Quantum Monte Carlo formalism for dynamical pions and nucleons

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Madeira, Lovato, Pederiva, and Schmidt. Quantum Monte Carlo formalism for dynamical pions and nucleons. *PRC*, 2018.

Objective

To include explicit pion degrees of freedom in quantum Monte Carlo simulations of nucleon systems

Usual assumptions

- Methods that are aimed at solving the Schrödinger equation associated with the nuclear Hamiltonian
  - Input: potentials and electroweak currents derived within some framework (pionless EFT, chiral EFT, phenomenology,...)
- Usual assumptions:
  - One meson exchange is instantaneous
  - Meson degrees of freedom can be integrated out $\rightarrow$ their contribution is encoded in nuclear potentials and electroweak currents
- Not much attention has been devoted to developing techniques capable of including mesonic degrees of freedom in these many-body calculations
- In this work we propose a formalism in which testing these assumptions is straightforward

What if instantaneous pions are fine?

- Even if few-nucleon sector calculations show that instantaneous pion interactions are justified
  - Our approach is enables us to compute quantities unavailable to other methods
  - In theories where pions are integrated out, current operators need to have the pion contributions calculated from the underlying theory
  - These pion contributions are immediately present in this work
- In this formalism m_π is an input
  - For this work, we employed the physical pion mass
  - It is straightforward to use different m_π, for example, to compare with LQCD calculations

Some previous works in this direction

- Nuclear lattice simulations with Chiral EFT: pions were treated as dynamical fields that coupled to the nucleon fields
- Explicit mesons (σ and π) as particles

Lee, Borasoy, and Schaefer. Nuclear lattice simulations with chiral effective field theory. *PRC*, 2004.

Fedorov. A Nuclear Model with Explicit Mesons. *Few-Body Syst.*, 2020.

Fedorov and Mikkelsen. Threshold Photoproduction of Neutral Pions Off Protons in Nuclear Model with Explicit Mesons. *Few-Body Syst.*, 2023.

Fedorov. The N(1440) Roper Resonance in the Nuclear Model with Explicit Mesons. *Few-Body Syst.*, 2024.

Chiral EFT Lagrangian

- Heavy baryon leading order chiral Lagrangian density

$$
\begin{aligned}
\mathcal{L}_0 = &\frac{1}{2}\partial_\mu \pi_i \partial^\mu \pi_i - \frac{1}{2} m_\pi^2 \pi_i \pi_i \\
&+ N^\dagger \left[i\partial_0 + \frac{\nabla^2}{2M_0} - \frac{1}{4f_\pi^2}\epsilon_{ijk}\tau_i \pi_j \partial_0 \pi_k - \frac{g_A}{2f_\pi}\tau_i \sigma^j \partial_j \pi_i - M_0 \right] N \\
&- \frac{1}{2} C_S (N^\dagger N)(N^\dagger N) - \frac{1}{2} C_T (N^\dagger \sigma_i N)(N^\dagger \sigma_i N)
\end{aligned}
$$

- The nucleon kinetic energy has been promoted since, with the nucleons on a continuum, the kinetic energy is required to have a well-behaved Hamiltonian with physical states
- Only nucleon and pion degrees of freedom are included
- Standard quantum Monte Carlo simulations: pion degrees of freedom are replaced with potentials

A few words about the power counting

- Establishing a rigorous power counting scheme in chiral EFT is currently a subject of debate
- Our power counting gives an expansion in the number of pion field variables, in this work truncated at the quadratic level
- We solve the Schrödinger equation for the states of our system using this truncated interaction at all orders $\rightarrow$ we consider this to be a leading-order calculation
- In principle, going to higher order is straightforward: higher-order Lagrangians would include more pion interactions

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Kaplan, Savage, and Wise. Nucleon-nucleon scattering from effective field theory. *Nucl. Phys. B*, 1996.

Nogga, Timmermans, and van Kolck. Renormalization of one-pion exchange and power counting. *PRC*, 2005.

Valderrama and Arriola. Renormalization of the NN interaction with a chiral two-pion-exchange potential: Central phases and the deuteron. *PRC*, 2006.

Epelbaum and Meißner. On the Renormalization of the One–Pion Exchange Potential and the Consistency of Weinberg's Power Counting. *Few-Body Syst.*, 2013.

Song, Lazauskas, and van Kolck. Triton binding energy and neutron-deuteron scattering up to next-to-leading order in chiral effective field theory. *PRC*, 2017.

Furnstahl, Hammer, and Schwenk. Nuclear Structure at the Crossroads. *Few-Body Syst.*, 2021.

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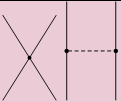
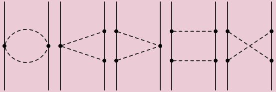
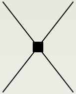
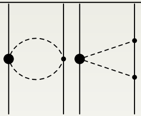
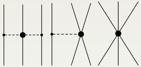
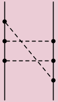
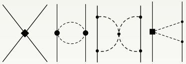
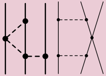
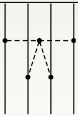
LO							…
NLO							…
N2LO							…
N3LO							…
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Pion fields in the Schrödinger picture

- Schrödinger picture: pion fields and their conjugate momenta are time independent
- Plane-wave expansion in a box of size L with periodic boundary conditions. The allowed momenta are discretized:

$$\boldsymbol{k} = \frac{2\pi}{L}(n_x, n_y, n_z) \text{ with } n_i = 0, \pm 1, \pm 2, \ldots$$

- EFTs have cutoffs
- To avoid infinities, the theory is regularized introducing an ultraviolet cutoff for the three-momentum of the pions, such that $k \equiv |\boldsymbol{k}| \leq k_c$

$$\pi_i(\boldsymbol{x}) = \sqrt{\frac{2}{L^3}} \sum_{\boldsymbol{k}}{}' [\pi^c_{i\boldsymbol{k}} \cos(\boldsymbol{k} \cdot \boldsymbol{x}) + \pi^s_{i\boldsymbol{k}} \sin(\boldsymbol{k} \cdot \boldsymbol{x})]$$

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Quantum Monte Carlo Hamiltonian

- Since the number of nucleons is conserved, the Hamiltonian for the sector with A nucleons and the pion field can be written down as

$$
\begin{aligned}
H &= H_N + H_{\pi\pi} + H_{AV} + H_{WT} \\
H_N &= \sum_{i=1}^{A} \left[\frac{P_i^2}{2M_P} + M_P + \beta_K P_i^2 + \delta M \right] + \sum_{i<j}^{A} \delta_{k_c}(\boldsymbol{r}_i - \boldsymbol{r}_j)[C_S + C_T \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j]
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H_{\pi\pi} &= \frac{1}{2} \sum_{\boldsymbol{k}}{}' \left[|\boldsymbol{\Pi}_{\boldsymbol{k}}^c|^2 + \omega_{\boldsymbol{k}}^2 |\boldsymbol{\pi}_{\boldsymbol{k}}^c|^2 + |\boldsymbol{\Pi}_{\boldsymbol{k}}^s|^2 + \omega_{\boldsymbol{k}}^2 |\boldsymbol{\pi}_{\boldsymbol{k}}^s|^2 \right]
\end{aligned}
$$

Quantum Monte Carlo Hamiltonian

- Pion-nucleon couplings

$$H_{AV} = \sum_{i=1}^{A} \frac{g_A}{2f_\pi} \sqrt{\frac{2}{L^3}} \sum_{\boldsymbol{k}}{}' \left\{ \boldsymbol{\sigma}_i \cdot \boldsymbol{k} \left[\boldsymbol{\tau}_i \cdot \boldsymbol{\pi}_{\boldsymbol{k}}^{s} \cos(\boldsymbol{k} \cdot \boldsymbol{r}_i) - \boldsymbol{\tau}_i \cdot \boldsymbol{\pi}_{\boldsymbol{k}}^{c} \sin(\boldsymbol{k} \cdot \boldsymbol{r}_i) \right] \right\}$$

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H_{WT} &= \sum_{i=1}^{A} \frac{1}{2f_\pi^2 L^3}\boldsymbol{\tau}_i \cdot \left[\sum_{\boldsymbol{k}}{}' \cos(\boldsymbol{k}\cdot\boldsymbol{r}_i)\boldsymbol{\pi}^c_{\boldsymbol{k}} \times \sum_{\boldsymbol{q}}{}' \cos(\boldsymbol{q}\cdot\boldsymbol{r}_i)\boldsymbol{\Pi}^c_{\boldsymbol{q}}\right. \\
&+ \sum_{\boldsymbol{k}}{}' \cos(\boldsymbol{k}\cdot\boldsymbol{r}_i)\boldsymbol{\pi}^c_{\boldsymbol{k}} \times \sum_{\boldsymbol{q}}{}' \sin(\boldsymbol{q}\cdot\boldsymbol{r}_i)\boldsymbol{\Pi}^s_{\boldsymbol{q}} \\
&+ \sum_{\boldsymbol{k}}{}' \sin(\boldsymbol{k}\cdot\boldsymbol{r}_i)\boldsymbol{\pi}^s_{\boldsymbol{k}} \times \sum_{\boldsymbol{q}}{}' \cos(\boldsymbol{q}\cdot\boldsymbol{r}_i)\boldsymbol{\Pi}^c_{\boldsymbol{q}} \\
&+ \left.\sum_{\boldsymbol{k}}{}' \sin(\boldsymbol{k}\cdot\boldsymbol{r}_i)\boldsymbol{\pi}^s_{\boldsymbol{k}} \times \sum_{\boldsymbol{q}}{}' \sin(\boldsymbol{q}\cdot\boldsymbol{r}_i)\boldsymbol{\Pi}^s_{\boldsymbol{q}}\right]
\end{aligned}
$$

- $\boldsymbol{\tau} \cdot \boldsymbol{\pi} \times \boldsymbol{\Pi}$ analog of $\boldsymbol{S} \cdot \boldsymbol{r} \times \boldsymbol{p}$

Trial wave functions: pions and nucleons

- We need to construct an accurate ground state trial wave function for the Hamiltonian
- In GFMC the trial function performs the dual role of lowering the statistical errors and controlling the sign problem
- Let us consider the case of fixed nucleons

$$
\begin{aligned}
H_{\pi\pi} + H_{AV} &= \frac{1}{2}\sum_{\boldsymbol{k}}{}' \left[|\boldsymbol{\Pi}_{\boldsymbol{k}}^{c}|^2 + \omega_{\boldsymbol{k}}^2|\boldsymbol{\pi}_{\boldsymbol{k}}^{c}|^2 + |\boldsymbol{\Pi}_{\boldsymbol{k}}^{s}|^2 + \omega_{\boldsymbol{k}}^2|\boldsymbol{\pi}_{\boldsymbol{k}}^{s}|^2\right] \\
&+ \sum_{i=1}^{A}\frac{g_A}{2f_\pi}\sqrt{\frac{2}{L^3}}\sum_{\boldsymbol{k}}{}' \left\{\boldsymbol{\sigma}_i\cdot\boldsymbol{k}\left[\boldsymbol{\tau}_i\cdot\boldsymbol{\pi}_{\boldsymbol{k}}^{s}\cos(\boldsymbol{k}\cdot\boldsymbol{r}_i) - \boldsymbol{\tau}_i\cdot\boldsymbol{\pi}_{\boldsymbol{k}}^{c}\sin(\boldsymbol{k}\cdot\boldsymbol{r}_i)\right]\right\}
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&+ \sum_{i=1}^{A} \frac{g_A}{2f_\pi} \sqrt{\frac{2}{L^3}} {\sum_{\boldsymbol{k}}}' \left\{ \boldsymbol{\sigma}_i \cdot \boldsymbol{k} \left[\boldsymbol{\tau}_i \cdot \boldsymbol{\pi}_{\boldsymbol{k}}^{s} \cos(\boldsymbol{k} \cdot \boldsymbol{r}_i) - \boldsymbol{\tau}_i \cdot \boldsymbol{\pi}_{\boldsymbol{k}}^{c} \sin(\boldsymbol{k} \cdot \boldsymbol{r}_i) \right] \right\}
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- For each pion mode, this looks like a harmonic oscillator with a linear term

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+ \quad & \sum_{i=1}^{A} \frac{g_A}{2f_\pi} \sqrt{\frac{2}{L^3}} \sum_{\boldsymbol{k}}{}' \left\{ \boldsymbol{\sigma}_i \cdot \boldsymbol{k} \left[\boldsymbol{\tau}_i \cdot \boldsymbol{\pi}_{\boldsymbol{k}}^{s} \cos(\boldsymbol{k}\cdot\boldsymbol{r}_i) - \boldsymbol{\tau}_i \cdot \boldsymbol{\pi}_{\boldsymbol{k}}^{c} \sin(\boldsymbol{k}\cdot\boldsymbol{r}_i) \right] \right\}
\end{aligned}
$$

- For each pion mode, this looks like a harmonic oscillator with a linear term

$$
H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{\omega^2 x^2}{2} + \lambda x \quad \xrightarrow{\tilde{x}=x+\lambda/\omega^2} \quad \boxed{H = -\frac{1}{2}\frac{\partial^2}{\partial \tilde{x}^2} + \frac{\omega^2 \tilde{x}^2}{2} - \frac{\lambda^2}{2\omega^2}}
$$

Trial wave functions: pions and nucleons

- Defining:

$$\boldsymbol{B}_{\boldsymbol{k}}^{c} \equiv \sqrt{\frac{2}{L^3}}\frac{g_A}{f_\pi}\sum_{i=1}^{A}\boldsymbol{\tau}_i \sin(\boldsymbol{k}\cdot\boldsymbol{r}_i)\boldsymbol{\sigma}_i\cdot\boldsymbol{k}, \qquad \boldsymbol{B}_{\boldsymbol{k}}^{s} \equiv -\sqrt{\frac{2}{L^3}}\frac{g_A}{f_\pi}\sum_{i=1}^{A}\boldsymbol{\tau}_i \cos(\boldsymbol{k}\cdot\boldsymbol{r}_i)\boldsymbol{\sigma}_i\cdot\boldsymbol{k}$$

- Allows us to complete the squares:

$$H_{\pi\pi} + H_{AV} = \frac{1}{2}\sum_{\boldsymbol{k}}{}' \left[|\boldsymbol{\Pi}_{\boldsymbol{k}}^{c}|^2 + \omega_{\boldsymbol{k}}^2 |\tilde{\boldsymbol{\pi}}_{\boldsymbol{k}}^{c}|^2 + |\boldsymbol{\Pi}_{\boldsymbol{k}}^{s}|^2 + \omega_{\boldsymbol{k}}^2 |\tilde{\boldsymbol{\pi}}_{\boldsymbol{k}}^{s}|^2 - \frac{1}{4\omega_k^2}\left(|\boldsymbol{B}_{\boldsymbol{k}}^{c}|^2 + |\boldsymbol{B}_{\boldsymbol{k}}^{s}|^2\right)\right]$$

- $\tilde{\boldsymbol{\pi}}_{\boldsymbol{k}}^{c,s} \equiv \boldsymbol{\pi}_{i\boldsymbol{k}}^{c,s} - \boldsymbol{B}_{\boldsymbol{k}}^{c,s}/2\omega_k^2$
- Trial wave function:

$$\langle RS\Pi|\Psi_T\rangle = \langle RS\Pi|\exp\left[-\sum_{\boldsymbol{k}}{}'\frac{\omega_k}{2}(|\tilde{\boldsymbol{\pi}}_{\boldsymbol{k}}^{c}|^2 + |\tilde{\boldsymbol{\pi}}_{\boldsymbol{k}}^{s}|^2)\right]|\Phi\rangle$$

Trial wave functions: pions and nucleons

- Going back to the original coordinates:

$$\langle RS\Pi|\Psi_T\rangle = \langle RS\Pi|\exp\left\{-\sum_{\boldsymbol{k}}{}' \left[\frac{\omega_k}{2}(|\boldsymbol{\pi}_{\boldsymbol{k}}^c|^2 + |\boldsymbol{\pi}_{\boldsymbol{k}}^s|^2) + \frac{\alpha_k}{2\omega_k}(\boldsymbol{\pi}_{\boldsymbol{k}}^c \cdot \boldsymbol{B}_{\boldsymbol{k}}^c + \boldsymbol{\pi}_{\boldsymbol{k}}^s \cdot \boldsymbol{B}_{\boldsymbol{k}}^s)\right.\right.$$

$$\left.\left. -\frac{1}{4}\omega_k\alpha_k^2 G_k^2 \sum_{i<j}^{A} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \boldsymbol{\sigma}_i \cdot \boldsymbol{k} \boldsymbol{\sigma}_j \cdot \boldsymbol{k} \cos(\boldsymbol{k} \cdot \boldsymbol{r}_{ij})\right]\right\}|\Phi\rangle$$

- $|\Phi\rangle$: nucleon model states

Nucleon model states

- One nucleon (4 components):

$$|\Phi\rangle \rightarrow \begin{pmatrix} p\uparrow \\ p\downarrow \\ n\uparrow \\ n\downarrow \end{pmatrix}$$

- Two nucleons (16 components)
  - Deuteron
  - Two neutrons
- We solve the two-body Schrödinger equation in a box with periodic boundary conditions:

$$V_{NN}(\boldsymbol{r}_{ij}) = \delta_{k_c}(\boldsymbol{r}_{ij})[C_S + C_T \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j] \text{ with } \delta_{k_c}(\boldsymbol{r}) = \frac{1}{L^3}\left(1 + 2{\sum_{\boldsymbol{k}}}' \cos(\boldsymbol{k}\cdot\boldsymbol{r})\right)$$

- A nucleons: 4^A components

Quantum Monte Carlo methods

- Variational Monte Carlo (VMC)
- Green's function Monte Carlo (GFMC)
  - Method for solving the imaginary-time many-body Schrödinger equation
  - Projects out the lowest energy eigenstate that has non-zero overlap with the initial state

$$\boxed{|\Phi_0\rangle \propto \lim_{\tau\to\infty} \exp\left[-(H-E_T)\tau\right]|\Psi_T\rangle}$$

$$\langle \mathbf{R}_N S_N \mathbf{\Pi}_N | \Phi_0\rangle = \sum_{S_0}\cdots\sum_{S_{N-1}}\int d^3\mathbf{R}_0 d^3\mathbf{\Pi}_0\cdots d^3\mathbf{R}_{N-1}d^3\mathbf{\Pi}_{N-1}$$

$$\left(\prod_{i=0}^{N-1}\langle \mathbf{R}_{i+1}S_{i+1}\mathbf{\Pi}_{i+1}|\exp\left[-(H-E_T)\delta\tau\right]|\mathbf{R}_i S_i \mathbf{\Pi}_i\rangle\right)\langle \mathbf{R}_0 S_0 \mathbf{\Pi}_0|\Psi_T\rangle$$

One nucleon: mass renormalization

- We introduced two counter terms due to our cutoff

$$H_N = \left[\frac{P^2}{2M_P} + M_P + \beta_K P^2 + \delta M \right]$$

- Diffusion

$$\frac{\partial C(\boldsymbol{r},\tau)}{\partial \tau} = D\nabla^2 C(\boldsymbol{r},\tau)$$

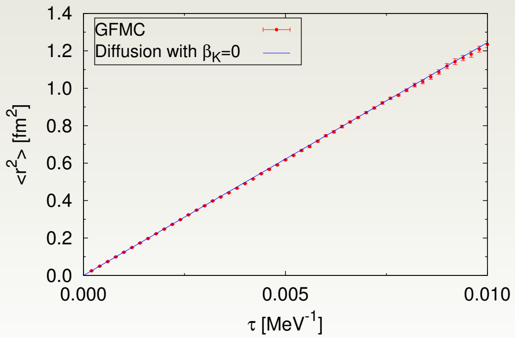
$$\langle r^2(\tau) \rangle = 6D\tau + \text{constant}$$

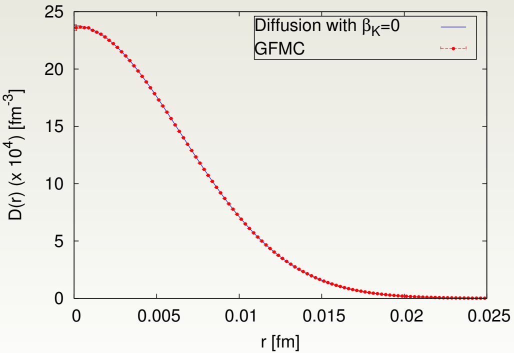
- Density correlation function

$$\mathcal{D}(\boldsymbol{r}) = \frac{\langle \Psi_T | \rho(\boldsymbol{r}) e^{-(H-E_T)\delta\tau} \rho(0) | \Psi_0 \rangle}{\langle \Psi_T | \Psi_0 \rangle}$$

One nucleon: mass renormalization

- We set $\beta_K = 0$
- This is in agreement with a nonrelativistic self-energy calculation we performed





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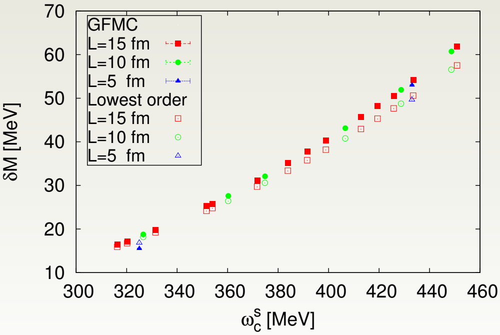
One nucleon: mass renormalization

- Rest mass counter term as a function of the cutoff for different box sizes

$$H_N = \left[\frac{P^2}{2M_P} + M_P + \beta_K P^2 + \delta M \right]$$



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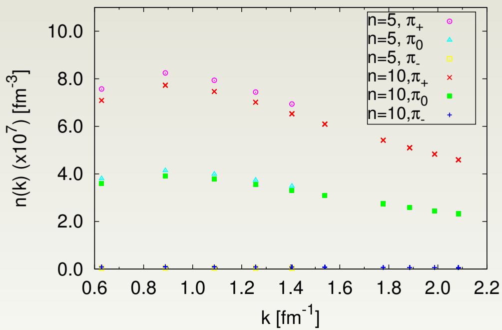
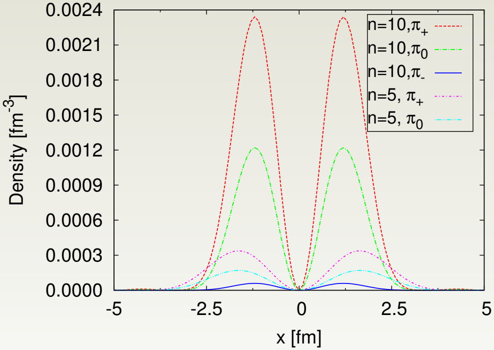
One nucleon: the pion cloud

- Model state is a spin-up proton





- Structure of the axial-vector coupling

$$\tau_i \pi_i = \frac{1}{2}\tau_+(\pi_x - i\pi_y) + \frac{1}{2}\tau_-(\pi_x + i\pi_y) + \tau_z \pi_0$$

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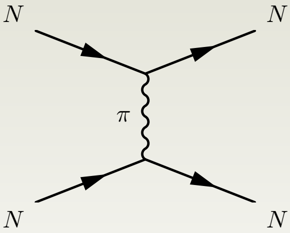
One pion exchange

- Long-range behavior of the nuclear force



$$V_{\mathrm{OPE}}(\boldsymbol{q}) = -\left(\frac{g_A}{2f_\pi}\right)^2 \frac{(\boldsymbol{\sigma}^1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}^2 \cdot \boldsymbol{q})}{q^2 + m_\pi^2} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$

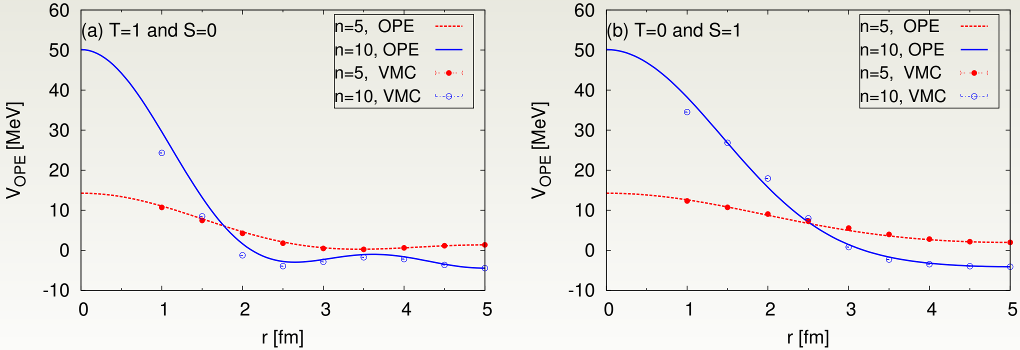
- In real space:

$$V_{\mathrm{OPE}}(\boldsymbol{r}) = \frac{m_\pi^2}{12\pi}\left(\frac{g_A}{2f_\pi}\right)^2 (\boldsymbol{\tau}^1 \cdot \boldsymbol{\tau}^2)$$
$$\left(\left[(3\hat{r}\cdot\boldsymbol{\sigma}^1\hat{r}\cdot\boldsymbol{\sigma}^2 - \boldsymbol{\sigma}^1\cdot\boldsymbol{\sigma}^2)\left(1 + \frac{3}{m_\pi r} + \frac{3}{(m_\pi r)^2}\right) + \boldsymbol{\sigma}^1\cdot\boldsymbol{\sigma}^2\right]\frac{e^{-m_\pi r}}{r} - \frac{4\pi}{3}\boldsymbol{\sigma}^1\cdot\boldsymbol{\sigma}^2\delta^3(r)\right)$$

Two nucleons: one pion exchange

- In the box and with a cutoff:

$$V_{\text{OPE}}(\boldsymbol{r}) = -\frac{1}{L^3}\frac{g_A^2}{2f_\pi^2}\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2\sum_{\boldsymbol{k}}{}'(\boldsymbol{\sigma}^1\cdot\boldsymbol{k})(\boldsymbol{\sigma}^2\cdot\boldsymbol{k})\frac{\cos(\boldsymbol{k}\cdot\boldsymbol{r})}{\omega_k^2}$$



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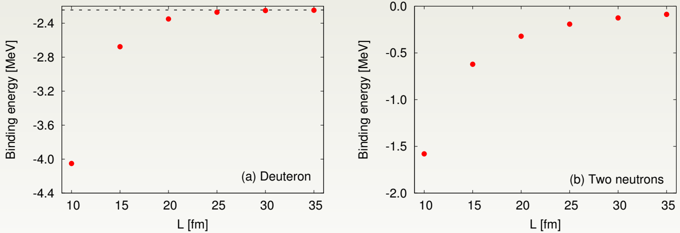
Two nucleons: LECs

- We need to fit the low-energy constants in the Hamiltonian

$$H_N = \sum_{i=1}^{A} \left[\frac{P_i^2}{2M_P} + M_P + \beta_K P_i^2 + \delta M \right] + \sum_{i<j}^{A} \delta_{R_0}(\boldsymbol{r}_i - \boldsymbol{r}_j)[C_S + C_T \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j]$$

- "Numerical experiment" → Energy of the deuteron and two neutrons in a box using a well-established phenomenological potential (AV6P)

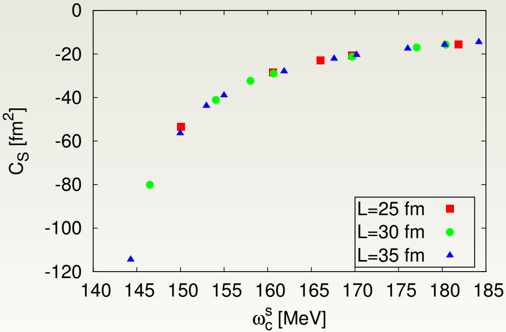


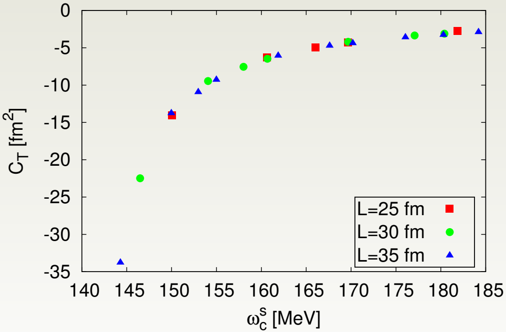
- We tuned C_S and C_T to reproduce the energies of the physical systems

Madeira, Lovato, Pederiva, and Schmidt. Quantum Monte Carlo formalism for dynamical pions and nucleons. *PRC*, 2018.

Two nucleons

- Now the *A*-nucleon Hamiltonian is completely determined





Madeira, Lovato, Pederiva, and Schmidt. Quantum Monte Carlo formalism for dynamical pions and nucleons. *PRC*, 2018.

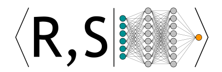
Outlook

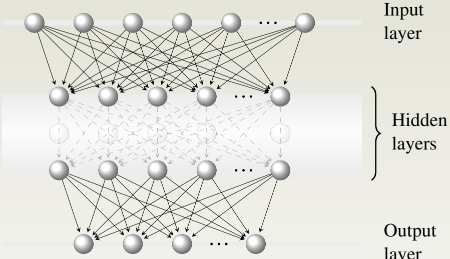
- Promising scheme to explicitly include pion contributions in QMC simulations
- One-nucleon properties
- Pion cloud: momentum and density distributions
- Two fixed nucleons $\rightarrow$ one pion exchange at large distances
- Low-energy constants
- Light-nuclei

Neural-Network Quantum States

- The objective of NNQS are to represent and approximate many-body wave functions by means of Neural Networks

$$\Psi_V(\mathbf{R},\mathbf{S}) \rightarrow \Psi_W(\mathbf{R},\mathbf{S}) =$$





Courtesy of Andrea Di Donna

- We will employ NNQS that take as input nucleon and pion degrees of freedom are have the correct symmetries

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Lovato, Adams, Carleo, and Rocco. Hidden-nucleons neural-network quantum states for the nuclear many-body problem. *Phys. Rev. Research*, 2022.

Gnech, Adams, Brawand, Carleo, Lovato, and Rocco. Nuclei with Up to $A = 6$ Nucleons with Artificial Neural Network Wave Functions. *Few-Body Syst.*, 2022.