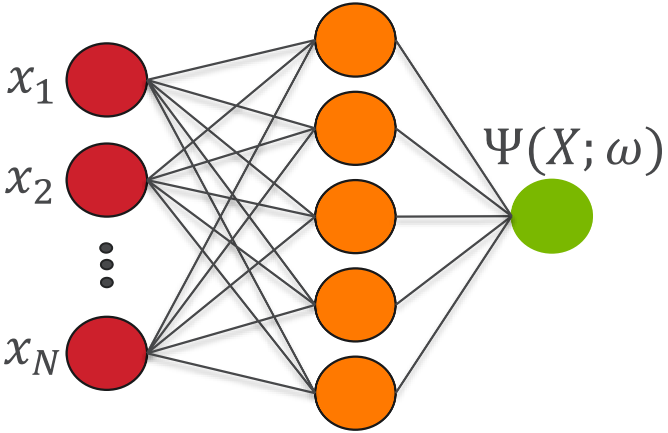
LIGHT NUCLEI WITH NEURAL-NETWORK QUANTUM STATES



BRYCE FORE

Light nuclei between single-particle and clustering features
December 2nd 2024

QUANTUM MANY-BODY METHODS

THE QUANTUM MANY-BODY PROBLEM

Many-body Schrödinger equation

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

Fermions have anti-symmetric wavefunction

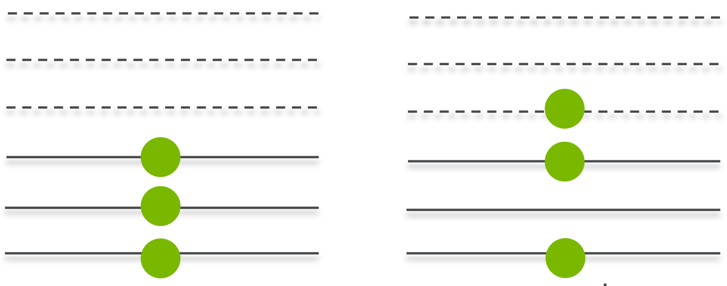
$$\Psi\left(x_1, \dots, x_i, \dots, x_j, \dots x_A\right) = -\Psi(x_1, \dots, x_j, \dots, x_i, \dots x_A)$$

THE NUCLEAR MANY BODY METHODS

Configuration-interaction

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

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



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

Quantum Monte Carlo

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

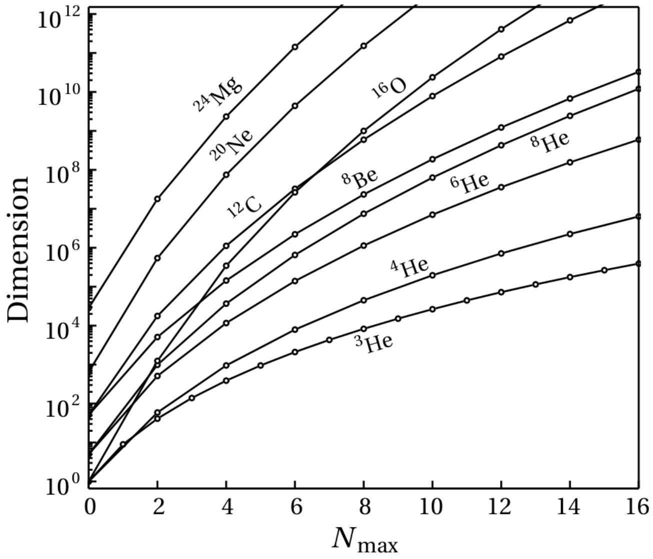
$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

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

CURSE OF DIMENSIONALITY

Configuration-interaction

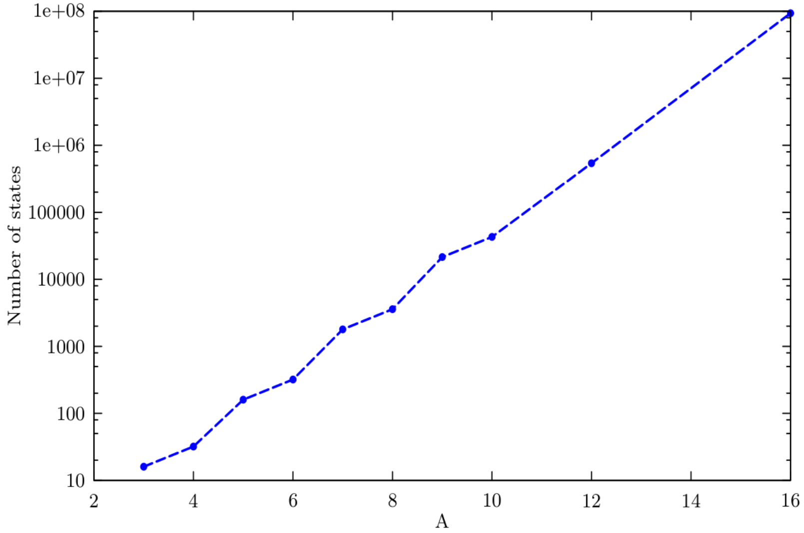
$$\binom{N}{A} = \frac{N!}{(N-A)!\,A!}$$



Credit: Patrick Fasano

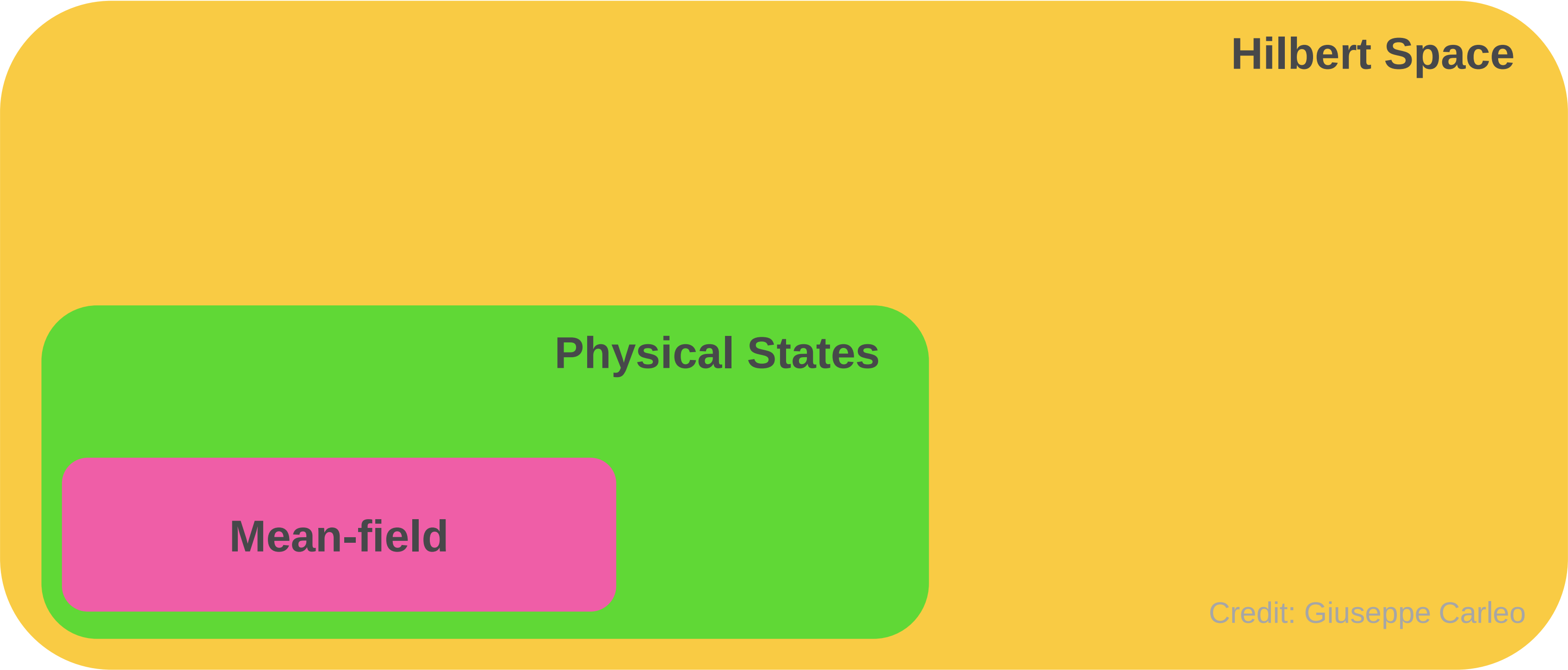
Green's function Monte Carlo

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

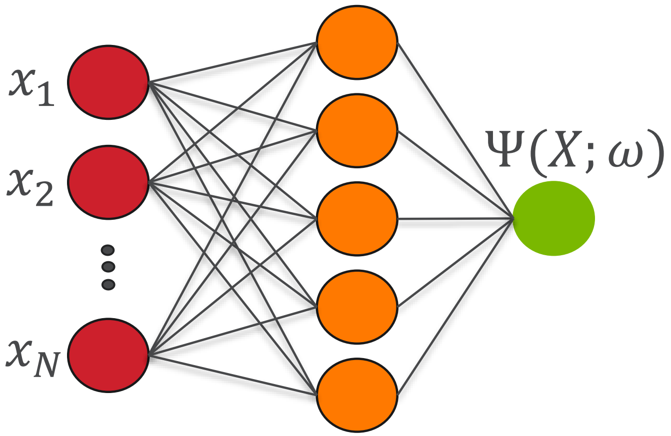


Credit: Alessandro Lovato

NEURAL QUANTUM STATES



NEURAL QUANTUM STATES



- Most quantum states of interest have distinctive features and intrinsic structures
- Artificial neural networks compactly represent complex high-dimensional functions
- Build in symmetries of quantum system to NQS architecture

SCALING AND COMPUTATIONAL PERFORMANCE

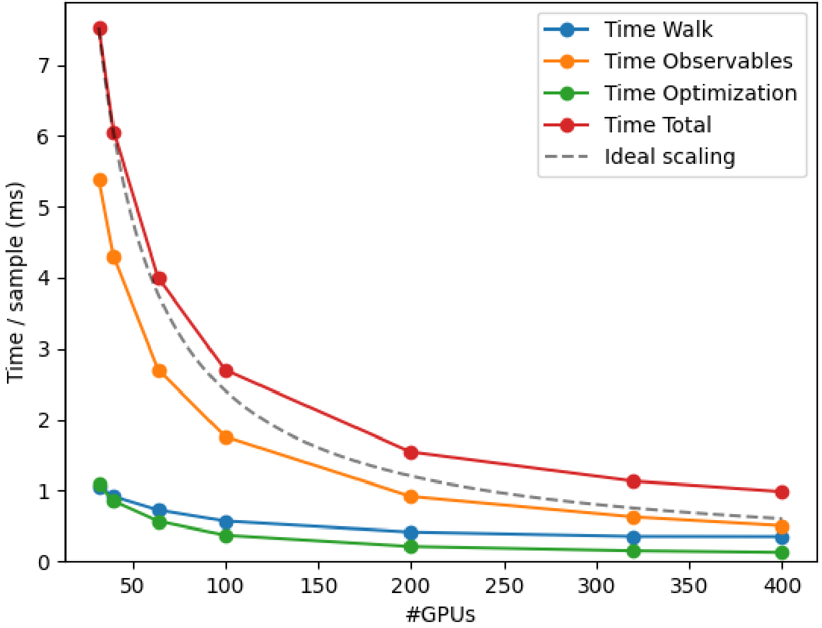
Scaling with system size

Conventional QMC: $O(2^A)$

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

A = Number of particles in system

Scaling with resources



VARIATIONAL MONTE CARLO WITH NQS

1. Create the NQS wavefunction

$$\Psi_V(R,S;\omega) = e^{U(R,S;\omega)}\Phi(R,S;\omega)$$

2. Compute its energy (Metropolis-Hastings algorithm)

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

3. Minimize the energy to get the ground state

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

METROPOLIS-HASTINGS SAMPLING

Sampling algorithm:

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

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

- 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

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

NQS WAVEFUNCTION ANSATZ OVERVIEW

- Neural Slater-Jastrow

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

- Hidden Fermion

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

- Neural Pfaffian

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

FERMIONIC WAVEFUNCTIONS

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

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

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

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

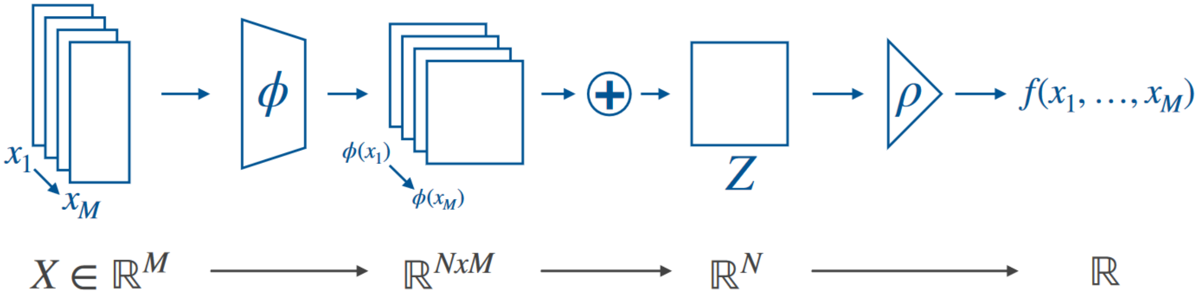
- Build in fermion antisymmetry for network compactness
- Permutation-invariant Jastrow function improves ansatz flexibility
- Build U and Φ functions from fully connected, deep neural networks

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)

NEURAL SLATER-JASTROW ANSATZ

- Slater determinants historically used to represent simple many-body states
- Slater determinant to enforce antisymmetry
- Single particle wavefunctions represented by neural networks

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

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

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 → Pfaffian
- Build in antisymmetry through a single pairing orbital rather than determinant of single-particle states

$$det(M) = pf(M)^2$$

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

$$\Phi(X) = pf\begin{bmatrix} 0 & \phi(x_1, x_2) & \cdots & \phi(x_1, x_N) \\ \phi(x_2, x_1) & 0 & \cdots & \phi(x_2, x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(x_N, x_1) & \phi(x_N, x_2) & \cdots & 0 \end{bmatrix}$$

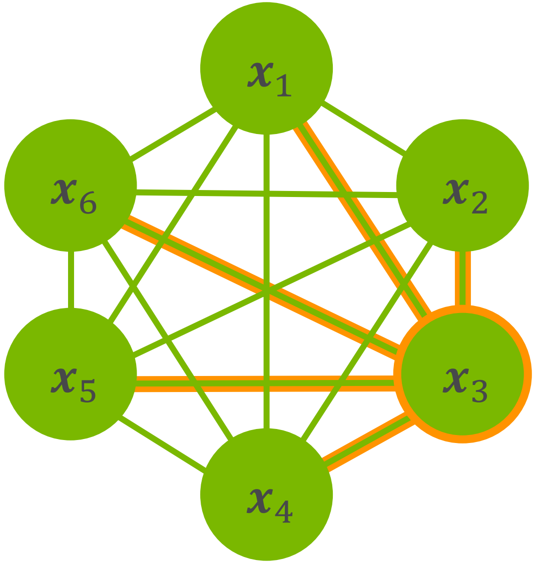
J. Kim, *Commun Phys* **7**, 148 (2024)

MESSAGE PASSING NEURAL NETWORK

Backflow transformation representable by updates to fully connected graph

$$\boldsymbol{x}_i \rightarrow f(\boldsymbol{x}_i; \{\boldsymbol{x}_j\}_{j \neq i})$$

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



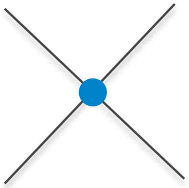
NQS RESULTS

PIONLESS EFT HAMILTONIAN

- Pionless-EFT Hamiltonian

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

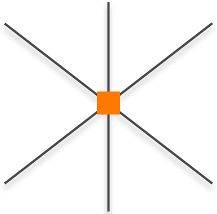
- NN potential fit to
  - np scattering lengths
  - effective radii
  - deuteron binding energy



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

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

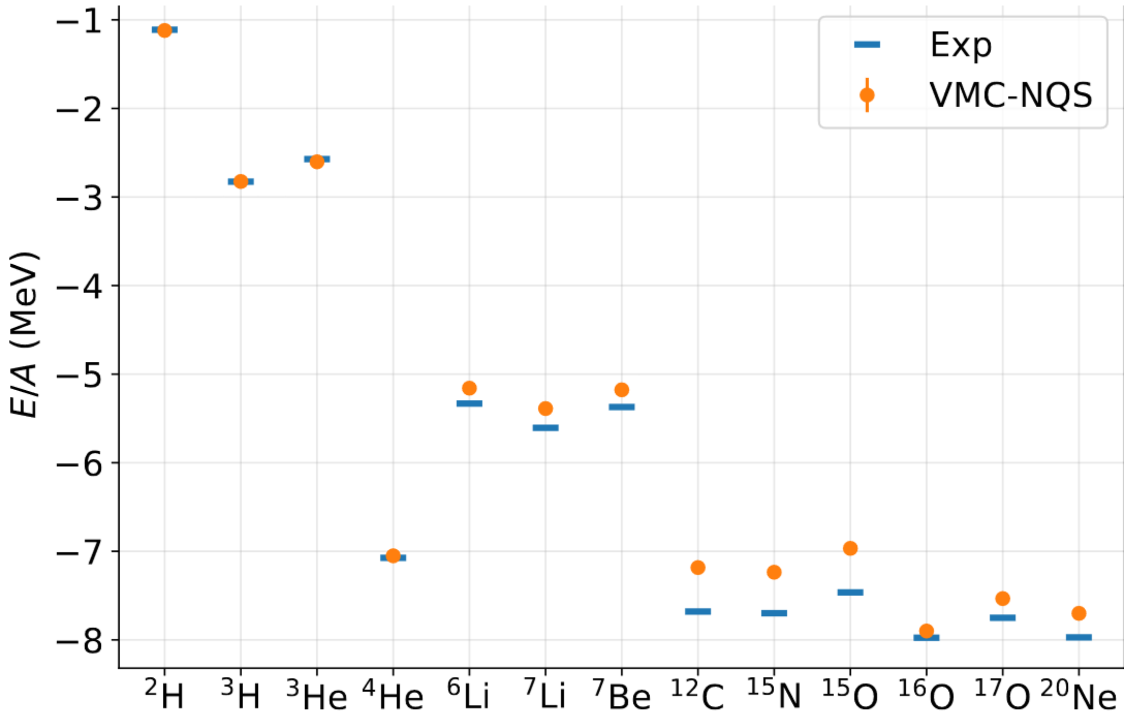
- Three body potential adjusted to reproduce ^{3}H binding



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

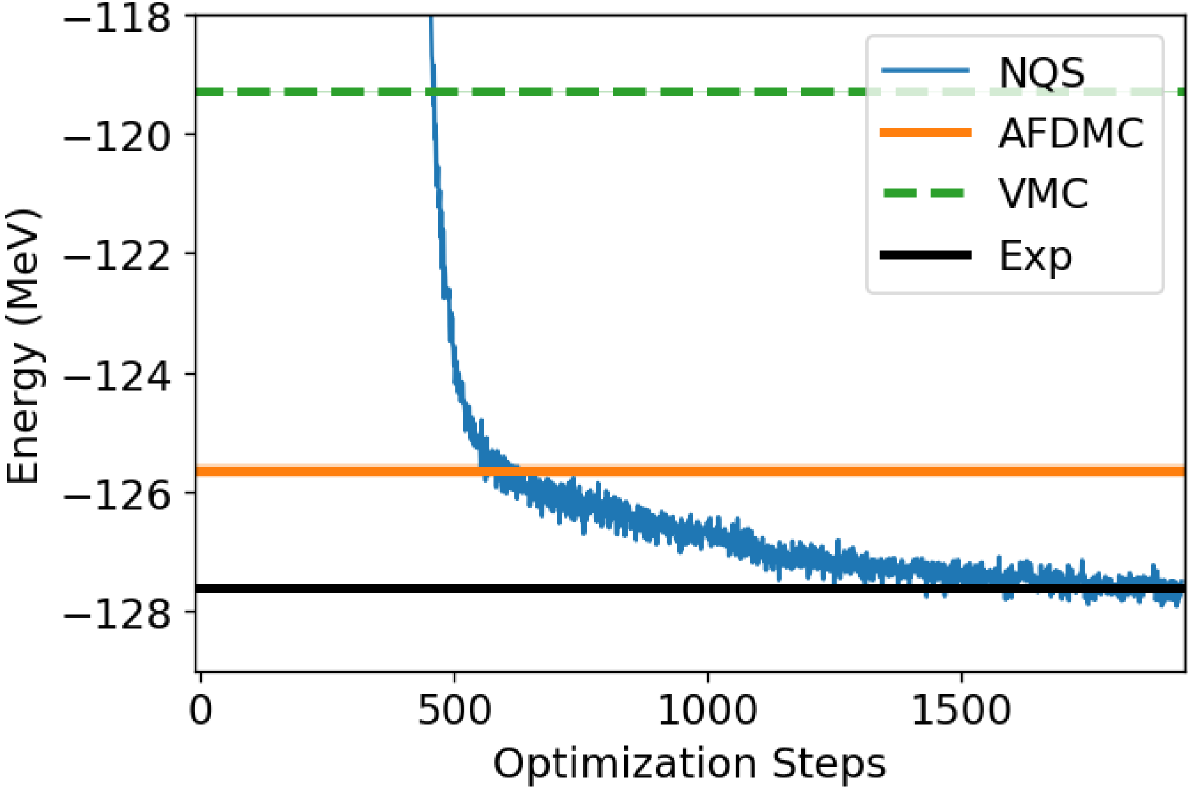
R. Schiavilla, PRC 103, 054003(2021)

NEURAL QUANTUM STATE RESULTS IN NUCLEI



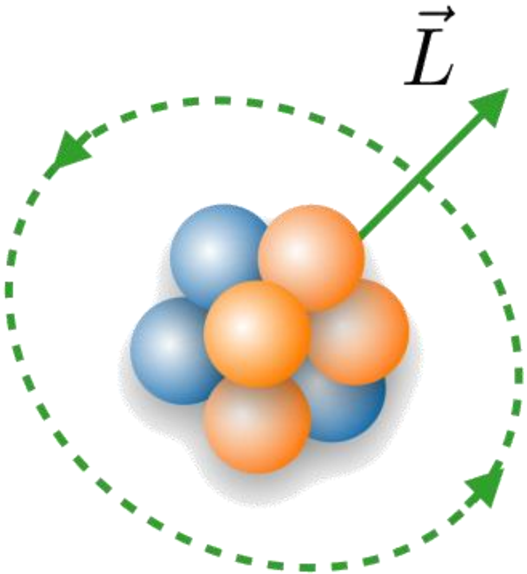
A. Gnech, Phys. Rev. Lett. 133, 142501

RESULTS IN 16O



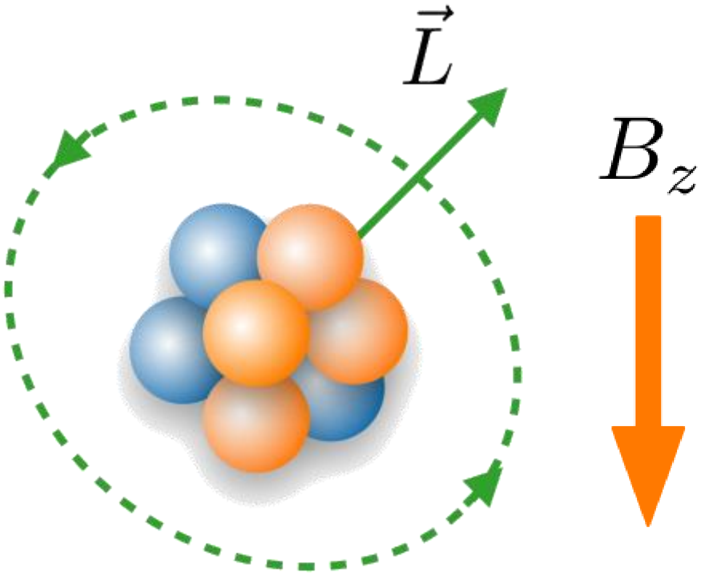
MAGNETIC MOMENTS

Ground state is degenerate in L_z



Break degeneracy using magnetic field B_z

$$H \to H - B_z L_Z$$



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

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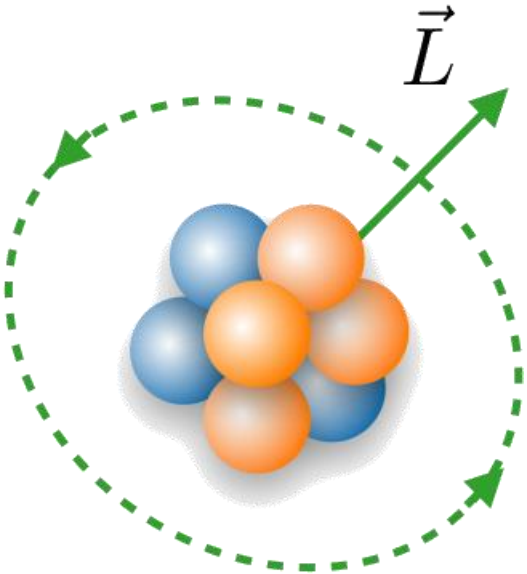

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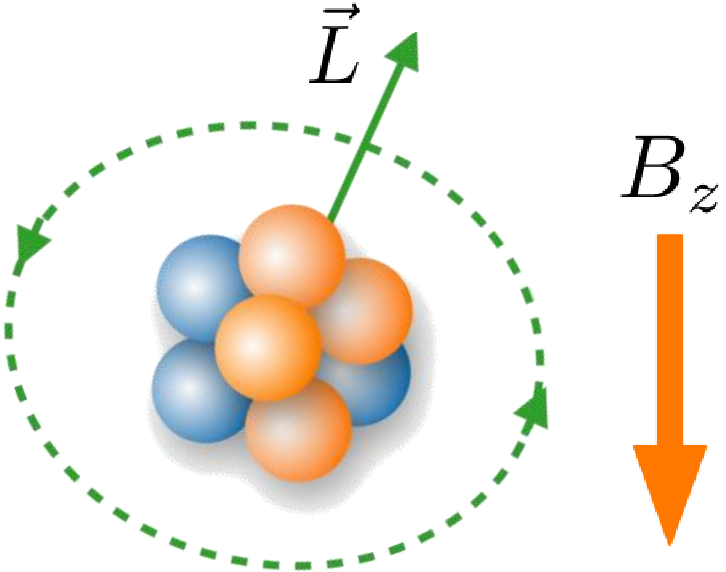

A. Gnech, B. Fore, Phys. Rev. Lett. 133, 142501

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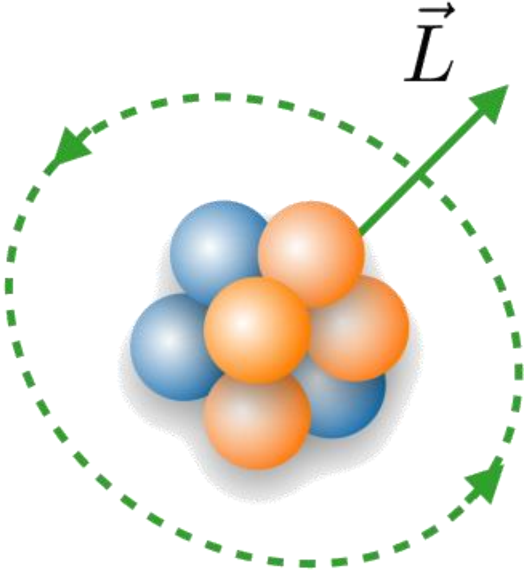

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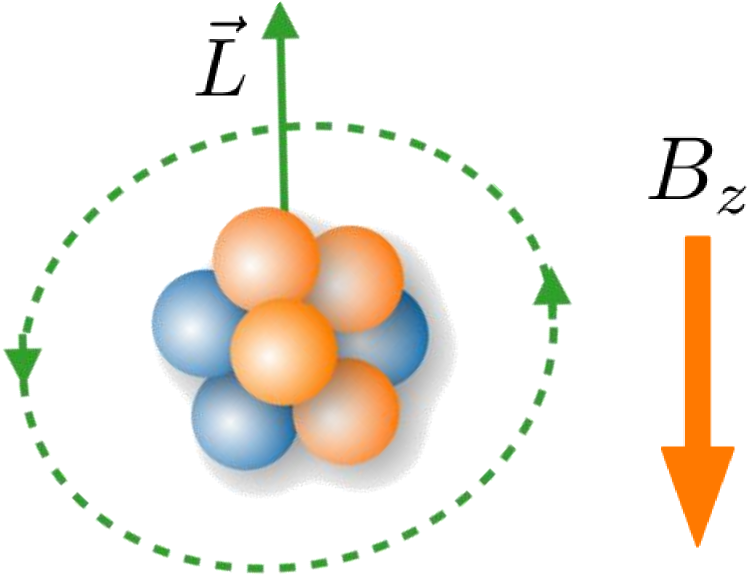

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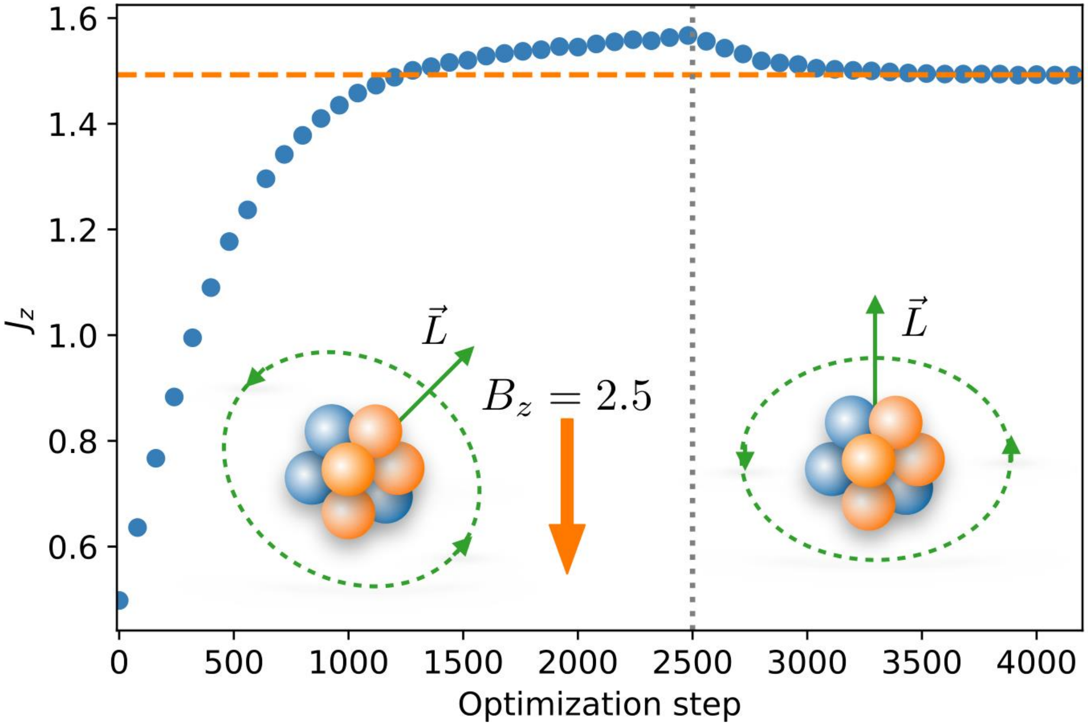

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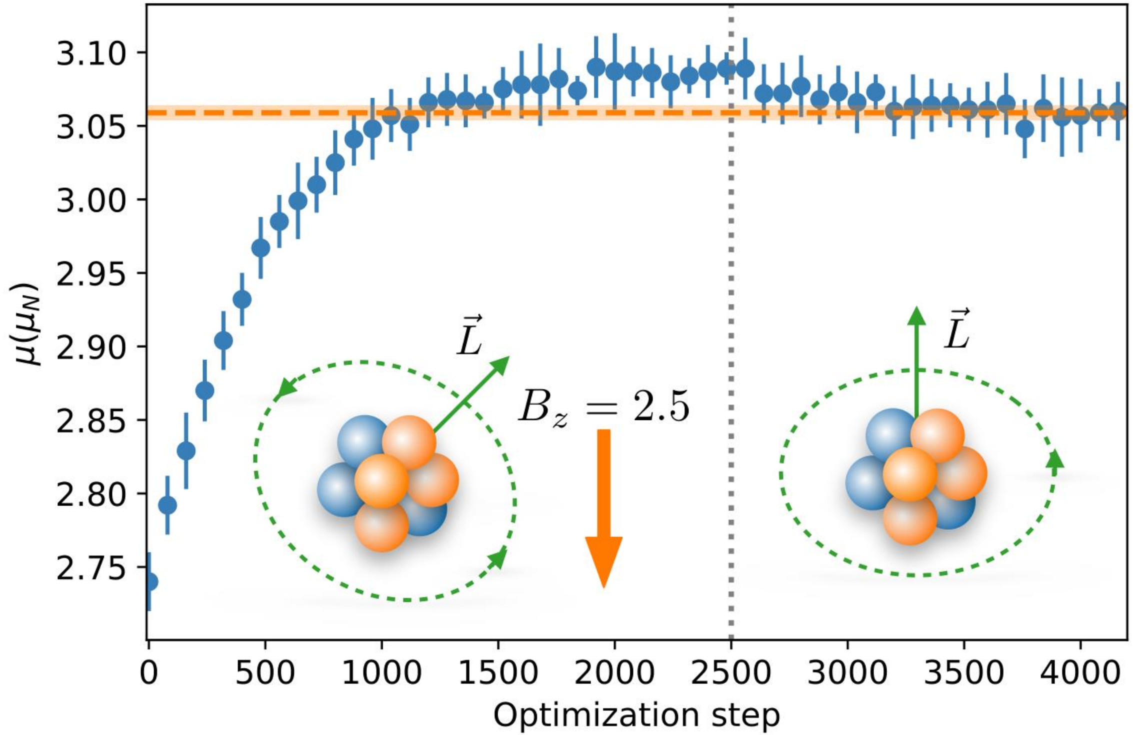

A. Gnech, B. Fore, Phys. Rev. Lett. 133, 142501

SLIGHTLY LESS MINIMAL POTENTIAL

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

- Charge symmetry breaking terms: V_{CC}, V_{MM}, V_{τ_z}, V_{T12}
- Charge-dependent (CD) and charge-asymmetric (CA) terms: V^{CD}, V^{CA}
- Three body force fit to ^{16}O instead of ^{3}H
- Projectors for three body force to exclude
    - nnn
    - ppp
    - ↑↑↑
    - ↓↓↓

CONCLUSIONS AND NEXT STEPS

- Conclusions:
  - Favorable scaling with number of fermions
  - Scaling to leadership-class computers
  - Universal and accurate approximations for fermion wavefunctions
  - NQS can access a variety of nuclear observables

- Next steps:
  - Improved nuclear potential including tensor term
  - Expanding to larger nuclei

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THANK YOU