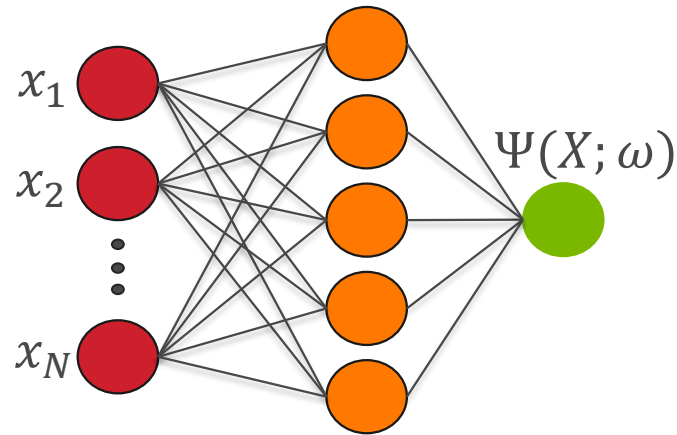


QUANTUM MONTE CARLO WITH NEURAL QUANTUM STATES

BRYCE FORE



EMMI Workshop: Light-ion collisions
Heidelberg, Germany
September 23st 2026

THE QUANTUM MANY-BODY PROBLEM

Many-body Schrödinger equation

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

Fermions have anti-symmetric wavefunction

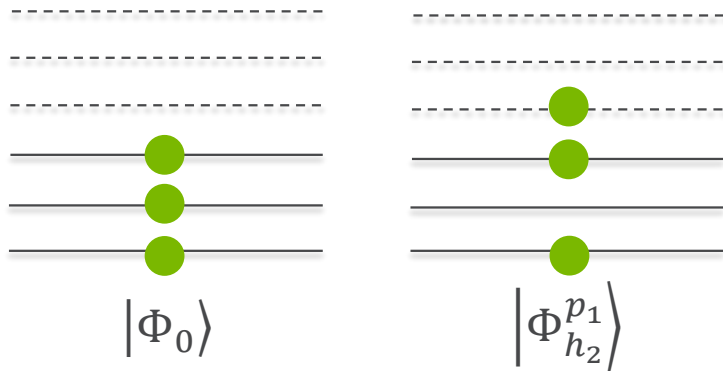
$$\Psi(x_1, \dots, x_i, \dots, x_j, \dots, x_A) = -\Psi(x_1, \dots, x_j, \dots, x_i, \dots, x_A)$$


THE NUCLEAR MANY BODY METHODS

Configuration-interaction

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

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



Quantum Monte Carlo

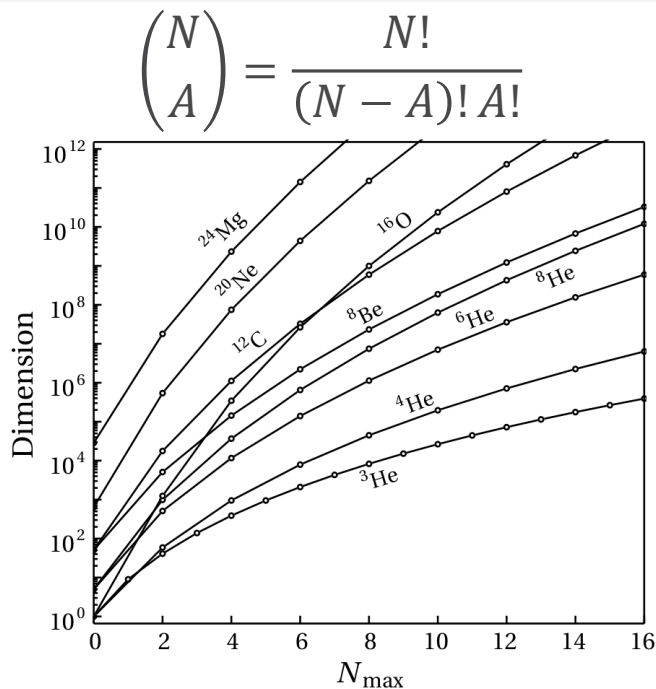
$$|\Psi_V\rangle = \sum_n c_n |\Psi_n\rangle$$

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

$$\lim_{\tau \rightarrow \infty} e^{-(H-E_0)\tau} |\Psi_V\rangle = c_0 |\Psi_0\rangle$$

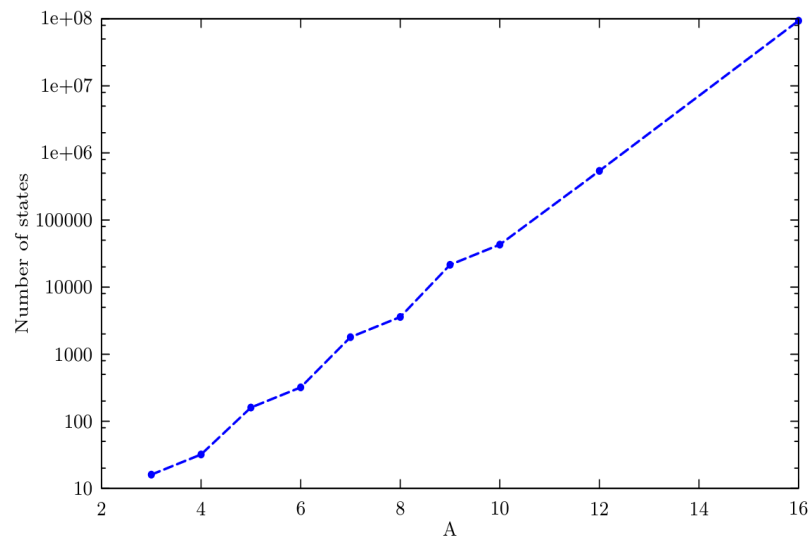
CURSE OF DIMENSIONALITY

Configuration-interaction



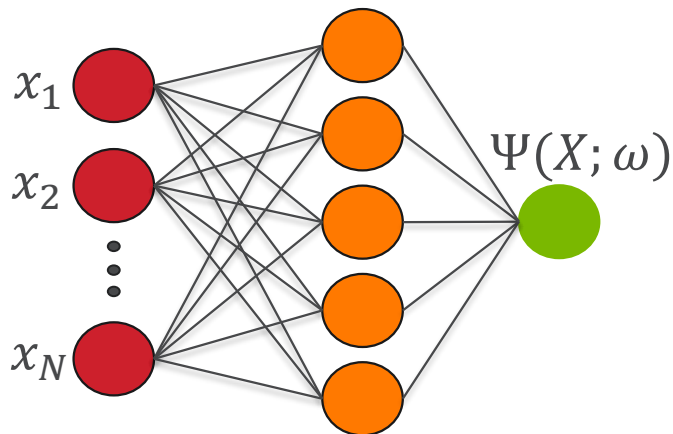
Green's function Monte Carlo

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



NEURAL QUANTUM STATES

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



Hilbert Space

Physical States

Mean-field

Credit: Giuseppe Carleo

SCALING AND COMPUTATIONAL PERFORMANCE

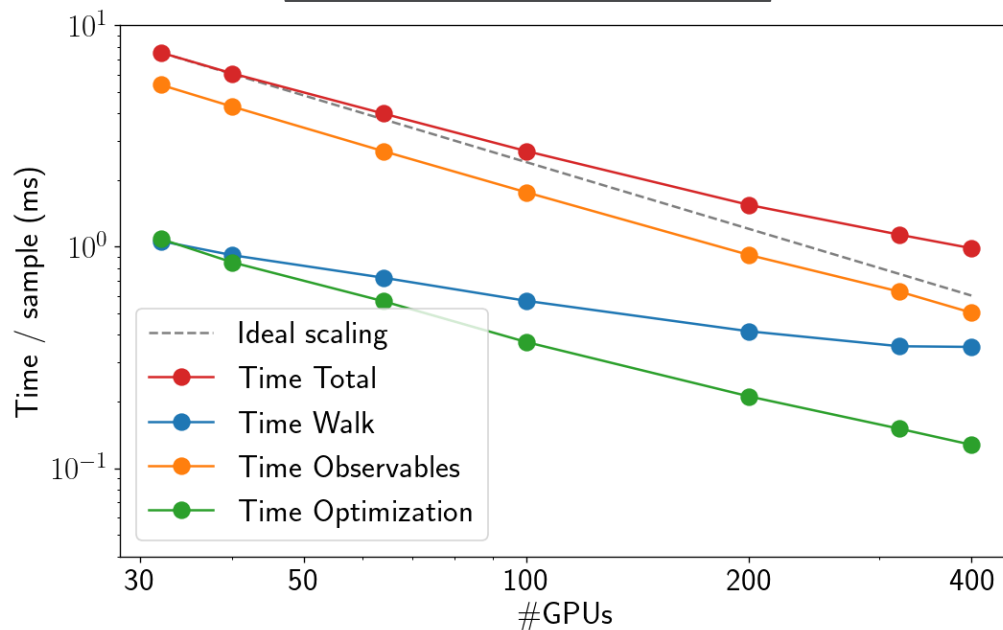
Scaling with system size

Conventional VMC: $O(2^A)$

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

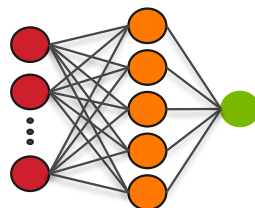
A = Number of particles in system

Scaling with resources



VARIATIONAL MONTE CARLO WITH NQS

1. Create the NQS wavefunction

$$\Psi_V(X; \omega) =$$


2. Sample (Metropolis-Hastings algorithm) and compute wavefunction energy

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

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

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

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

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

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

- 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

FERMIONIC WAVEFUNCTIONS

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

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

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

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

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

NQS WAVEFUNCTION ANSATZ OVERVIEW

- Neural Slater-Jastrow

$$\Psi_V = e^{U(\bullet)} \det(\phi_{\bullet}(\bullet))$$

- Hidden Fermion

$$\Psi_V = \det \begin{pmatrix} \phi_{\bullet}(\bullet) & \phi_{\bullet}(\bullet) \\ \phi_{\bullet}(\bullet) & \phi_{\bullet}(\bullet) \end{pmatrix}$$

- Neural Pfaffian

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

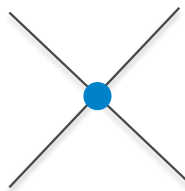
PIONLESS EFT HAMILTONIAN

- Pionless-EFT Hamiltonian

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

- NN potential fit to

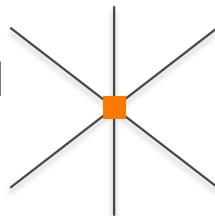
- np scattering lengths
- effective radii
- deuteron binding energy



$$v_{ij}^{\text{CI}} = \sum_{p=1}^4 e^{-r_{ij}^2/R^2} O_{ij}^p$$

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

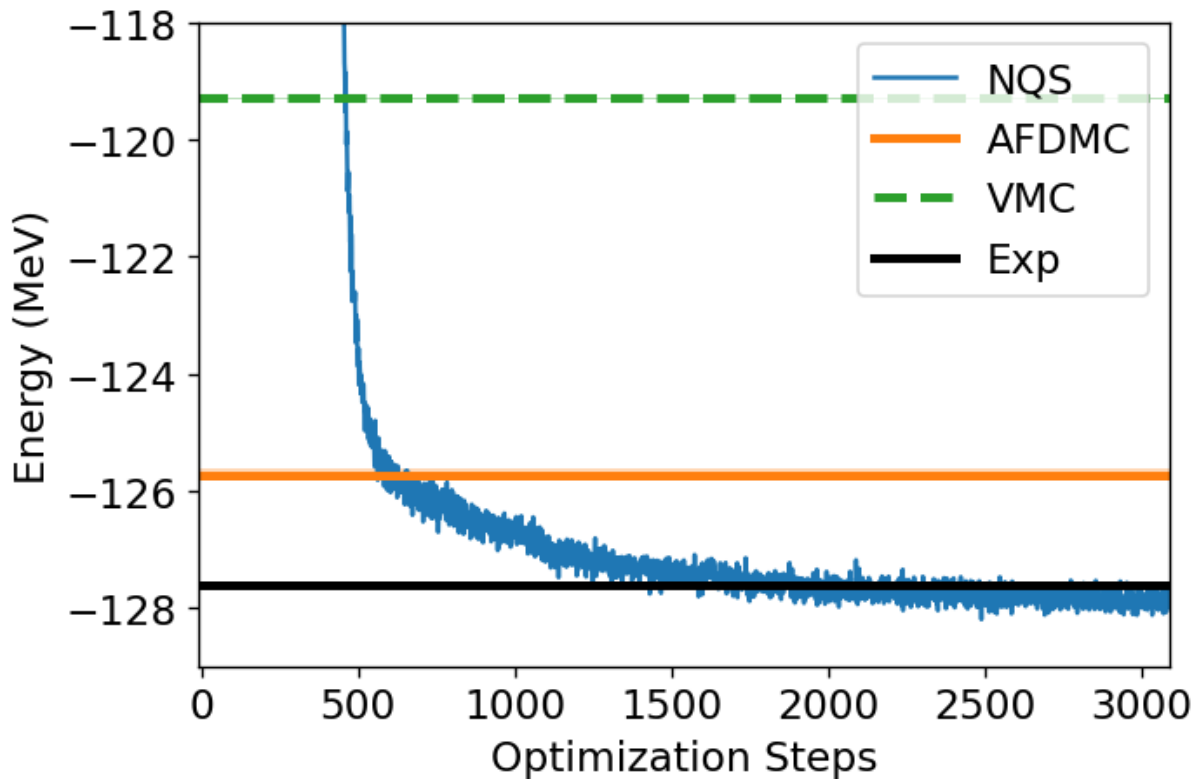
- Three body potential adjusted to reproduce ^3H binding



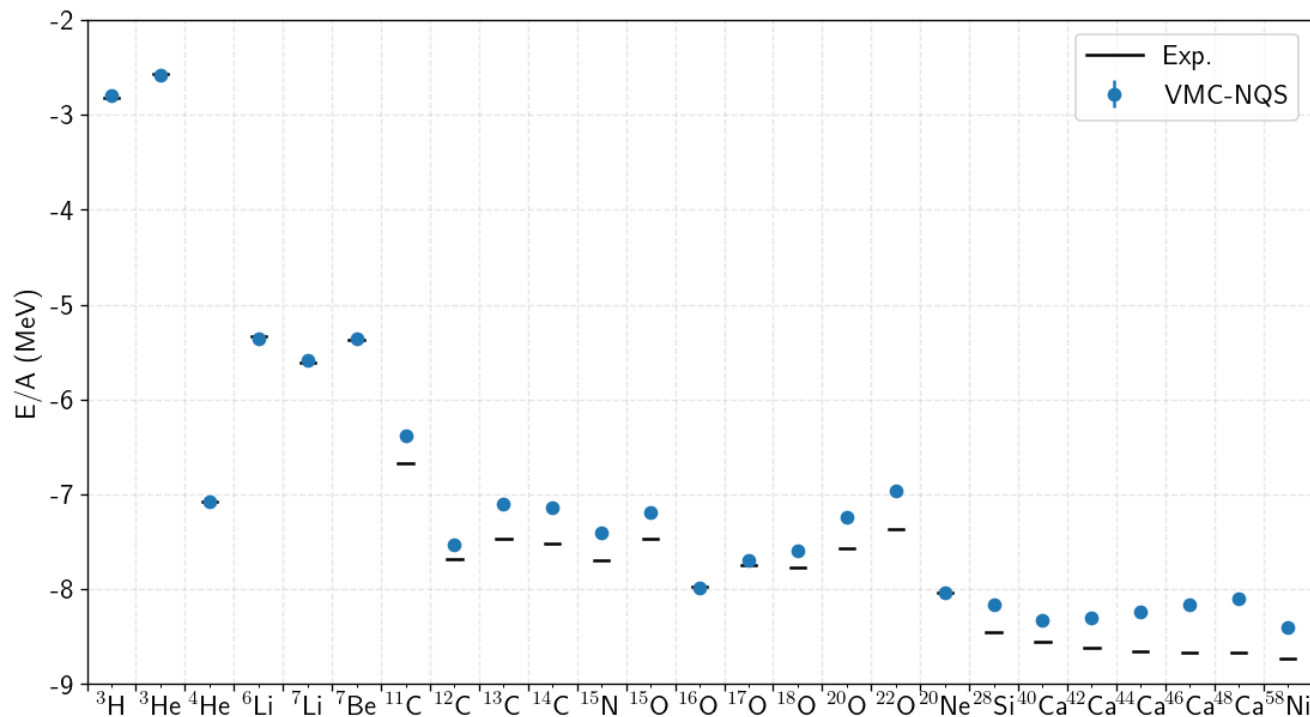
$$V_{ijk} = c_E \sum_{\text{cyc}} e^{-(r_{ij}^2 + r_{jk}^2)/R_3^2}$$

R. Schiavilla, PRC 103, 054003(2021)

RESULTS IN 16O

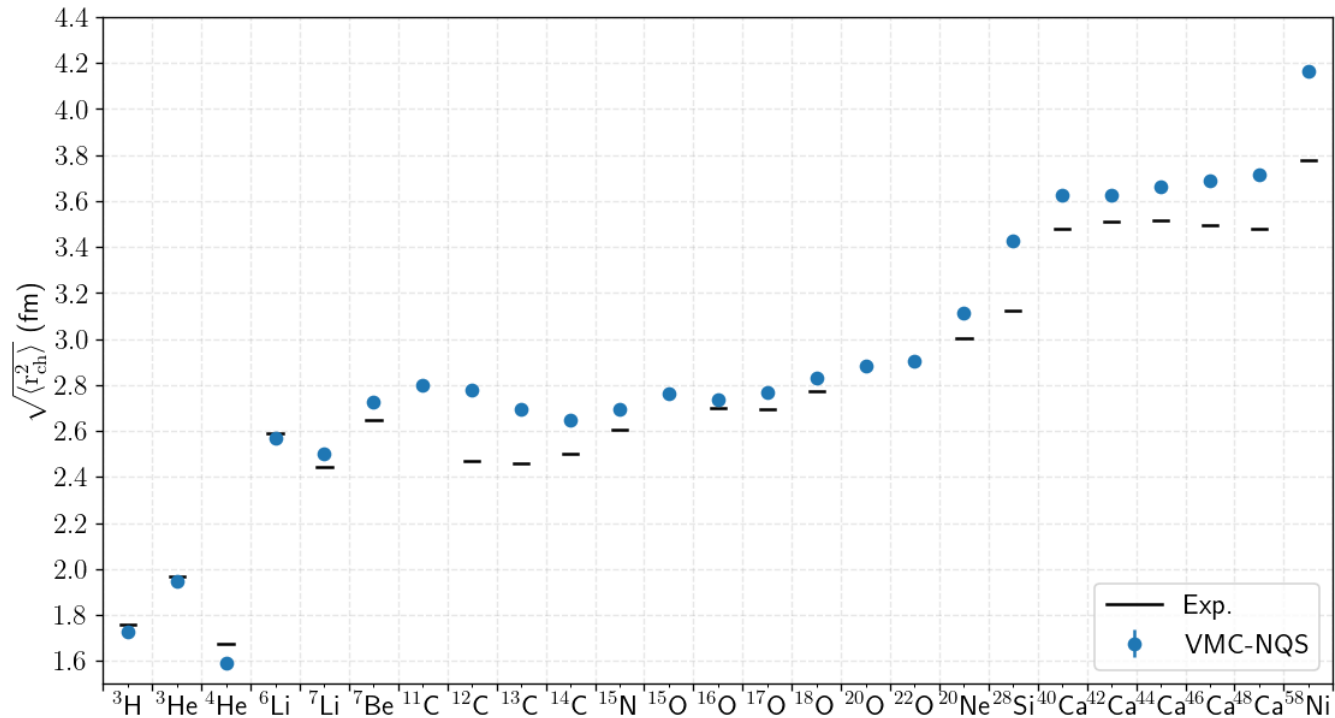


NEURAL QUANTUM STATE RESULTS IN NUCLEI



B. Fore, Arxiv:2607.09223

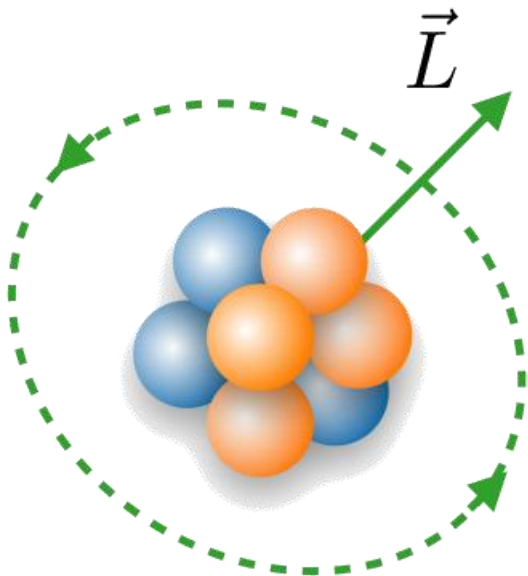
NEURAL QUANTUM STATE RESULTS IN NUCLEI



B. Fore, Arxiv:2607.09223

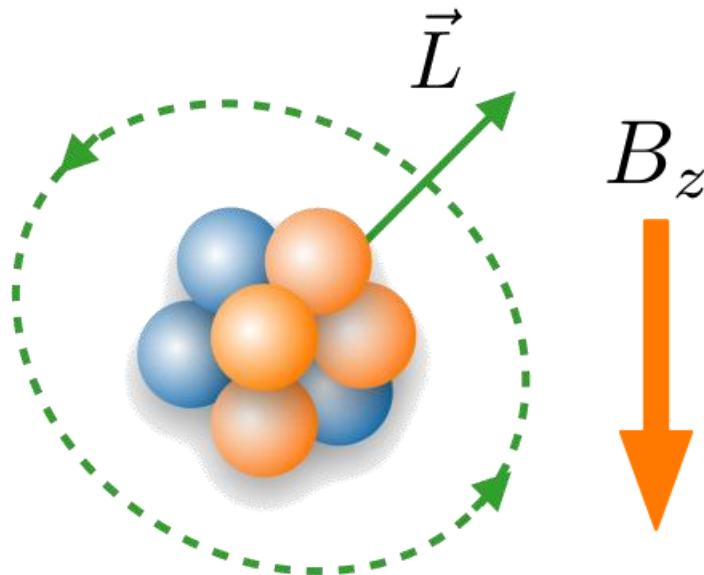
MAGNETIC MOMENTS

Ground state is degenerate in L_z



Break degeneracy using magnetic field B_z

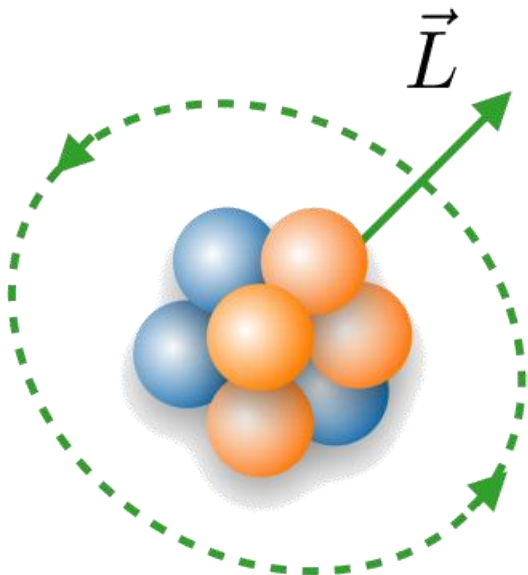
$$H \rightarrow H - B_z L_z$$



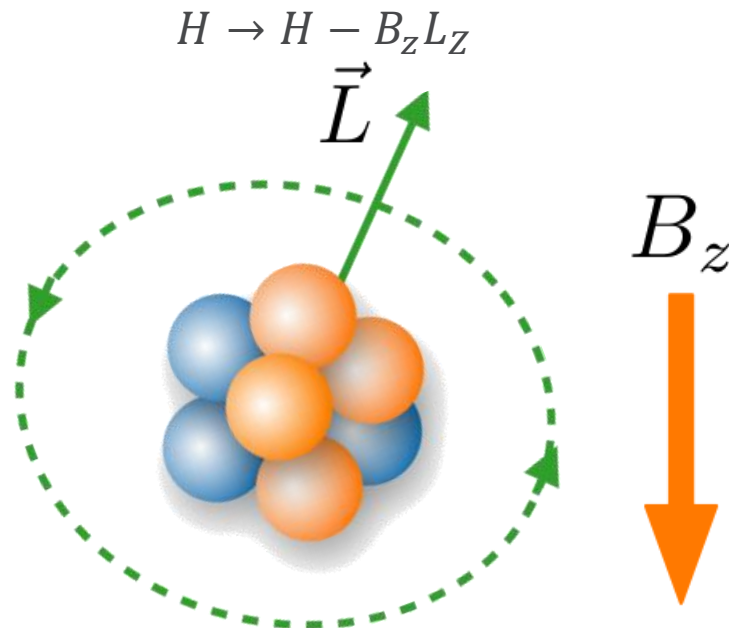
A. Gnech, B. Fore, Phys. Rev. Lett. 133, 142501

MAGNETIC MOMENTS

Ground state is degenerate in L_z



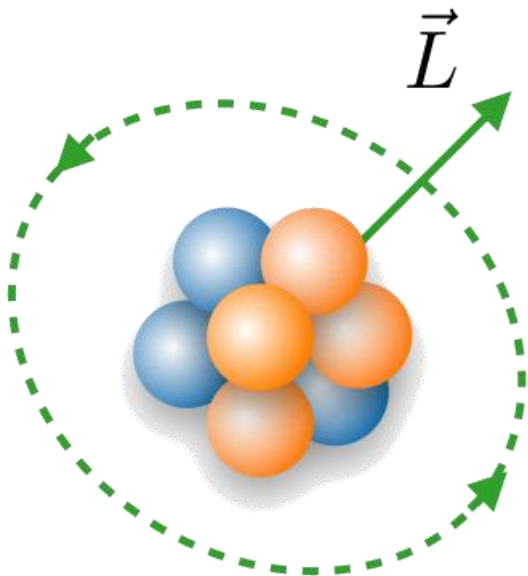
Break degeneracy using magnetic field B_z



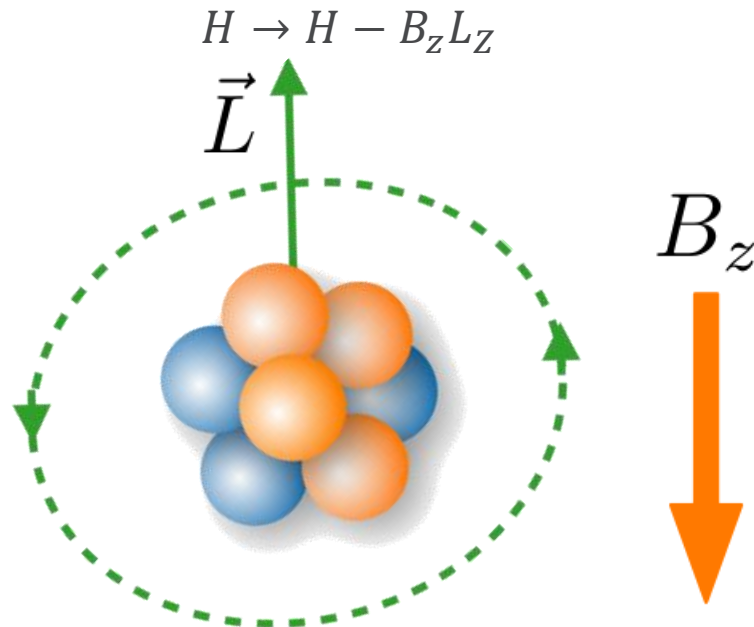
A. Gnech, B. Fore, Phys. Rev. Lett. 133, 142501

MAGNETIC MOMENTS

Ground state is degenerate in L_z

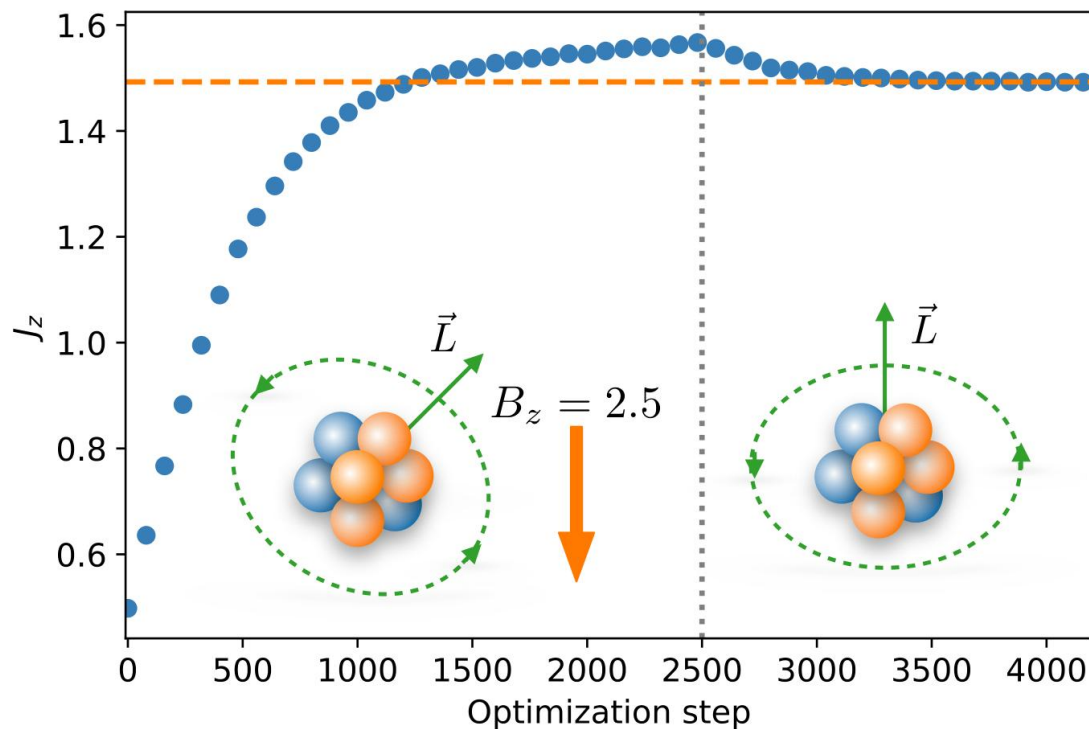


Break degeneracy using magnetic field B_z



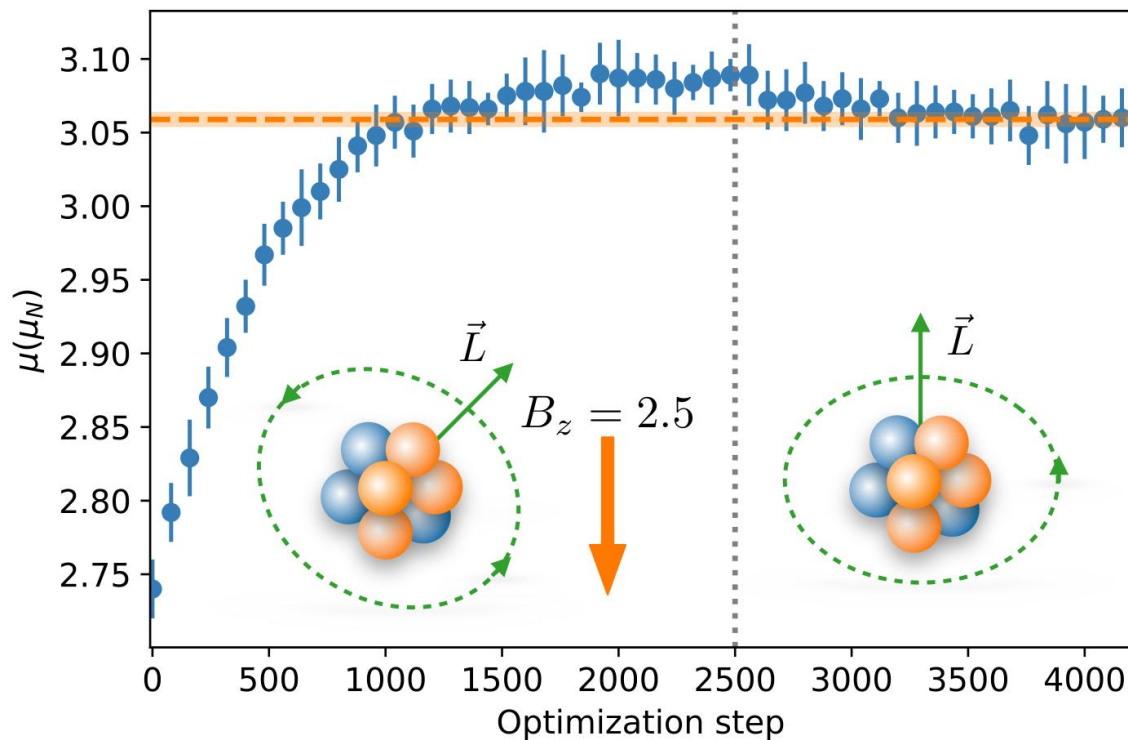
A. Gnech, B. Fore, Phys. Rev. Lett. 133, 142501

MAGNETIC MOMENTS



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

MAGNETIC MOMENTS



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

CONCLUSIONS AND NEXT STEPS

- Conclusions:
 - Universal and accurate approximations for fermion wavefunctions
 - No assumptions applied to nuclear structure
 - Favorable scaling with number of fermions
- Next steps:
 - Ground state calculations including tensor term
 - DMC calculations beginning from NQS results
 - Excited state calculations
 - Real time dynamics

COLLABORATORS



A. Lovato and J.Kim



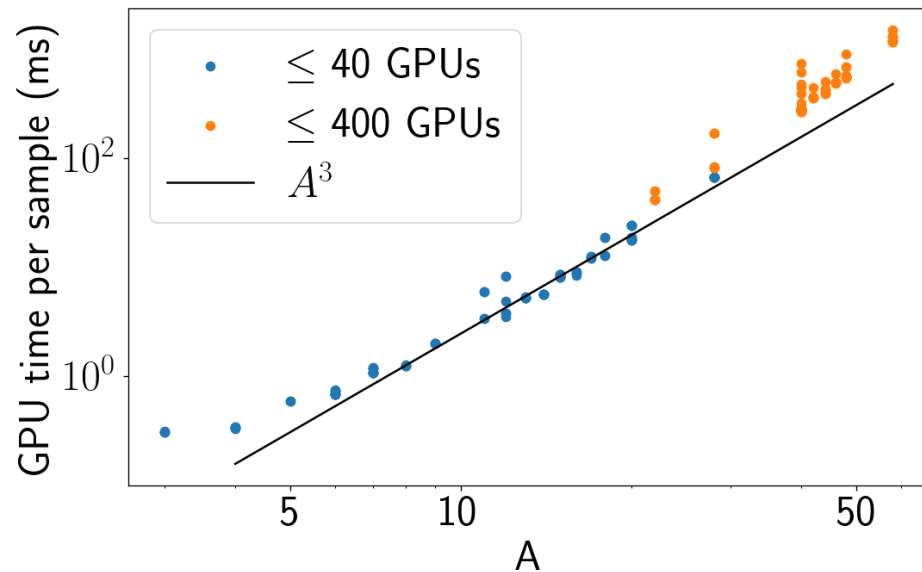
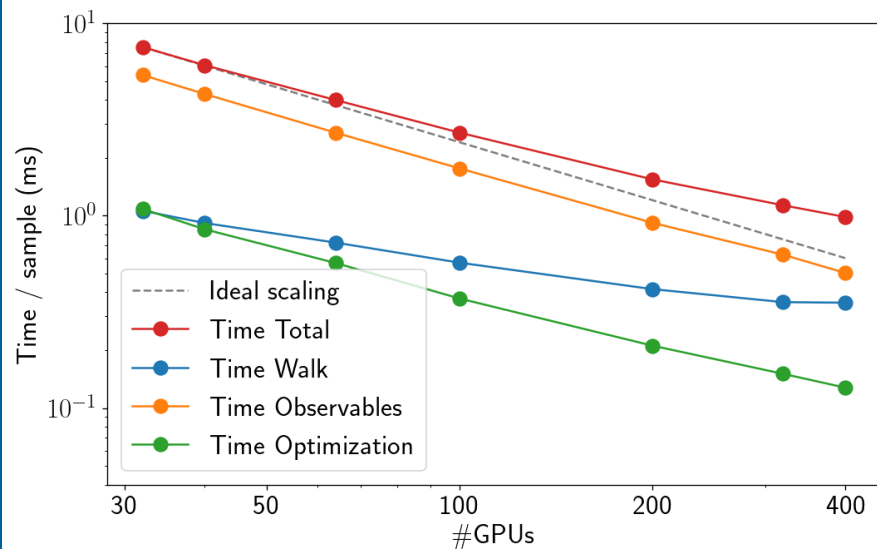
UNIVERSITY
OF OSLO

M. Hjorth-Jensen

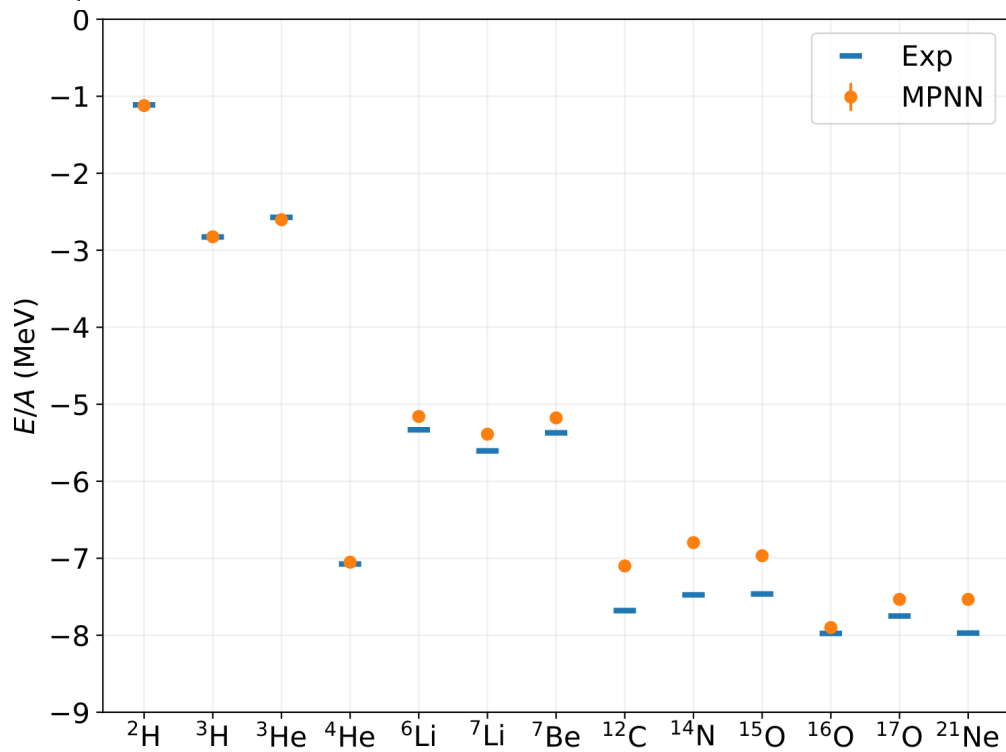
THANK YOU

SUPPLEMENTAL SLIDES

LARGER NUCLEI SCALING

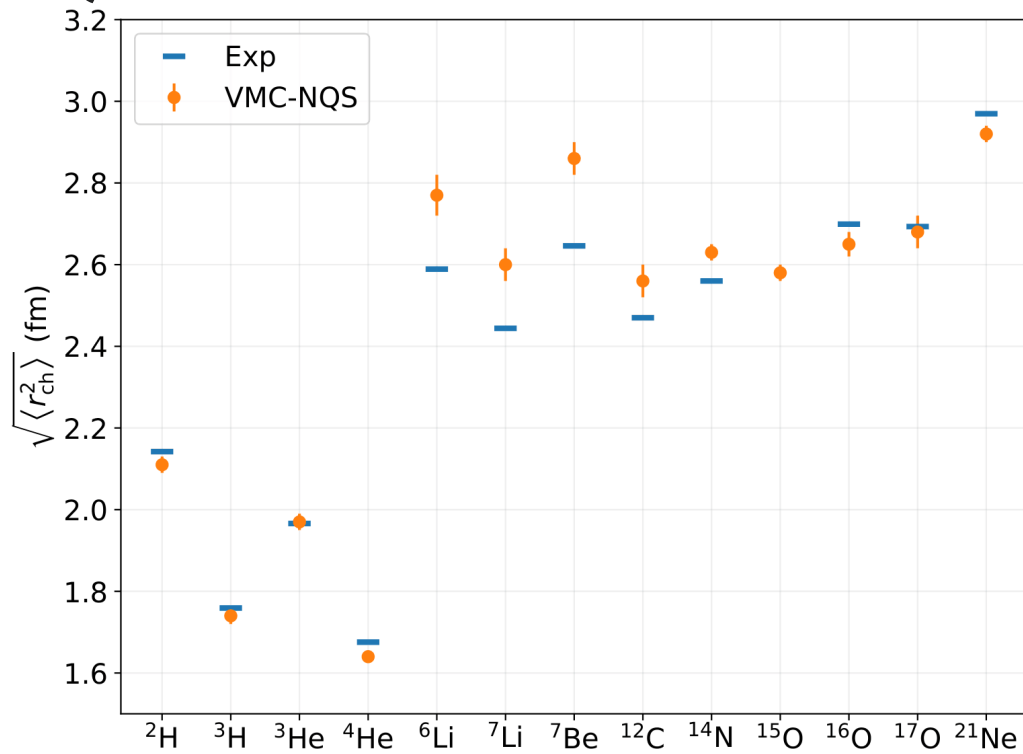


NEURAL QUANTUM STATE RESULTS IN NUCLEI



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

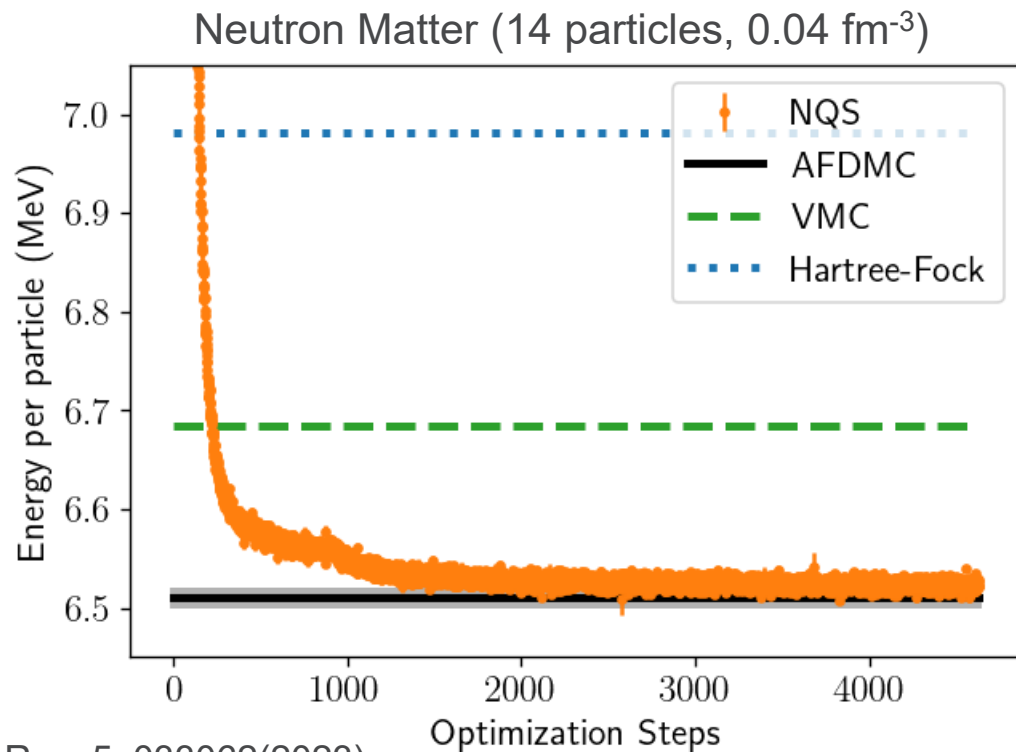
NEURAL QUANTUM STATE RESULTS IN NUCLEI



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

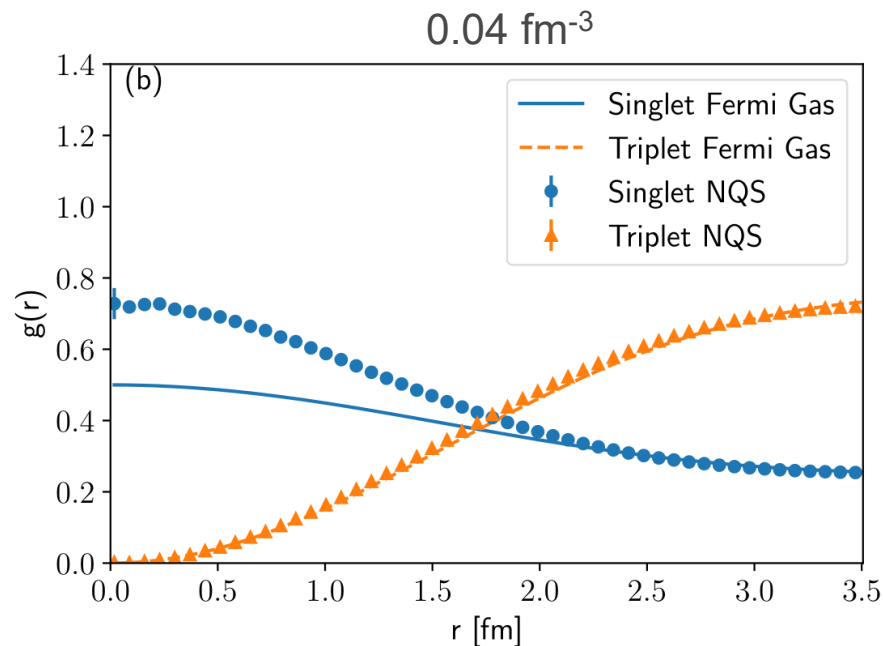
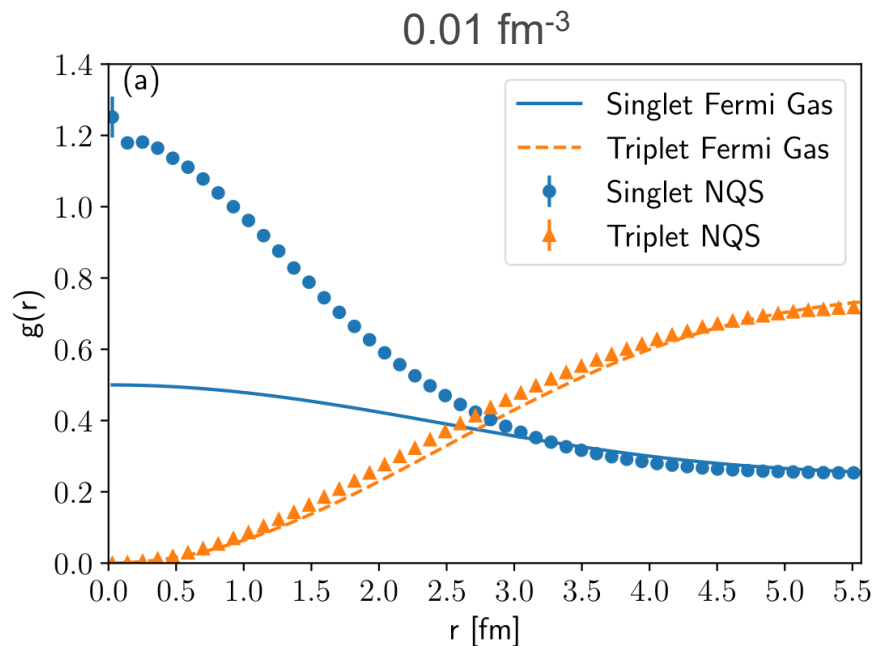
NUCLEAR MATTER RESULTS

PURE NEUTRON MATTER



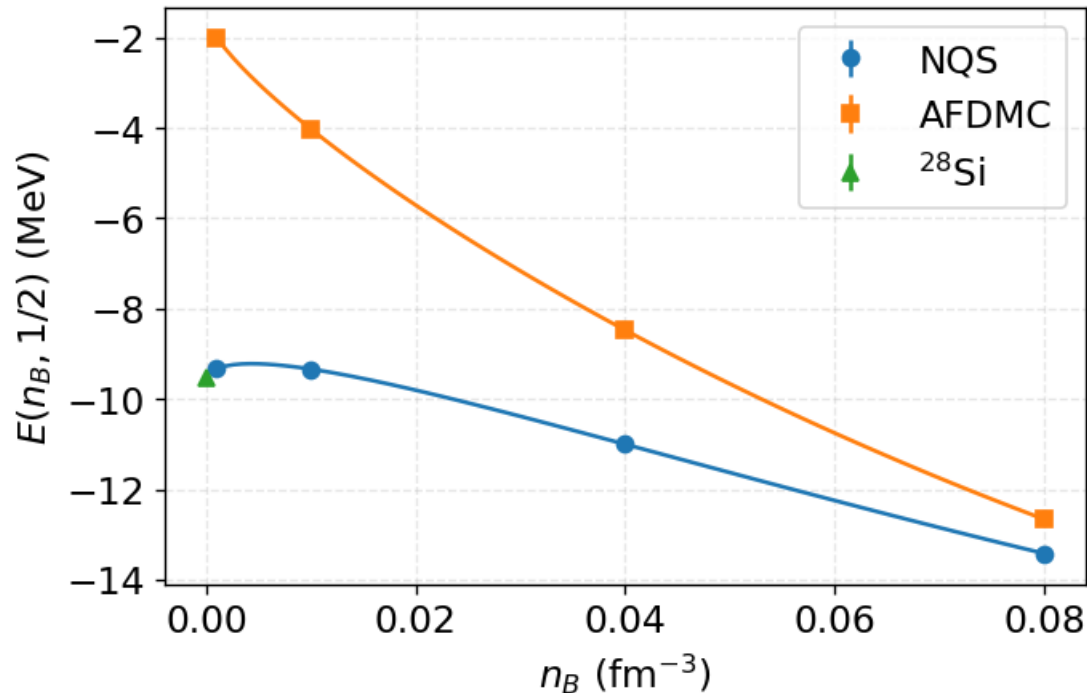
B. Fore, Phys. Rev. Res. 5, 033062(2023)

TWO-BODY PAIR DISTRIBUTIONS



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

SYMMETRIC NUCLEAR MATTER

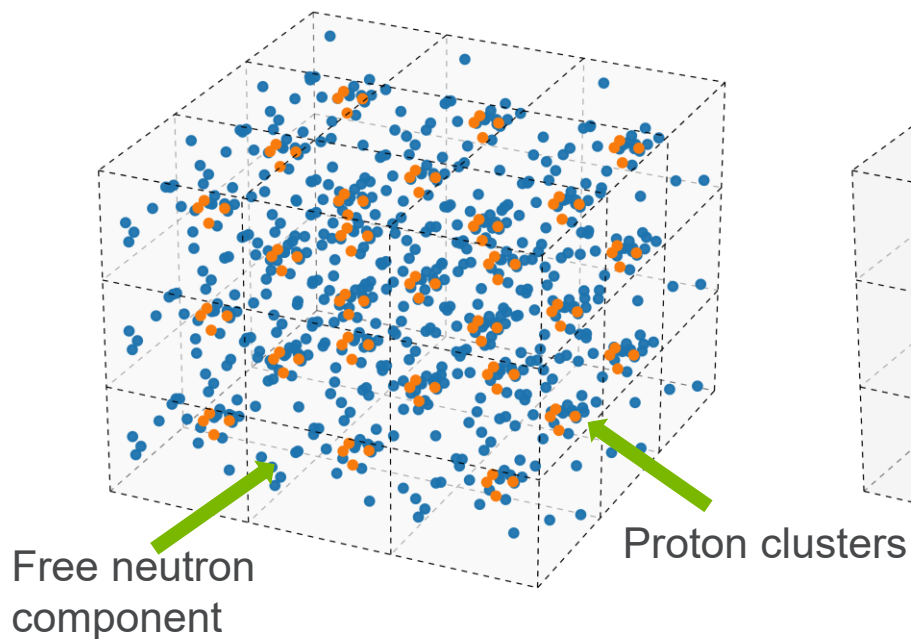


B. Fore, *Commun Phys* **8**, 108 (2025)

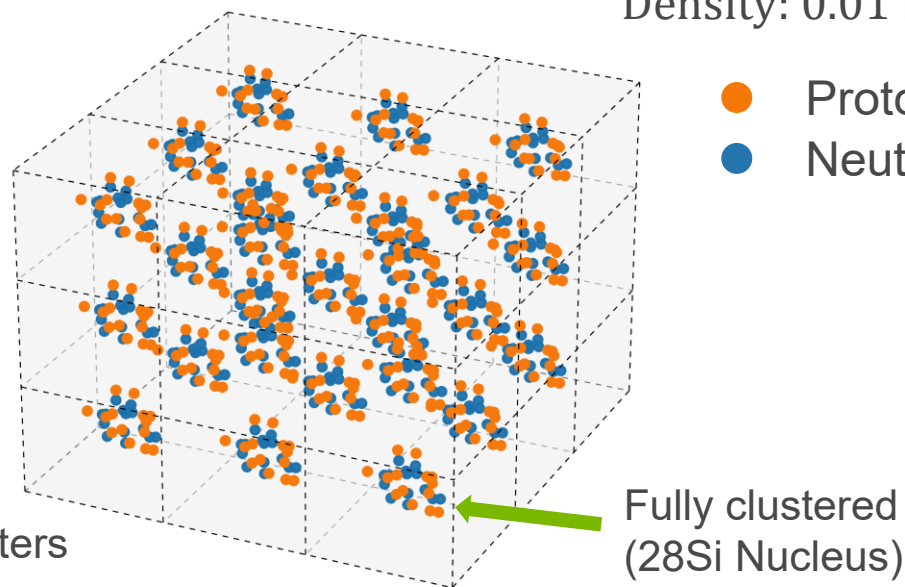
SELF EMERGING CLUSTERING

Density: 0.01 fm^{-3}

● Proton
● Neutron



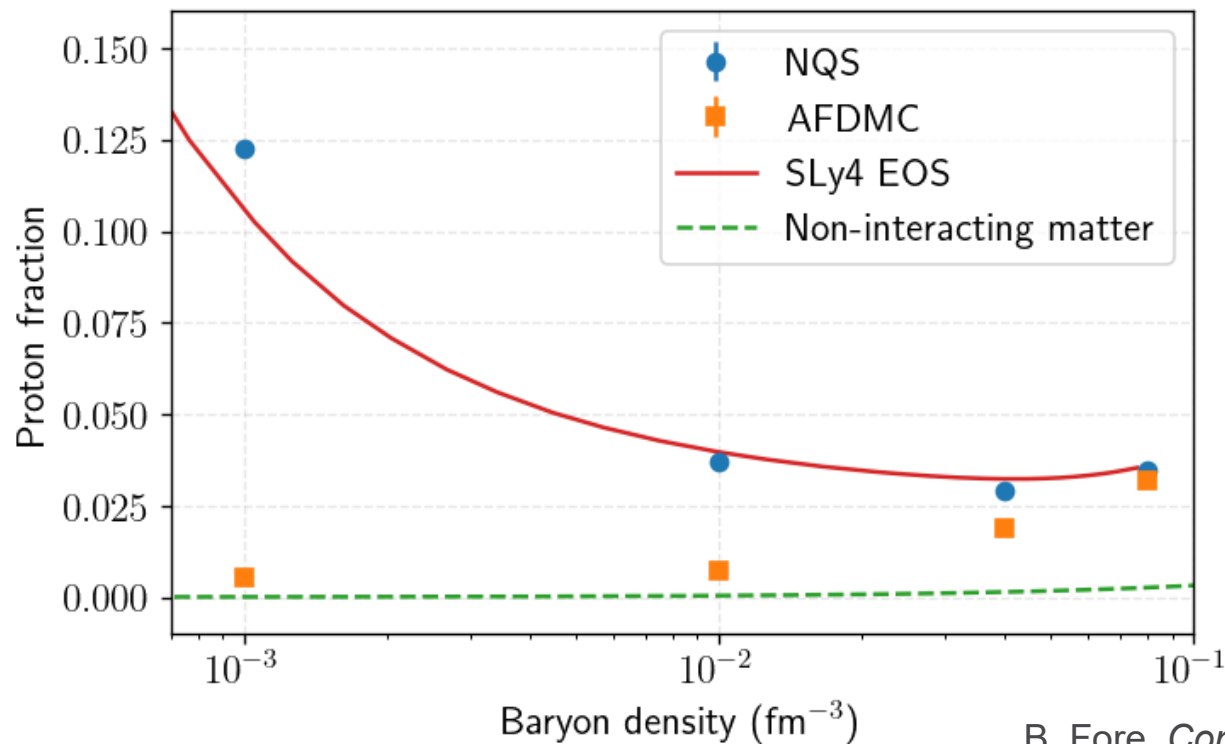
4 protons; 24 neutrons



14 protons; 14 neutrons

B. Fore, *Commun Phys* **8**, 108 (2025)

NUCLEAR MATTER PROTON FRACTION



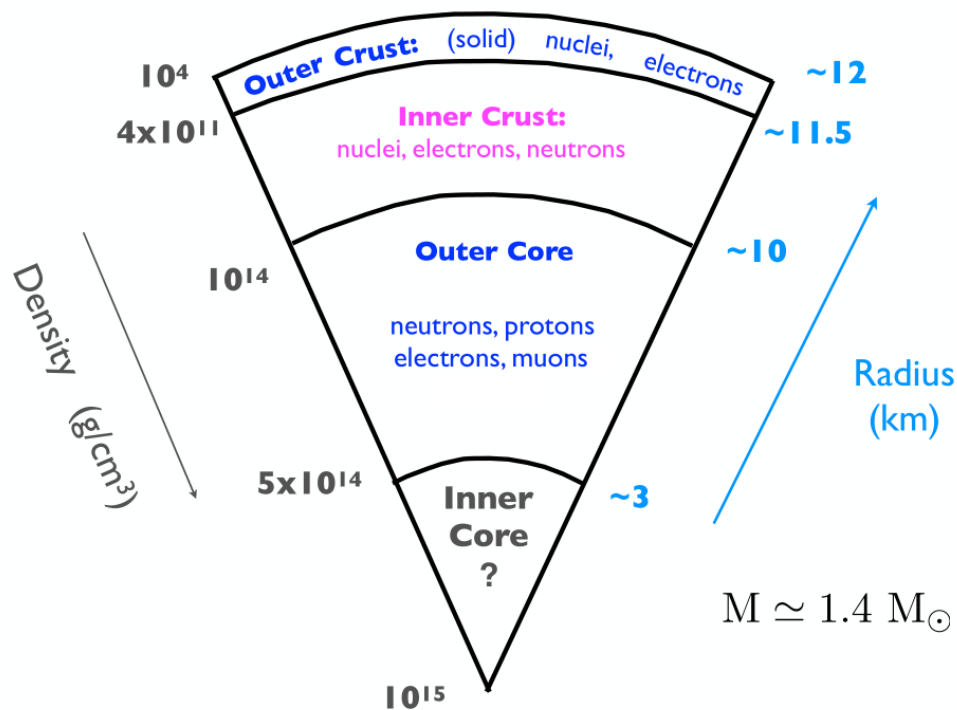
Assumptions:

- Energy expansion in neutron richness
- Charge neutrality
 $n_p = n_e$
- Beta equilibrium
 $\mu_e = \mu_n - \mu_p$

B. Fore, *Commun Phys* **8**, 108 (2025)

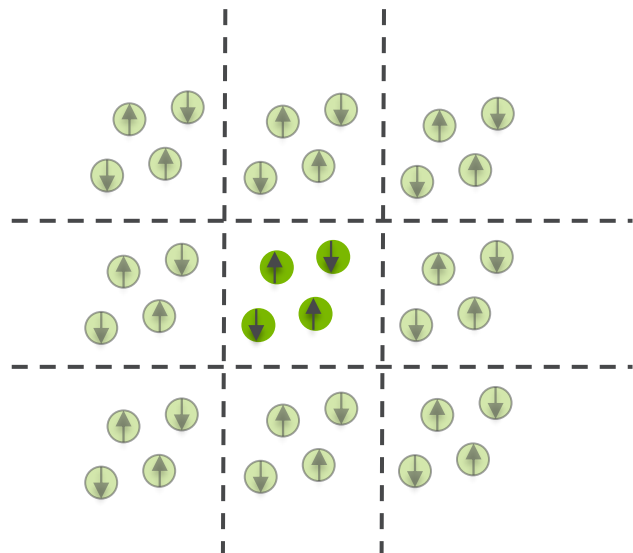
NUCLEAR MATTER BACKGROUND

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

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
- Assume Coulomb potential is screened by electrons

MEDIUM MASS NUCLEI

CHARGE DEPENDENT TERMS

- Includes charge-dependent and charge-asymmetric terms
- Includes additional EM terms
- Three body potential adjusted to reproduce ^4H and ^{16}O binding
- Two potentials:
 - CD (standard three body)
 - CD-triangle (experimental three body force)

$$C_{CD}(3\tau_{1z}\tau_{2z} - \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)$$

$$C_{CA}(\tau_{1z} + \tau_{2z})$$

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

$$V_{ijk} = c_E \sum_{cyc} e^{-(r_{ij}^2 + r_{jk}^2 + r_{ik}^2)/R_3^2}$$

P-WAVE TERMS

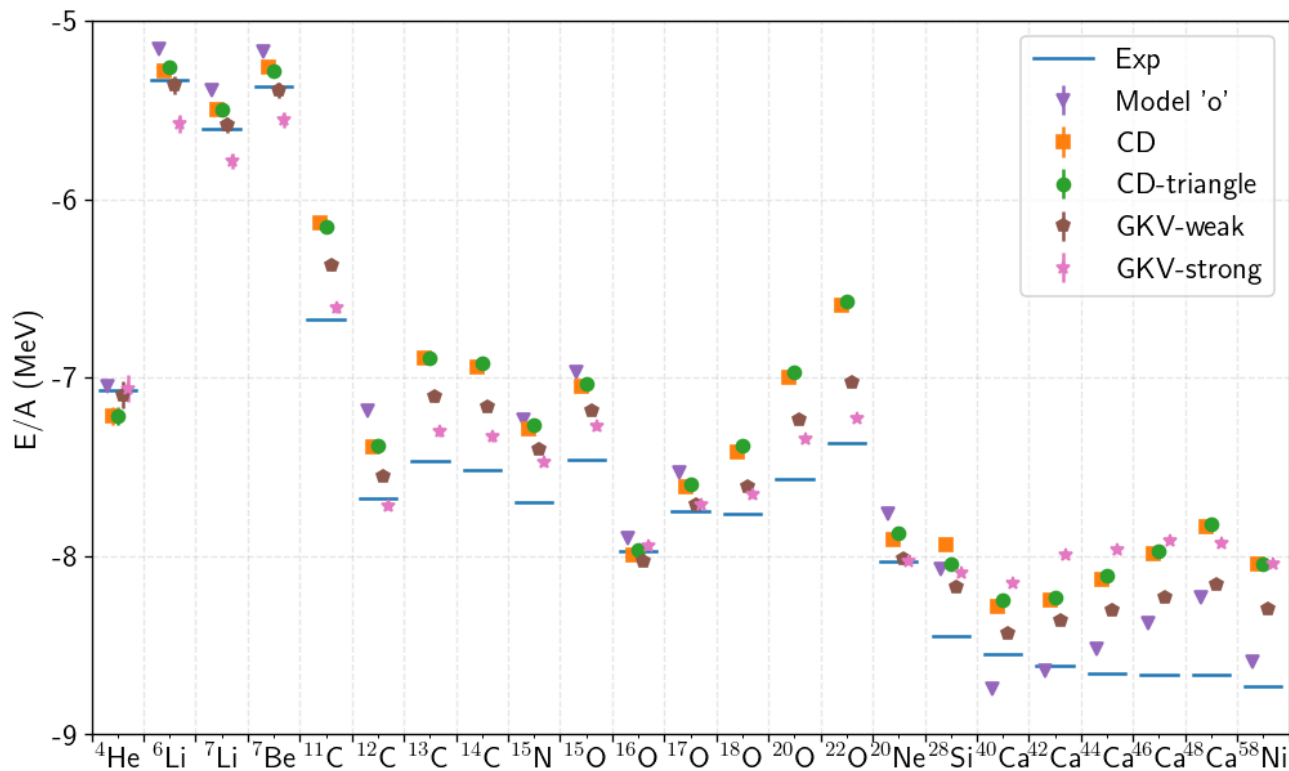
- Includes v_{00} and v_{11} terms
- Three body potential adjusted to reproduce ^4H and ^{16}O binding
- Two potentials:
 - GKV-weak ($v_{11} = -1.78$)
 - GKV-strong ($v_{11} = -3.857$)

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

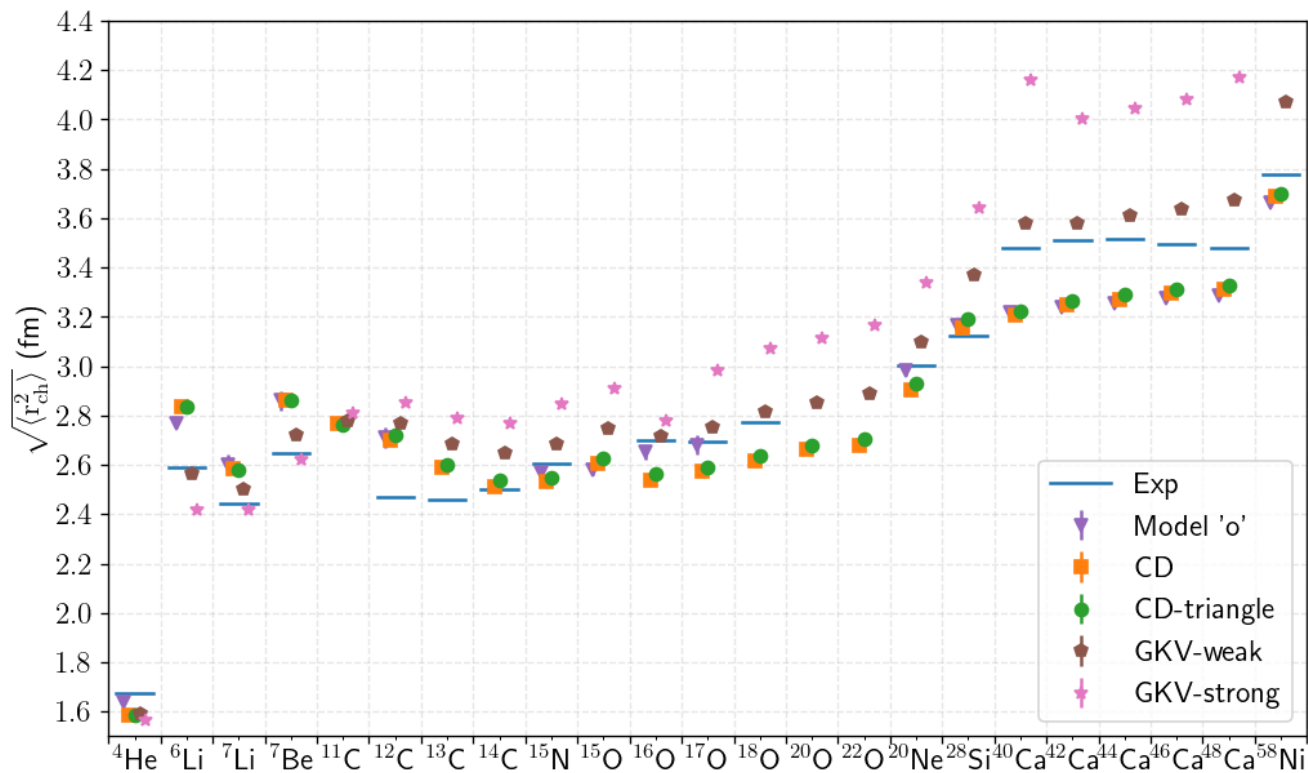
$$V_{ijk} = c_E \sum_{cyc} e^{-(r_{ij}^2 + r_{jk}^2)/R_3^2}$$

M. Gattobigio, Phys. Rev. C 100, 034004

LARGER NUCLEI ENERGY



LARGER NUCLEI RADII



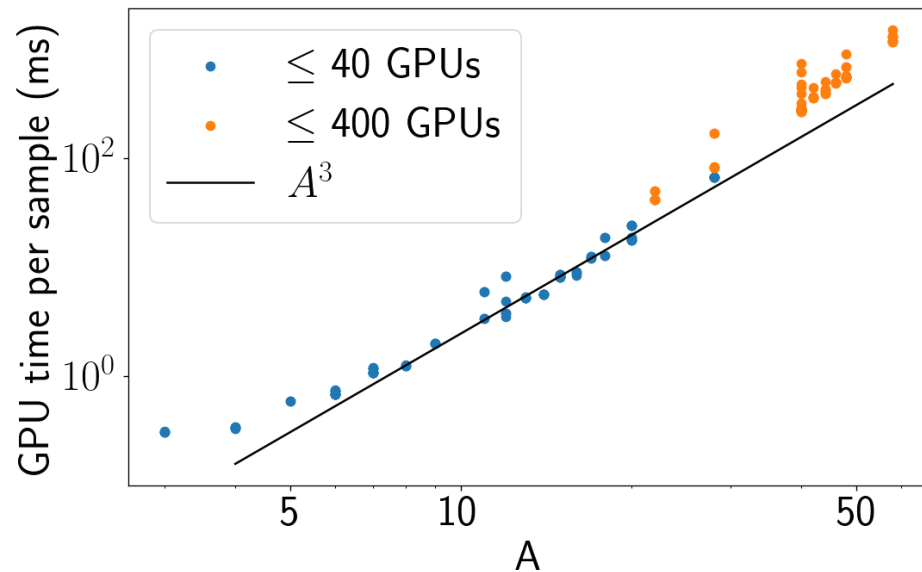
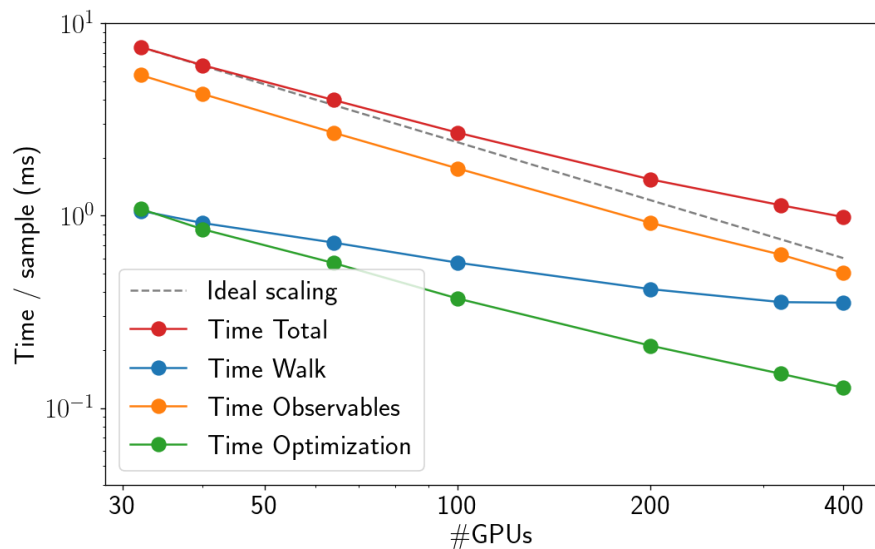
LARGER NUCLEI RESULTS

Nucleus	Expected L^2	Measured L^2
^4He	0	0.0000(1)
^6Li	0	0.0012(2)
^7Li	2	2.0028(2)
^7Be	2	2.0043(2)
^{11}C	2	2.1206(11)
^{12}C	0	0.0117(4)
^{13}C	2	2.0702(9)
^{14}C	0	0.0227(4)
^{15}N	2	2.0364(7)
^{15}O	2	2.0516(7)
^{16}O	0	0.0233(5)
^{17}O	6	0.3005(33)
^{18}O	0	0.0851(13)
^{20}O	0	0.0391(5)
^{22}O	0	0.0482(5)
^{20}Ne	0	0.0458(13)
^{28}Si	0	0.1835(15)
^{40}Ca	0	0.2224(8)
^{48}Ca	0	0.3084(10)

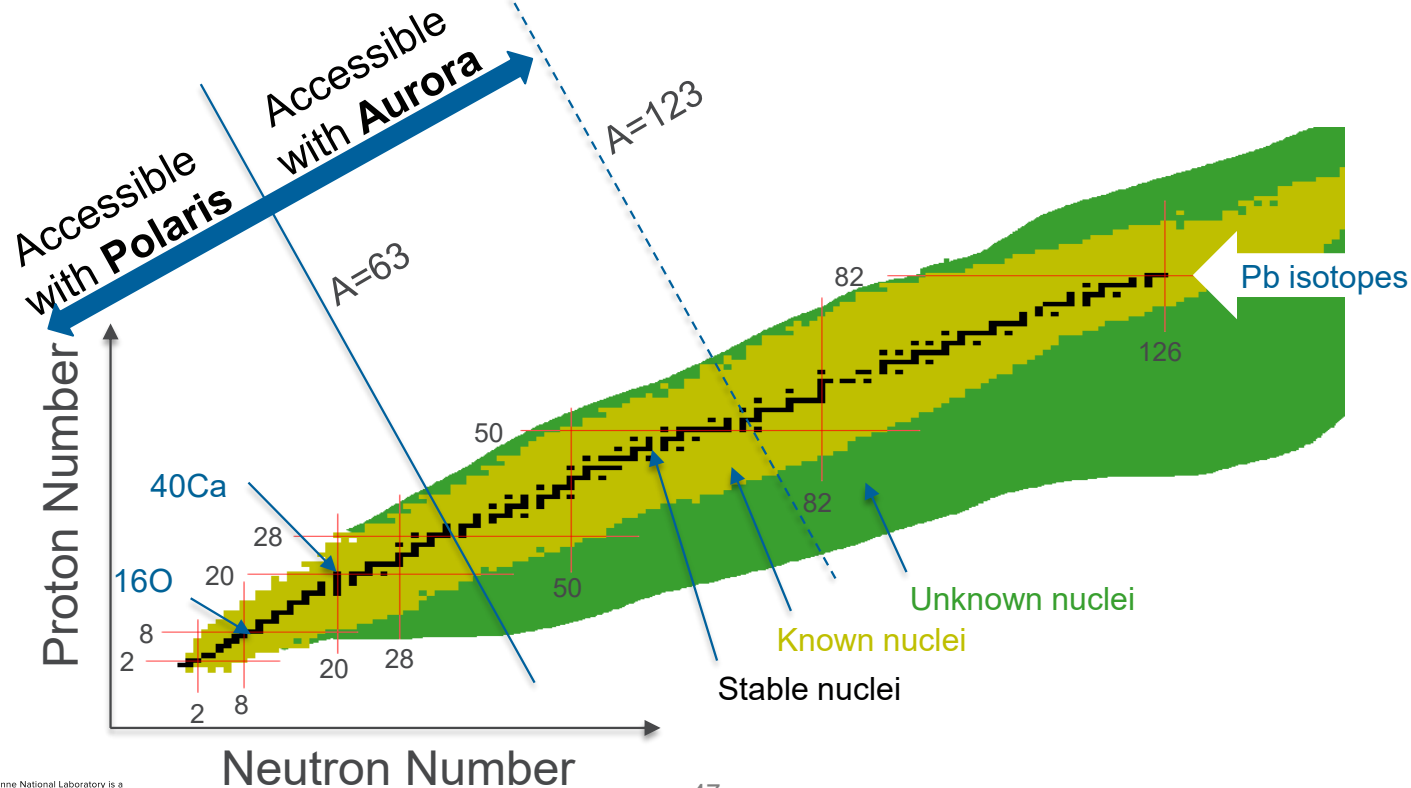
48Ca point radii

Potential	R_n	R_p	R_{skin}
model 'o'	3.4462(5)	3.1983(4)	0.2480(5)
CD	3.4277(7)	3.2224(5)	0.2054(10)
CD-triangle	3.4414(5)	3.2366(5)	0.2048(8)
GKV-weak	3.7323(5)	3.5935(5)	0.1388(9)
GKV-strong	4.1410(11)	4.0984(15)	0.0427(20)
Exp.			0.121(35)

LARGER NUCLEI SCALING



LARGER NUCLEI SCALING



OTHER NUCLEI RESULTS

FERMIONIC NQS CONSTRUCTION

FERMIONIC WAVEFUNCTIONS

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

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

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

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

- 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

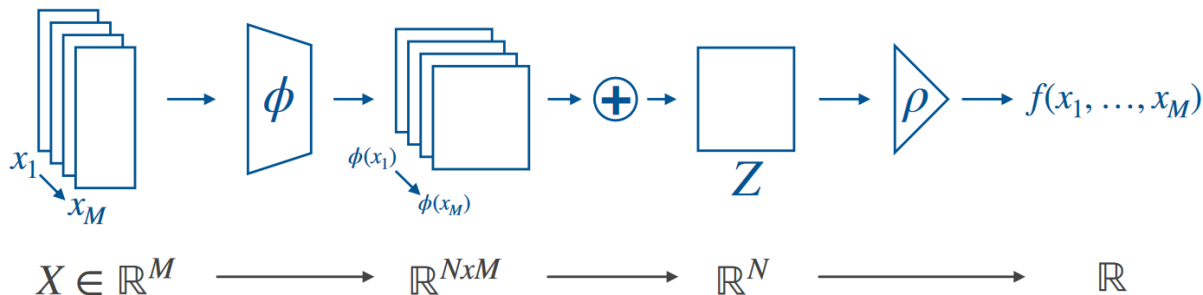
DEEP SET ARCHITECTURE

- Generic permutation invariant function

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

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

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



Wagstaff et al., arXiv:1901.09006 (2019)

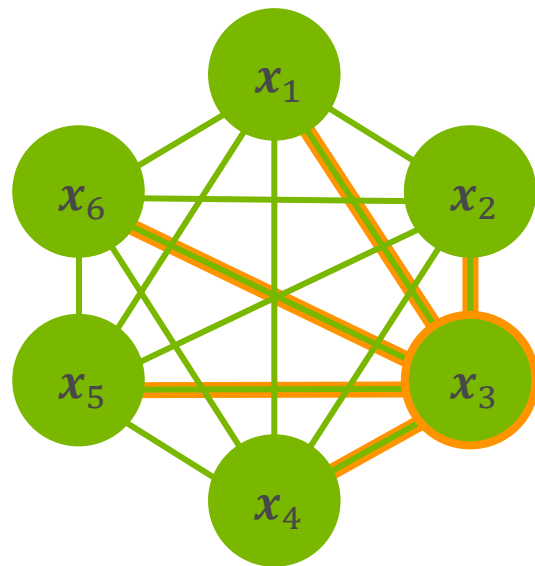
Zaheer et al., arXiv:1703.06114 (2017)

MESSAGE PASSING NEURAL NETWORK

Backflow transformation representable by updates to fully connected graph

$$x_i \rightarrow f(x_i; \{x_j\}_{j \neq i})$$

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



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

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

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

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

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

NEURAL PFAFFIAN ANSATZ

- Slater determinant $\rightarrow$ 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)

NQS WAVEFUNCTION ANSATZ OVERVIEW

- Neural Slater-Jastrow

$$\Psi_V = e^{U(\bullet)} \phi_{\bullet}(\bullet)$$

- Hidden Fermion

$$\Psi_V = \det \begin{pmatrix} \phi_{\bullet}(\bullet) & \phi_{\bullet}(\bullet) \\ \phi_{\bullet}(\bullet) & \phi_{\bullet}(\bullet) \end{pmatrix}$$

- Neural Pfaffian

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

DETERMINANT VS PFAFFIAN

Defined for $n \times n$ matrices

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

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

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

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

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

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

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

OTHER SPECIFICS ON NQS-VMC

METROPOLIS-HASTINGS SAMPLING

Sampling algorithm:

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

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

- 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

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

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

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

Parameters at step s are updated as

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

STOCHASTIC RECONFIGURATION

Improve wavefunction by minimizing energy expectation value

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

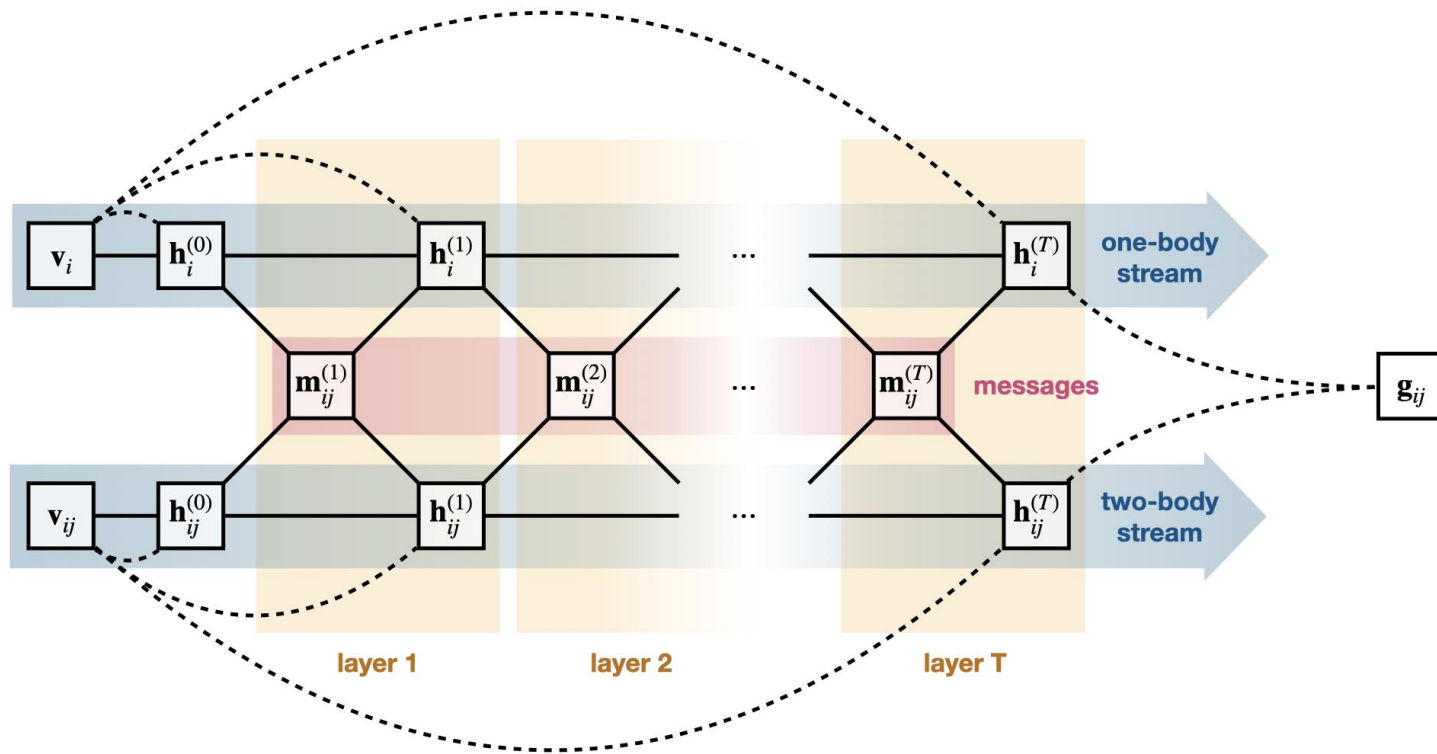
Gradient of energy ($G_i = \frac{dE_V}{d\omega_i}$), supplemented by Quantum Fisher Information S_{ij}

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

Parameters at step s are updated as

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

MESSAGE PASSING NEURAL NETWORK



MESSAGE PASSING NEURAL NETWORK

