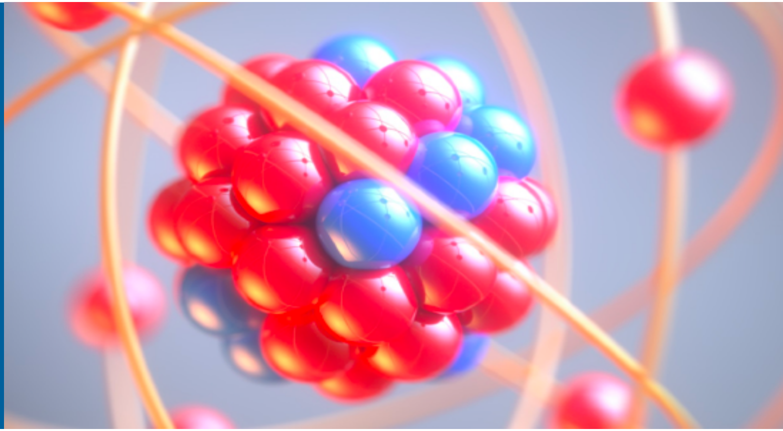
VARIATIONAL LEARNING NUCLEI AND HYPER NUCLEI



ALESSANDRO LOVATO

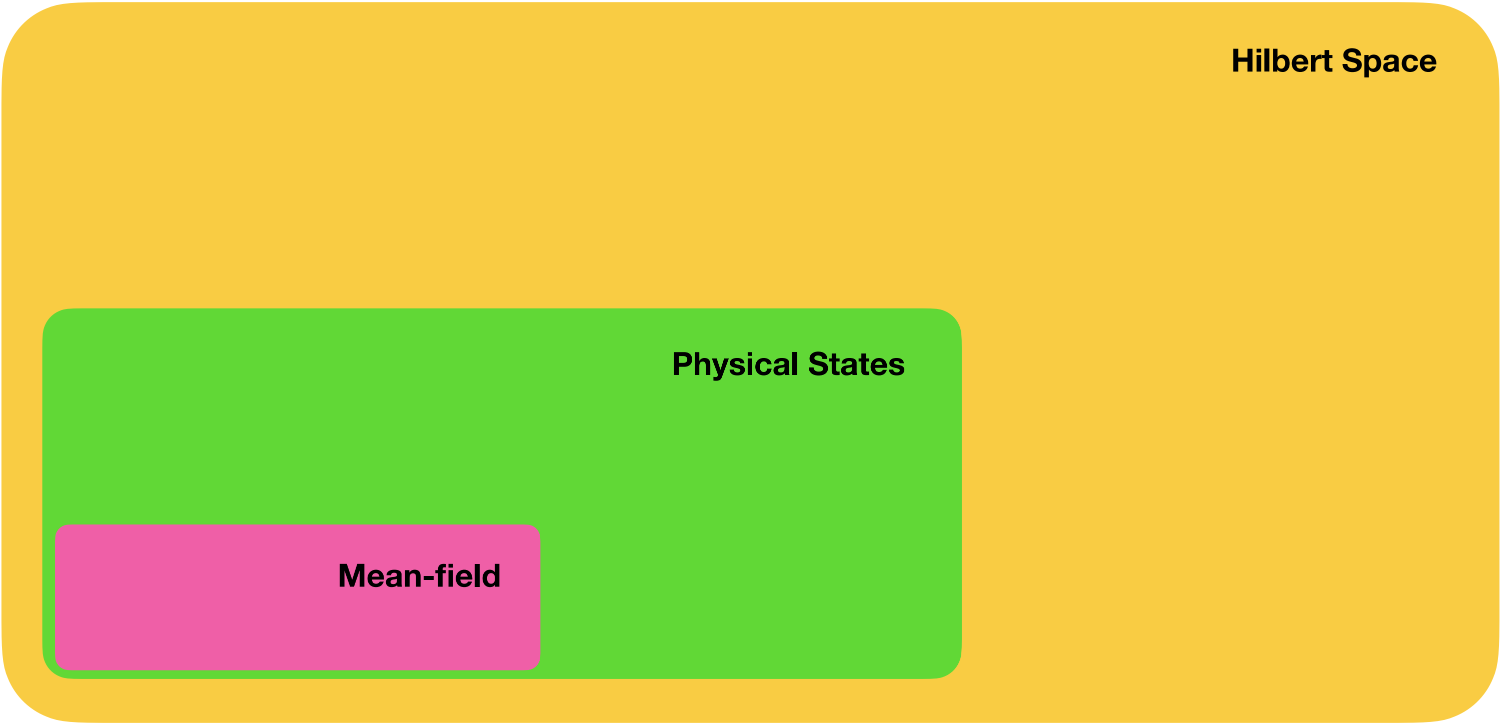
STREAMLINE Collaboration Symposium

Michigan State University & FRIB

May 10, 2024

Argonne NATIONAL LABORATORY

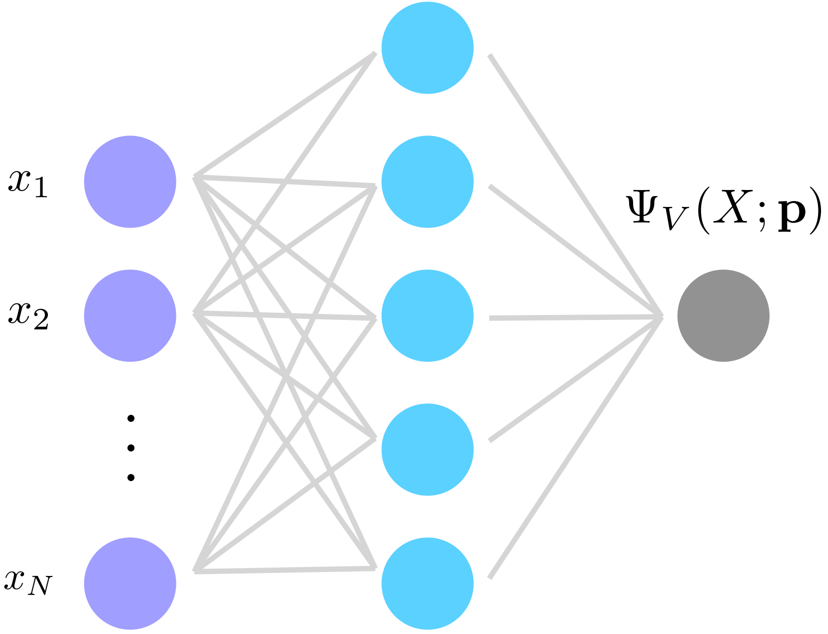
NEURAL-NETWORK QUANTUM STATES



Credit: G. Carleo

NEURAL-NETWORK QUANTUM STATES

Originally introduced by Carleo and Troyer for spin systems, NQS are now widely and successfully applied to study condensed-matter systems



$$E_V \equiv \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} > E_0$$

$$E_V \simeq \frac{1}{N} \sum_{X \in |\Psi_V(X)|^2} \frac{\langle X | H | \Psi_V \rangle}{\langle X | \Psi_V \rangle}$$

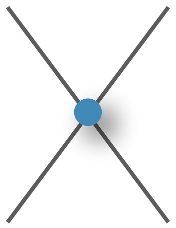
$$\mathbf{p}_{\tau+\delta\tau} = \mathbf{p}_\tau - \eta (S_\tau + \epsilon I)^{-1} \mathbf{g}_\tau$$

PIONLESS EFT HAMILTONIAN

Input: Hamiltonian inspired by a LO pionless-EFT expansion

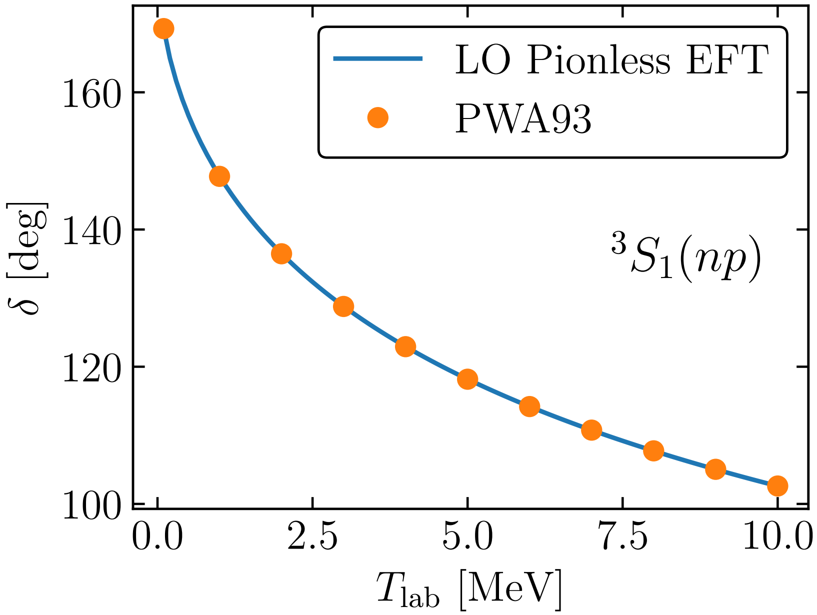
$$H_{LO} = -\sum_i \frac{\vec{\nabla}_i^2}{2m_N} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

- NN potential fit to s-wave np scattering lengths and effective ranges



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

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



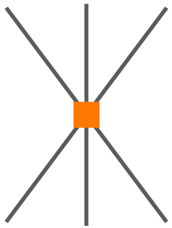
R. Schiavilla, AL, PRC **103**, 054003 (2021)

PIONLESS EFT HAMILTONIAN

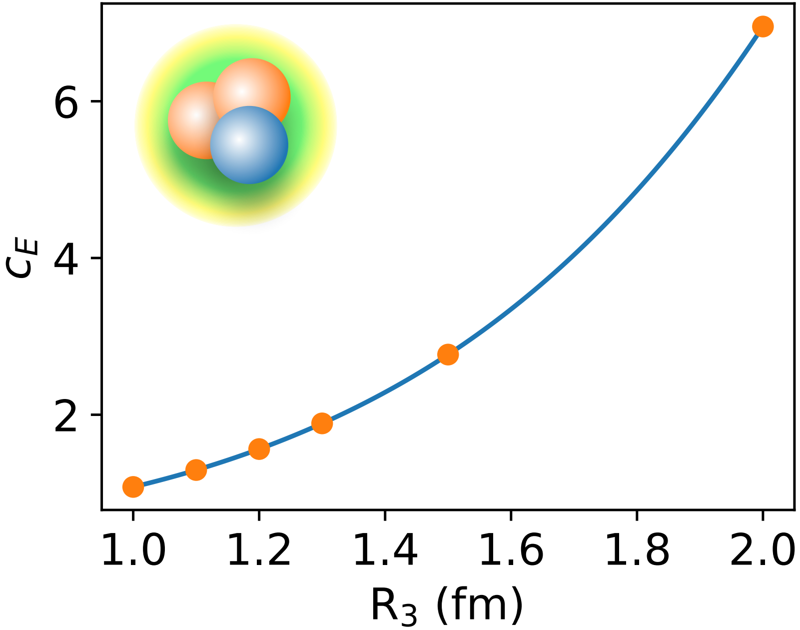
Input: Hamiltonian inspired by a LO pionless-EFT expansion

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

- 3NF adjusted to reproduce the energy of ^{3}H.



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



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

HIDDEN NUCLEONS ANSATZ

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

Visible orbitals on visible coordinates

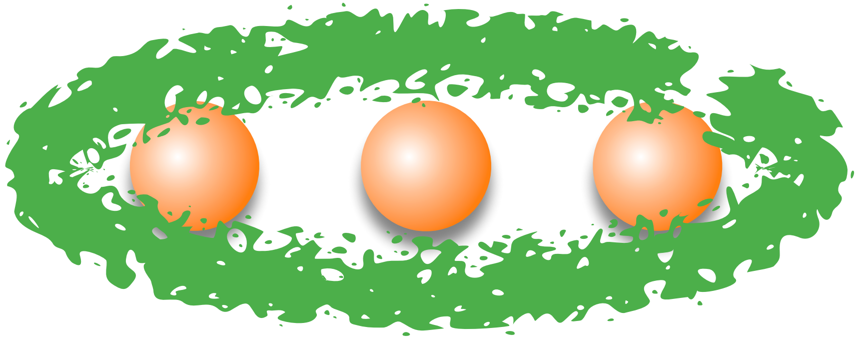
Visible orbitals on hidden coordinates

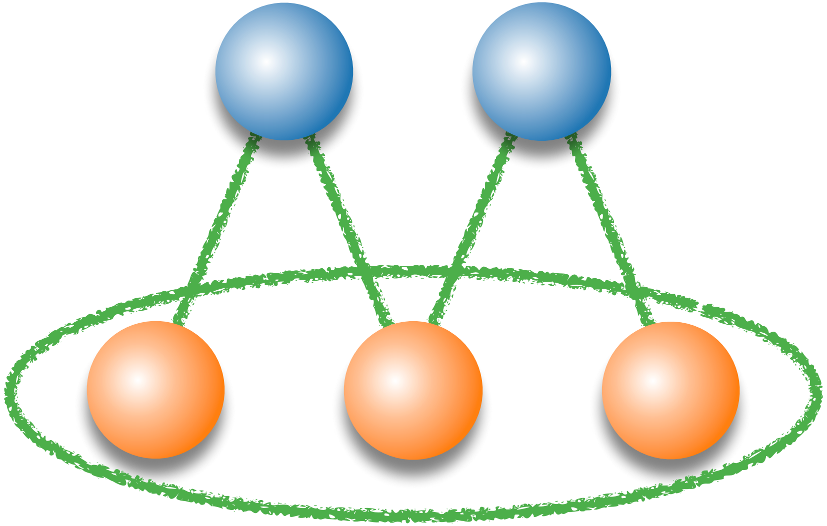
Hidden orbitals on visible coordinates

Hidden orbitals on hidden coordinates

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

HIDDEN NUCLEONS ANSATZ

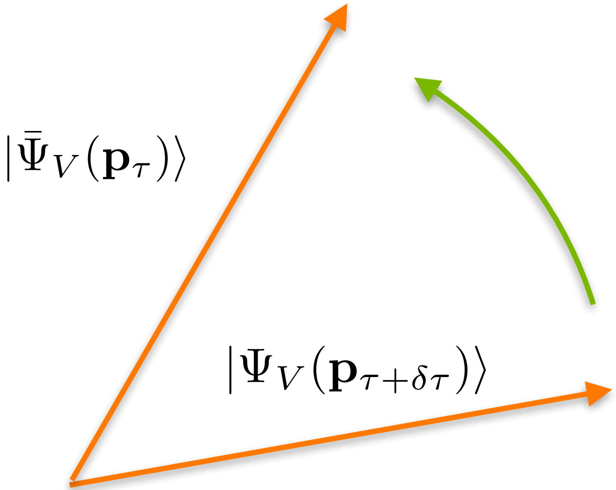




WAVE FUNCTION OPTIMIZATION

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

$$\begin{cases} |\bar{\Psi}_V(\mathbf{p}_\tau\rangle \equiv (1 - H\delta\tau)|\Psi_V(\mathbf{p}_\tau)\rangle \\ \mathbf{p}_{\tau+\delta\tau} = \underset{\mathbf{p}\in R^d}{\arg\max} \left(\left| \langle \bar{\Psi}_V(\mathbf{p}_\tau) | \Psi_V(\mathbf{p}_{\tau+\delta\tau}) \rangle \right|^2 \right) \end{cases}$$



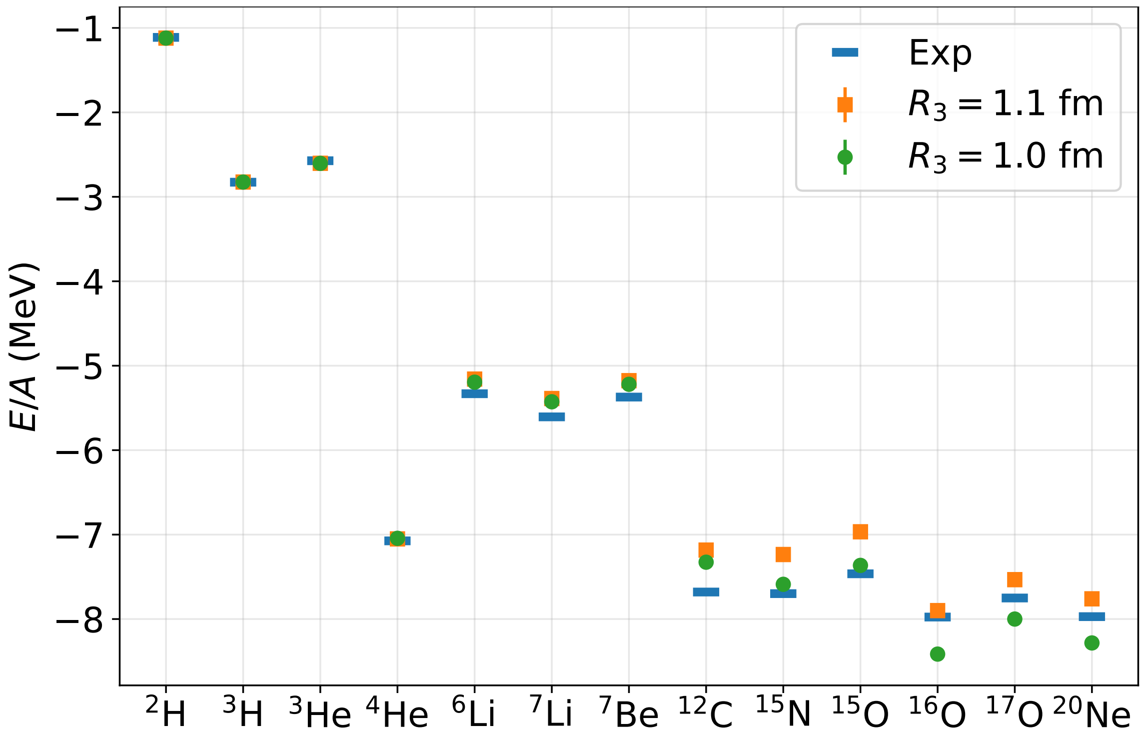
The parameters are updated as

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

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

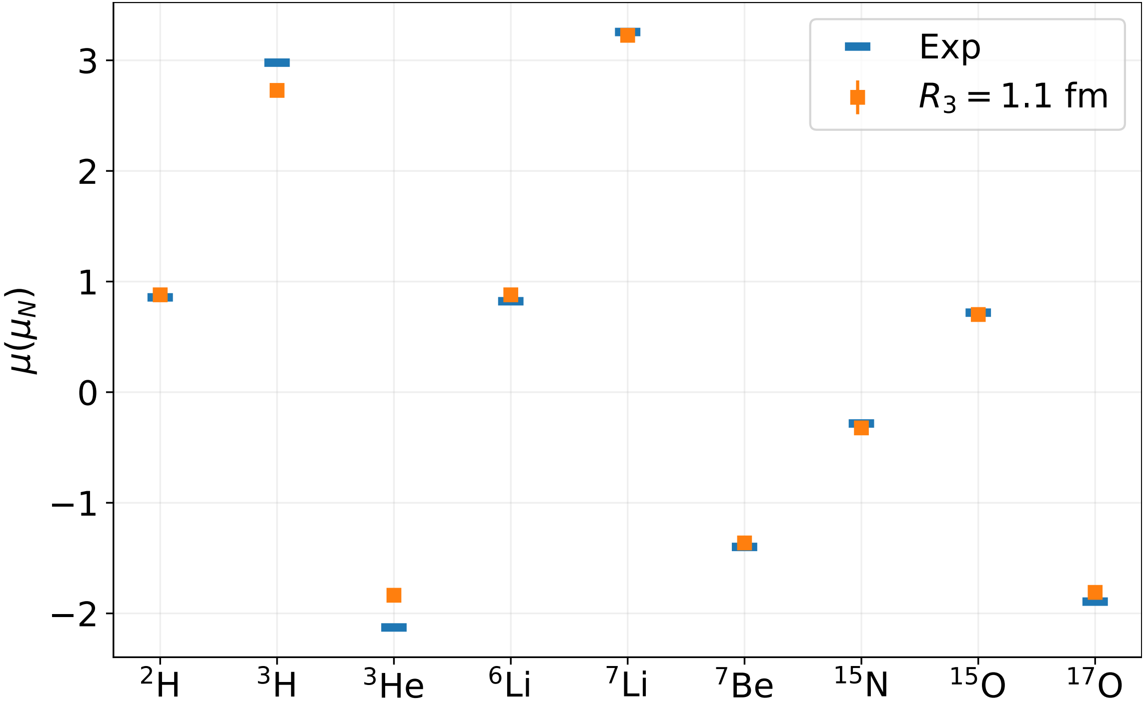
S. Sorella, Phys. Rev. B 64, 024512 (2001)

BINDING ENERGIES



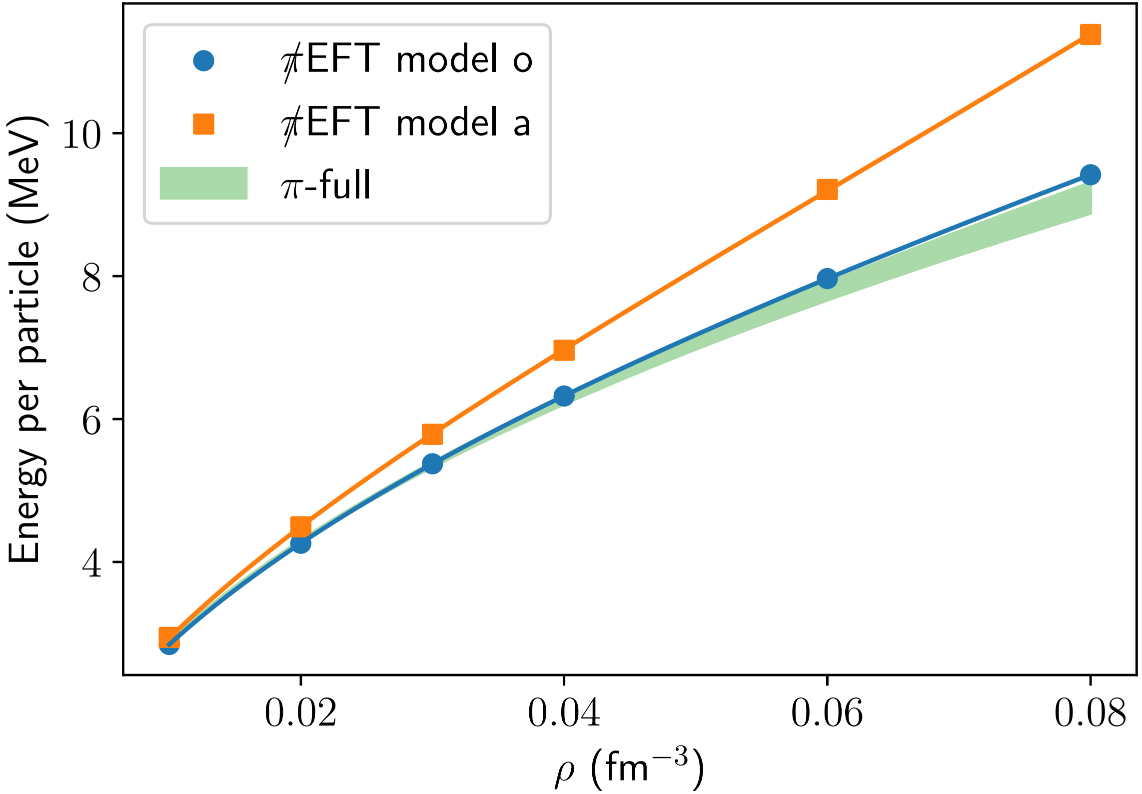
A. Gnech, AL, et al., 2308.16266

MAGNETIC MOMENTS



A. Gnech, et al., 2308.16266

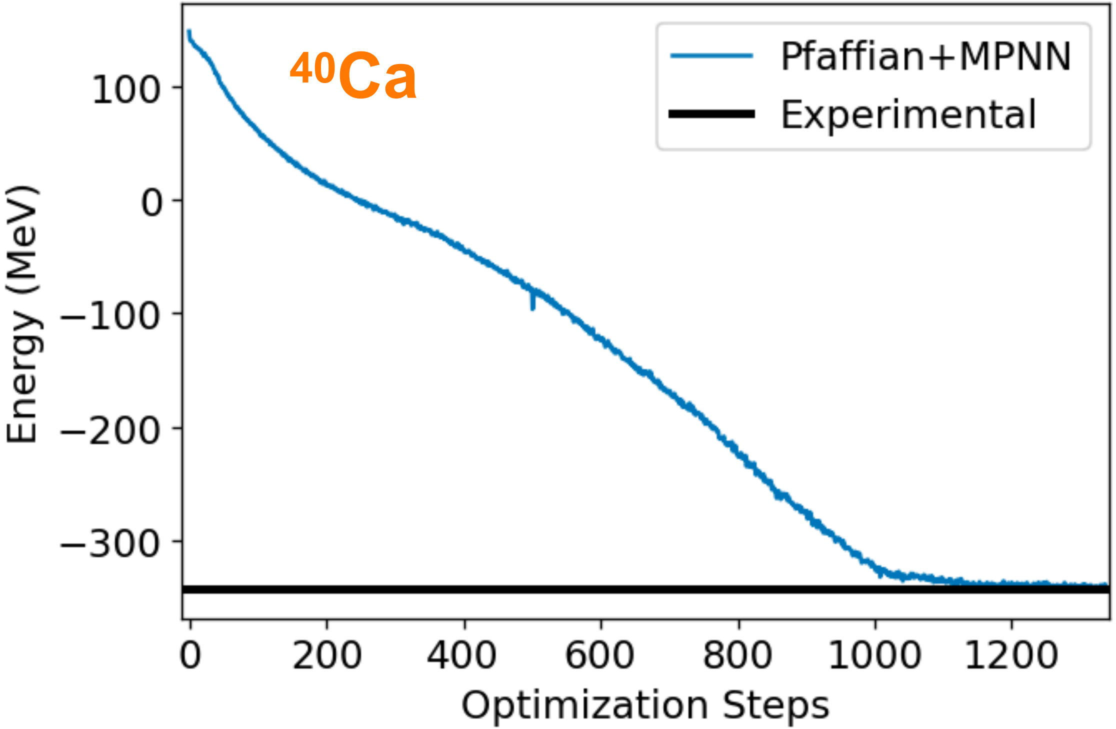
DILUTE NEUTRON MATTER



B. Fore, AL et al., *Phys. Rev. Res.* **5**, 033062 (2023)

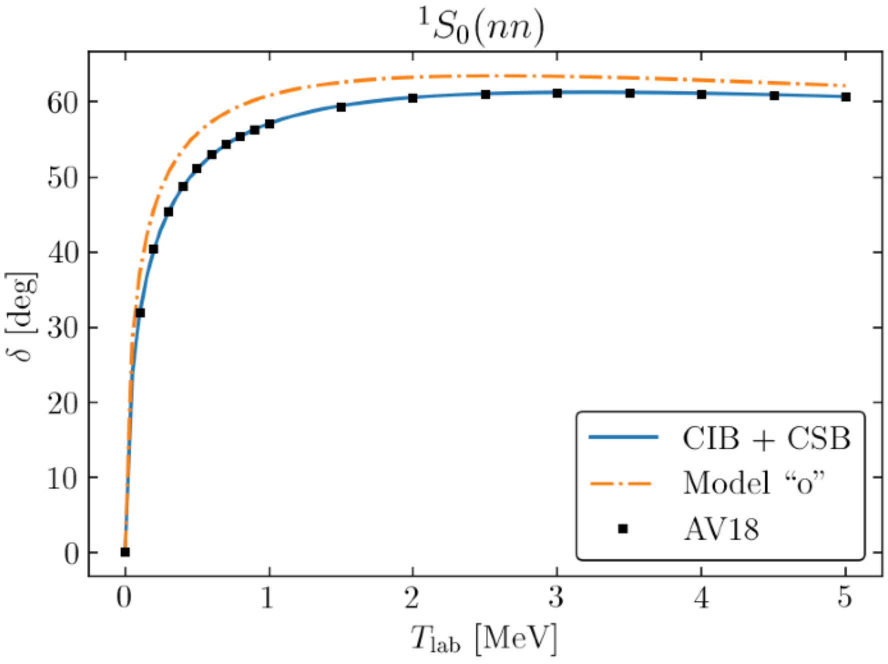
FIRST GOAL: EXTENSION TO LARGER NUCLEI

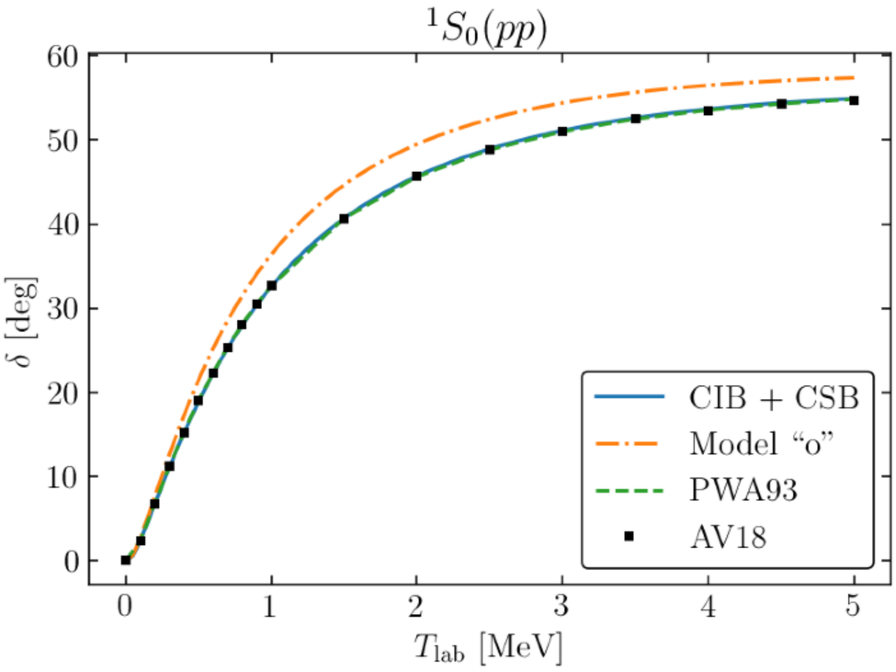
Bryce Fore has significantly improved the scalability of the code to multiple GPU nodes



SECOND GOAL: MORE REALISTIC POTENTIALS

Anthony Tropiano has included CIB and CSB terms in the Hamiltonian

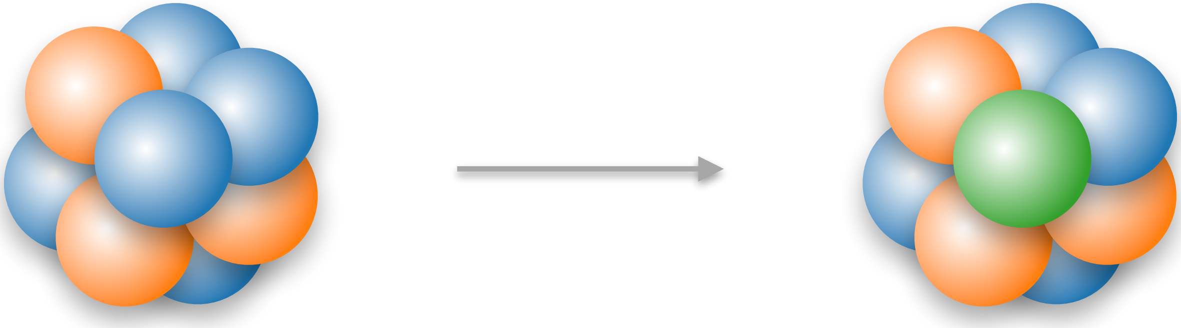




ADDITIONAL GOAL: TACKLE STRANGENESS

Hypernuclei: bound state between an ordinary nucleus with one (or more) hyperons

Our work: consider single-Λ hypernuclei to begin with

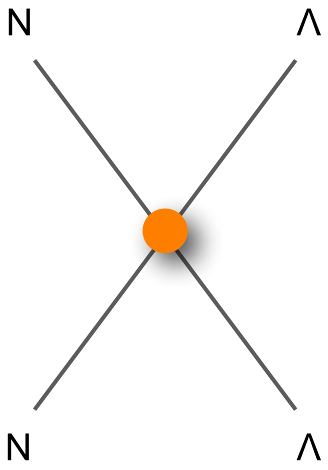


$^{12}\mathrm{C}$ $\longrightarrow$ $^{12}_{\Lambda}\mathrm{C}$

6 protons, 6 neutrons — 6 protons, 5 neutrons, 1 lambda

PIONLESS EFT FOR HYPER-NUCLEI

Input: Hamiltonian inspired by a LO pionless-EFT expansion



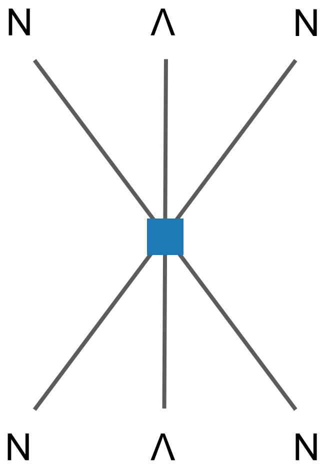
$$V_{\Lambda N} = \sum_{S,T} v_{ST}(r_{ij}) \hat{P}_{ST}$$

- ➡ T=1/2, S=1
- ➡ T=1/2, S=0

Parameters are determined by fitting proton-Λ scattering length and effective range

PIONLESS EFT FOR HYPER-NUCLEI

Input: Hamiltonian inspired by a LO pionless-EFT expansion



$$V_{\Lambda NN} = \sum_{S,T} D_{S,T} v_{ST}(r_{i\Lambda}) v_{ST}(r_{j\Lambda}) \hat{Q}_{ST}$$

- T=0, S=1/2
- T=0, S=3/2
- T=1, S=1/2

Parameters are determined by fitting ${}^{3}_{\Lambda}\mathrm{H}$, ${}^{4}_{\Lambda}\mathrm{H}(S=0)$, ${}^{4}_{\Lambda}\mathrm{H}(S=1)$, and ${}^{5}_{\Lambda}\mathrm{He}$.

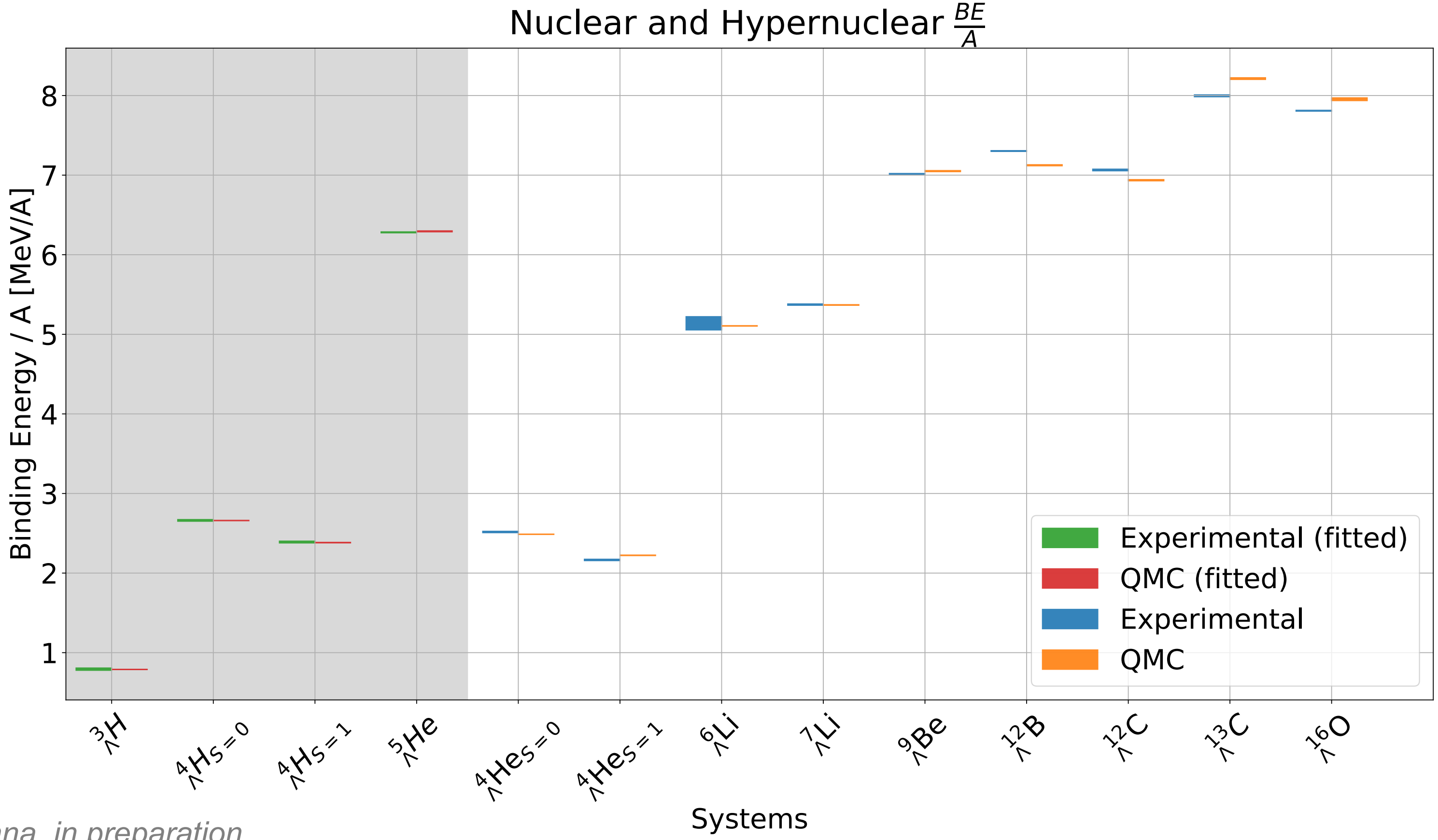
NQS FOR HYPER-NUCLEI

No terms in the Hamiltonian mix lambda and nucleons: **distinguishable**

Andrea Di Donna proposed the following ansatz

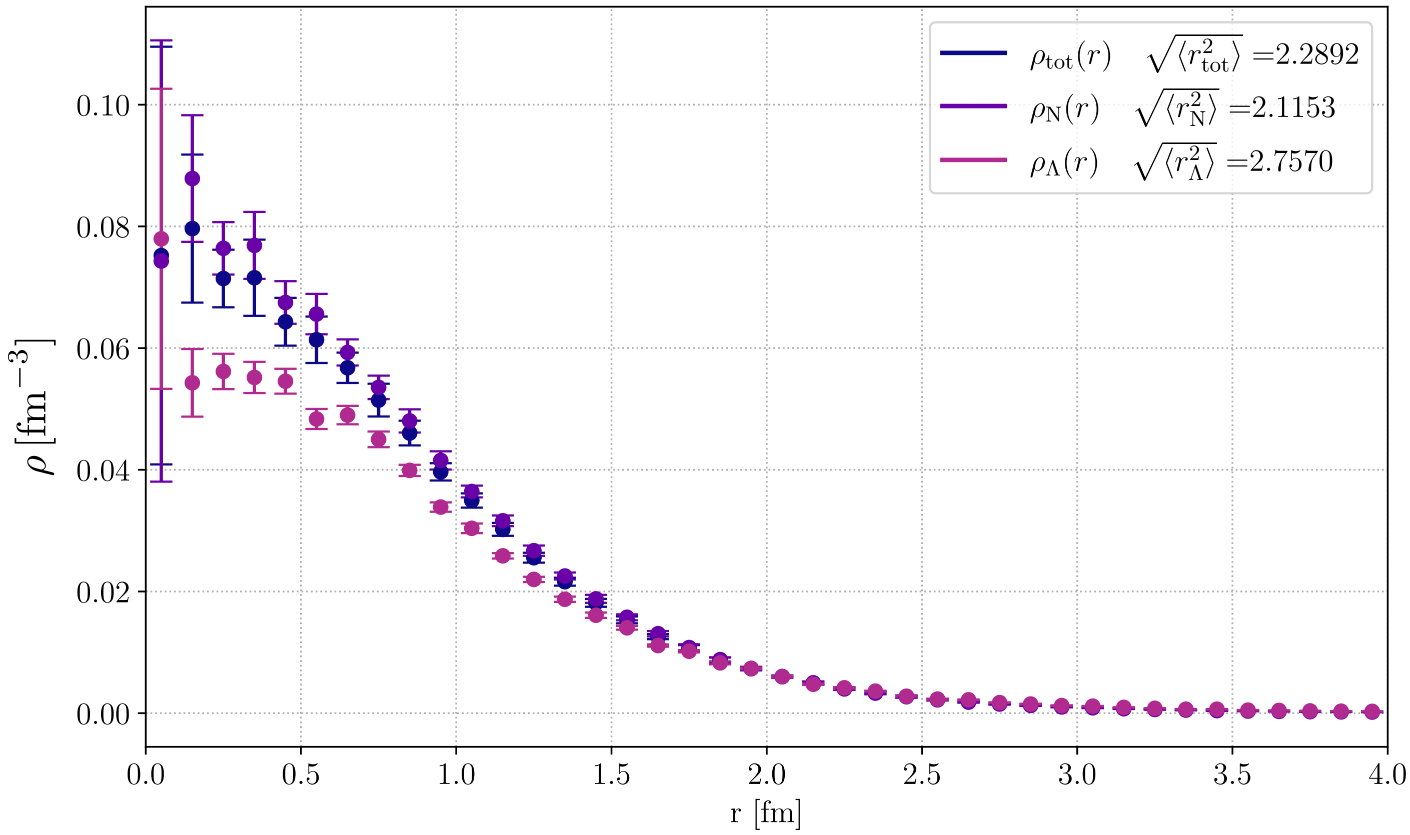
$$\Psi(x_\Lambda, x_1, \ldots, x_A) = \mathcal{U}(x_\Lambda; x_1, \ldots, x_A) \times \Psi_{HN}(x_1, \ldots, x_A)$$

GROUND-STATE ENERGIES



A. Di Donna, in preparation

SINGLE-PARTICLE DENSITIES

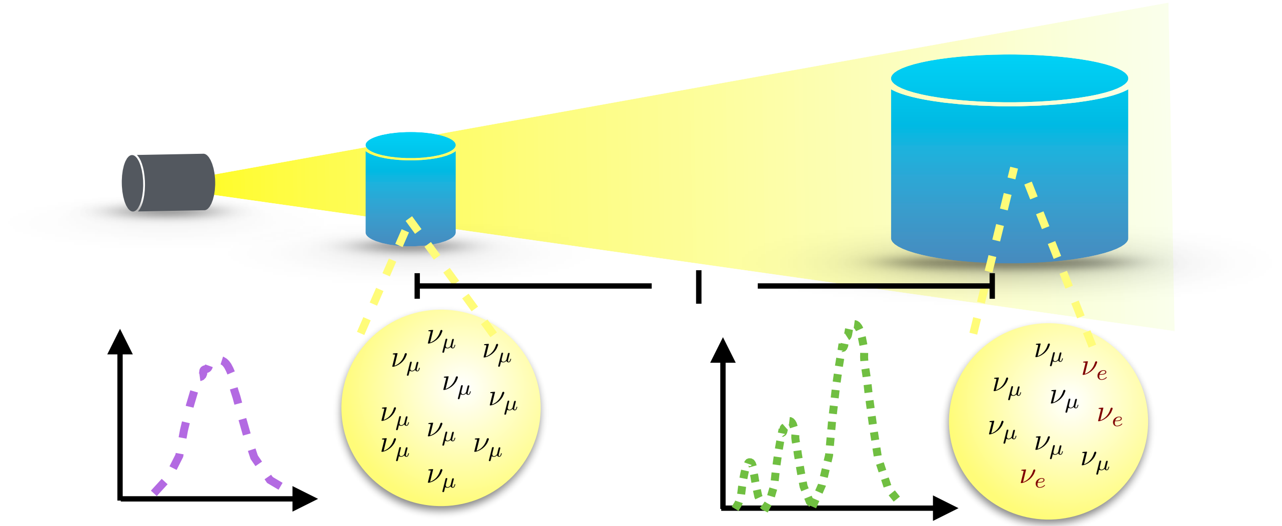


A. Di Donna, in preparation

REAL-TIME QUANTUM DYNAMICS

Real-time quantum dynamics is the prototypal exponentially-hard problem

➡ Relevant for: fission, fusion lepton- and hadron-nucleus scattering, collective neutrino oscillations



Credit: N. Rocco

REAL-TIME QUANTUM DYNAMICS

Initial goal: compute the linear response function:

$$R(\omega) = \sum_n \langle \Psi_0 | D^\dagger | \Psi_n \rangle \langle \Psi_n | D | \Psi_0 \rangle \delta(\omega - E_f + E_0)$$

$$D = \frac{NZ}{A}\Big(\frac{1}{Z} \sum_{p=1}^{A} \vec{r}_p - \frac{1}{N} \sum_{n=1}^{N} \vec{r}_n \Big) = \frac{NZ}{A} (\vec{R}_p - \vec{R}_n)$$

With N. Rocco and K. Godbye, we re-derived off the expressions for the linear response

$$R(\omega) = \mathrm{Im}\left[\int dt\, e^{i\omega t} \left(\langle \Psi(t) | D | \Psi(t) \rangle - \langle \Psi_0 | D | \Psi_0 \rangle \right) \right]$$

REAL-TIME QUANTUM DYNAMICS

The time-evolved state is given by

$$|\Psi(t)\rangle = e^{-iHt}e^{-ibD}|\Psi_0\rangle$$

Two options:

- ➡ Use the TDVP to evolve $|\Psi_0\rangle$ with $H' = D$ for a time b.
- ➡ Maximize the fidelity between $e^{-ibD}|\Psi_0\rangle$ and $|\hat{\Psi}(\mathbf{p})\rangle_b$

Real time evolution with the nuclear Hamiltonian

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

THANK YOU