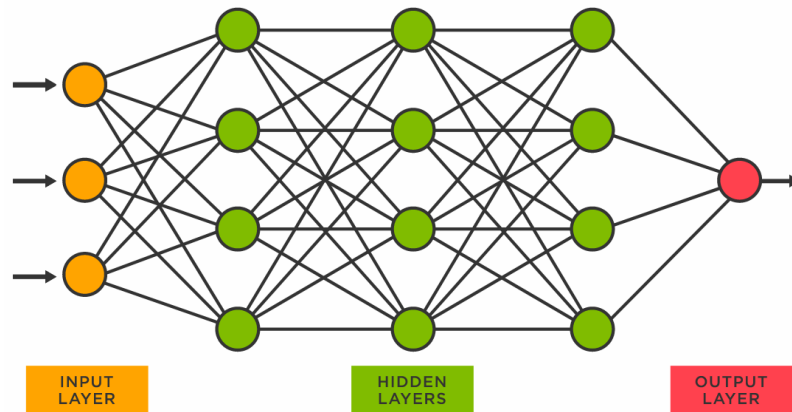


NEURAL QUANTUM STATES FOR NEUTRON STARS

BRYCE FORE



OUTLINE

- Overview of nuclei results
- Neutron star background
 - Structure
 - Why they are interesting
 - Observation
 - Modeling as a continuous periodic system
- 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

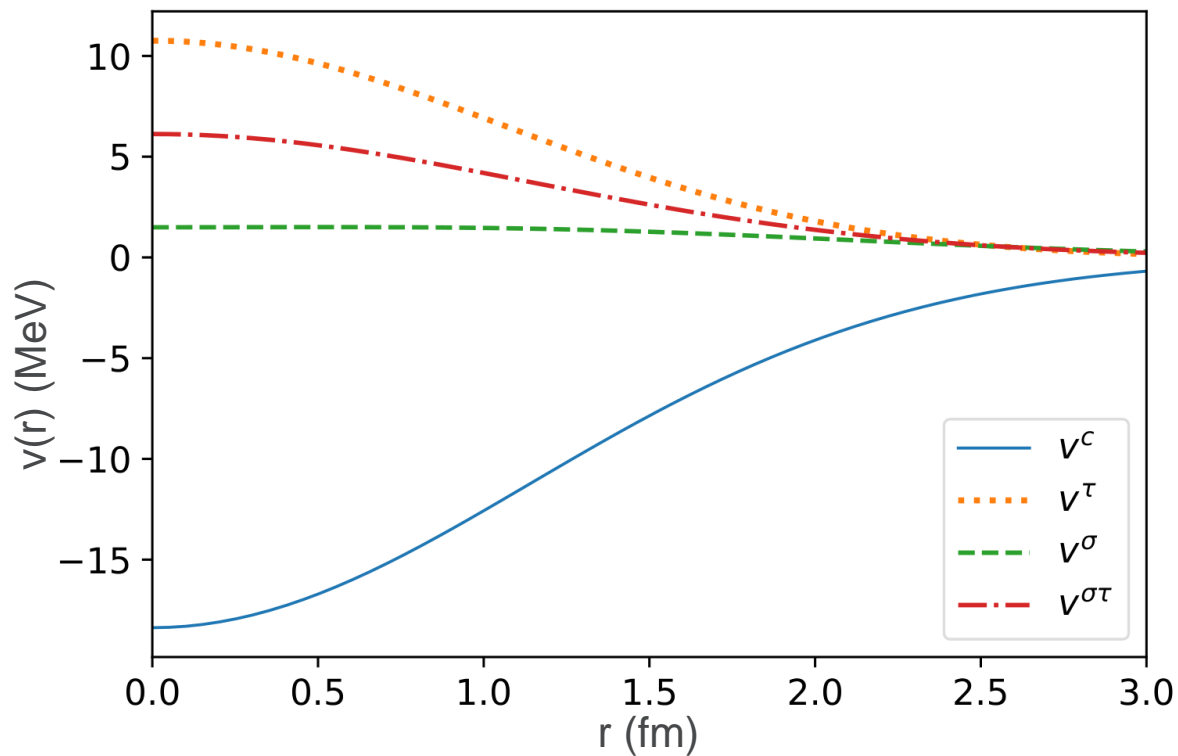
$$v_{ij}^{\text{CI}} = \sum_{p=1}^4 v^p(r_{ij}) O_{ij}^p$$

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

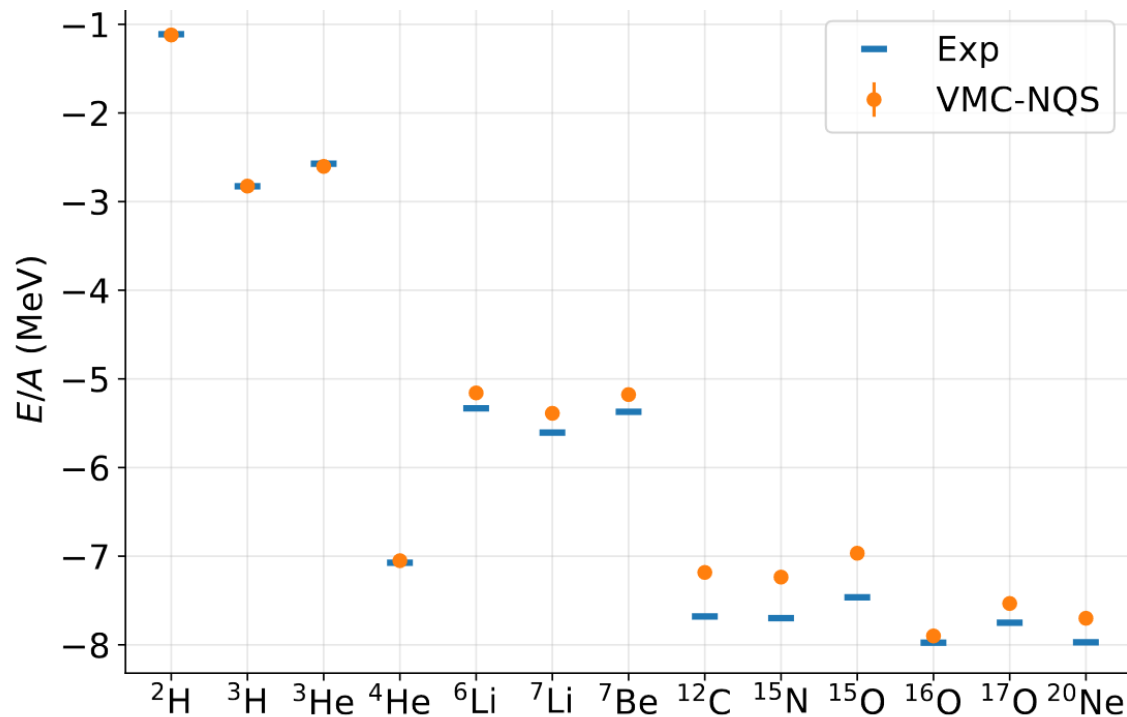
$$\sigma_{ij} = \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, \quad \tau_{ij} = \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$$

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

PIONLESS EFT HAMILTONIAN

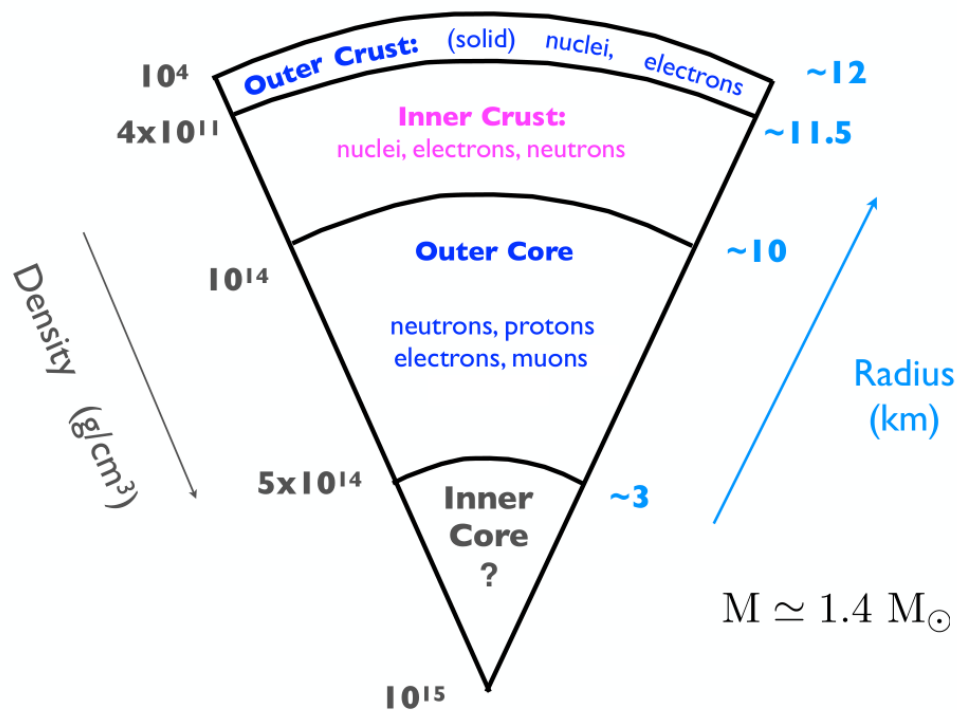


NEURAL QUANTUM STATE RESULTS IN NUCLEI



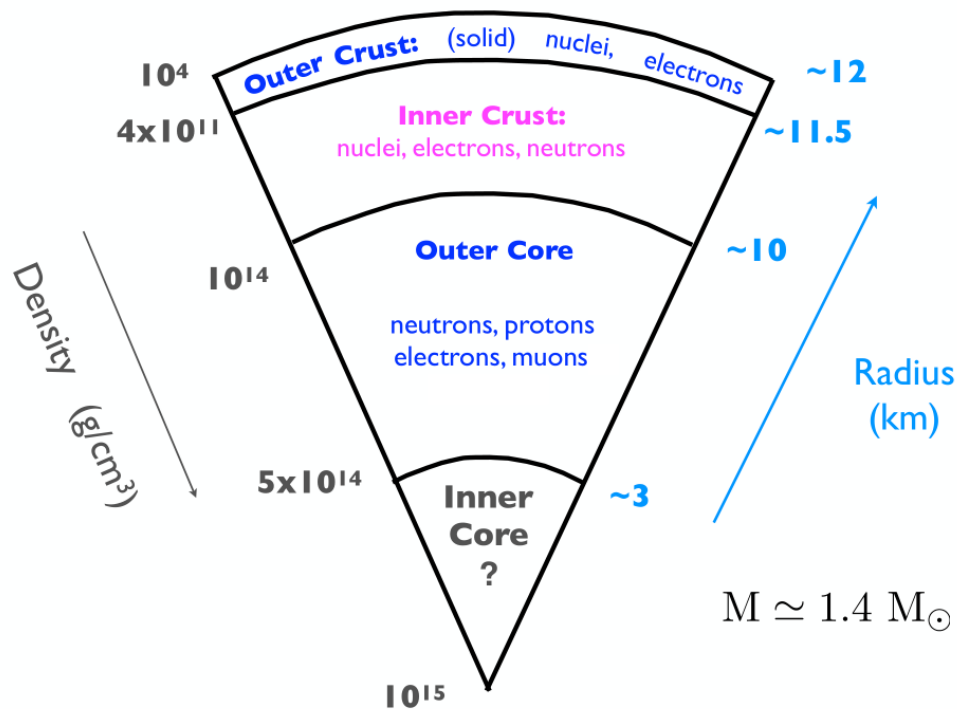
A. Gnech, arXiv:2308.16266

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
- Calculations currently focus on inner crust/outer core boundary

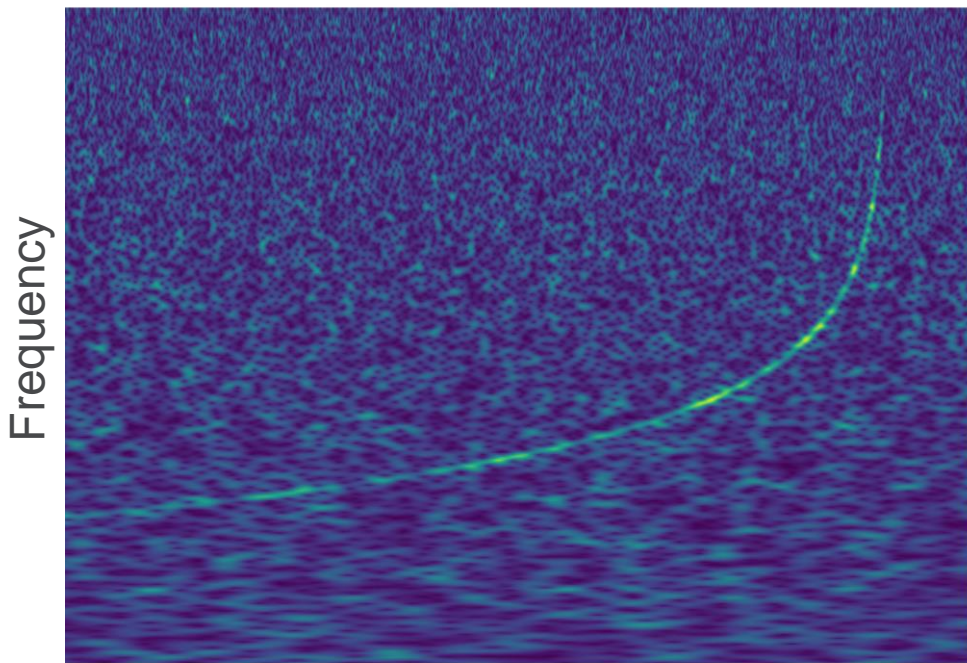
NEUTRON STAR INTEREST



- 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

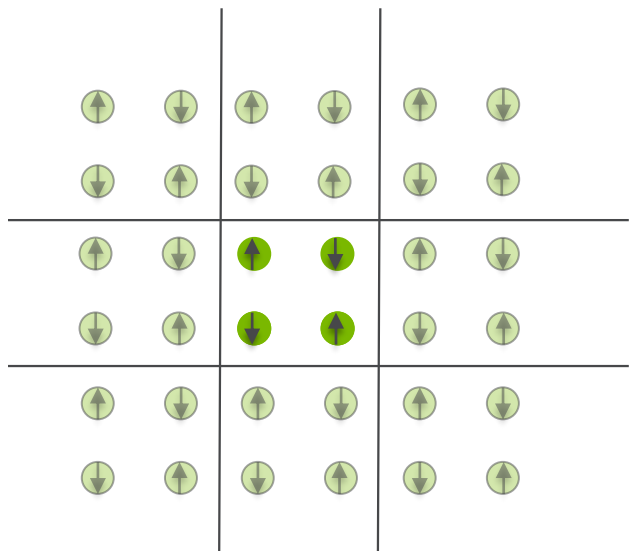
NEUTRON STAR OBSERVATION

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



Time
GW170817 signal

BULK NUCLEAR MATTER SETUP



- Periodic boundary conditions and coordinate system

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

- Continuous positions
- Discrete spins
- Potential energy contribution from particle images

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

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

- 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

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

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

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

Parameters at step s are updated as

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

FERMIONIC TRIAL WAVEFUNCTIONS

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

$$\begin{aligned} \Psi(\dots, x_i, \dots x_j \dots) &= -\Psi(\dots, x_j, \dots x_i \dots) \\ U(\dots, x_i, \dots x_j \dots) &= U(\dots, x_j, \dots x_i \dots) \\ \Phi(\dots, x_i, \dots x_j \dots) &= -\Phi(\dots, x_j, \dots x_i \dots) \end{aligned}$$

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

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

DEEP SET ARCHITECTURE

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

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

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

$$U(X) = \rho \left(\sum_i \vec{\phi}(x_i) \right) \quad \begin{array}{l} \vec{\phi}: \mathbb{R}^5 \rightarrow \mathbb{R}^{latent} \\ \rho: \mathbb{R}^{latent} \rightarrow \mathbb{R} \end{array}$$

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

HIDDEN FERMIONS

$$\Psi_T(X) = \left[\begin{array}{cccc|cccc} \phi_1(x_1) & \phi_1(x_2) & \phi_1(x_3) & \phi_1(x_4) & \phi_1(y_1) & \phi_1(y_2) & \phi_1(y_3) & \phi_1(y_4) \\ \phi_2(x_1) & \phi_2(x_2) & \phi_2(x_3) & \phi_2(x_4) & \phi_2(y_1) & \phi_2(y_2) & \phi_2(y_3) & \phi_2(y_4) \\ \phi_3(x_1) & \phi_3(x_2) & \phi_3(x_3) & \phi_3(x_4) & \phi_3(y_1) & \phi_3(y_2) & \phi_3(y_3) & \phi_3(y_4) \\ \phi_4(x_1) & \phi_4(x_2) & \phi_4(x_3) & \phi_4(x_4) & \phi_4(y_1) & \phi_4(y_2) & \phi_4(y_3) & \phi_4(y_4) \\ \chi_1(x_1) & \chi_1(x_2) & \chi_1(x_3) & \chi_1(x_4) & \chi_1(y_1) & \chi_1(y_2) & \chi_1(y_3) & \chi_1(y_4) \\ \chi_2(x_1) & \chi_2(x_2) & \chi_2(x_3) & \chi_2(x_4) & \chi_2(y_1) & \chi_2(y_2) & \chi_2(y_3) & \chi_2(y_4) \\ \chi_3(x_1) & \chi_3(x_2) & \chi_3(x_3) & \chi_3(x_4) & \chi_3(y_1) & \chi_3(y_2) & \chi_3(y_3) & \chi_3(y_4) \\ \chi_4(x_1) & \chi_4(x_2) & \chi_4(x_3) & \chi_4(x_4) & \chi_4(y_1) & \chi_4(y_2) & \chi_4(y_3) & \chi_4(y_4) \end{array} \right]$$

Visible wavefunctions
on visible coordinates

Hidden wavefunctions
on visible coordinates

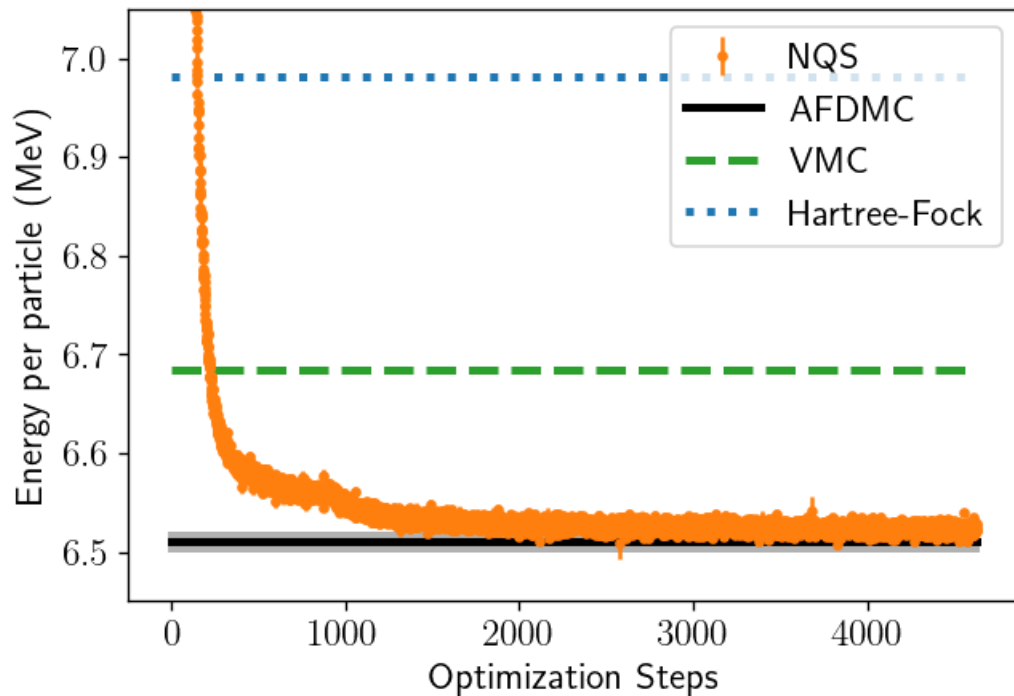
Visible wavefunctions
on hidden coordinates

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

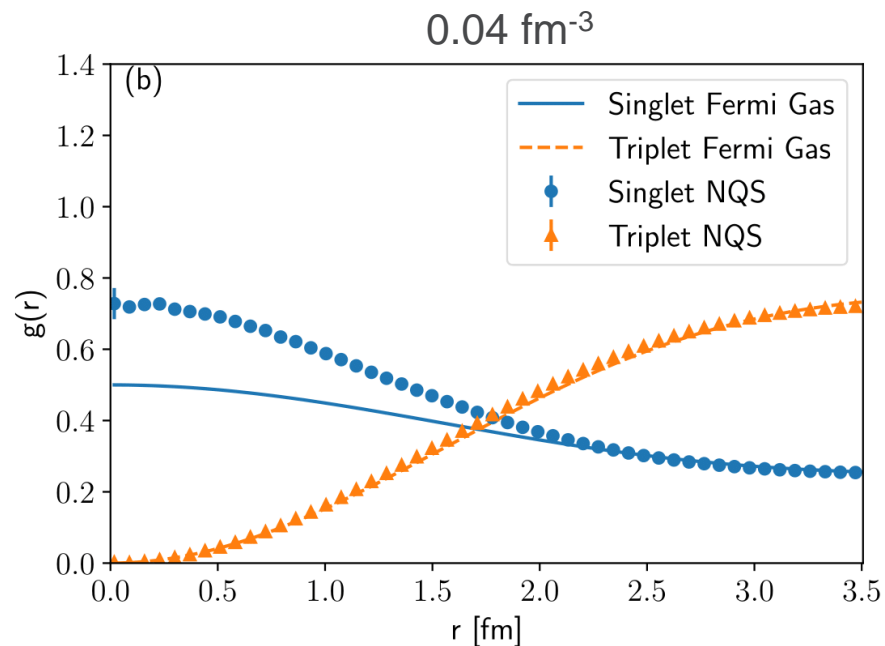
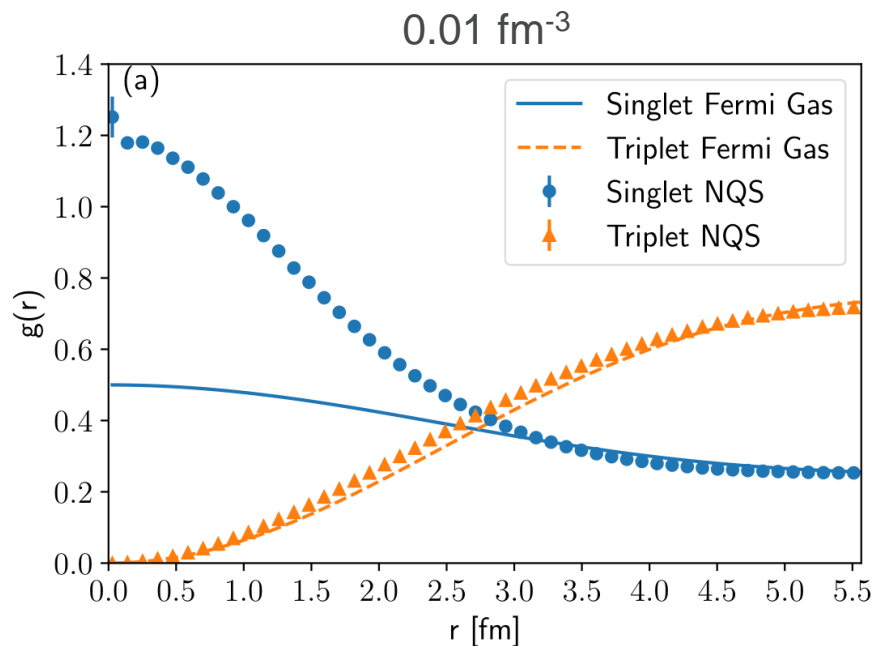
$$g_c(\mathbf{r}) = \frac{1}{2\pi r^2 \rho N} \sum_{i < j} \frac{\langle \psi | \delta(\mathbf{r}_{ij} - \mathbf{r}) | \psi \rangle}{\langle \psi | \psi \rangle}$$

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

Spin singlet and triplet channel two body densities

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

TWO BODY DENSITY



IMPROVED TRIAL WAVEFUNCTION ANSATZ

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

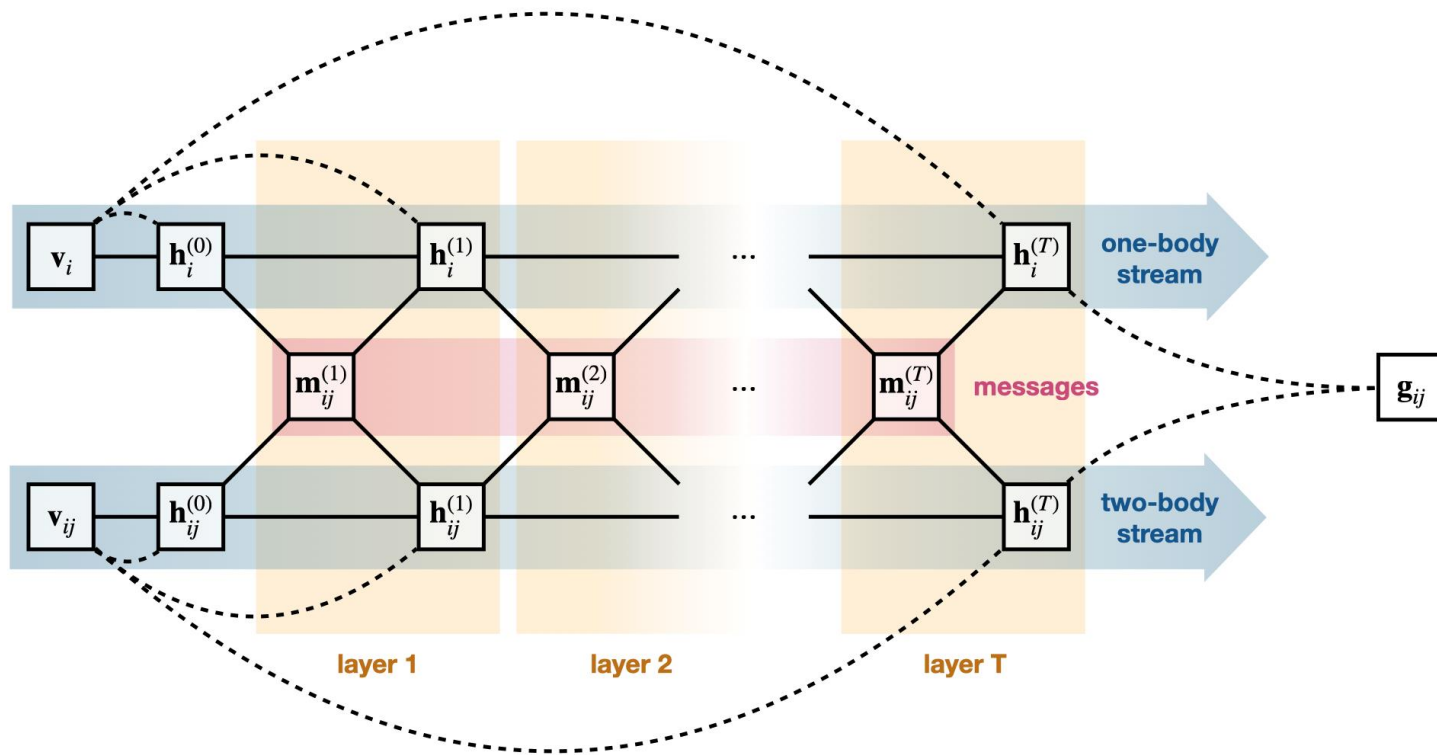
$$\Phi_{pf}(X) = pf[M]$$

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

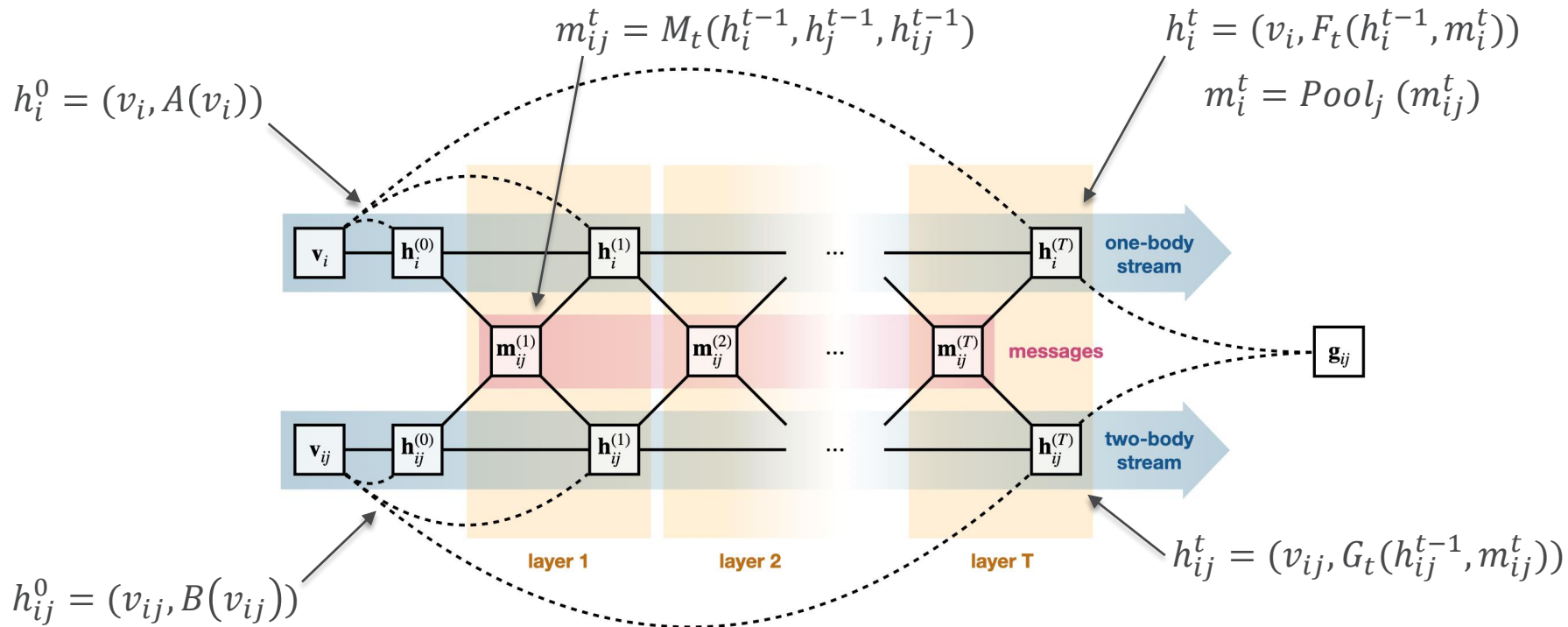
- Input, X , preprocessed by MPNN to give X^*
- Slater determinant \rightarrow Pfaffian
- M must be skew symmetric, $A = -A^T$, and square with even size
- Built in pairwise structure
- Pfaffian requires only one MLP so uses far fewer parameters
- Extra row and column can be added for odd numbers of particles

<https://arxiv.org/abs/2305.08831>

MESSAGE PASSING NEURAL NETWORK

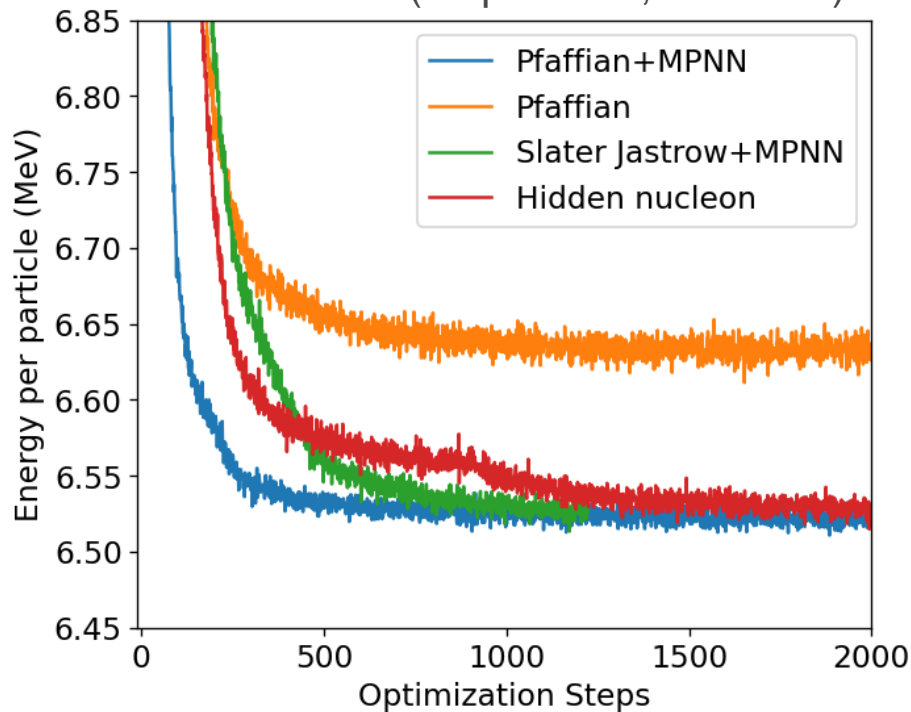


MESSAGE PASSING NEURAL NETWORK



ANSATZ COMPARISONS

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



**Optimization step time
(4 A100 GPUs, 32000 samples)**

Pfaffian+MPNN ~42 (s)

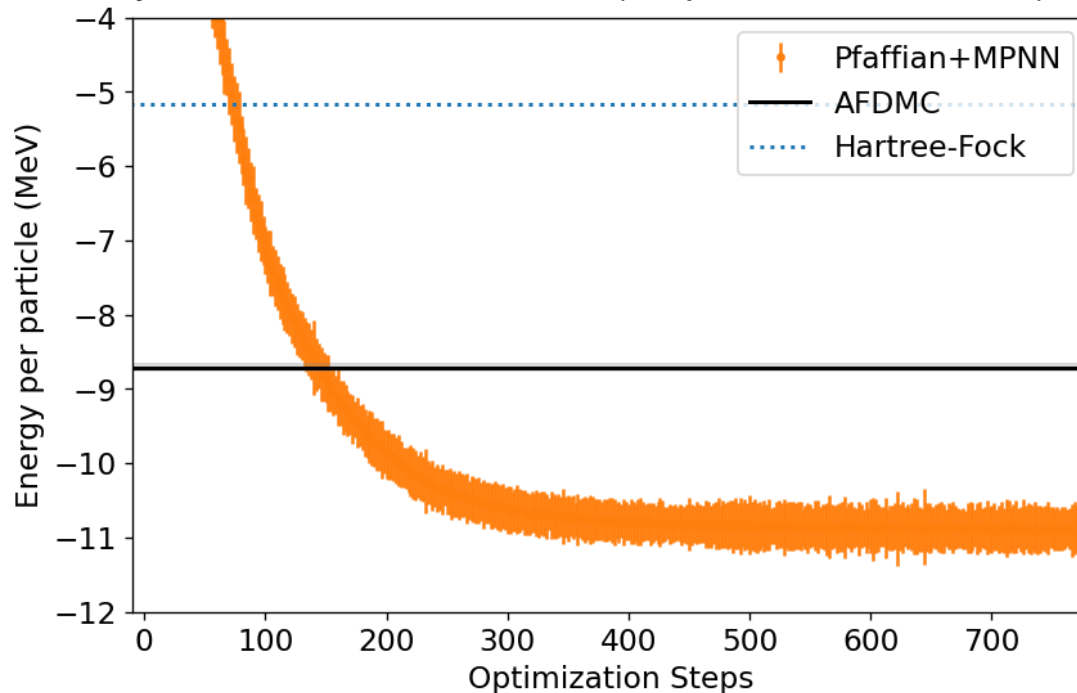
Pfaffian ~21 (s)

Slater Jastrow+MPNN ~35 (s)

Hidden fermion ~46 (s)

PRELIMINARY 14 NEUTRONS + 14 PROTONS

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



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 $\frac{1}{2}$ initially focusing on the emergence of clustering
 - Implement more sophisticated nuclear potentials
 - Larger systems possibly up to $A=40$ for nuclei

THANK YOU