Rising Researchers Seminar Series

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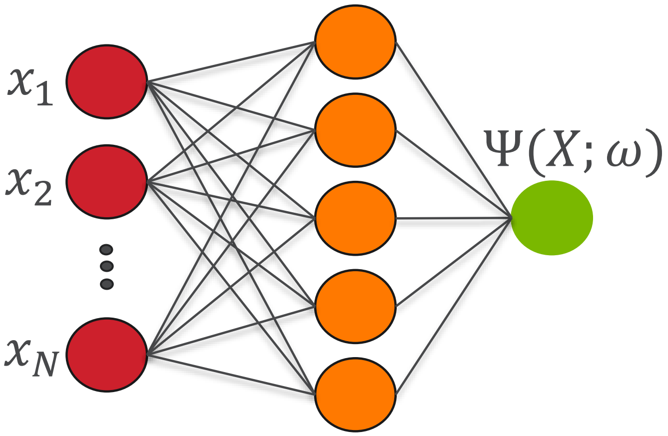
Participants shall **treat each other professionally and respectfully**. Participants shall refrain from any inappropriate behaviour, including discriminatory actions and comments based on individual characteristics such as age, race, ethnicity, sexual orientation, gender identity, gender expression, marital status, nationality, immigration status, political affiliation, ability status, or educational background. Disruptive or harassing behavior will not be tolerated including but not limited to inappropriate or intimidating language and unwelcome jokes or comments.

Violations of this code of conduct should be reported to any member of the executive committee (see About Us page on the website). The Executive committee may also act of their own accord should they notice violations. Sanctions may range from verbal warning, to ejection from the meeting or, in severe cases, partial or total bans from future meetings.

References: This code of conduct is based heavily on that of the INT and the APS. We are also grateful to Roxanne Springer for valuable discussion and guidance.

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



BRYCE FORE

U.S. DEPARTMENT OF ENERGY
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Rising Researchers Seminar Series
October 15^{th} 2024

OUTLINE

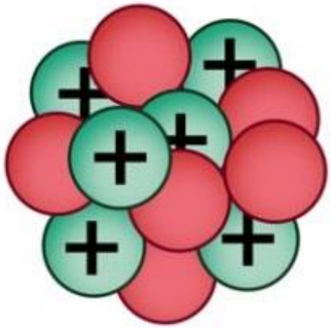
- Nuclear many body problem
  - Many body methods
  - Curse of dimensionality
- Overview of variational Monte Carlo (VMC)
  - Metropolis-Hastings Sampling
  - Parameter optimization
  - Fermionic trial wavefunctions
- Results
  - Nuclei
  - Pure neutron matter
  - Symmetric nuclear matter
  - Self emergence of clustering

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



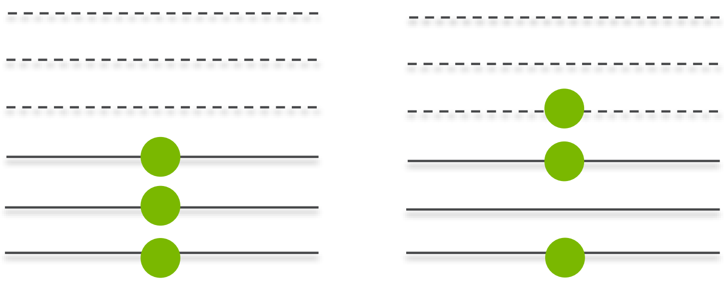
Neutron stars

THE NUCLEAR MANY BODY METHODS

Configuration-interaction

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

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



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

Quantum Monte Carlo

$$\left|\Psi_T\right\rangle = \sum_n c_n \left|\Psi_n\right\rangle$$

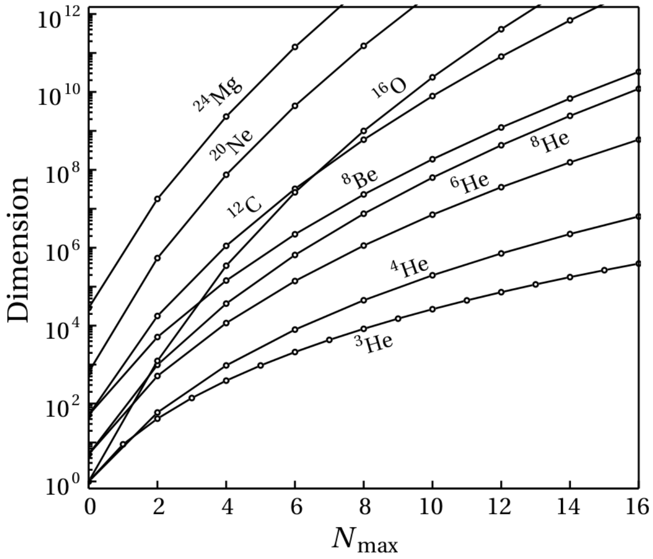
$$H\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle$$

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

CURSE OF DIMENSIONALITY

Configuration-interaction

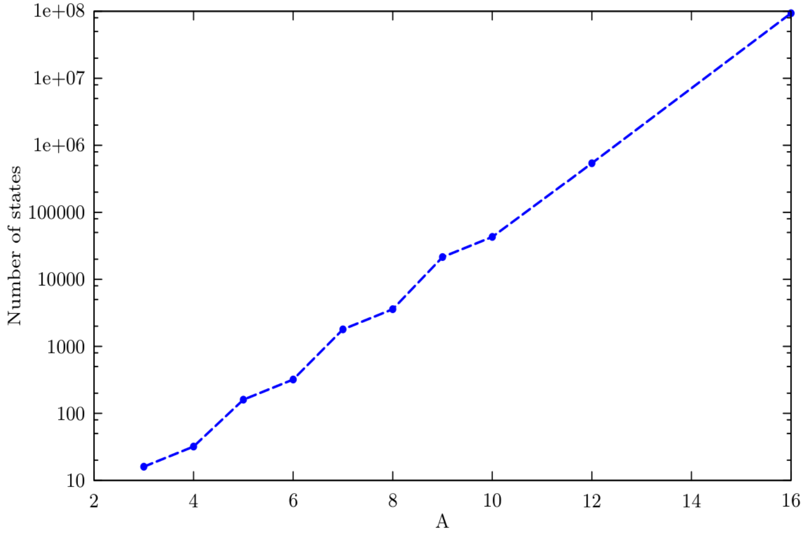
$$\binom{N}{A} = \frac{N!}{(N-A)!\,A!}$$



Credit: Patrick Fasano

Green's function Monte Carlo

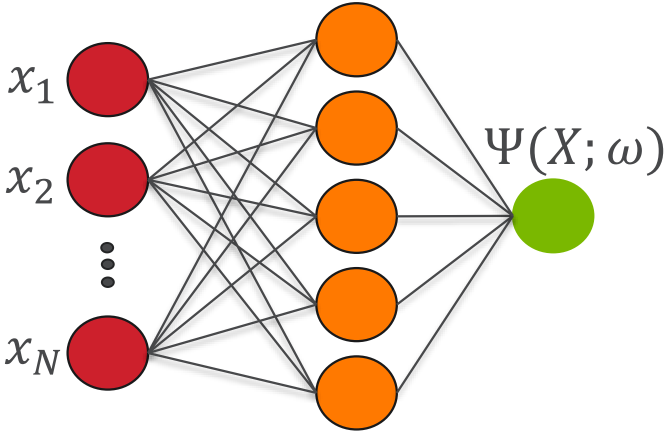
$$\lim_{\tau\to\infty} e^{-(H-E_0)\tau}\left|\Psi_T\right\rangle = c_o\left|\Psi_0\right\rangle$$

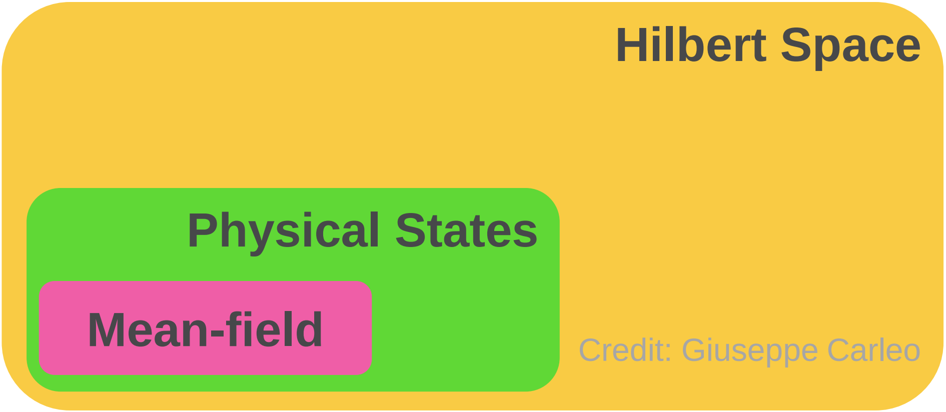


Credit: Alessandro Lovato

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

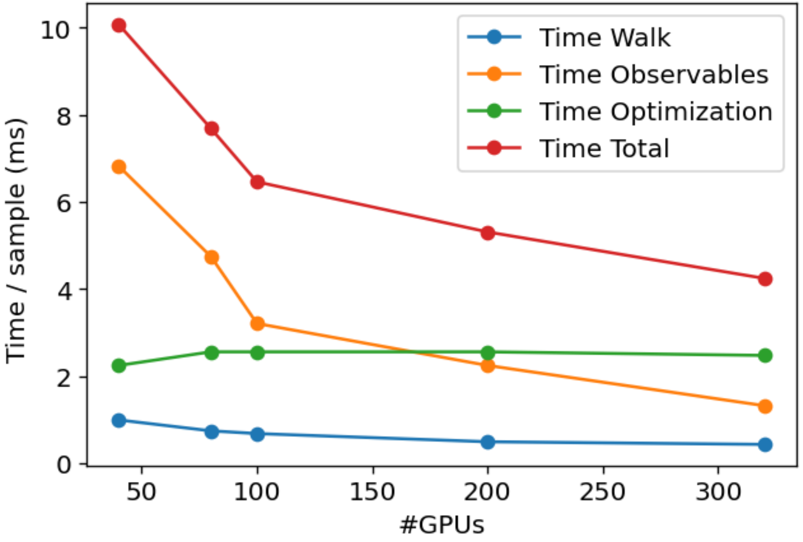
Scaling with system size

Conventional QMC: $O(2^A)$

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

A = Number of particles in system

Scaling with resources



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

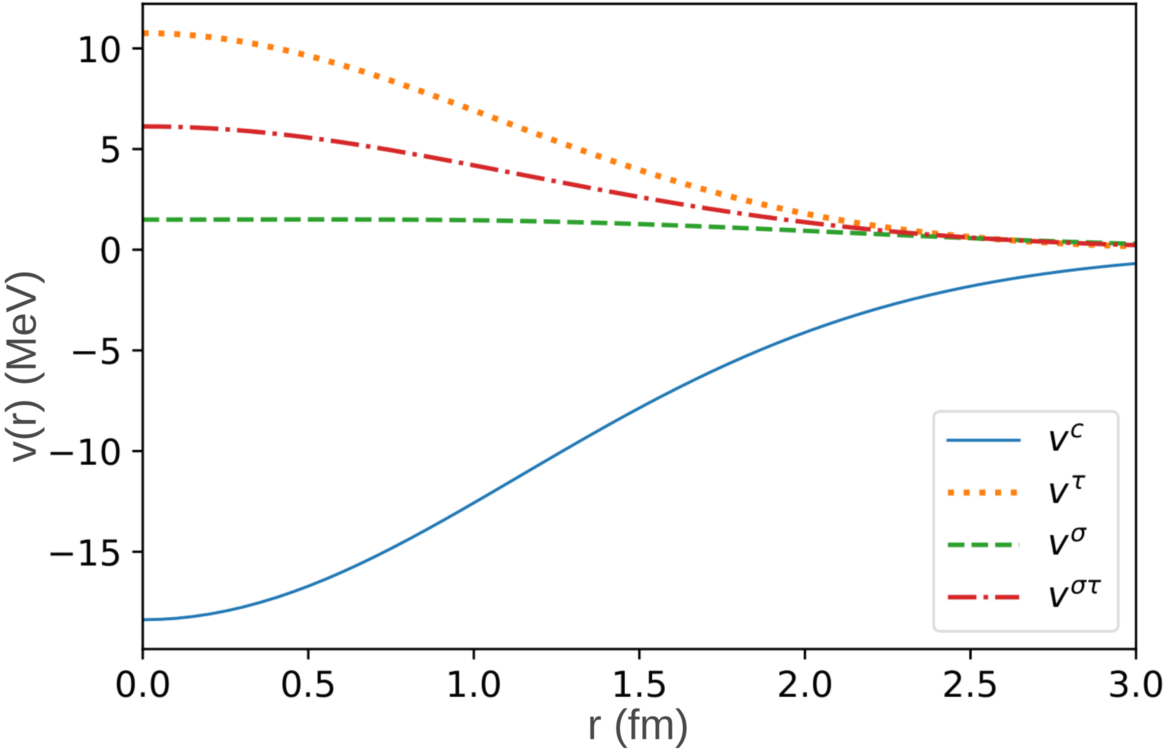
$$v_{ij}^{\mathrm{CI}} = \sum_{p=1}^{4} v^p(r_{ij}) O_{ij}^p$$

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

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

R. Schiavilla, PRC 103, 054003(2021)

PIONLESS EFT HAMILTONIAN



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

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

FERMIONIC TRIAL WAVEFUNCTIONS

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

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

- 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 function independent of particle ordering

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

- Map configuration for each particle to a latent space, sum results, map to real numbers

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

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

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

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

NEURAL SLATER-JASTROW ANSATZ

- Use Slater determinant to enforce antisymmetry
- Single particle wavefunctions represented by neural networks

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

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

NEURAL PFAFFIAN ANSATZ

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

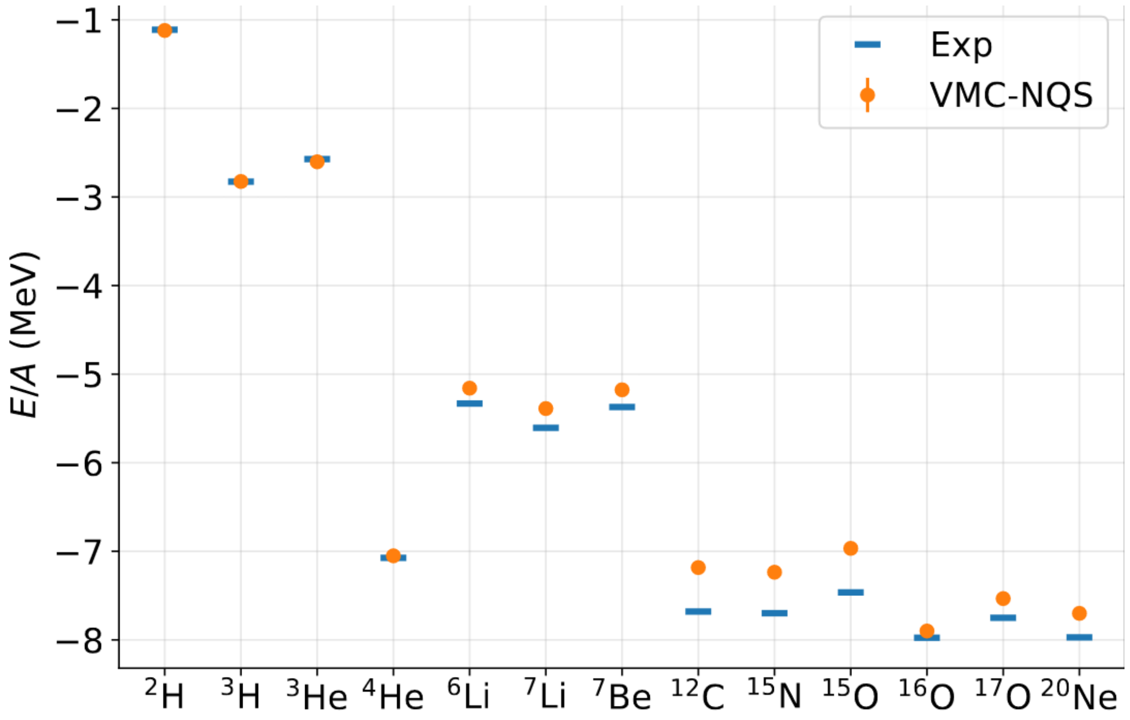
$$\Phi_{pf}(X) = pf[M]$$

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

- 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 neural net, ϕ, so uses far fewer parameters

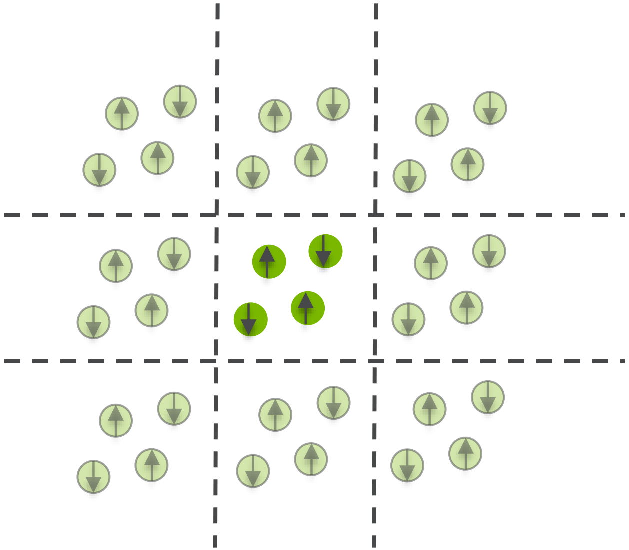
J. Kim, *Commun Phys* **7**, 148 (2024)

NEURAL QUANTUM STATE RESULTS IN NUCLEI



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

BULK NUCLEAR MATTER SETUP

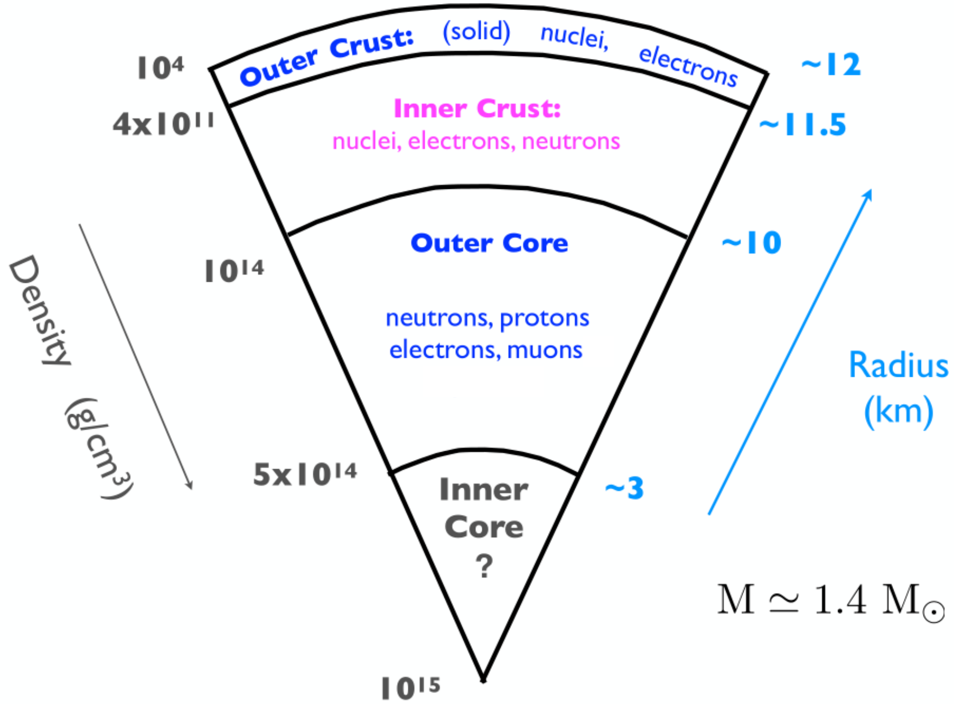


- Periodic boundary conditions and coordinate system

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

- Potential energy contribution from particle images
- Remove Coulomb potential

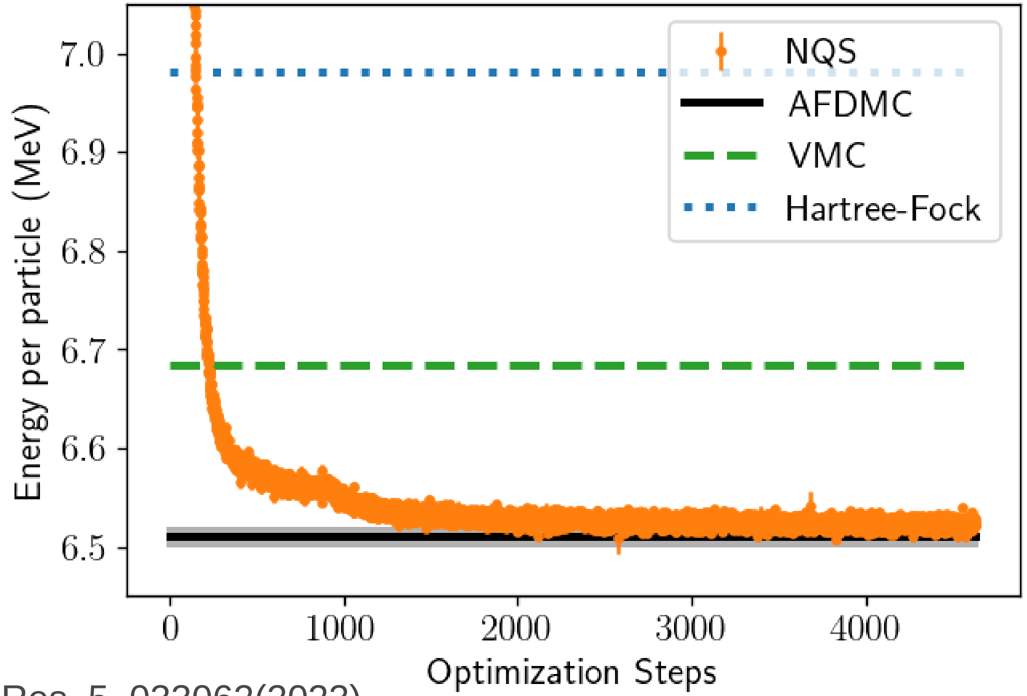
NEUTRON STAR STRUCTURE



- 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

PURE NEUTRON MATTER

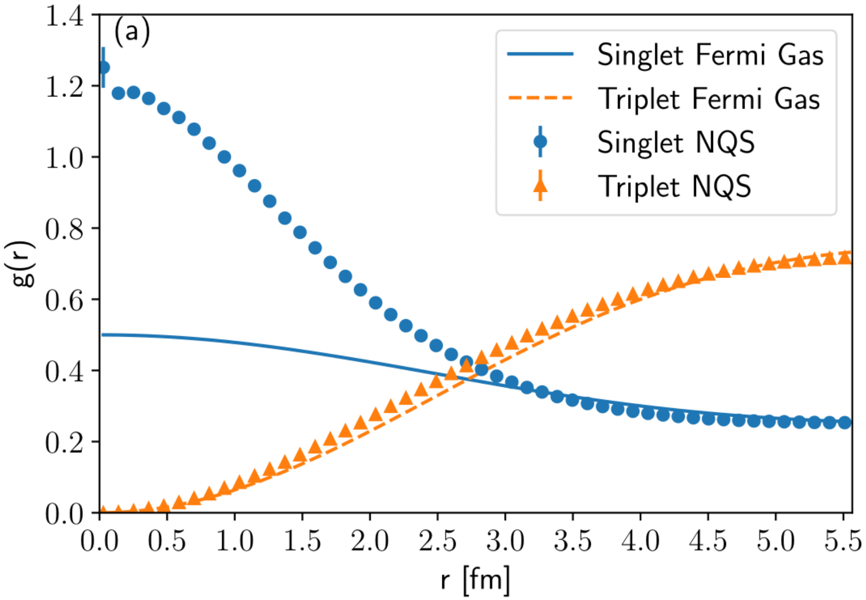
Neutron Matter (14 particles, 0.04 fm^{-3})



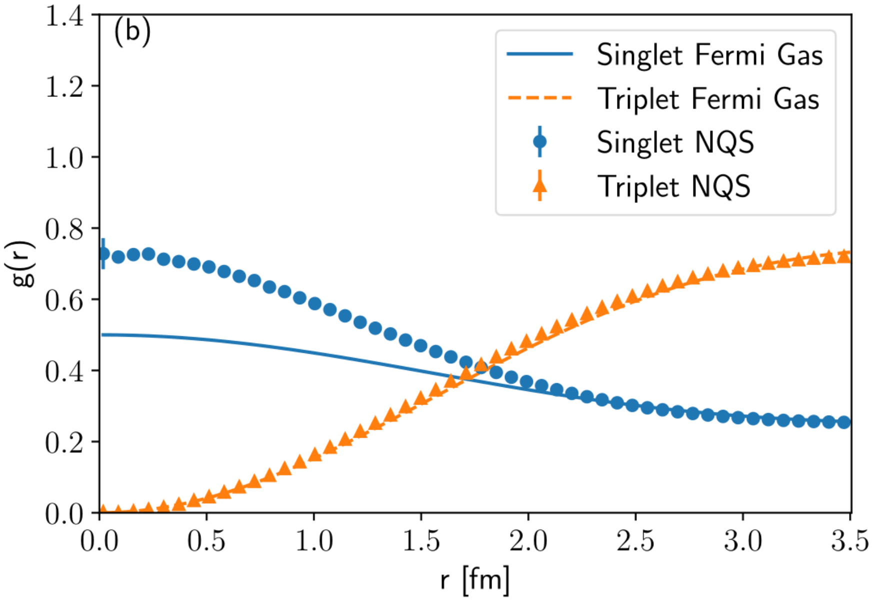
B. Fore, Phys. Rev. Res. 5, 033062(2023)

TWO-BODY PAIR DISTRIBUTIONS

0.01 fm^{-3}

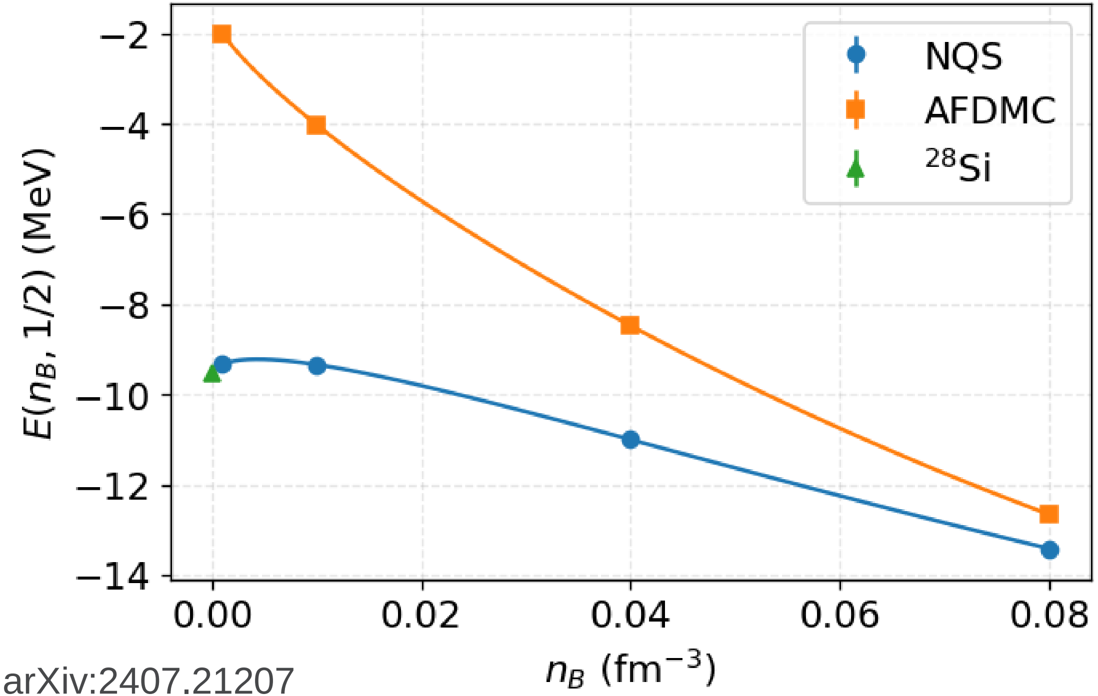


0.04 fm^{-3}



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

SYMMETRIC NUCLEAR MATTER

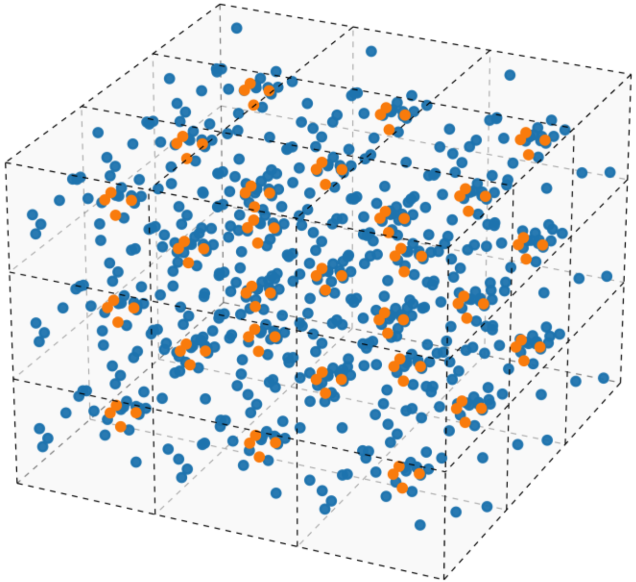


B. Fore, arXiv:2407.21207

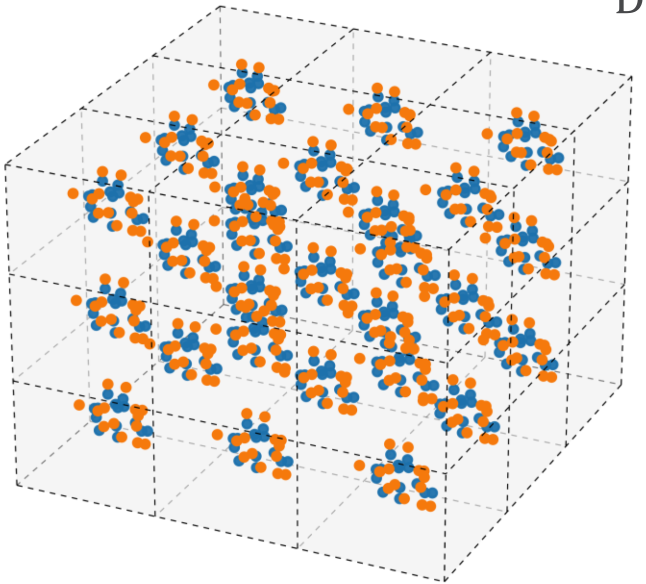
SELF EMERGING CLUSTERING

Density: 0.01 fm^{-3}

Proton
Neutron



4 protons; 24 neutrons

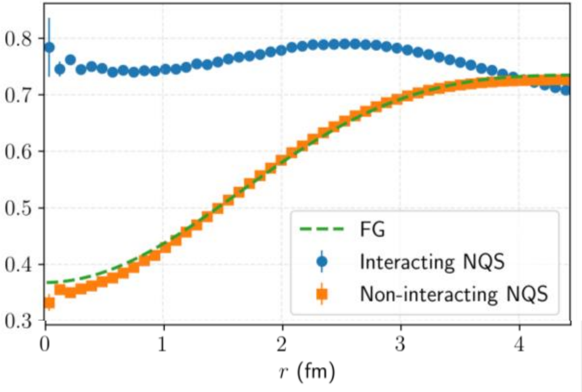


14 protons; 14 neutrons

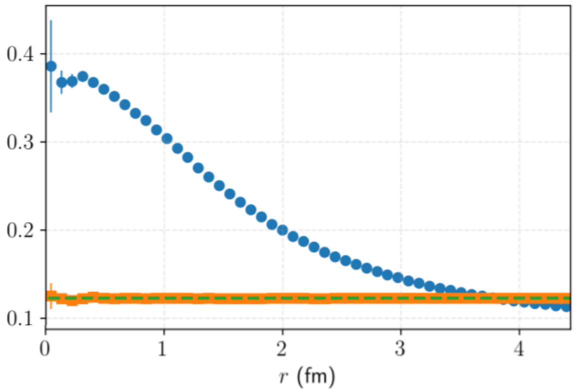
B. Fore, arXiv:2407.21207

CLUSTERING: TWO-BODY PAIR DISTRIBUTIONS

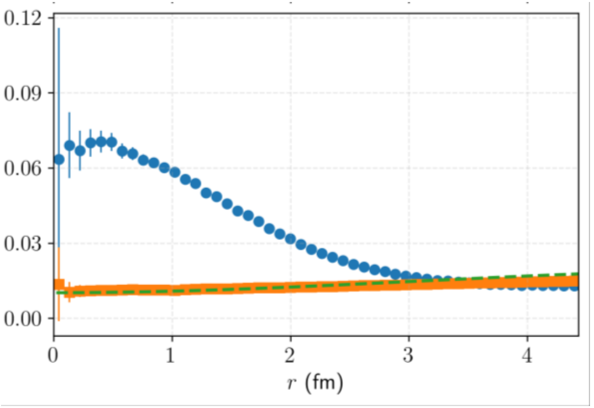
Neutron-neutron



Neutron-proton



Proton-proton



B. Fore, arXiv:2407.21207

ASYMMETRIC MATTER ENERGY

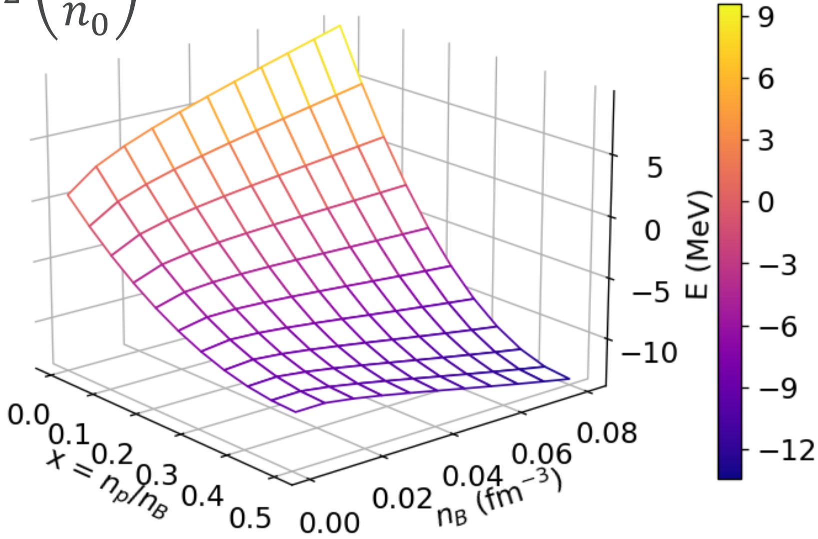
- Fit $E(n_B, 0)$ and $E(n_B, 1/2)$

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

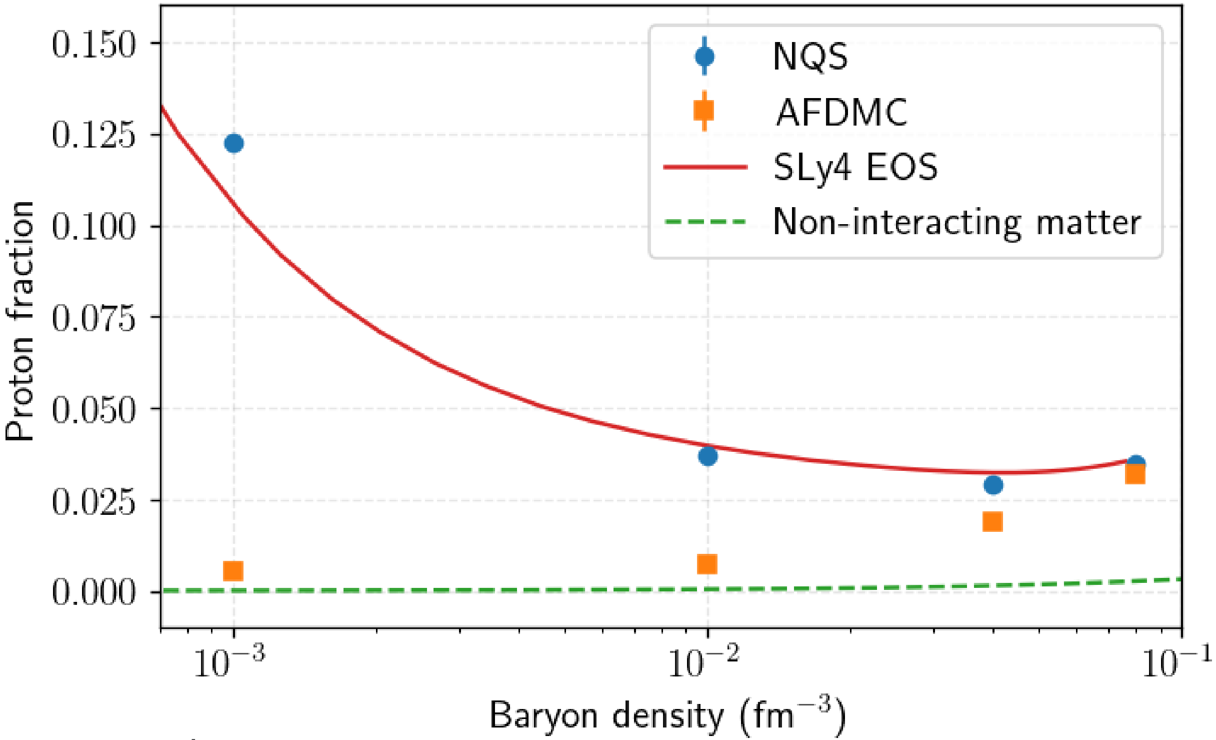
- Model energy by symmetry energy expansion

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

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



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

COLLABORATORS

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THANK YOU