NUCLEI AND NUCLEONIC MATTER WITH NEURAL-NETWORK QUANTUM STATES



ALESSANDRO LOVATO

Workshop on Progress in Ab Initio Nuclear Theory

TRIUMF, Vancouver, BC



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COLLABORATORS



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THE QUANTUM MANY-BODY PROBLEM

$$H = \sum_{i} \frac{p_i^2}{2m} + \sum_{i < j} v_{ij} + \sum_{i < j < k} V_{ijk}$$

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



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CONFIGURATION-INTERACTION METHODS



GREEN'S FUNCTION MONTE CARLO

The GFMC projects out the lowest-energy state using an imaginary-time propagation



CONVENTIONAL QUANTUM MONTE CARLO



HOW TO TACKLE (EVEN) LARGER NUCLEI?



ENERGY





$$H_{TIF} = -h\sum_{i}\sigma_{i}^{x} - \sum_{\langle i,j\rangle}\sigma_{i}^{z}\sigma_{j}^{z}$$

Finding the exact ground-state is, in principle, exponentially hard

 $|\Psi\rangle = c_{\uparrow\uparrow\uparrow\dots}|\uparrow\uparrow\uparrow\dots\rangle + c_{\downarrow\uparrow\uparrow\dots}|\downarrow\uparrow\uparrow\dots\rangle + \dots + c_{\downarrow\downarrow\downarrow\dots}|\downarrow\downarrow\downarrow\dots\rangle$

Quantum states of physical interest have distinctive features and intrinsic structures



$$c_{\uparrow\uparrow\uparrow\dots} \equiv \langle\uparrow\uparrow\uparrow\dots|\Psi\rangle \equiv \Psi(\uparrow\uparrow\uparrow\dots)$$

$$c_{\downarrow\uparrow\uparrow\dots} \equiv \langle\downarrow\uparrow\uparrow\dots|\Psi\rangle \equiv \Psi(\downarrow\uparrow\uparrow\dots)$$

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Idea: use neural networks to represent the quantum many-body wave function

$$\hat{\Psi}(S) = \sum_{h_i=0,1} e^{\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j}$$

G. Carleo et al. Science 355, 602 (2017)



G. Carleo and M. Troyer proved that Restricted Boltzmann machines outperform traditional Jastrow



G. Carleo et al. Science 355, 602 (2017)



MACHINE-LEARNING THE DEUTERON

ANNs solve the deuteron using the N3LO Entem-Machleidt chiral-EFT NN potential



The parameters of the ANN are optimized minimizing the variational energy using RMSprop





Keeble, Rios, PLB 809, 135743 (2020)

PIONLESS EFT HAMILTONIAN

We take as input a LO 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 s-wave np scattering lengths and effective ranges

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

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



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• 3NF adjusted to reproduce the energy of ³H.

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

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



Product of mean-field state modulated by a flexible correlator factor

$$\Psi_{SJ}(X) = e^{J(X)}\Phi(X)$$

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Mean-field: Slater determinant of single-particle orbitals

$$\det \begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_1(\mathbf{x}_2) & \cdots & \phi_1(\mathbf{x}_N) \\ \phi_2(\mathbf{x}_1) & \phi_2(\mathbf{x}_2) & \cdots & \phi_2(\mathbf{x}_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(\mathbf{x}_1) & \phi_N(\mathbf{x}_2) & \cdots & \phi_N(\mathbf{x}_N) \end{bmatrix}$$

Each orbital is a FFNN that takes as input

$$\bar{\mathbf{r}}_i = \mathbf{r}_i - \mathbf{R}_{CM}$$



"Manually" imposing permutation-invariance scales factorially with A

 $J(X) = j(x_1, x_2, x_3) + j(x_1, x_3, x_2) + j(x_2, x_1, x_3) + j(x_2, x_3, x_1) + j(x_3, x_1, x_2) + j(x_3, x_2, x_1)$

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Solution: "deep-sets"
$$\longrightarrow J(X) = \rho_F \left[\sum_i \vec{\phi}_F(\bar{\mathbf{r}}_i, \mathbf{s}_i) \right]$$



Wagstaff et al., arXiv:1901.09006 (2019)

SAMPLING COORDINATES AND SPIN

$$E_V = \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} = \frac{\sum_S \int dR |\Psi_V(R, S)|^2 \frac{\langle RS | H | \Psi_V \rangle}{\langle RS | \Psi_V \rangle}}{\sum_S \int dR |\Psi_V(R, S)|^2}$$

Markov Chain Mote Carlo algorithm to sample the Hilbert space

$$P_{\rm acc} = \min\left(1, \frac{|\Psi_V(R', S')|^2}{|\Psi_V(R, S)|^2}\right)$$

Observables estimated by averaging over the sampled configurations

$$\frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} \simeq \frac{1}{N} \sum_{R,S} \frac{\langle R, S | H | \Psi_V \rangle}{\langle R, S | \Psi_V \rangle}$$

WAVE FUNCTION OPTIMIZATION

ANN trained by performing an imaginary-time evolution in the variational manifold

$$\begin{split} |\bar{\Psi}_{V}(\mathbf{p}_{\tau}) &\equiv (1 - H\delta\tau) |\Psi_{V}(\mathbf{p}_{\tau})\rangle \\ \mathbf{p}_{\tau+\delta\tau} &= \operatorname*{arg\,max}_{\mathbf{p}\in R^{d}} \left(\left| \langle \bar{\Psi}_{V}(\mathbf{p}_{\tau}) | \Psi_{V}(\mathbf{p}_{\tau+\delta\tau}) \rangle \right|^{2} \right) \end{split}$$



The parameters are updated as

$$\mathbf{p}_{\tau+\delta\tau} = \mathbf{p}_{\tau} - \delta\tau S^{-1}\mathbf{g}_{\tau}$$

J. Stokes, at al., Quantum 4, 269 (2020).

S. Sorella, Phys. Rev. B 64, 024512 (2001)

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STOCHASTIC RECONFIGURATION



COMPARISON WITH GFMC

• The ANN Slater Jastrow ansatz outperforms conventional Jastrow correlations

| | Λ | VMC-ANN | VMC-JS | GFMC | GFMC_{c} |
|-----------------|---------------------|-----------|-----------|-----------|---------------------------|
| ² H | $4 {\rm fm}^{-1}$ | -2.224(1) | -2.223(1) | -2.224(1) | - |
| | 6 fm^{-1} | -2.224(4) | -2.220(1) | -2.225(1) | - |
| 311 | $4 {\rm fm}^{-1}$ | -8.26(1) | -7.80(1) | -8.38(2) | -7.82(1) |
| 11 | 6 fm^{-1} | -8.27(1) | -7.74(1) | -8.38(2) | -7.81(1) |
| ⁴ He | 4 fm^{-1} | -23.30(2) | -22.54(1) | -23.62(3) | -22.77(2) |
| | $6 \ {\rm fm}^{-1}$ | -24.47(3) | -23.44(2) | -25.06(3) | -24.10(2) |

Differences with the GFMC due to deficiencies in the Slater-Jastrow ansatz

$$\Psi_{SJ}(X) = e^{J(X)}\Phi(X)$$

C. Adams, AL, et al, PRL 127, 022502 (2021)

$$\Phi(X) = \det \begin{bmatrix} \phi_1(x_1) & \phi_1(x_2) & \phi_1(x_3) & \phi_1(x_4) \\ \phi_2(x_1) & \phi_2(x_2) & \phi_2(x_3) & \phi_2(x_4) \\ \phi_3(x_1) & \phi_3(x_2) & \phi_3(x_3) & \phi_3(x_4) \\ \phi_4(x_1) & \phi_4(x_2) & \phi_4(x_3) & \phi_4(x_4) \end{bmatrix}$$

$$\Psi_{\rm HN}(X) = \det \begin{bmatrix} \phi_1(x_1) & \phi_1(x_2) & \phi_1(x_3) & \phi_1(x_4) \\ \phi_2(x_1) & \phi_2(x_2) & \phi_2(x_3) & \phi_2(x_4) \\ \phi_3(x_1) & \phi_3(x_2) & \phi_3(x_3) & \phi_3(x_4) \\ \phi_4(x_1) & \phi_4(x_2) & \phi_4(x_3) & \phi_4(x_4) \\ \chi_1(x_1) & \chi_1(x_2) & \chi_1(x_3) & \chi_1(x_4) \\ \chi_2(x_1) & \chi_2(x_2) & \chi_2(x_3) & \chi_2(x_4) \end{bmatrix} \begin{pmatrix} \phi_1(y_1) & \phi_1(y_2) \\ \phi_2(y_1) & \phi_1(y_2) \\ \phi_3(y_1) & \phi_1(y_2) \\ \phi_4(y_1) & \phi_1(y_2) \\ \chi_1(y_1) & \chi_2(y_2) \\ \chi_2(y_1) & \chi_2(y_2) \end{bmatrix}$$

| Visible orbitals on visible coordinates | Visible orbitals on hidden coordinates |
|---|--|
| Hidden orbitals on visible coordinates | Hidden orbitals on hidden coordinates |

J. R. Moreno, et al., PNAS 119, 2122059119(2022)



We extend the reach of neural quantum states to ¹⁶O

In addition to its ground-state energy, we evaluate the point-nucleon density of ¹⁶O with A_h=16



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DILUTE NEUTRON MATTER

Periodic hidden-nucleons ansatz to model low-density neutron matter

- NQS: 100 GPU hours
- AFDMC: 1.2 million CPU hours



DILUTE NEUTRON MATTER



CONDENSED-MATTER DETOUR



Periodic-NQS to solve the two-components Fermi gas in the BCS- BEC crossover region



We model the 3D unpolarized gas of fermions with the Hamiltonian

$$H = \sum_{i} \frac{p_i^2}{2m} + \sum_{i < j} v_{ij}$$

 Modified Pöschl-Teller potential between opposite-spin particles

$$v_{ij} = (\delta_{s_i, s_j} - 1) v_0 \frac{2\hbar^2}{m} \frac{\mu^2}{\cosh^2(\mu r_{ij})}$$



We introduce a Pfaffian-Jastrow ansatz

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

In order for the above matrix to be skew-symmetric, the neural pairing orbitals are taken to be

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

Example: pf
$$\begin{bmatrix} 0 & \phi_{12} & \phi_{13} & \phi_{14} \\ -\phi_{12} & 0 & \phi_{23} & \phi_{24} \\ -\phi_{13} & -\phi_{23} & 0 & \phi_{34} \\ -\phi_{14} & -\phi_{24} & -\phi_{34} & 0 \end{bmatrix} = \phi_{12}\phi_{34} - \phi_{13}\phi_{24} + \phi_{14}\phi_{23}$$

HOMOGENOUS ELECTRON GAS

The nodal structure is improved with neural back-flow transformations $\mathbf{x}_i \longrightarrow \phi(\mathbf{x}_i; \mathbf{x}_{j \neq i})$



Translation-invariant (and periodic) by construction: $\longrightarrow \mathbf{x}_i^{(0)} = \mathbf{e}, \quad \mathbf{x}_{ij}^{(0)} = [\mathbf{r}_{ij}, ||\mathbf{r}_{ij}||, s_i \cdot s_j].$



$$\left(\frac{E}{E_{FG}}\right)_{\rm exp} = \xi = 0.376(5)$$



J. Kim, B. Fore, AL, et al. arXiv:2305.08831

BACK TO NUCLEAR PHYSICS







Liquid phase

40



²H clusters

41



⁸Be clusters



⁴He clusters

43

24 Neutrons, 4 Protons @ ρ =0.01 fm⁻³



24 Neutrons, 4 Protons @ ρ =0.01 fm⁻³





Physics Letters 3 732 (2019) 134652



Essential elements for nuclear binding



Bing-Nan Lu⁴, Ning Li⁴, Serdar Elhatisari^{b,2}, Dean Lee^{4,4}, Evgeny Epelbaum⁴, Ulf-G. Meißner^{b,c,1}

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* Institute for Advanced Environment for Receipting and PERA Control for Hard on Physics, For advancement and Hard, do S1001 (Mich. See many Wilds Environments, C100 (Polis), Complex

PHYSICAL REVIEW C 103, 054003 (2021)

Two- and three-nucleon contact interactions and ground-state energies of light- and medium-mass nuclei

B. Schinvilla, 12 L. Girlanda, M. A. Grech, 6,23 A. Kievsky 6,5 A. Lovato 6,73 L. E. Marcucci, 56 M. Picralli, 2 and M. Viviani 2.

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¹DHPI-Fica, 35127 Fite, Italy ²Physics Emission, Argonne National Enhancing, Argonne, Rimais 50429, USA ⁴BIEN TIPPA Dents Institute of Fundamental Physics and Applications, 35123 Trento, Italy ⁹Department of Physics, Washington University In St. Louis, St. Louis, Missouri 68130, USA

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A simple pionless-EFT Hamiltonian reproduces well the spectrum of different nuclei



Deviations from experiments are more pronounced for charge radii



The ground-state is generate in L_z

$$|\Psi_{HN};L,S\rangle = \sum_{L_z S_z} c_{L_z S_z}^{L,S} |L,L_z;S,S_z\rangle.$$



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Remove this degeneracy by

 $H \to H - B_z L_z$





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 \vec{B}

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Remove this degeneracy by

 $H \to H - B_z L_z$







A. Gnech, et al., 2308.16266

MAGNETIC MOMENTS WITH MPNN

In addition to energies and single-particle densities, we compute electroweak properties



A. Gnech, et al., 2308.16266

A simple pionless-EFT Hamiltonian reproduces well the spectrum of different nuclei



HIGH-PERFORMANCE COMPUTING

The variational Monte Carlo with neural network quantum state code is by design scalable to leadership-class hybrid CPU/GPU computers





PERSPECTIVES

• Larger nuclei are within reach on leadership-class machines

Optimized version of the code reaches
 ⁷⁶Ge on Polaris @ANL

 Work in progress to port it to Intel Ponte Vecchio (¹⁰⁰Sn and beyond on Aurora @ANL)



PERSPECTIVES

- **Real-time dynamics** is the prototypal exponentially-hard problem in many-body theory
 - Relevant for: fission, fusion lepton- and hadron-nucleus scattering
 - Learn from TDHF calculations: collaboration with K. Godbey, W. Nazarewicz, and N. Rocco.

$$\mathcal{D}\left(|\Psi(\mathbf{p}_{t+\delta t})\rangle, e^{-iHt}|\Psi(\mathbf{p}_{t})\right)^{2} = \arccos\left(\sqrt{\frac{\langle\Psi(\mathbf{p}_{t+\delta t})|e^{-iHt}|\Psi(\mathbf{p}_{t})\rangle\langle\Psi(\mathbf{p}_{t})|e^{iHt}|\Psi(\mathbf{p}_{t+\delta t})\rangle}{\langle\Psi(\mathbf{p}_{t+\delta t})|\Psi(\mathbf{p}_{t+\delta t})\rangle\langle\Psi(\mathbf{p}_{t})|\Psi(\mathbf{p}_{\tau+\delta t})\rangle}}\right)^{2}$$

Alternative approach based on integral transform, with N. Barnea, E. Parnes, and N. Rocco

SOME PERSPECTIVES:

• Occupation number formalism allows to naturally satisfy Pauli's exclusion principle



THANK YOU