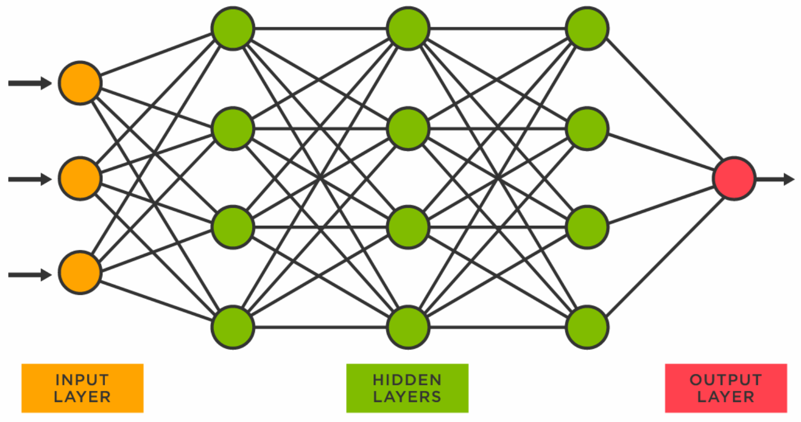
NEURAL QUANTUM STATES FOR NEUTRON STARS



BRYCE FORE

Many-Body quantum physics with machine learning

September 6th 2023

U.S. DEPARTMENT OF ENERGY
Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

OUTLINE

- Recent nuclei results
- Neutron star background
  - Structure
  - Why they are interesting
  - Observation
  - Continuous periodic systems
- Monte Carlo and neural quantum state details
  - Variational Monte Carlo methods
  - Hidden fermion ansatz
- Results
  - Pure neutron matter
  - Pfaffian + MPNN ansatz
  - Preliminary symmetric matter

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

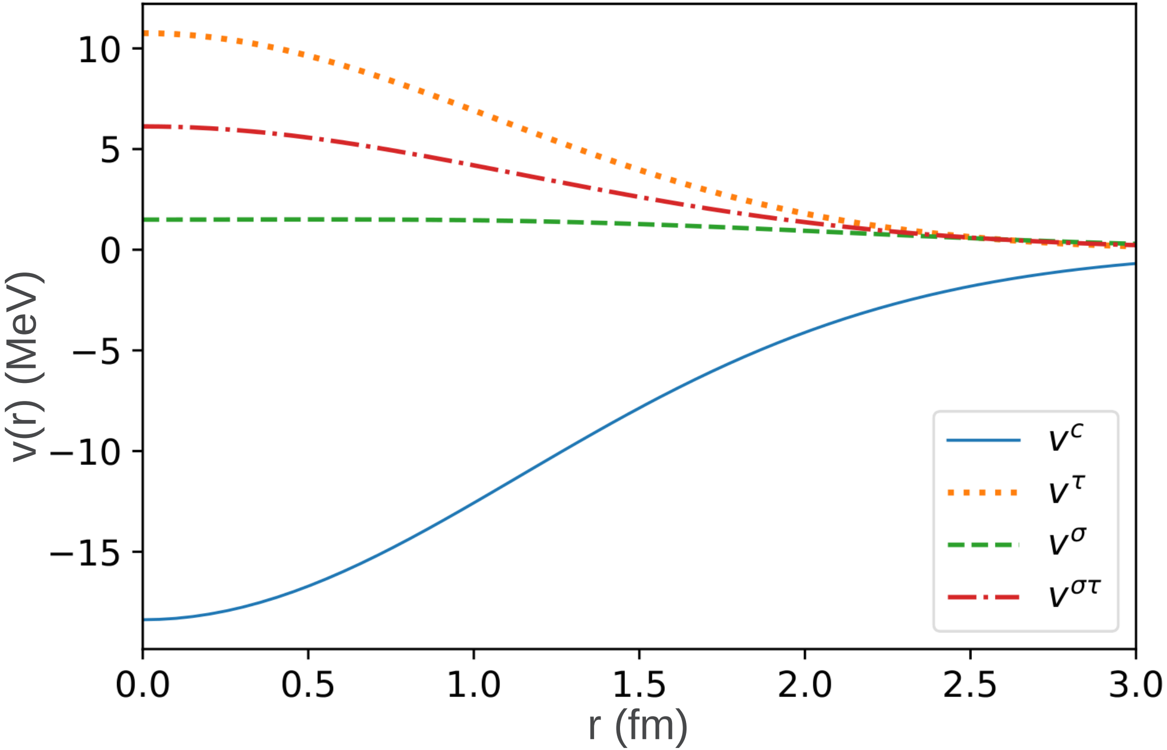
$$v_{ij}^{\mathrm{CI}} = \sum_{p=1}^{4} v^p(r_{ij}) O_{ij}^p$$

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

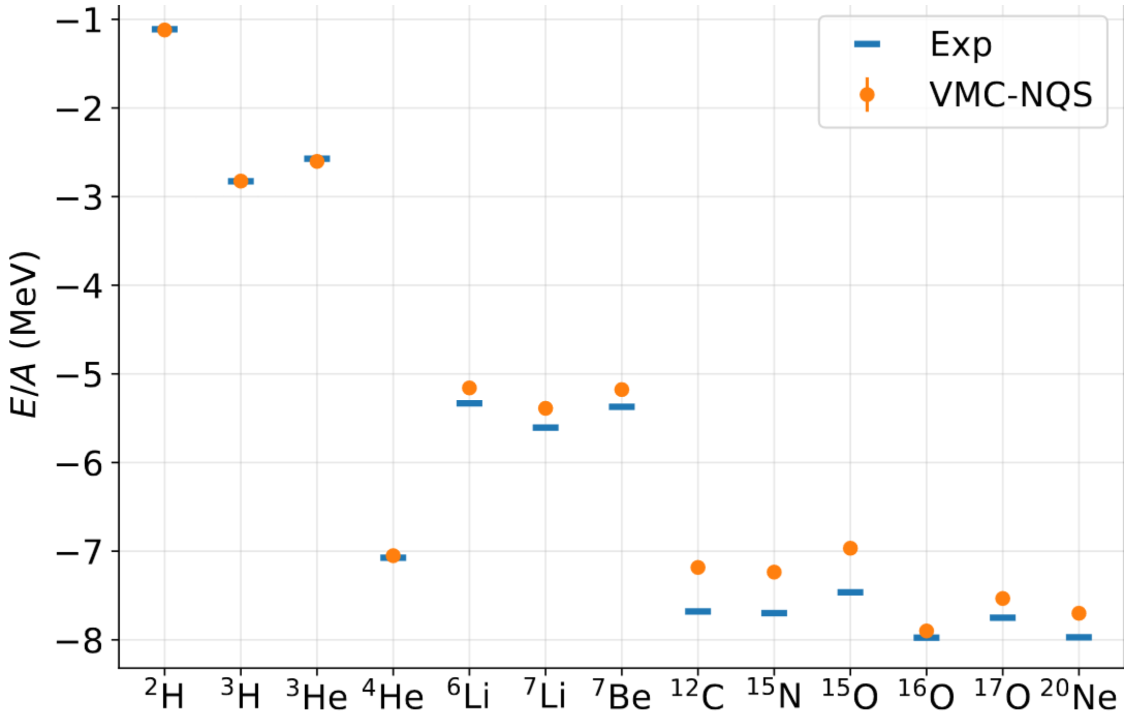
$$\sigma_{ij} = \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\,, \quad \tau_{ij} = \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$$

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

PIONLESS EFT HAMILTONIAN

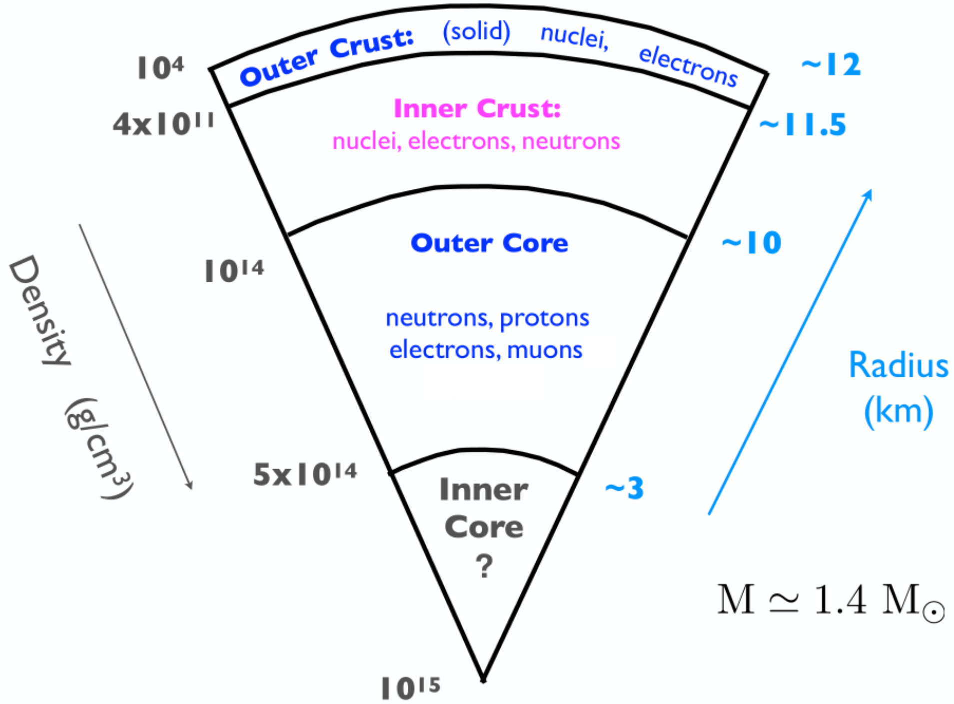


NEURAL QUANTUM STATE RESULTS IN NUCLEI



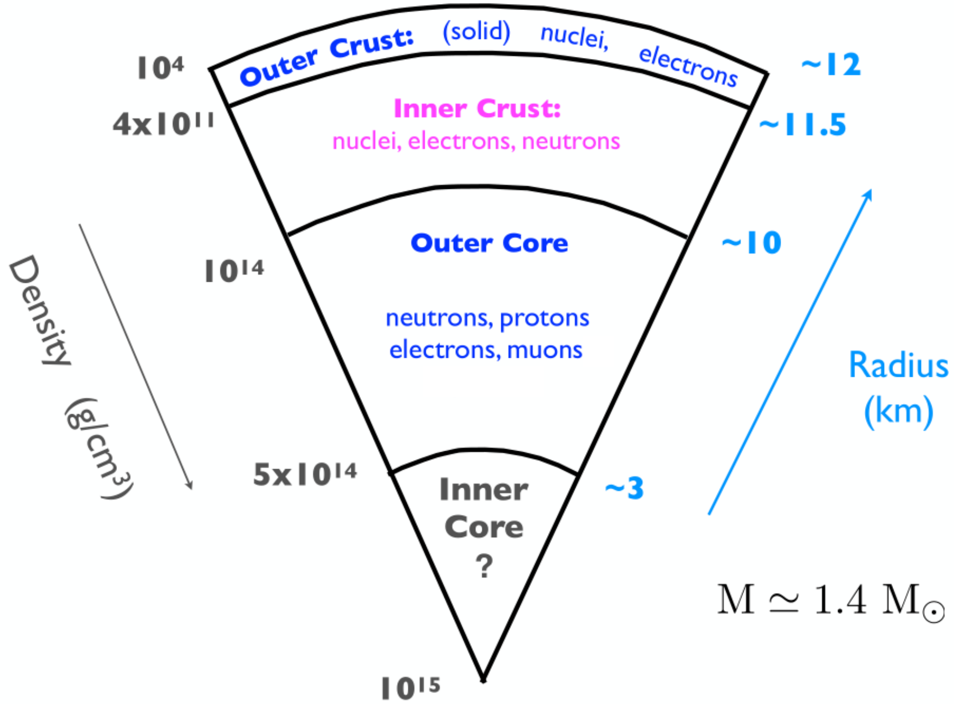
A. Gnech, arXiv:2308.16266

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
- More exotic hadrons and leptons possible in outer core
- Inner core composition largely uncertain

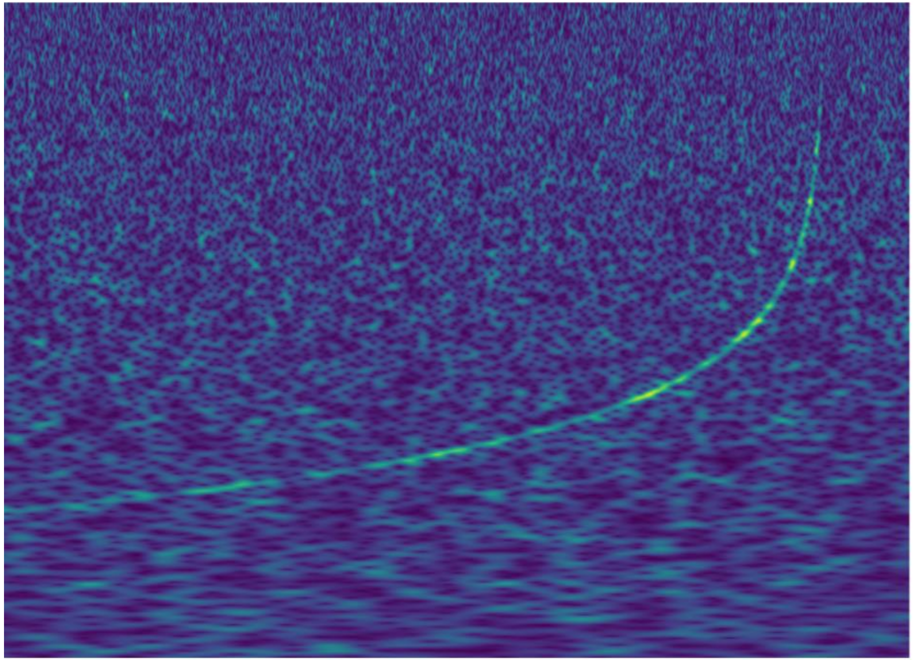
NEUTRON STAR INTEREST



- 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

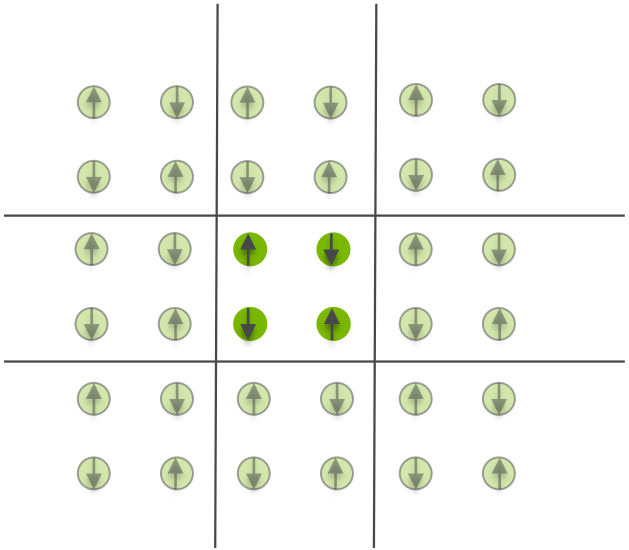
NEUTRON STAR OBSERVATION

- Gravitational waves
- Kilonova light curves
- Pulsars
- Pulsar glitches
- Neutron star cooling



GW170817 signal

BULK NUCLEAR MATTER SETUP



- Periodic boundary conditions and coordinate system
- Continuous positions
- Discrete spins
- Low densities where pionless Hamiltonian is accurate
- Unpolarized

CONTINUOUS PERIODIC SYSTEMS

- Requirements for periodic systems
  - Uniform position initialization over simulation box
  - Periodic 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 from particle images
- Filled shells used for comparison to single determinant results
  - First closed shell of neutron matter will have 14 particles since there are 7 momentum states and 2 spin states

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

- Given our trial wavefunction we can sample coordinates and spin using the Metropolis-Hastings algorithm

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

- Accept move if P greater than uniform random variable from 0 to 1
- 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

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

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

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

Parameters at step s are updated as

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

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
- Artificial neural networks compactly represent high-dimensional functions
- Single particle orbitals and Jastrow function can be represented by neural networks

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

DEEP SET ARCHITECTURE

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

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

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

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

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

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

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

HIDDEN FERMIONS

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

Visible wavefunctions on visible coordinates

Visible wavefunctions on hidden coordinates

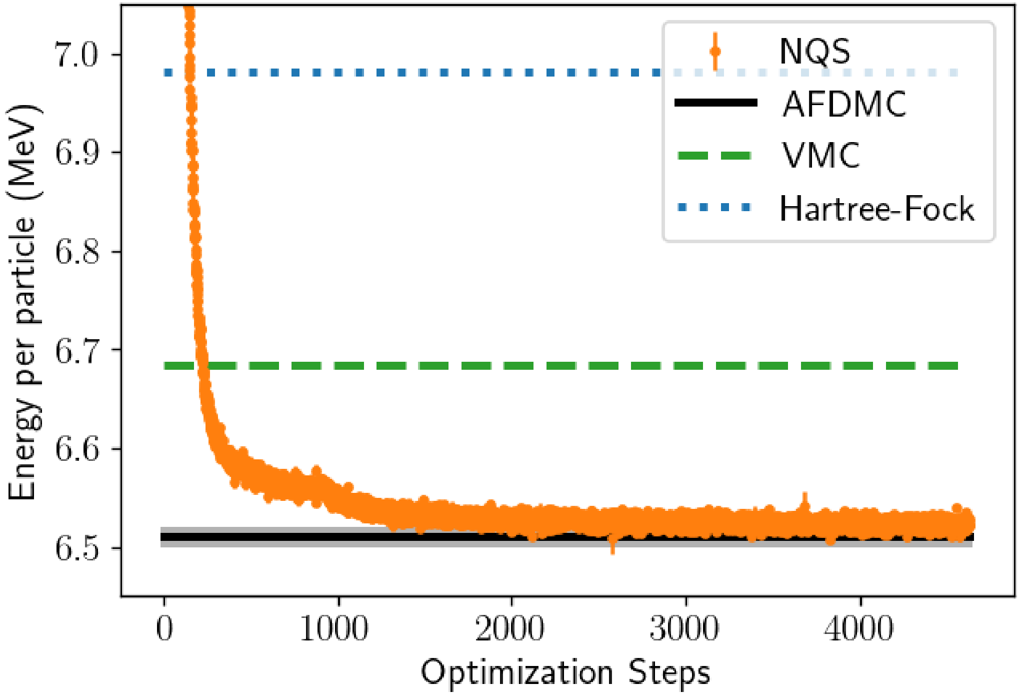
Hidden wavefunctions on visible coordinates

Hidden wavefunctions on hidden coordinates

J. R. Moreno, et al., arXiv:2111.10420

PURE NEUTRON MATTER

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



TWO BODY DENSITY

Central and spin two body densities

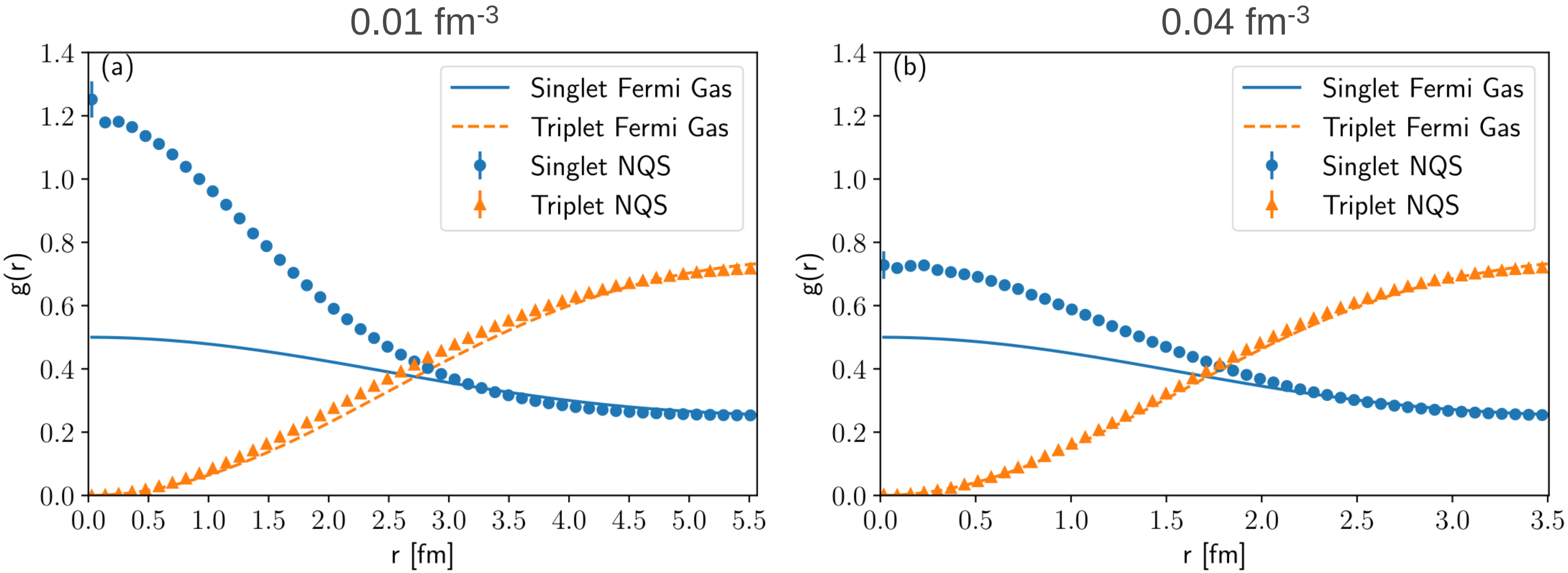
$$g_c(r) = \frac{1}{2\pi r^2 \rho N} \sum_{i<j} \frac{\langle \psi | \delta(r_{ij} - r) | \psi \rangle}{\langle \psi | \psi \rangle}$$

$$g_\sigma(r) = \frac{1}{2\pi r^2 \rho N} \sum_{i<j} \frac{\langle \psi | \delta(r_{ij} - r) \sigma_i \cdot \sigma_j | \psi \rangle}{\langle \psi | \psi \rangle}$$

Spin singlet and triplet channel two body densities

$$g_0(r) = \tfrac{1}{4}[g_c(r) - g_\sigma(r)] \qquad g_1(r) = \tfrac{1}{4}[3g_c(r) + g_\sigma(r)]$$

TWO BODY DENSITY



IMPROVED TRIAL WAVEFUNCTION ANSATZ

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

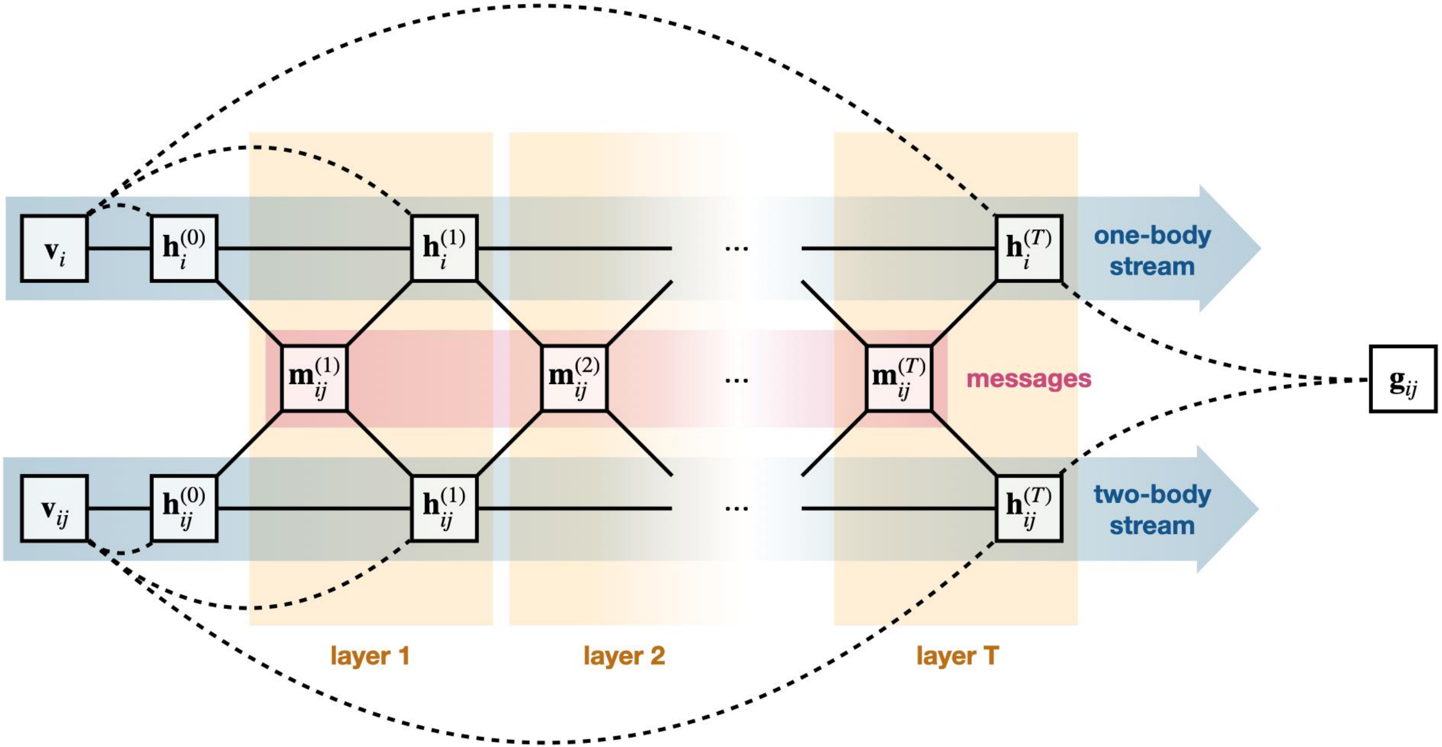
$$\Phi_{pf}(X) = pf[M]$$

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

- Input, X, preprocessed by MPNN to give 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
- Extra row and column can be added for odd numbers of particles

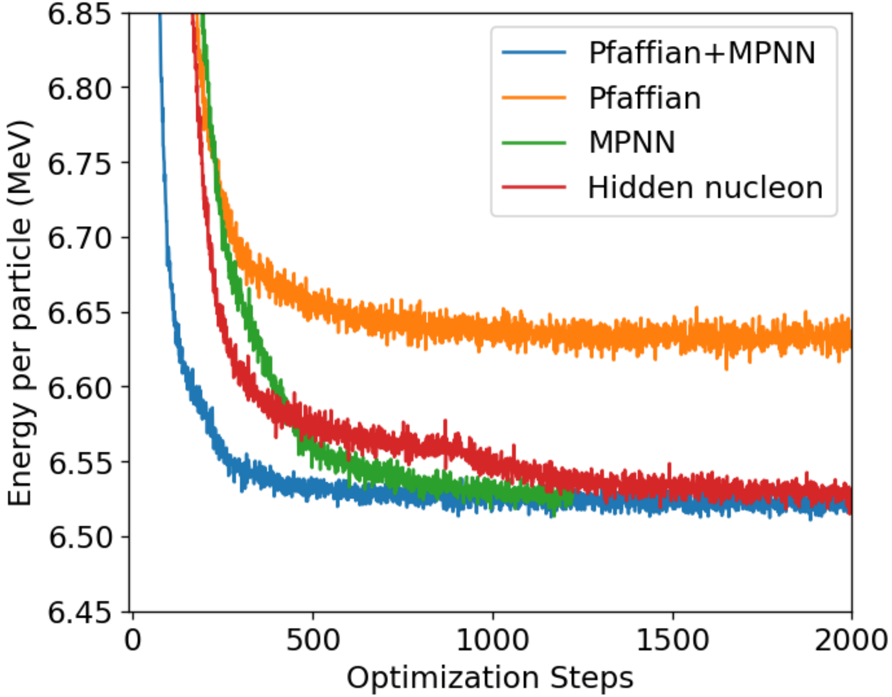
https://arxiv.org/abs/2305.08831

MESSAGE PASSING NEURAL NETWORK



ANSATZ COMPARISONS

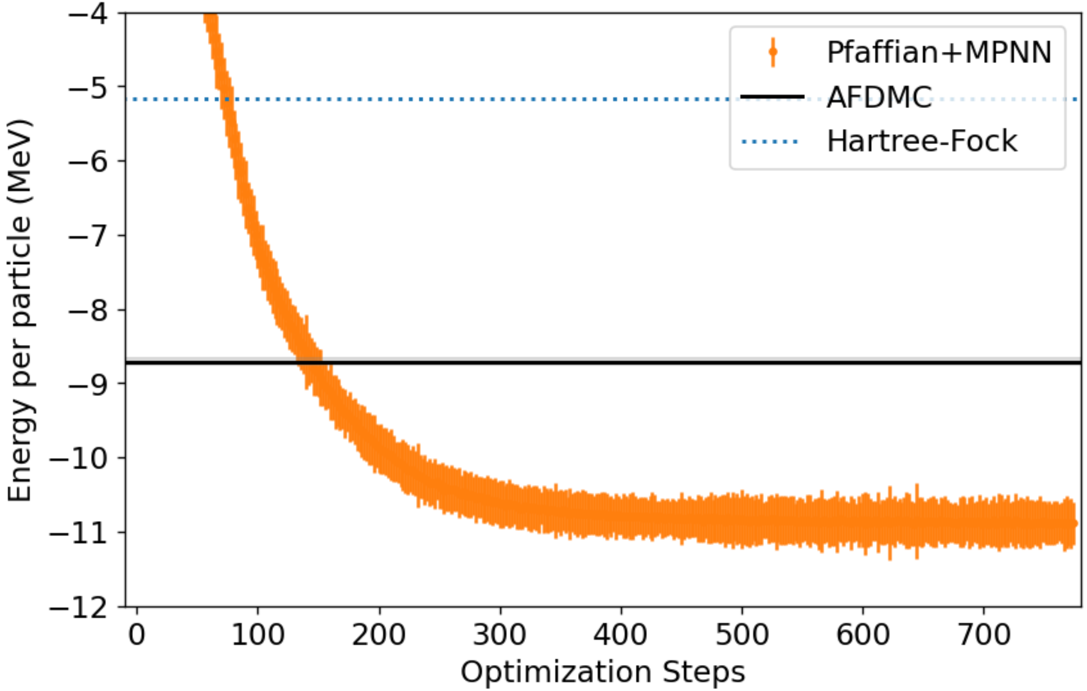
Neutron Matter (14 particles, 0.04 fm^{-3})



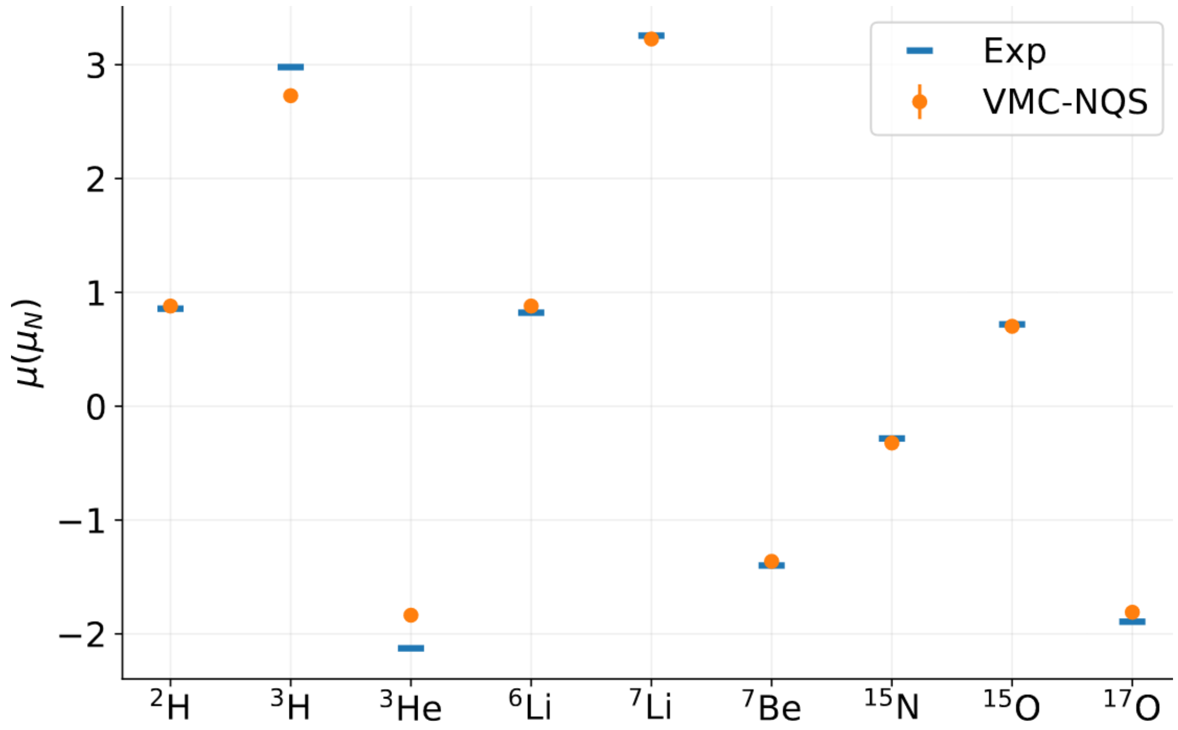
Optimization step time (4 A100 GPUs, 32000 samples)	
Pfaffian+MPNN	~42 (s)
Pfaffian	~21 (s)
MPNN	~35 (s)
Hidden nucleon	~46 (s)

PRELIMINARY 14 NEUTRONS + 14 PROTONS

Symmetric Nuclear Matter (28 particles, 0.04 fm^{-3})

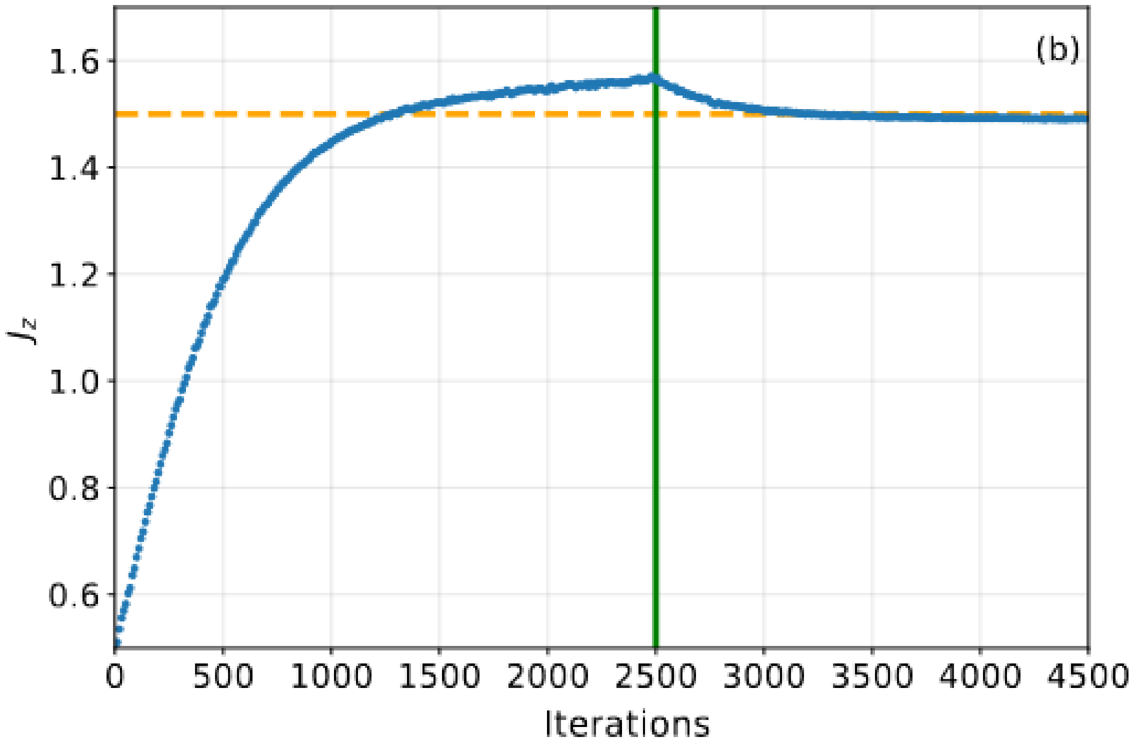


MAGNETIC MOMENTS



A. Gnech, arXiv:2308.16266

MAGNETIC MOMENTS



A. Gnech, arXiv:2308.16266

CONCLUSIONS AND NEXT STEPS

- Questions:
  - Determine if Jastrow function is needed for Pfaffian + MPNN ansatz
  - How does the size of the Pfaffian+MPNN ansatz need to scale with increasing particle number?

- Next steps
  - Investigations of nuclear matter with proton fractions between 0 and ½ initially focusing on the emergence of clustering
  - Implement more sophisticated nuclear potentials
  - Larger systems possibly up to A=40 for nuclei

MPNN EQUATIONS

$h_i^0 = (v_i, A(v_i))$ $\quad h_{ij}^0 = (v_{ij}, B(v_{ij}))$

$$m_{ij}^t = M_t(h_i^{t-1}, h_j^{t-1}, h_{ij}^{t-1})$$

$$m_i^t = Pool_j\,(m_{ij}^t)$$

$$h_i^t = (v_i, F_t(h_i^{t-1}, m_i^t))$$

$$h_{ij}^t = (v_{ij}, G_t(h_{ij}^{t-1}, m_{ij}^t))$$