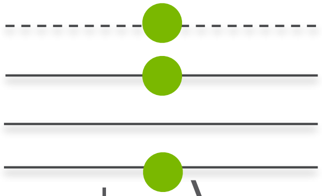
THE NUCLEAR MANY BODY METHODS

Configuration-interaction

$$\left|\Psi_0\right\rangle = \sum_{h_1,\ldots,p_1,\ldots} c^{p_1\ldots}_{h_1\ldots}\left|\Phi^{p_1\ldots}_{h_1\ldots}\right\rangle$$

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

$$\left|\Phi_0\right\rangle$$



$$\left|\Phi^{p_1}_{h_2}\right\rangle$$

Quantum Monte Carlo

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

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

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

SCALING AND COMPUTATIONAL PERFORMANCE

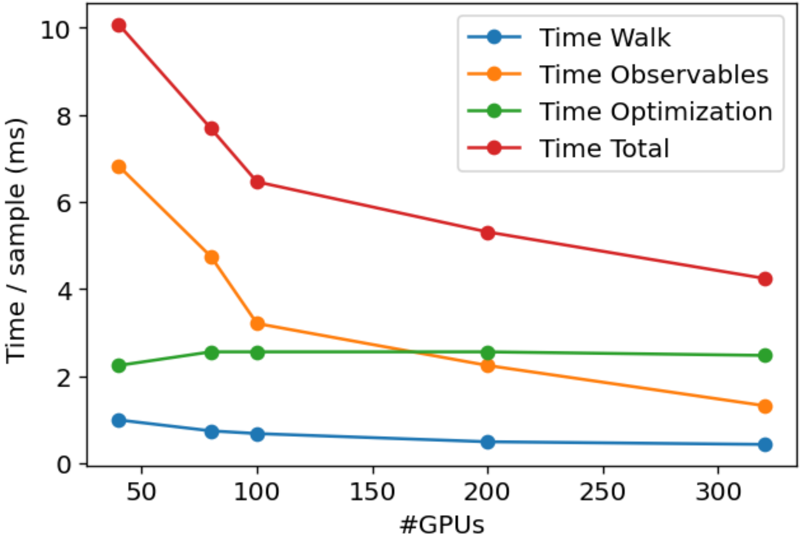
Scaling with system size

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

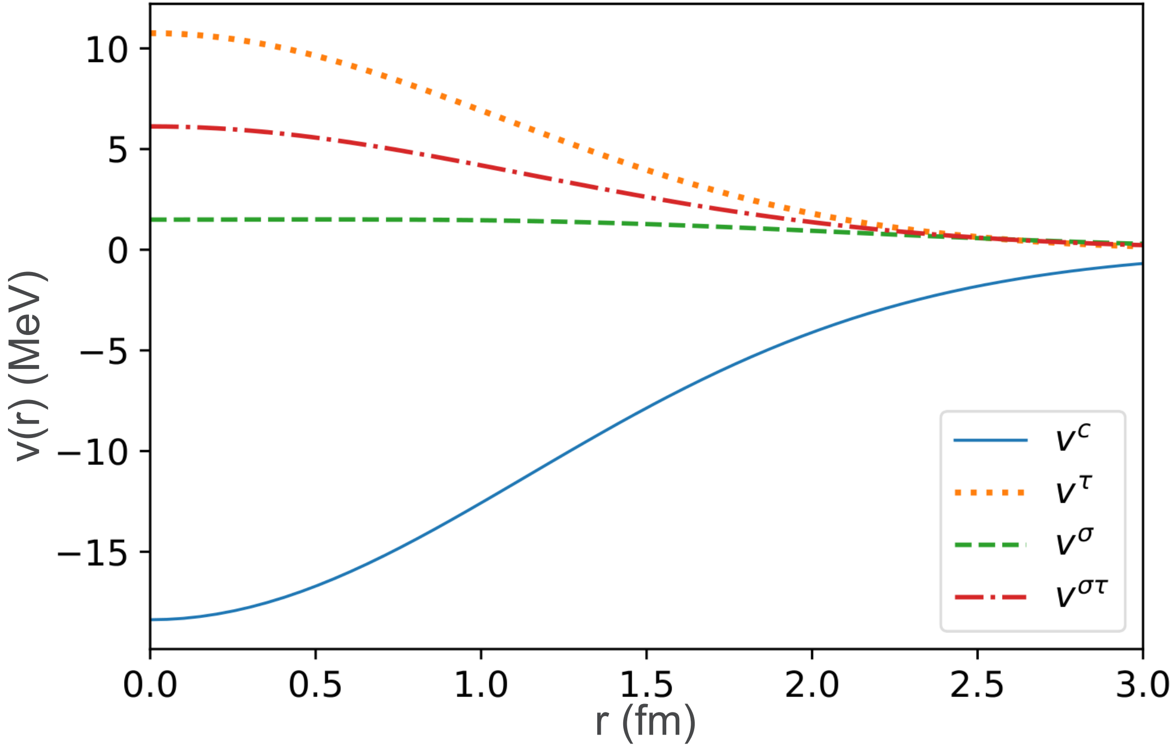
$$v_{ij}^{\mathrm{CI}} = \sum_{p=1}^{4} v^p(r_{ij}) O_{ij}^p$$

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

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

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

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

3. Optimize parameters of trial wavefunction to obtain lower energy

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

METROPOLIS-HASTINGS SAMPLING

Sampling algorithm:

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

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

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

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

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

STOCHASTIC RECONFIGURATION

Improve trial wavefunction by minimizing energy expectation value

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

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

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

Parameters at step s are updated as

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

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

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

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

NEURAL PFAFFIAN ANSATZ

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

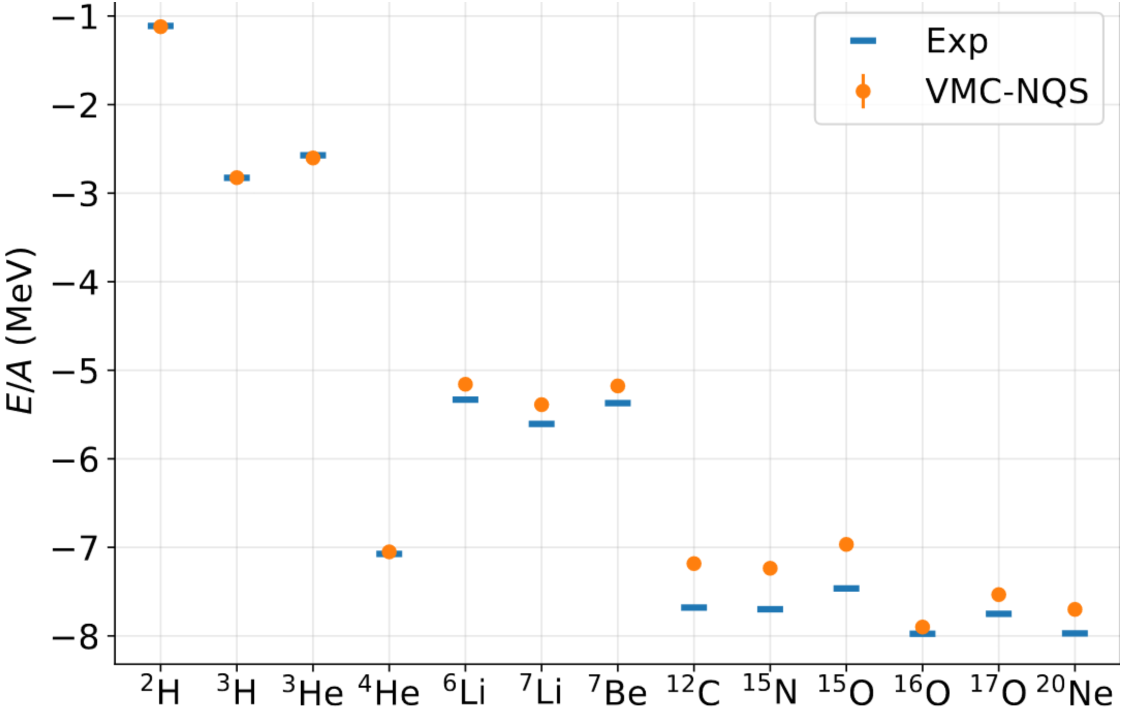
$$\Phi_{pf}(X) = pf[M]$$

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

- 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