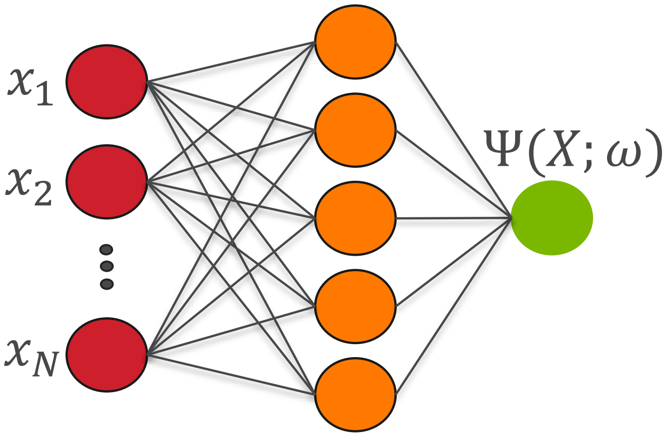
Argonne NATIONAL LABORATORY

MODELING LOW-DENSITY NUCLEAR MATTER WITH NEURAL-NETWORK QUANTUM STATES



BRYCE FORE

Physics in the AI Era
University of Pisa
September 25th 2023

OUTLINE

- Overview of nuclei results
- Neutron star background
  - Structure
  - Observation
  - Modeling
- Overview of variational Monte Carlo (VMC)
  - Metropolis-Hastings Sampling
  - Parameter optimization
- Neural-network quantum states for fermions
  - Deep set architecture
  - Pfaffian NQS wavefunction
- Results

PIONLESS EFT HAMILTONIAN

- Pionless-EFT Hamiltonian

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

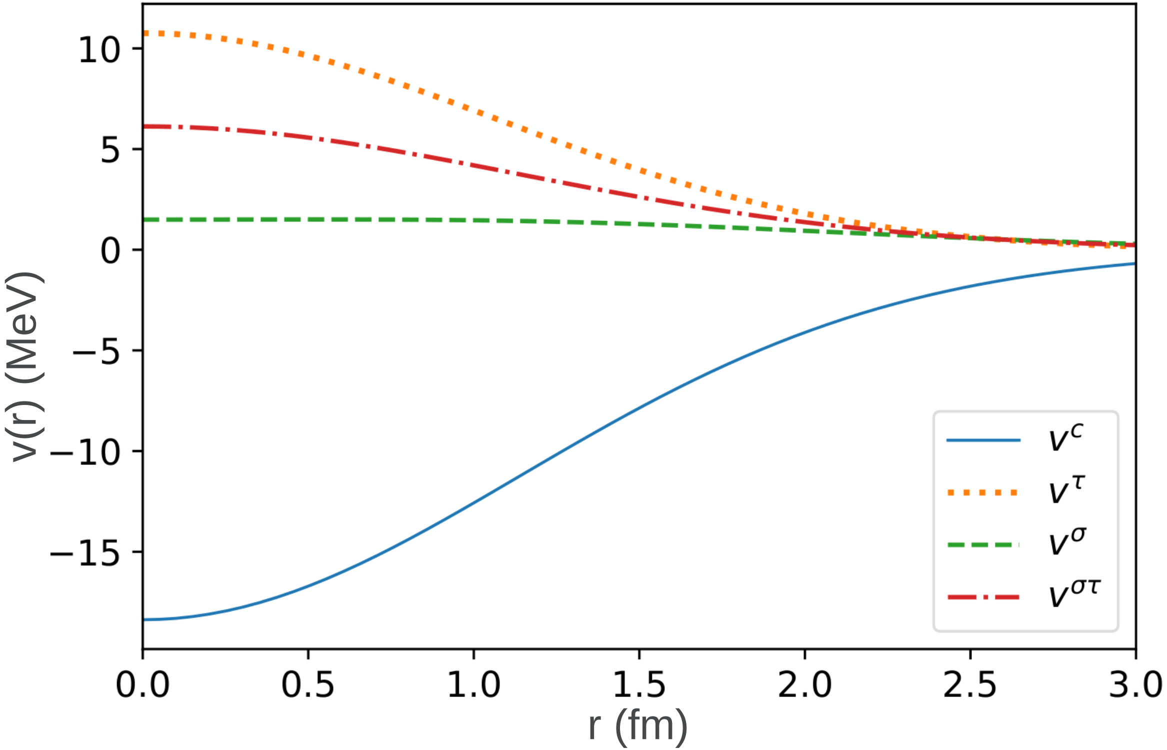
- Two body operators including spin and isospin dependence

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

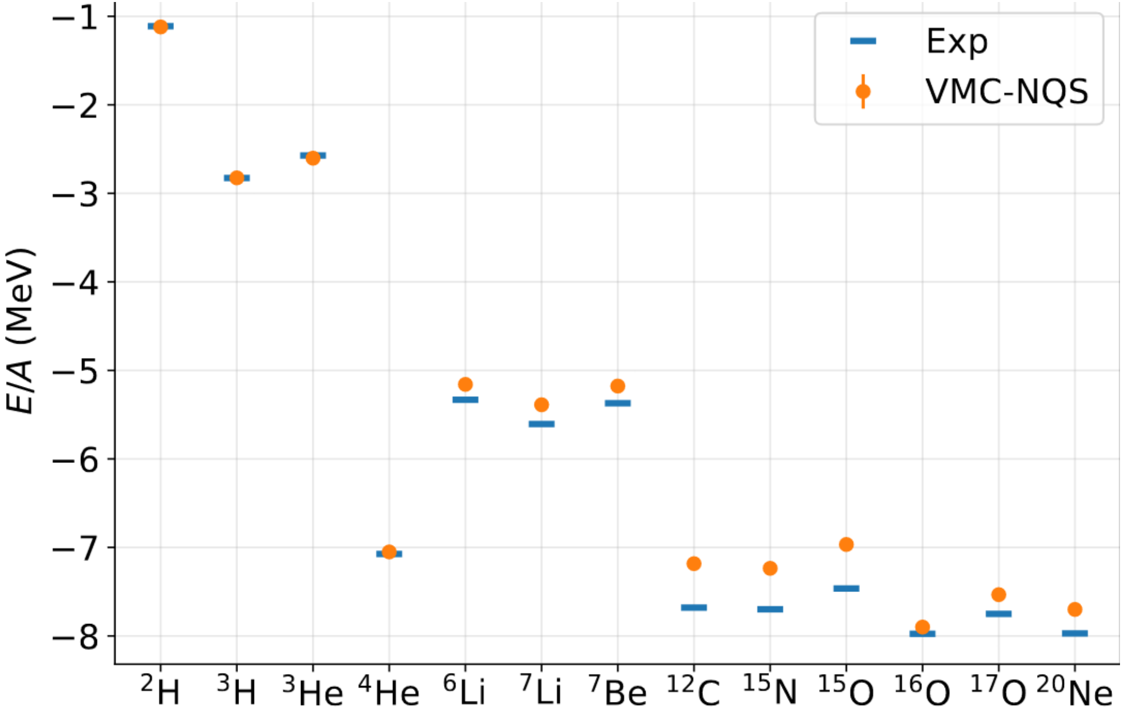
$$\sigma_{ij} = \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\,, \quad \tau_{ij} = \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$$

R. Schiavilla, PRC 103, 054003(2021)

PIONLESS EFT HAMILTONIAN

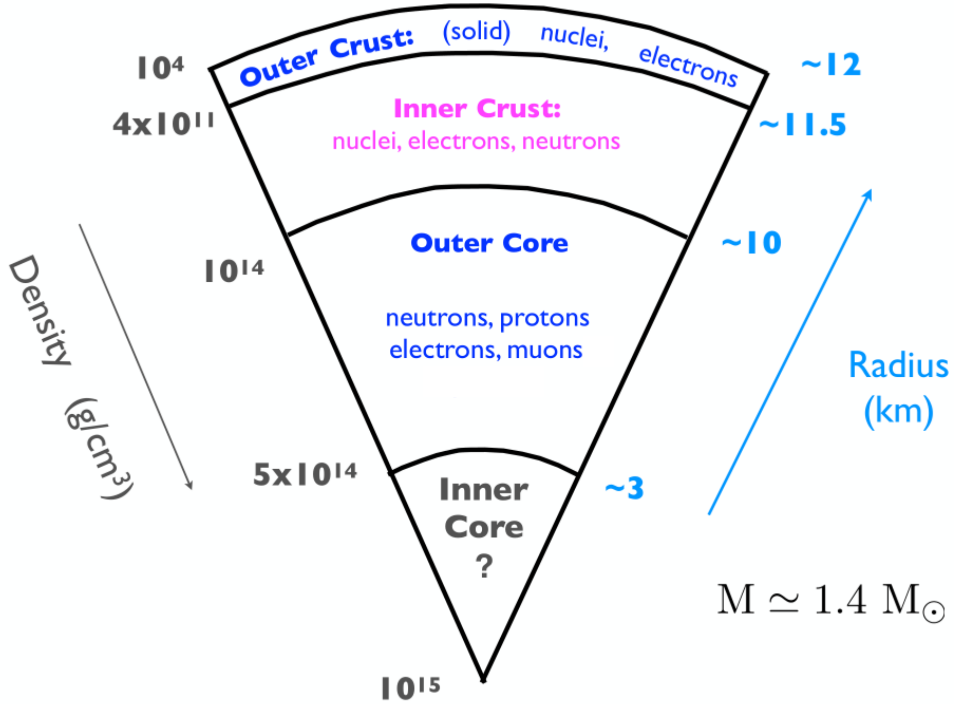


NEURAL QUANTUM STATE RESULTS IN NUCLEI



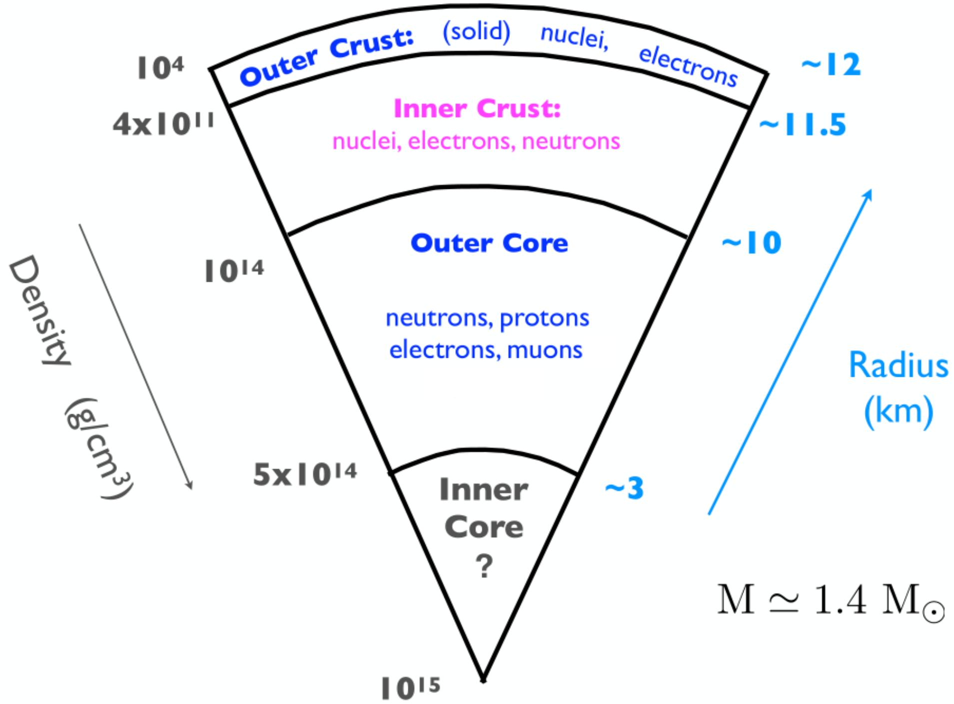
A. Gnech, arXiv:2308.16266

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

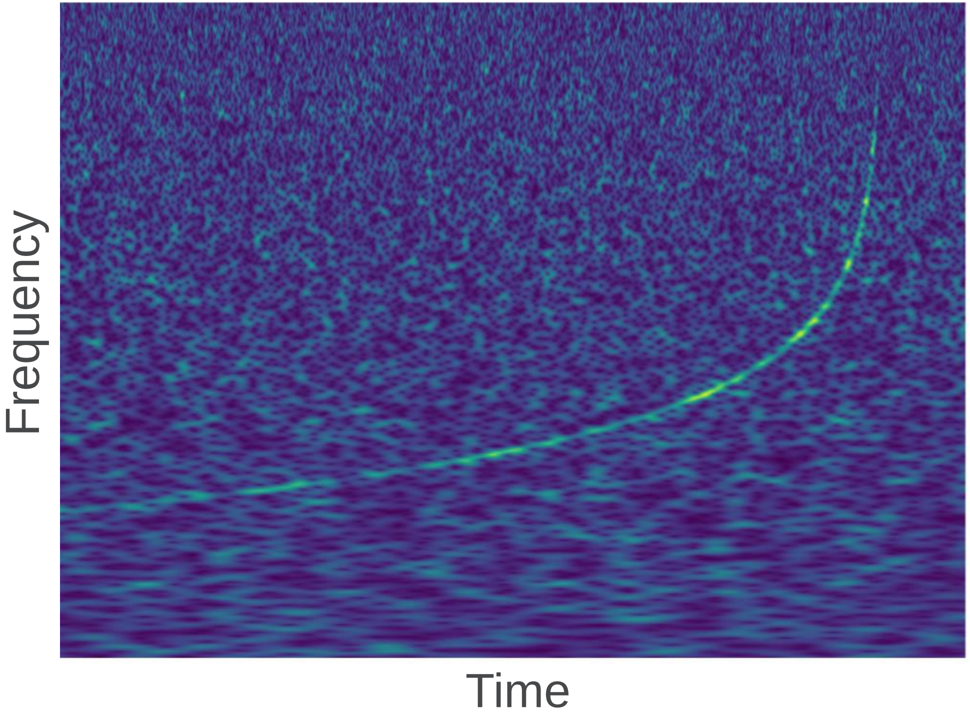
NEUTRON STAR INTEREST



- Unique system for accessing nuclear EOS info
  - High densities
  - High isospin asymmetries
- Mergers result in creation of very heavy elements
- Relation between mass and radius controlled by nuclear EOS

NEUTRON STAR OBSERVATION

- Gravitational waves
- Kilonova light curves
- Pulsars
- Pulsar glitches



GW170817 signal

VARIATIONAL MONTE CARLO (VMC)

1. Specify a parameterized function to act as the trial wavefunction

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

2. Use Metropolis-Hastings algorithm to sample trial wavefunction

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

3. Optimize parameters of trial wavefunction to obtain lower energy

$$E_0 \leq E_T = \frac{\langle\Psi_T|\hat{H}|\Psi_T\rangle}{\langle\Psi_T|\Psi_T\rangle}$$

METROPOLIS-HASTINGS SAMPLING

Sampling algorithm:

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

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

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

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

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

STOCHASTIC RECONFIGURATION

Improve trial wavefunction by minimizing energy expectation value

$$E_0 \leq E_T = \frac{\langle \Psi_T | \hat{H} | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$$

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

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

Parameters at step s are updated as

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

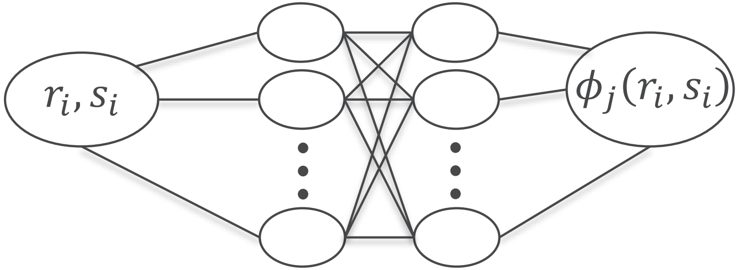
NEURAL NETWORK QUANTUM STATES

- Artificial neural networks compactly represent complex high-dimensional functions

$$\langle RS|\Psi_T\rangle = e^{U(R,S)}\langle RS|\Phi\rangle$$

- Slater determinant enforces antisymmetry and single particle wavefunctions can be represented by neural networks

$$\langle RS|\Phi\rangle = \begin{vmatrix} \phi_1(r_1,s_1) & \phi_1(r_2,s_2) & \cdots & \phi_1(r_n,s_n) \\ \phi_2(r_1,s_1) & & & \vdots \\ \vdots & & & \\ \phi_n(r_1,s_1) & \cdots & & \phi_n(r_n,s_n) \end{vmatrix}$$



FERMIONIC TRIAL WAVEFUNCTIONS

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

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

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

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

- Slater determinant enforces antisymmetry
- Jastrow function makes wavefunction more general
- Single particle orbitals and Jastrow function can be represented by neural networks

$$\Phi(R,S) = \begin{vmatrix} \phi_1(r_1,s_1) & \phi_1(r_2,s_2) & \ldots & \phi_1(r_n,s_n) \\ \phi_2(r_1,s_1) & & & \vdots \\ \vdots & & & \\ \phi_n(r_1,s_1) & \ldots & & \phi_n(r_n,s_n) \end{vmatrix}$$

DEEP SET ARCHITECTURE

- We require a generic function which is independent of particle ordering for the Jastrow function.

$$U(\ldots, x_i, \ldots x_j \ldots) = U(\ldots, x_j, \ldots x_i \ldots)$$

- By mapping the configuration for each particle to a latent space and summing the results we remove the particle ordering information.

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

$$\vec{\phi}\colon \mathbb{R}^5 \to \mathbb{R}^{latent}$$

$$\rho\colon \mathbb{R}^{latent} \to \mathbb{R}$$

- $\vec{\phi}$ and ρ are represented by neural networks

IMPROVED TRIAL WAVEFUNCTION ANSATZ

$$\Psi_T(X) = e^{U(X^*)}\Phi_{\text{pf}}(X^*)$$

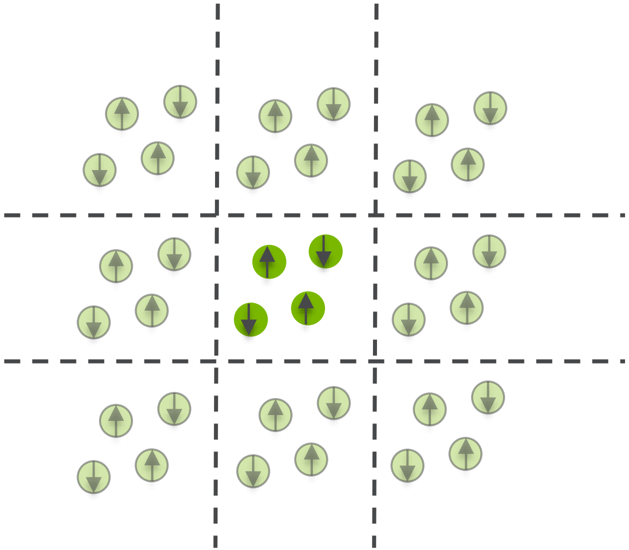
$$\Phi_{pf}(X) = pf[M]$$

$$M_{ij} = \phi(x_i, x_j) - \phi(x_j, x_i)$$

- Input, X, with backflow preprocessing gives X^*
- Slater determinant → Pfaffian
- M must be skew symmetric, $A = -A^T$, and square with even size
- Built in pairwise structure
- Pfaffian requires only one MLP so uses far fewer parameters

J. Kim, arXiv:2305.08831

BULK NUCLEAR MATTER SETUP



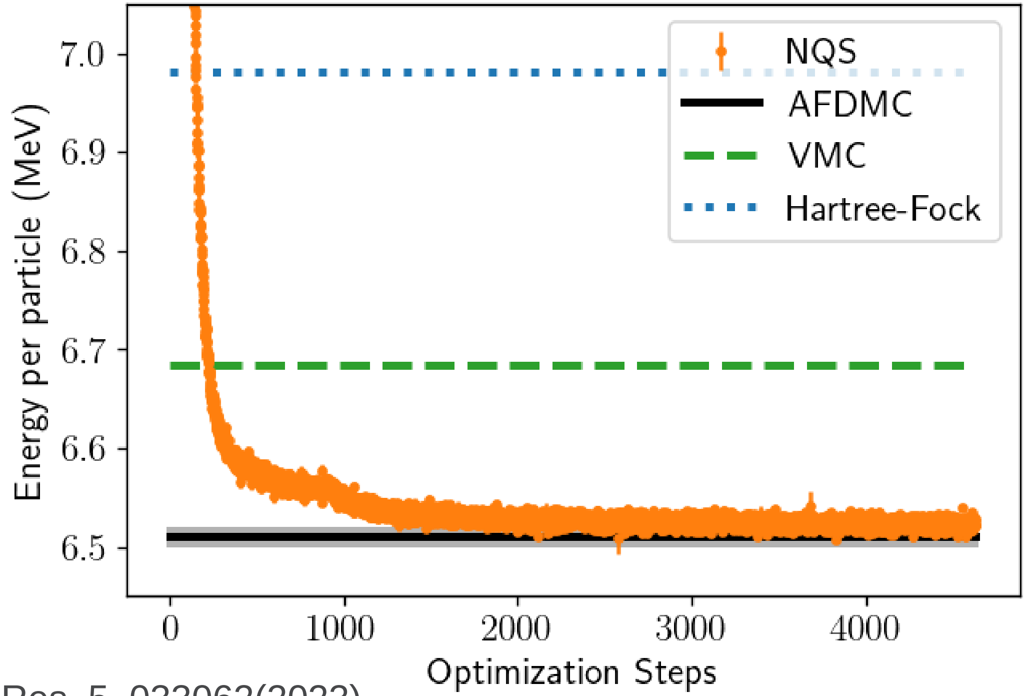
- Periodic boundary conditions and coordinate system

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

- Potential energy contribution from particle images

PURE NEUTRON MATTER

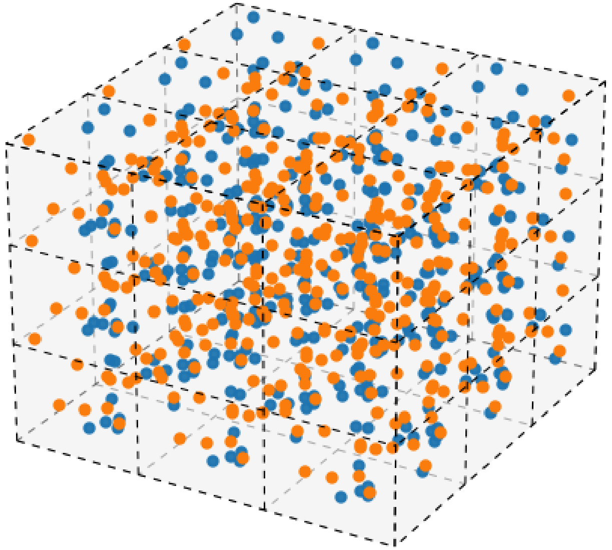
Neutron Matter (14 particles, 0.04 fm^{-3})



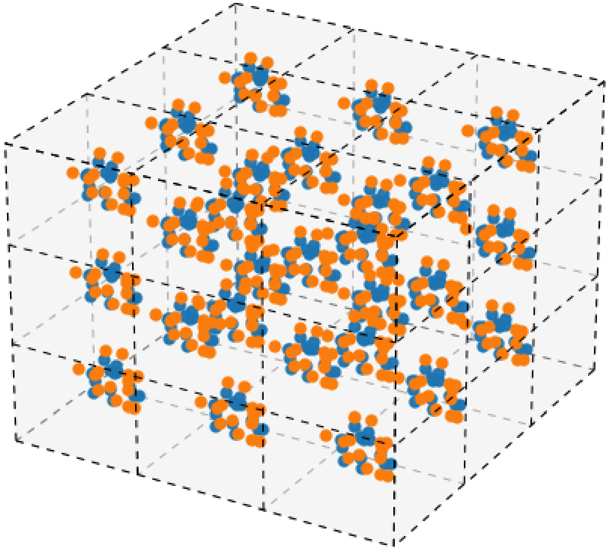
B. Fore, Phys. Rev. Res. 5, 033062(2023)

CLUSTERING

Conventional QMC

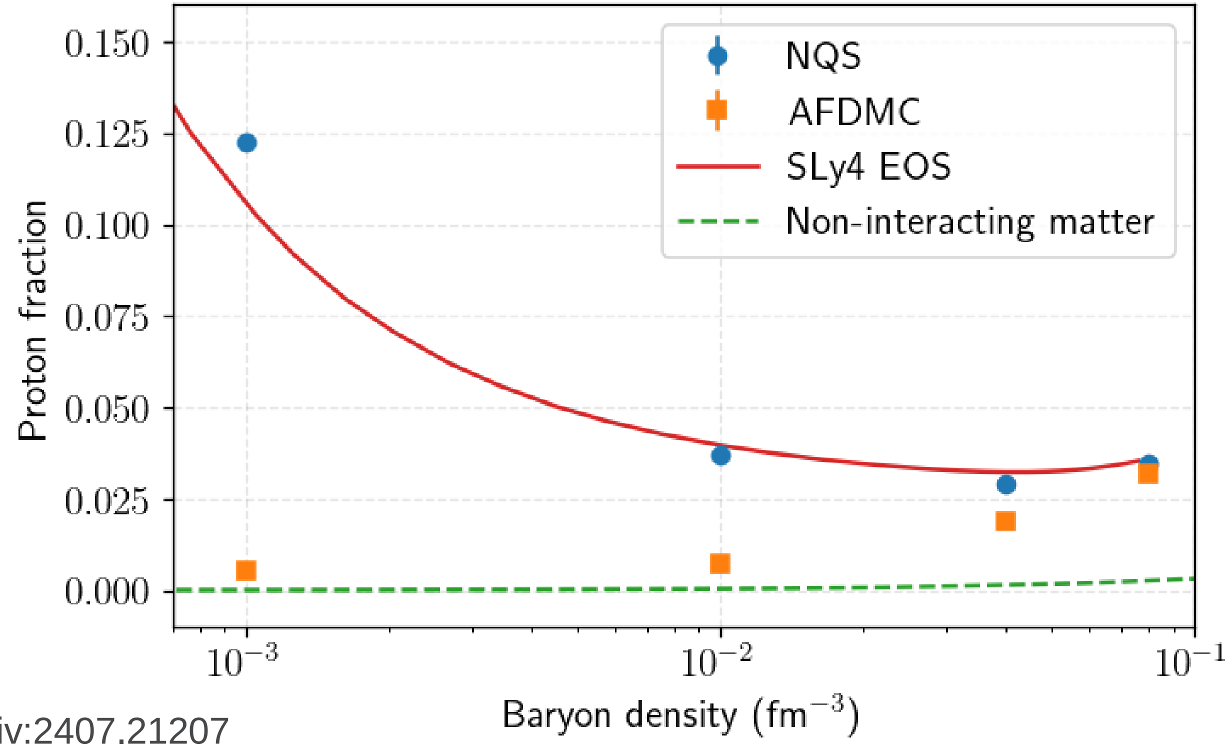


Neural quantum states



B. Fore, arXiv:2407.21207

NUCLEAR MATTER PROTON FRACTION



B. Fore, arXiv:2407.21207

CONCLUSIONS AND NEXT STEPS

- Conclusions:
  - Neural quantum states preform as well or better than conventional quantum Monte Carlo methods
  - Neural quantum states has a unique access to nuclear matter at subnuclear densities

- Next steps
  - Add more complex terms to nuclear potential
  - Larger systems: access larger nuclei and better simulations of nuclear matter

THANK YOU