QMC with dynamical pions and nucleons

A neural quantum state approach

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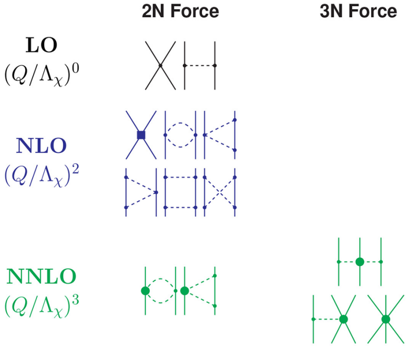
From chiral EFT diag. expansion to Hamiltonian dynamical pions

$$\nu = -2 + 2A - 2C + 2L + \sum_i V_i \Delta_i, \qquad \Delta_i = d_i + \frac{n_i}{2} - 2,$$

$$V_{NN}^{(\nu)} \sim \left(\frac{Q}{\Lambda_\chi}\right)^\nu, \quad Q \sim \{p, m_\pi\} \ll \Lambda_\chi$$



Potential route: diagrams → potential

Assign the order. Power counting assigns ν to each irreducible diagram.

Build the potential. Nucleon contacts + Pion propagation encoded into **instantaneous nPE operators**

Truncate. All irreducible diagrams till order ν are collected in $V^{(\leq\nu)}$.

Iterate it. Solve the LS equation $T = V + VG_0T$ in the **nucleonic Hilbert space** resum this potential non-perturbatively in the nucleonic Hilbert space.

Explicit-pion route: operators → Hamiltonian

Retain a selected set* of chiral interaction vertices of the Lagrangian in the Hamiltonian **Resum non-perturbatively** all processes they generate in the **extended Hilbert space** by solving the Schrödinger equation.

Exchange paths (OPE/∼TPE):

$$NN \overset{H_{AV}}{\longleftrightarrow} NN\pi \overset{H_{AV}}{\longleftrightarrow} NN\pi\pi$$

Figure adapted from D. R. Entem, R. Machleidt, and Y. Nosyk, *Frontiers in Physics* **8**, 57 (2020), Fig. 1.

LO χEFT in Hamiltonian formalism

Madeira *et al.*, Phys. Rev. C **98**, 034005 (2018)

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

Field amplitudes as coordinates

In the Schrödinger picture, the operators are time independent. In a periodic box, expand

$$\pi_i(\mathbf{x}) \simeq \sum_{\mathbf{k}}{}' \left[\pi^c_{i\mathbf{k}}\cos(\mathbf{k}\cdot\mathbf{x}) + \pi^s_{i\mathbf{k}}\sin(\mathbf{k}\cdot\mathbf{x})\right],$$

$$\Pi_i(\mathbf{x}) \simeq \sum_{\mathbf{k}}{}' \left[\Pi^c_{i\mathbf{k}}\cos(\mathbf{k}\cdot\mathbf{x}) + \Pi^s_{i\mathbf{k}}\sin(\mathbf{k}\cdot\mathbf{x})\right].$$

Each real coefficient $\pi^{c,s}_{i\mathbf{k}}$ is therefore an ordinary quantum-mechanical coordinate.

Canonical quantization

The equal-time relations are

$$[\pi_i(\mathbf{x}), \pi_j(\mathbf{y})] = [\Pi_i(\mathbf{x}), \Pi_j(\mathbf{y})] = 0,$$

$$[\pi_i(\mathbf{x}), \Pi_j(\mathbf{y})] = i\delta_{ij}\delta^{(3)}(\mathbf{x}-\mathbf{y}).$$

Hence, for the independent modes ($i \neq j$),

$$[\pi^c_{i\mathbf{k}}, \Pi^c_{j\mathbf{k}'}] = i\delta_{ij}\delta_{\mathbf{k}\mathbf{k}'}, \qquad [\pi^s_{i\mathbf{k}}, \Pi^s_{j\mathbf{k}'}] = i\delta_{ij}\delta_{\mathbf{k}\mathbf{k}'}.$$

$\pi^\alpha_{i\mathbf{k}}$-conjugate coordinates are: $\rightarrow \boxed{\Pi^{c,s}_{i\mathbf{k}} = -i\frac{\partial}{\partial \pi^{c,s}_{i\mathbf{k}}}}$.

Monte Carlo coordinates: each nonzero $\mathbf{k}$ carries $2 \times 3 = 6$ real amplitudes (cos/sin $\times$ isospin); the zero mode carries only 3 $\pi^c_{a,\mathbf{k}}$.

Schrödinger-picture free pion field in a finite box

$$\mathbf{k} = \frac{2\pi}{L}\mathbf{n}, \qquad \omega_k = \sqrt{\mathbf{k}^2 + m_\pi^2}, \qquad \mathbf{n} \in \mathbb{Z}^3.$$

A real field is represented by one momentum from each $\{\mathbf{k}, -\mathbf{k}\}$ pair:

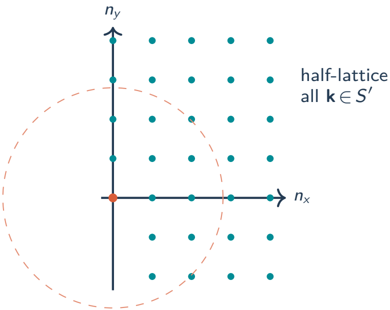
$$\pi_a(\mathbf{x}) = \sqrt{\frac{2}{L^3}} \sum_{\mathbf{k}\in S^+}' \left[\pi^c_{a\mathbf{k}} \cos(\mathbf{k}\cdot\mathbf{x}) + \pi^s_{a\mathbf{k}} \sin(\mathbf{k}\cdot\mathbf{x})\right].$$

where S^+ is the set of independent half-lattice momenta.
After Legendre transformation, the free field becomes a set of independent oscillators,

$$H_\pi = \sum_{a,\mathbf{k}\in S^+}' \left[-\frac{1}{2}\frac{\partial^2}{\partial(\pi^c_{a\mathbf{k}})^2} - \frac{1}{2}\frac{\partial^2}{\partial(\pi^s_{a\mathbf{k}})^2} + \frac{\omega_k^2}{2}\left((\pi^c_{a\mathbf{k}})^2 + (\pi^s_{a\mathbf{k}})^2\right)\right].$$

with free-pion vacuum

$$\Psi_{\pi,0}(\boldsymbol{\pi}) = \mathcal{N} \exp\left[-\frac{1}{2}\sum_{a,\mathbf{k}\in S^+}' \omega_k \left(|\pi^c_{a,\mathbf{k}}|^2 + |\pi^s_{a,\mathbf{k}}|^2\right)\right],$$



Nonrelativistic nucleons. The nucleon sector uses $\epsilon_N(\mathbf{p}) = M_N + \mathbf{p}^2/(2M_N) + \cdots$, while pions keep $\omega_k = \sqrt{k^2 + m_\pi^2}$.

Hamiltonian: interaction structure and counterterms

$$\boxed{H = H_N + H_\pi + H_{AV} + H_{WT}}$$

Nucleon Hamiltonian

$$H_N = \sum_i \left[\frac{\mathbf{P}_i^2}{2M_N} + \beta_K^{\mathrm{ct}} \mathbf{P}_i^2 + \delta M_{\mathrm{ct}} \right] + \sum_{i<j} \delta_\Lambda(\mathbf{r}_{ij}) \left(C_S + C_T \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \right) .$$

Keeping the nucleon physical: δM_{ct} fixes the pole; β_K^{ct} fixes the dispersion curvature. Both run with the pion cutoff.

The ingredient: axial pion-nucleon vertex

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

Each application creates or annihilates one pion.

How to represent the enlarged Hilbert space?

Standard nuclear description

$$\Psi_N(R, S, T)$$

Pion dynamics is encoded in
effective interactions and currents.

$\xrightarrow{\text{enlarge the Hilbert space}}$

This work

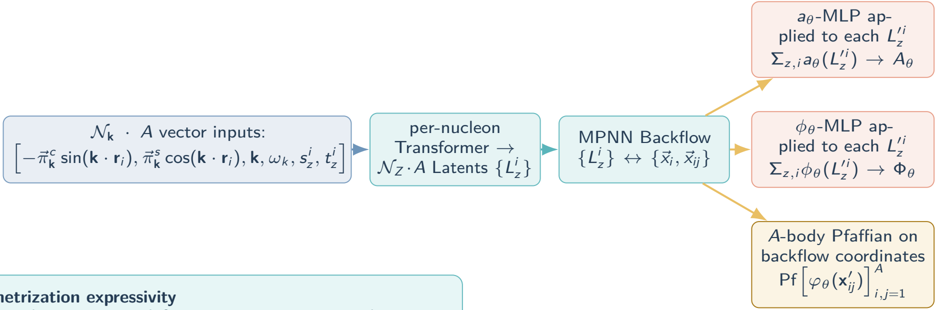
$$\Psi(R, S, T, \Pi)$$

The pion field is sampled
together with the nucleons.

Can we give a parametrization
in terms of neural networks?

Neural ansatze: π-vacuum $\times$ π-cloud deformation $\times$ A-pfaffian

$$\log \Psi_\theta = \underbrace{-\frac{1}{2}\sum_k \omega_k \pi_k^2}_{\pi\text{-vacuum}} + \underbrace{A_\theta(\{L_z'^i\}) + i\Phi_\theta(\{L_z'^i\})}_{\pi\text{-cloud deformation}} + \underbrace{\log \mathrm{Pf}\left[\varphi_\theta(\mathbf{x}'_{ij})\right]_{i,j=1}^{A}}_{A\text{-body antisymmetry}} .$$



Parametrization expressivity
The complex π-vacuum deformation generates excited states:

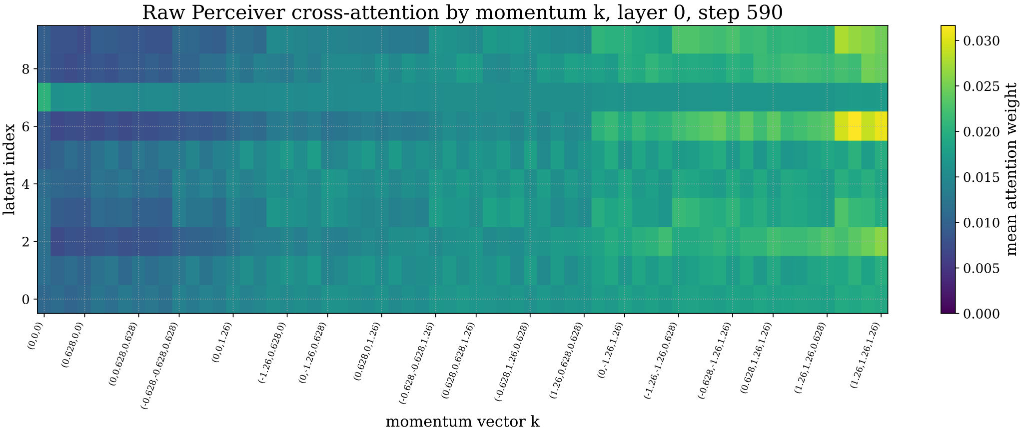
$$A(\pi_k) = \log|\pi_k|\,, \qquad \Phi(\pi_k) = \arg(\pi_k),$$

gives

$$\Psi(\pi_k) \propto \pi_k\, e^{-\omega_k \pi_k^2/2} \propto \psi_1(\pi_k),$$

the first excited harmonic-oscillator state.

Neural ansatze: π-vacuum $\times$ π-cloud deformation $\times$ A-pfaffian



Neural ansatze: π-vacuum $\times$ π-cloud deformation $\times$ A-pfaffian

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$\mathcal{N}_{\mathbf{k}} \cdot A$ vector inputs: $\left[-\vec{\pi}^c_{\mathbf{k}} \sin(\mathbf{k}\cdot\mathbf{r}_i), \vec{\pi}^s_{\mathbf{k}} \cos(\mathbf{k}\cdot\mathbf{r}_i), \mathbf{k}, \omega_k, s_z^i, t_z^i\right]$

per-nucleon Transformer $\to$ $\mathcal{N}_Z \cdot A$ Latents $\{L_z^i\}$

MPNN Backflow $\{L_z^i\} \leftrightarrow \{\vec{x}_i, \vec{x}_{ij}\}$

a_θ-MLP applied to each $L_z'^i$ $\Sigma_{z,i} a_\theta(L_z'^i) \to A_\theta$

ϕ_θ-MLP applied to each $L_z'^i$ $\Sigma_{z,i} \phi_\theta(L_z'^i) \to \Phi_\theta$

A-body Pfaffian on backflow coordinates $\mathrm{Pf}\left[\varphi_\theta(\mathbf{x}_{ij}')\right]_{i,j=1}^{A}$

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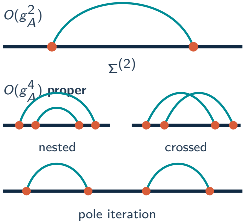
Fourth order tracks the variational result as the cutoff grows

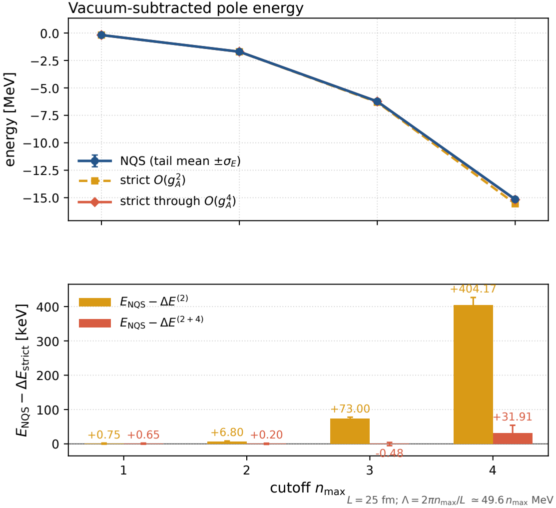
Terms retained in the Self Energy



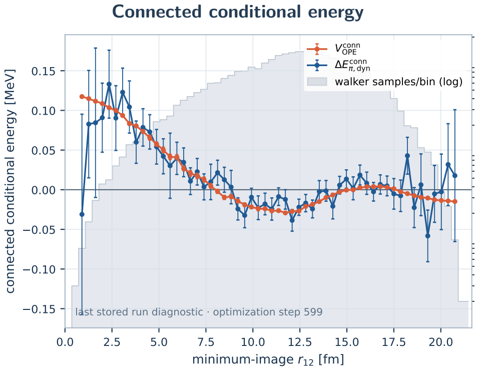
Expansion of Σ at 4-th Order

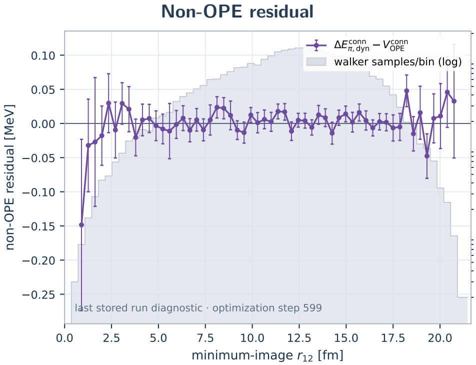
$$\Delta E^{(2+4)}_{\mathrm{pole}} = \Sigma^{(2)} + \Sigma^{(4)}_{\mathrm{nested}} + \Sigma^{(4)}_{\mathrm{crossed}} + \Sigma^{(2)}\,\partial_E \Sigma^{(2)}.$$

The last term is generated by expanding the pole equation; it is not a new proper topology.



The dynamical pion field reproduces the sampled OPE contribution





$$V_{\mathrm{OPE}}(\mathbf{r}) = -\frac{1}{L^3}\frac{g_A^2}{2f_\pi^2}\,\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \sum_{\mathbf{k}}{}' \frac{(\boldsymbol{\sigma}_1\cdot\mathbf{k})(\boldsymbol{\sigma}_2\cdot\mathbf{k})}{\omega_{\mathbf{k}}^{,2}}\cos(\mathbf{k}\cdot\mathbf{r}), \qquad \omega_{\mathbf{k}}^{,2} = \mathbf{k}^2 + m_\pi^2$$

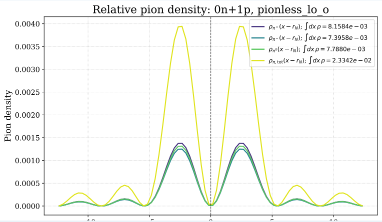
$$\Delta E_{\pi,\mathrm{dyn}} \equiv H_{\mathrm{full}} - T_N$$

Connected Expectation value: $X^{\mathrm{conn}}(r) = \langle X\rangle_r - \langle X\rangle_{\mathrm{ref}}.$

What becomes accessible once the pion is dynamical?

Already accessible

ground-state and elastic information



Charge-resolved pion density $\rho_{\pi^+}, \rho_{\pi^0}, \rho_{\pi^-}$ from $|\Psi_0|^2$; $L = 10$ fm, $n_{\max} = 3$

Equal-time connected correlation

$$C_O(q) = \langle \delta O^\dagger(q) \delta O(q) \rangle$$

total connected strength, without resolving ω

Elastic form factors

axial $G_A(Q^2)$, isovector charge $F_C^{(V)}(Q^2)$

Requires energy resolution

how the strength is distributed in ω

For a chosen current or operator $O(q)$:

Lorentz integral transform (LIT)

$$L_O(\sigma_R, \sigma_I) \xrightarrow{\text{inversion}} R_O(q, \omega)$$

continuum information without constructing each final state

Responses determine the cross section

$$\frac{d^2\sigma}{d\Omega\, d\omega} = \sigma_0 \sum_\alpha v_\alpha R_\alpha(q, \omega)$$

Neutrino–nucleus
inclusive R_V, R_A, R_{VA}

Pion production
spectral strength above the $N\pi$ threshold

Takeaways

01 **Recovered at $O(g_A^4)$ nucleon self energy**

02 **A scalable N-body representation**
for the pion-nuclon neural ansatze

03 **The long-range mechanism emerges**
The dynamical effect of OPE emerges at small cutoffs, without inserting it as an instantaneous NN potential.

→ **NEXT** contact refit and deuteron ⟶ consistent currents and response functions

Thank you