Psi_V \rangle \langle \Psi_V | \Psi_V \rangle}$$

Parameters at step s are updated as

$$\omega^{s+1} = \omega^s - \eta (S + \Lambda)^{-1} G$$

HIDDEN FERMIONS

$$\Psi_V(X) = \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \phi_1(x_3) & \phi_1(x_4) & \phi_1(y_1) & \phi_1(y_2) & \phi_1(y_3) & \phi_1(y_4) \\ \phi_2(x_1) & \phi_2(x_2) & \phi_2(x_3) & \phi_2(x_4) & \phi_2(y_1) & \phi_2(y_2) & \phi_2(y_3) & \phi_2(y_4) \\ \phi_3(x_1) & \phi_3(x_2) & \phi_3(x_3) & \phi_3(x_4) & \phi_3(y_1) & \phi_3(y_2) & \phi_3(y_3) & \phi_3(y_4) \\ \phi_4(x_1) & \phi_4(x_2) & \phi_4(x_3) & \phi_4(x_4) & \phi_4(y_1) & \phi_4(y_2) & \phi_4(y_3) & \phi_4(y_4) \\ \chi_1(x_1) & \chi_1(x_2) & \chi_1(x_3) & \chi_1(x_4) & \chi_1(y_1) & \chi_1(y_2) & \chi_1(y_3) & \chi_1(y_4) \\ \chi_2(x_1) & \chi_2(x_2) & \chi_2(x_3) & \chi_2(x_4) & \chi_2(y_1) & \chi_2(y_2) & \chi_2(y_3) & \chi_2(y_4) \\ \chi_3(x_1) & \chi_3(x_2) & \chi_3(x_3) & \chi_3(x_4) & \chi_3(y_1) & \chi_3(y_2) & \chi_3(y_3) & \chi_3(y_4) \\ \chi_4(x_1) & \chi_4(x_2) & \chi_4(x_3) & \chi_4(x_4) & \chi_4(y_1) & \chi_4(y_2) & \chi_4(y_3) & \chi_4(y_4) \end{vmatrix}$$

Visible wavefunctions on visible coordinates

Visible wavefunctions on hidden coordinates

Hidden wavefunctions on visible coordinates

Hidden wavefunctions on hidden coordinates

Comparison to Neural SJ Ansatz

$$\Psi_V(X) = e^{U(X)}\Phi(X)$$

J. R. Moreno, PNAS 119 (32) e2122059119

DETERMINANT VS PFAFFIAN

Defined for $n \times n$ matrices

$$\det(A) = \sum_{\sigma \in S_n} \operatorname{sgn}(\sigma) \prod_{i=1}^{n} a_{i,\sigma(i)}$$

$$\det(A^T) = \det(A)$$

$$\det(A)\det(B) = \det(AB)$$

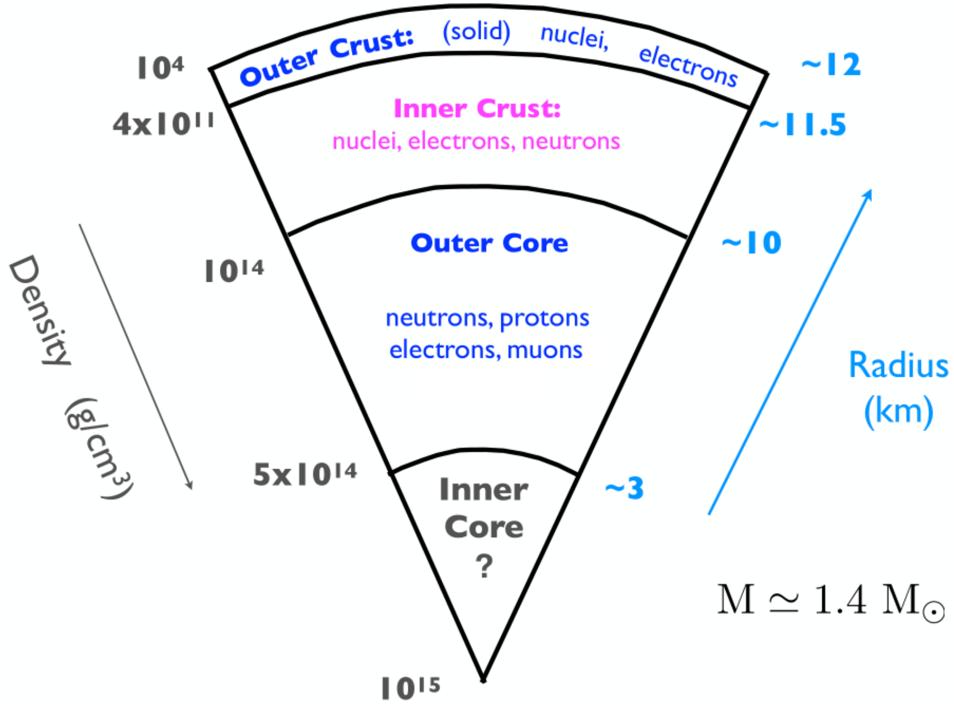
Defined for $2n \times 2n$ skew-symmetric matrices

$$\operatorname{pf}(A) = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \operatorname{sgn}(\sigma) \prod_{i=1}^{n} a_{\sigma(2i-1),\sigma(2i)}$$

$$\operatorname{pf}(A^T) = (-1)^n \operatorname{pf}(A)$$

$$\operatorname{pf}(A)\operatorname{pf}(B) = \exp\left(\frac{1}{2}\operatorname{tr}\log(A^T B)\right)$$

NEUTRON STAR STRUCTURE



- Mostly neutrons but composition varies with density
- Nuclei in crust are squeezed into uniform matter in core
- Likely neutron superfluid in inner crust and outer core
- Calculations currently focus on inner crust

ASYMMETRIC MATTER ENERGY

- Fit $E(n_B, 0)$ and $E(n_B, 1/2)$

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

- Model energy by symmetry energy expansion

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

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