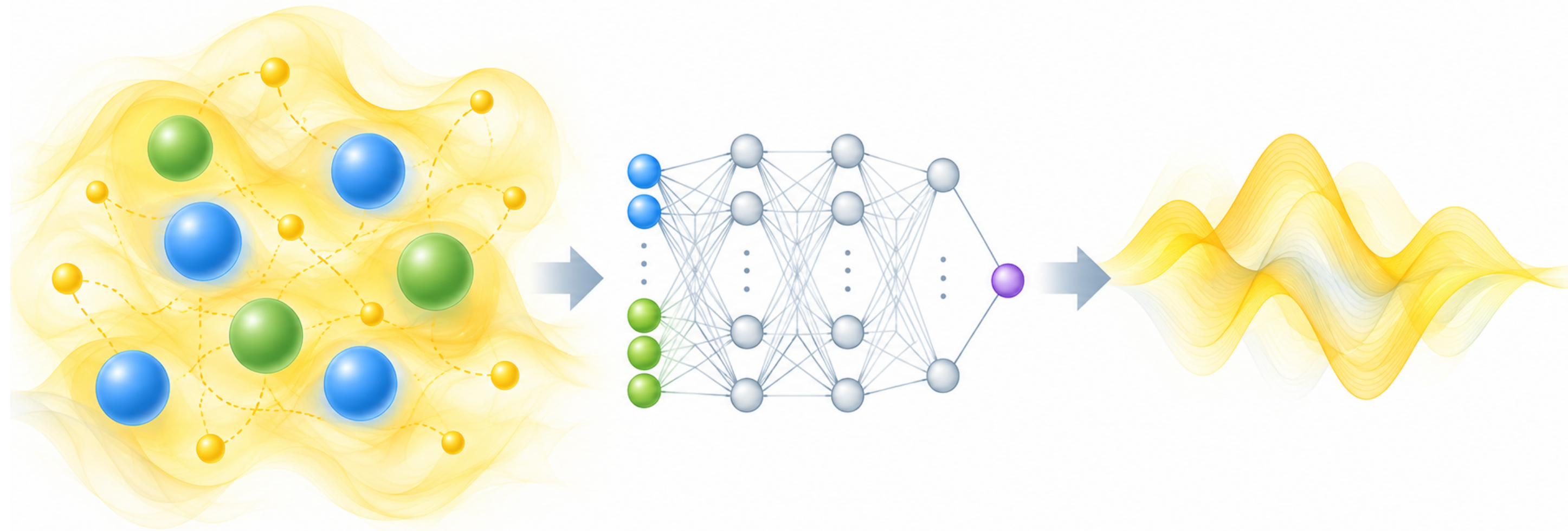


Neural Quantum States for Dynamical Pions and Nucleons



Alessandro Lovato

The 15th International Workshop on the Physics of Excited Nucleons

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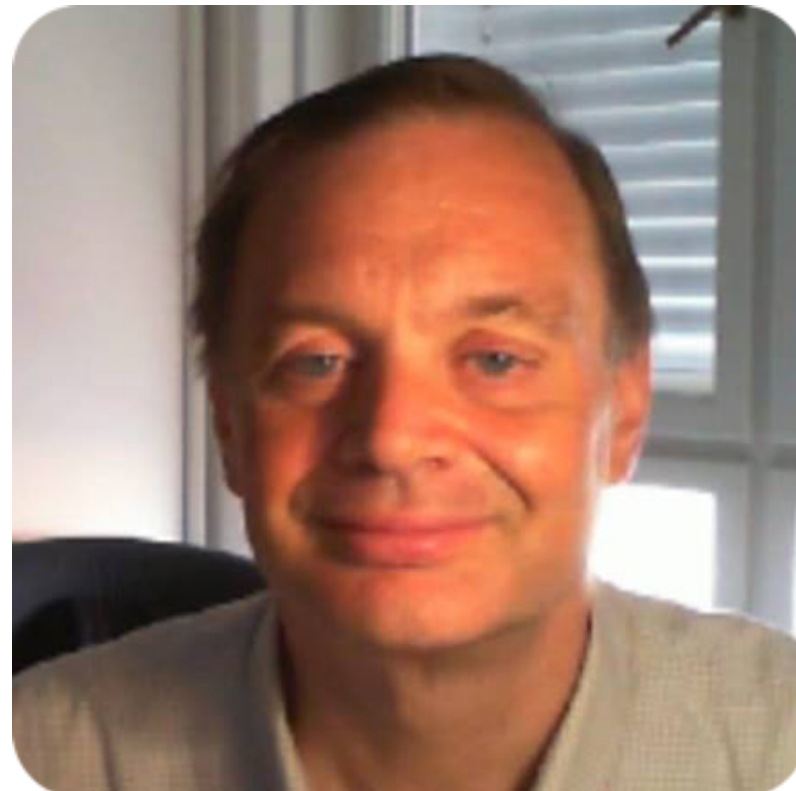
Collaborators



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Lucas Madeira, ECT*

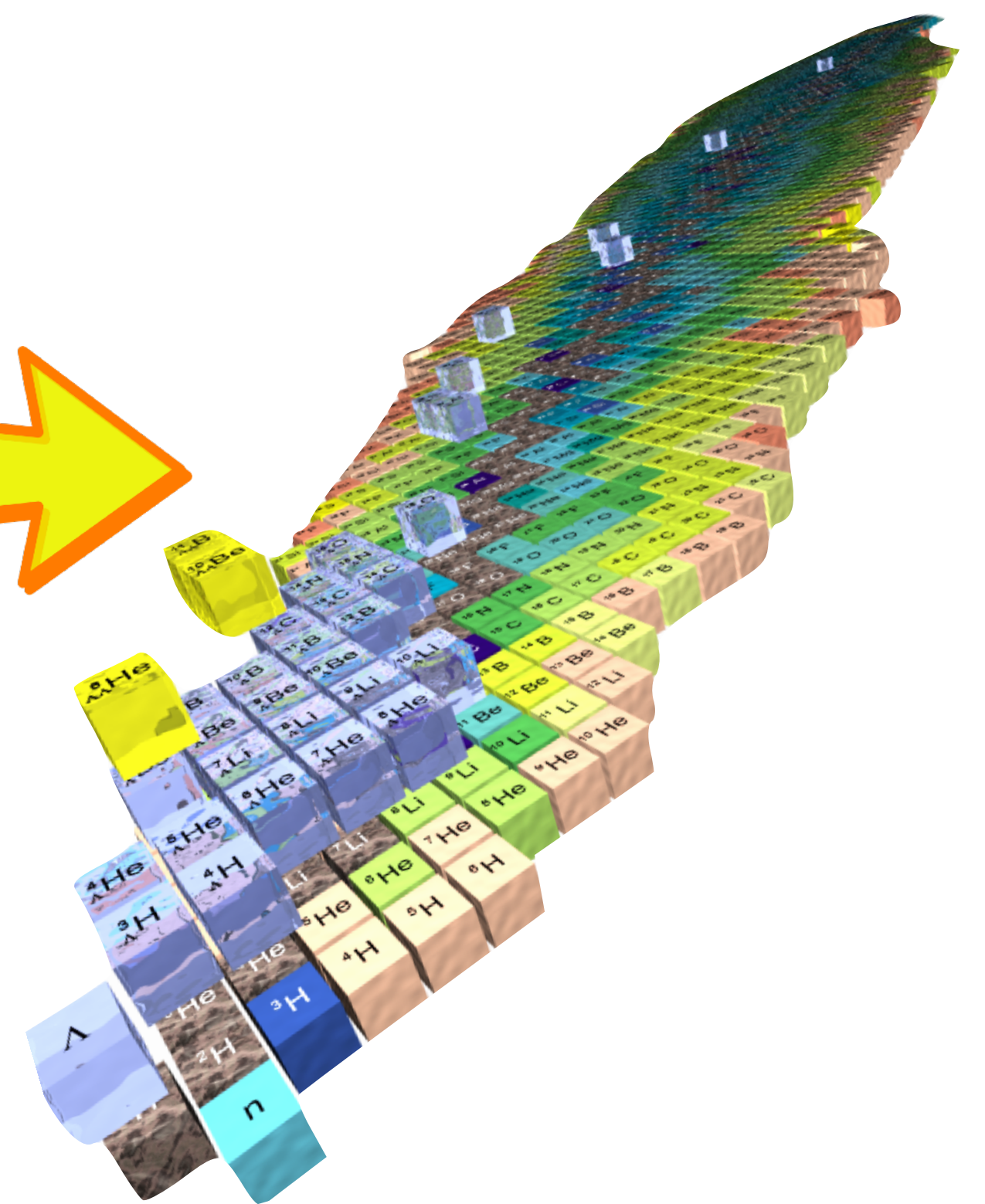
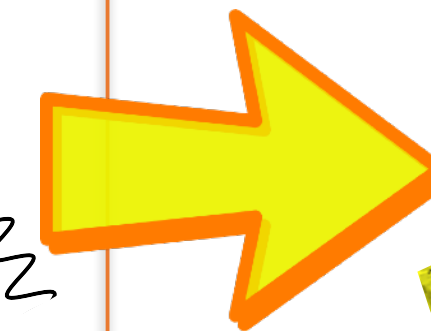
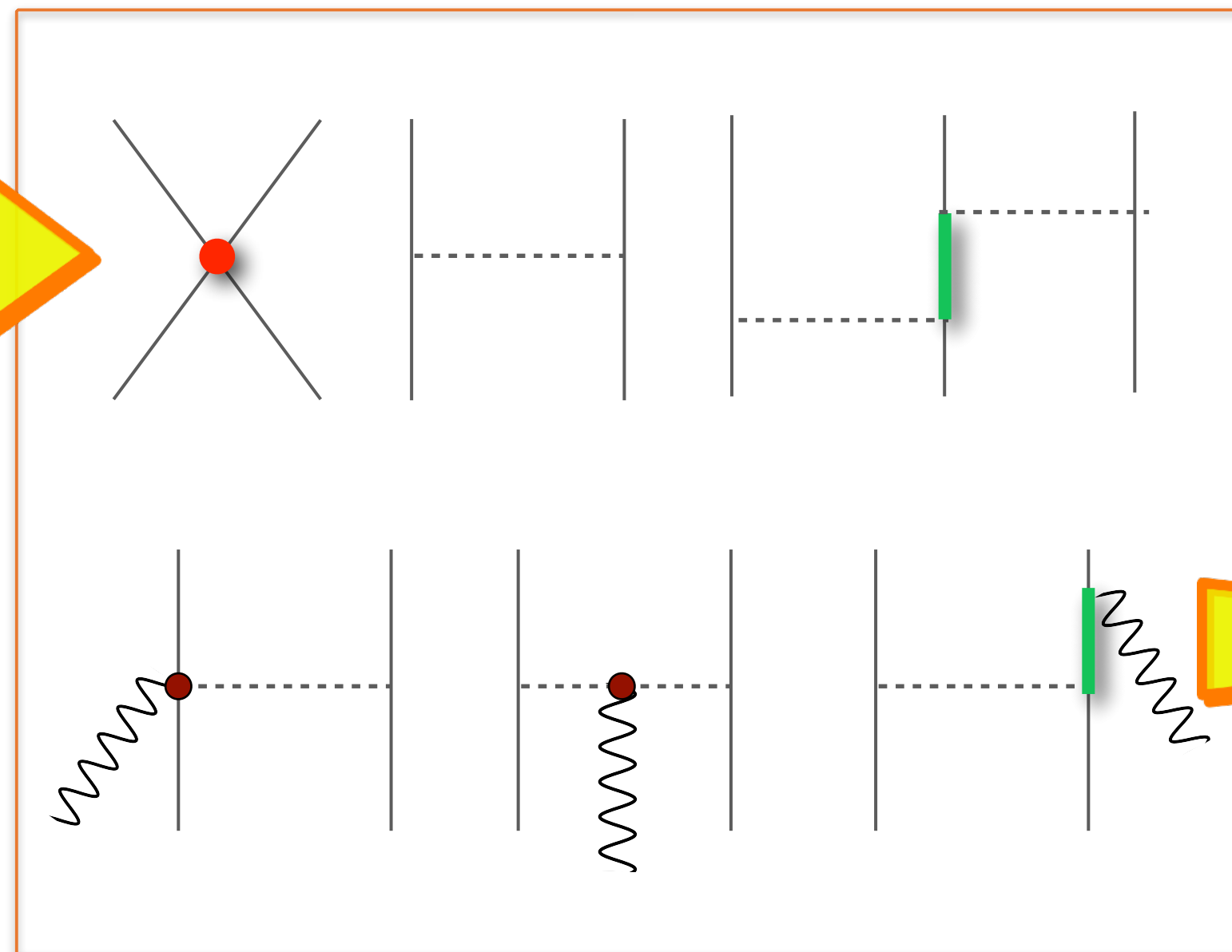
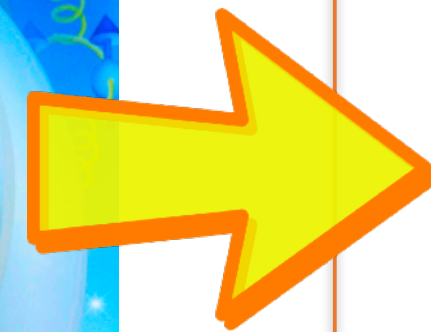
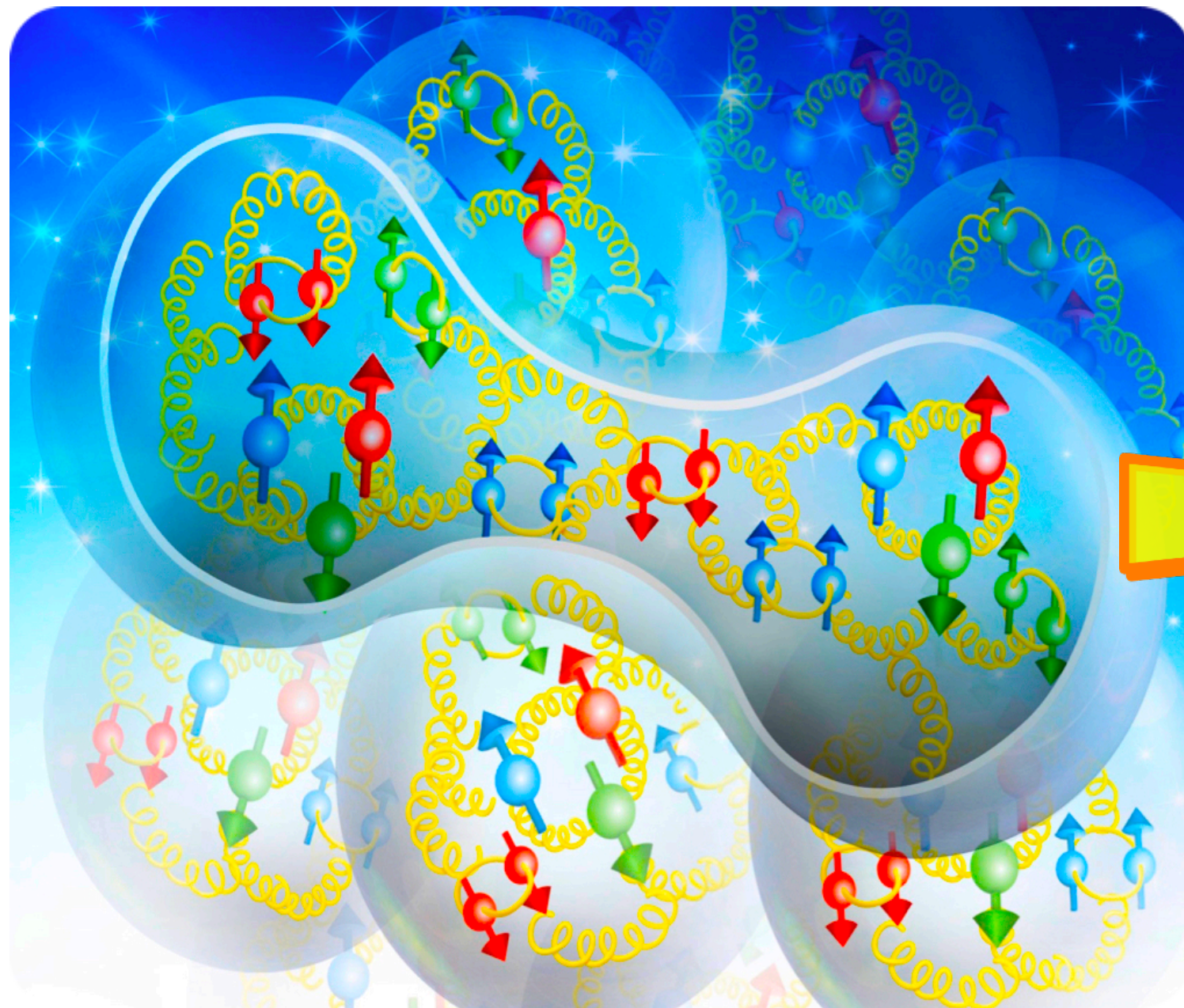


Francesco Pederiva, University of Trento



Kevin Schmidt, Arizona State University

“Ab initio” nuclear physics



“Ab initio” nuclear physics

- Main input: nucleon-only Hamiltonians and consistent currents

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} \quad ; \quad J = \sum_i j_i + \sum_{i<j} j_{ij}$$

- Sophisticated quantum many-body methods solve the corresponding Schrödinger equation

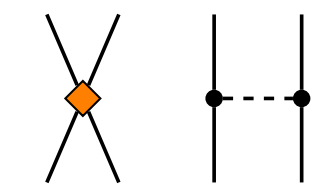
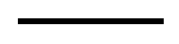
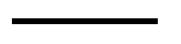
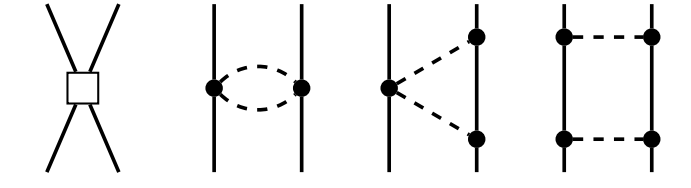
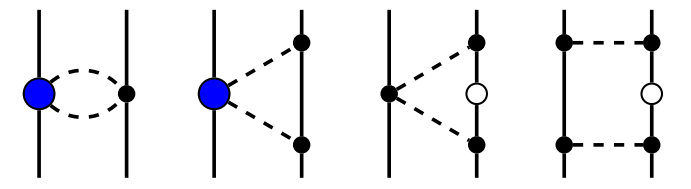
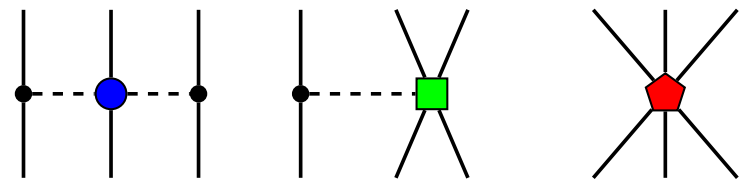
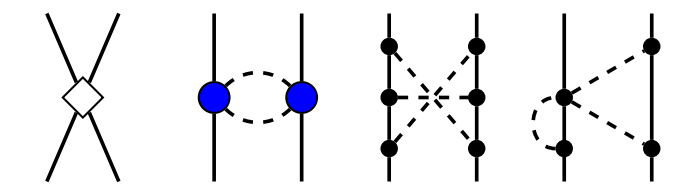
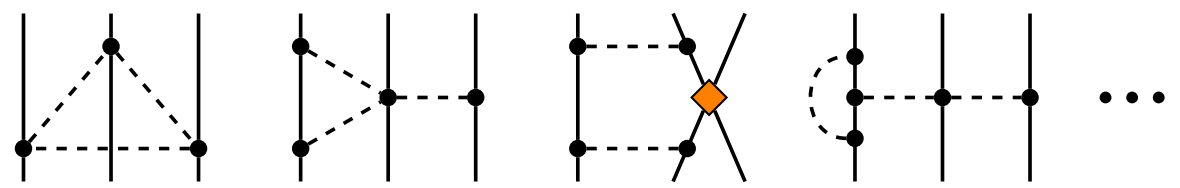
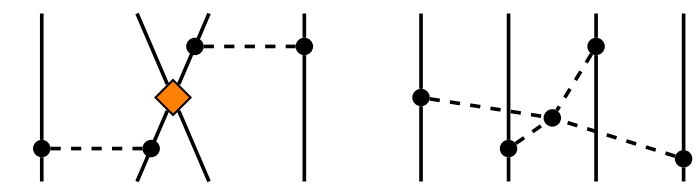
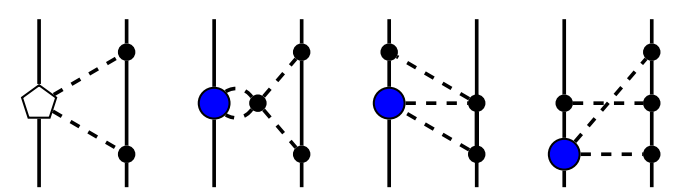
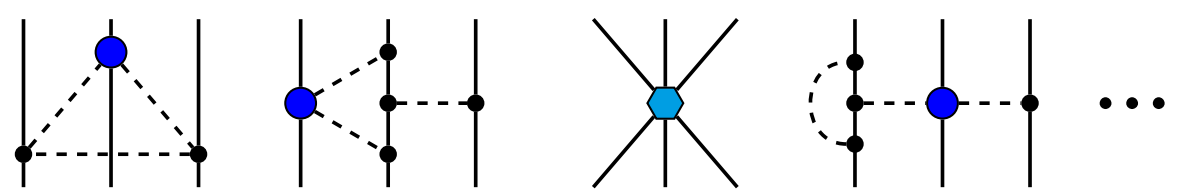
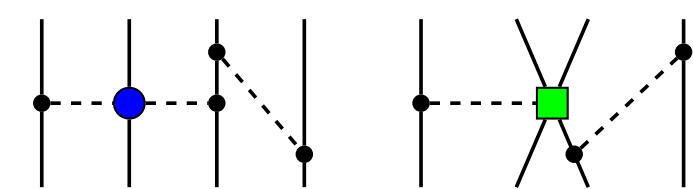
$$H|\Psi_n\rangle = E_n|\Psi_n\rangle \quad ; \quad M_{mn} = \langle\Psi_m|J|\Psi_n\rangle$$

- The “active” Hilbert space comprises the coordinates of the nucleons only (spatial plus spin/isospin)

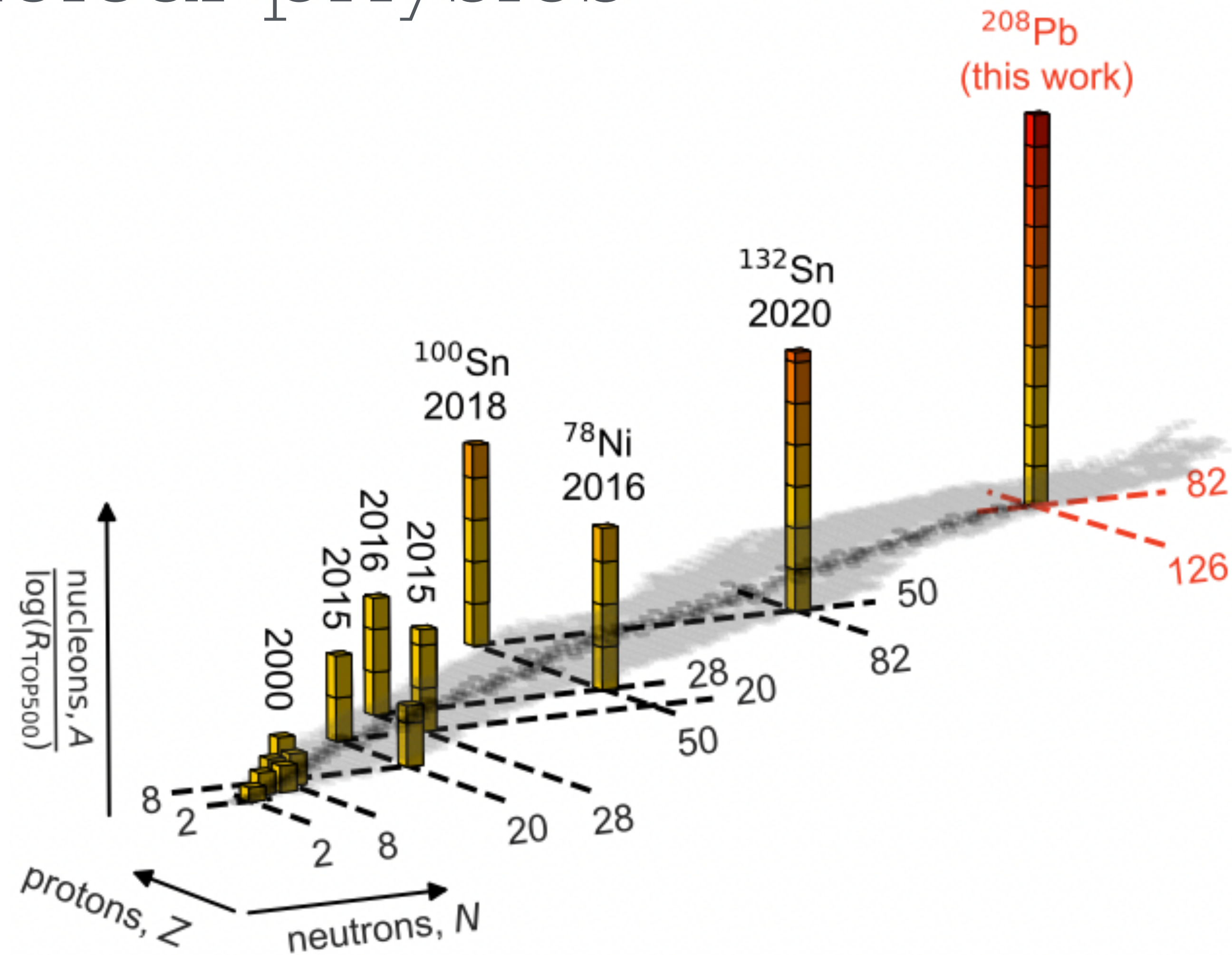
$$\Psi_n(\mathbf{R}, S, T) \equiv \langle\mathbf{R}, S, T|\Psi_n\rangle \quad ; \quad \mathbf{R} \equiv \{\mathbf{r}_1, \dots, \mathbf{r}_A\}, \quad S \equiv \{s_1^z, \dots, s_A^z\}, \quad T \equiv \{t_1^z, \dots, t_A^z\}$$

“Ab initio” nuclear physics

- Pion effects are typically encoded in interactions and currents.

	NN	3N	4N
LO $\mathcal{O}(Q^0/\Lambda^0)$	1990 [151,152] 2 		
NLO $\mathcal{O}(Q^2/\Lambda^2)$	1992 [164,165] 7 	1992,1994 [166-169] 	
N^2LO $\mathcal{O}(Q^3/\Lambda^3)$	1992 [164,165] 0 	1994 [167,170] 2 	
N^3LO $\mathcal{O}(Q^4/\Lambda^4)$	2000–2002 [179-182] 12 	2008–2011 [183-185] 0 	2006 [186] 0 
N^4LO $\mathcal{O}(Q^5/\Lambda^5)$	2015 [188,189] 0 	2011– [190-192] ? 	

“Ab initio” nuclear physics



Why treat pions explicitly?

Goal: include pions as active degrees of freedom in the Hilbert space

$$\Psi_n(\mathbf{R}, S, T) \equiv \langle \mathbf{R}, S, T | \Psi_n \rangle \quad \longrightarrow \quad \Psi_n(\mathbf{R}, S, T; \boldsymbol{\pi}^{c,s}) \equiv \langle \mathbf{R}, S, T; \boldsymbol{\pi}^{c,s} | \Psi_n \rangle$$

- Test the “conventional” potential chiral-EFT power counting
- Automatically obtain the long-range part of nuclear interactions and currents
- Study pion-nucleus scattering
- Additional insights in the EMC effect
- Real pion-production in lepton-nucleus scattering experiments

Few-Body Sys. **61**, 40 (2020), *Phys. Rev. C* **101**, 035202 (2020), *Phys. Rev. C* **53**, 3097 (1996)

Phys. Rev. C **50**, 2761 (1994), *Phys. Rev. C* **70**, 014007 (2004)

Why treat pions explicitly?

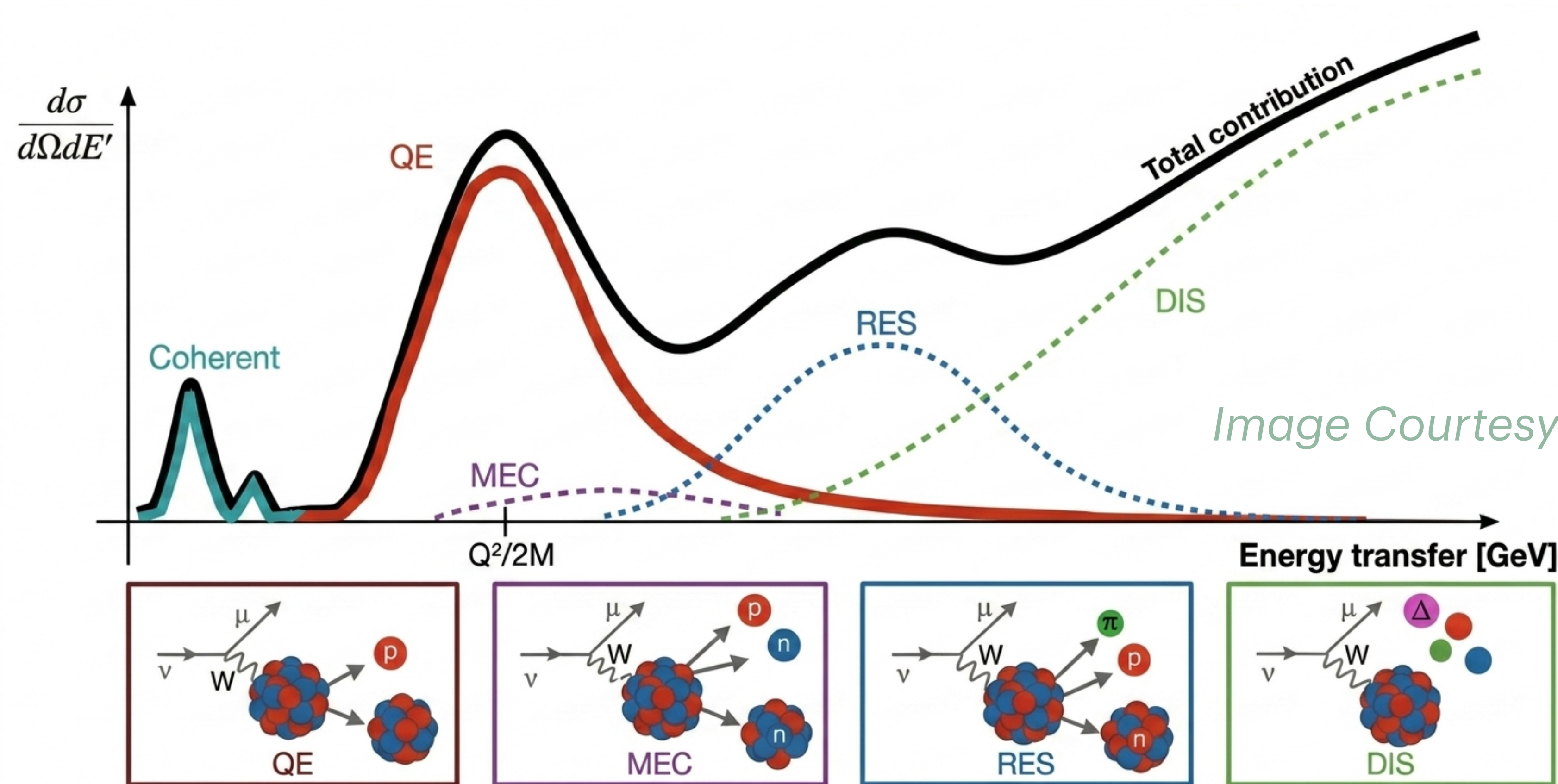


Image Courtesy of Noemi Rocco

Alexis' and Seisho's talks yesterday

Rocco's talk tomorrow

How to include pions?

- Nucleons are heavy; they can be treated as non-relativistic, point-like particles.
- Pions are light, need to treat them as relativistic quantum fields.
- Start from leading-order chiral-EFT Lagrangian in the heavy-baryon formalism

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

How to include pions?

- To leverage a variational principle, we need the Hamiltonian

$$\Pi_N \equiv \frac{\partial \mathcal{L}_0}{\partial(\partial_0 N)} = iN^\dagger \quad ; \quad \Pi_{N^\dagger} \equiv \frac{\partial \mathcal{L}_0}{\partial(\partial_0 N^\dagger)} = 0 \quad ; \quad \Pi_k \equiv \frac{\partial \mathcal{L}_0}{\partial(\partial_0 \pi_k)} = \partial_0 \pi_k - \frac{1}{4f_\pi^2} \epsilon_{ijk} \pi_j N^\dagger \tau_i N.$$

- The Hamiltonian splits into three components

$$H = H_{\pi\pi} + H_{\pi N} + H_{NN} \quad \left\{ \begin{array}{l} H_{\pi\pi} = \frac{1}{2} \int d^3x \left[\Pi_i^2 + (\nabla \pi_i)^2 + m_\pi^2 \pi_i^2 \right]. \\ H_{\pi N} = \int d^3x N^\dagger \left[\frac{g_A}{2f_\pi} \tau_i (\boldsymbol{\sigma} \cdot \nabla) \pi_i + \frac{1}{4f_\pi^2} \epsilon_{ijk} \tau_i \pi_j \Pi_k \right] N. \\ H_{NN} = \int d^3x \left[N^\dagger \left(-\frac{\nabla^2}{2M_0} + M_0 \right) N + \frac{C_S}{2} (N^\dagger N)^2 + \frac{C_T}{2} (N^\dagger \boldsymbol{\sigma} N)^2 \right]. \end{array} \right.$$

Pure pionic sector

- In the Cartesian basis, the pion fields are Hermitian

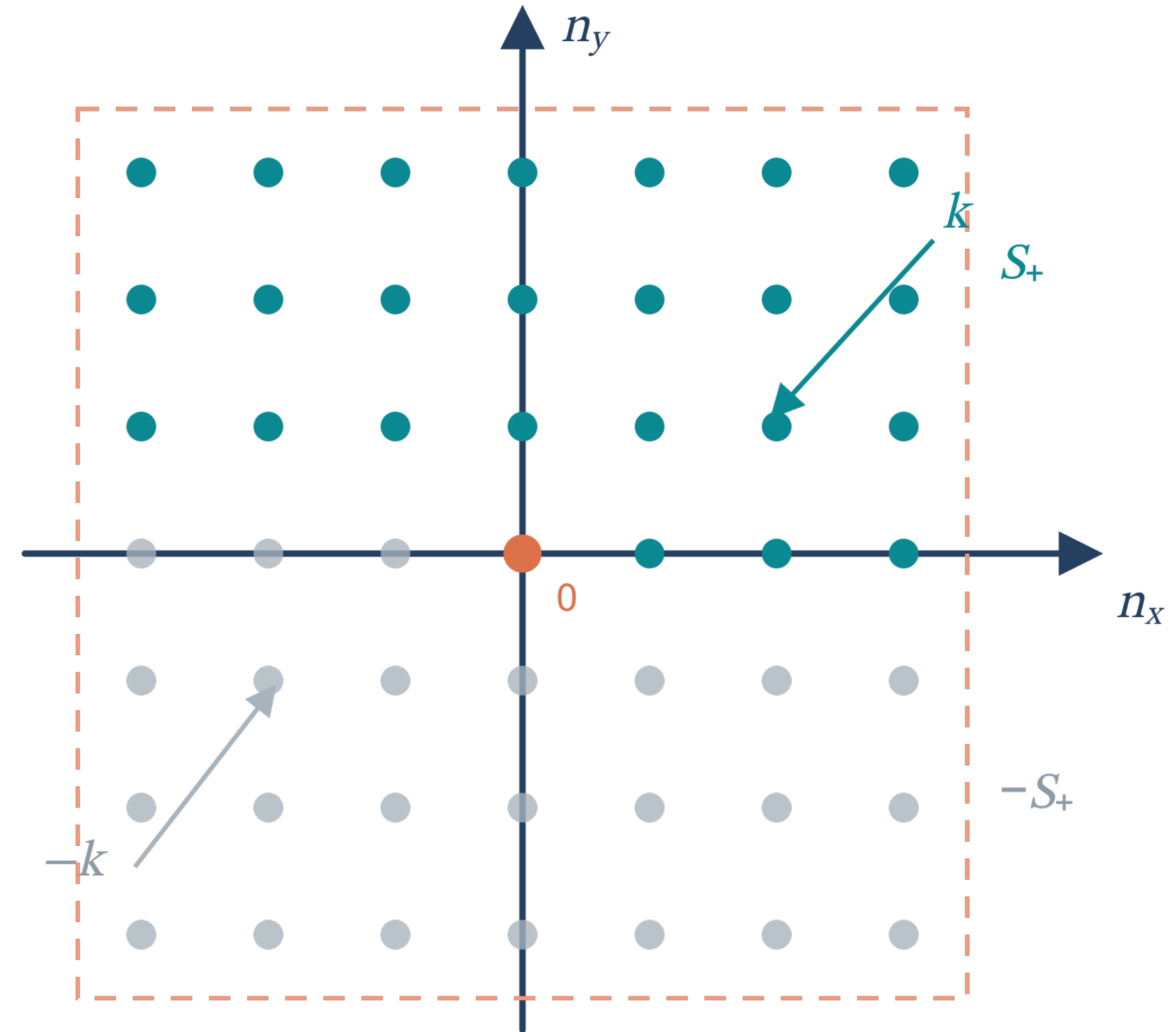
$$\pi_i^\dagger(\mathbf{x}) = \pi_i(\mathbf{x}), \quad \mathbf{k} = \frac{2\pi}{L}\mathbf{n}, \quad V = L^3.$$

- The normalized expansions are

$$\left\{ \begin{array}{l} \pi_i(\mathbf{x}) = \sqrt{\frac{2}{L^3}} \sum_{\mathbf{k} \in \mathcal{S}_+} [\pi_{i\mathbf{k}}^c \cos(\mathbf{k} \cdot \mathbf{x}) + \pi_{i\mathbf{k}}^s \sin(\mathbf{k} \cdot \mathbf{x})] \\ \Pi_i(\mathbf{x}) = \sqrt{\frac{2}{L^3}} \sum_{\mathbf{k} \in \mathcal{S}_+} [\Pi_{i\mathbf{k}}^c \cos(\mathbf{k} \cdot \mathbf{x}) + \Pi_{i\mathbf{k}}^s \sin(\mathbf{k} \cdot \mathbf{x})] \end{array} \right.$$

- The Hamiltonian is a collection of harmonic oscillators

$$H_{\pi\pi} = \sum'_{\mathbf{k} \in \mathcal{S}_+} \sum_{i=x,y,z} \left[\frac{1}{2} \Pi_{i\mathbf{k}}^c{}^2 + \frac{1}{2} \Pi_{i\mathbf{k}}^s{}^2 + \frac{1}{2} \omega_{\mathbf{k}}^2 (\pi_{i\mathbf{k}}^c{}^2 + \pi_{i\mathbf{k}}^s{}^2) \right].$$



Pure pionic sector

- Let us quantize the fields

$$\begin{aligned} [\pi_i(\mathbf{x}), \pi_j(\mathbf{y})] &= [\Pi_i(\mathbf{x}), \Pi_j(\mathbf{y})] = 0, \\ [\pi_i(\mathbf{x}), \Pi_j(\mathbf{y})] &= i \delta_{ij} \delta_L^{(3)}(\mathbf{x} - \mathbf{y}). \end{aligned} \quad \longrightarrow \quad \left\{ \begin{aligned} [\pi_{i\mathbf{k}}^c, \Pi_{j\mathbf{k}'}^c] &= i \delta_{ij} \delta_{\mathbf{k},\mathbf{k}'}, \\ [\pi_{i\mathbf{k}}^s, \Pi_{j\mathbf{k}'}^s] &= i \delta_{ij} \delta_{\mathbf{k},\mathbf{k}'}, \\ [\pi_{i\mathbf{k}}^c, \Pi_{j\mathbf{k}'}^s] &= [\pi_{i\mathbf{k}}^s, \Pi_{j\mathbf{k}'}^c] = 0. \end{aligned} \right.$$

- Analogously to the quantum harmonic oscillator

$$\Pi_{i\mathbf{k}}^{c,s} \longrightarrow -i \frac{\partial}{\partial \pi_{i\mathbf{k}}^{c,s}}. \quad \longrightarrow \quad H_{\pi\pi} = \sum'_{\mathbf{k} \in \mathcal{S}_+} \sum_{i=x,y,z} \left[-\frac{1}{2} \frac{\partial^2}{\partial \pi_{i\mathbf{k}}^{c2}} - \frac{1}{2} \frac{\partial^2}{\partial \pi_{i\mathbf{k}}^{s2}} + \frac{1}{2} \omega_{\mathbf{k}}^2 (\pi_{i\mathbf{k}}^{c2} + \pi_{i\mathbf{k}}^{s2}) \right].$$

- The ground-state is a product of gaussians

$$\Psi_0(\boldsymbol{\pi}^{c,s}) \propto \exp \left[- \sum'_{\mathbf{k} \in \mathcal{S}_+} \sum_{i=x,y,z} \frac{\omega_{\mathbf{k}}}{2} (\pi_{i\mathbf{k}}^{c2} + \pi_{i\mathbf{k}}^{s2}) \right].$$

Adding nucleons

- The axial-vector part of the Hamiltonian reads:

$$H_{AV} = \sum_{a=1}^A \frac{g_A}{2f_\pi} \sqrt{\frac{2}{L^3}} \sum_{\mathbf{k} \in \mathcal{S}_+} (\boldsymbol{\sigma}_a \cdot \mathbf{k}) \left[(\boldsymbol{\tau}_a \cdot \boldsymbol{\pi}_{\mathbf{k}}^s) \cos(\mathbf{k} \cdot \mathbf{r}_a) - (\boldsymbol{\tau}_a \cdot \boldsymbol{\pi}_{\mathbf{k}}^c) \sin(\mathbf{k} \cdot \mathbf{r}_a) \right].$$

- The nucleonic part is given by:

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


Kinetic mass counter-term

Rest mass counter-term

Solve the many-body problem (“old” way)

- **Goal:** solve the Schrödinger equation for the full Hamiltonian

$$H = H_{\pi\pi} + H_N + H_{\pi N} \quad \longleftrightarrow \quad \langle \mathbf{R}, \mathcal{S}, \mathcal{T}; \boldsymbol{\pi} | \hat{H} | \Psi_0 \rangle = E_0 \Psi_0(\mathbf{R}, \mathcal{S}, \mathcal{T}; \boldsymbol{\pi})$$

- Trial wave function: collection of shifted harmonic oscillators

$$\Psi_T(\mathbf{R}, S, T; \boldsymbol{\pi}^{c,s}) = \left\langle \mathbf{R}, S, T; \boldsymbol{\pi}^{c,s} \left| \exp \left[- \sum_{\mathbf{k} \in \mathcal{S}_+} \frac{\omega_{\mathbf{k}}}{2} \left(|\tilde{\boldsymbol{\pi}}_{\mathbf{k}}^c|^2 + |\tilde{\boldsymbol{\pi}}_{\mathbf{k}}^s|^2 \right) \right] \right| \Phi \right\rangle$$

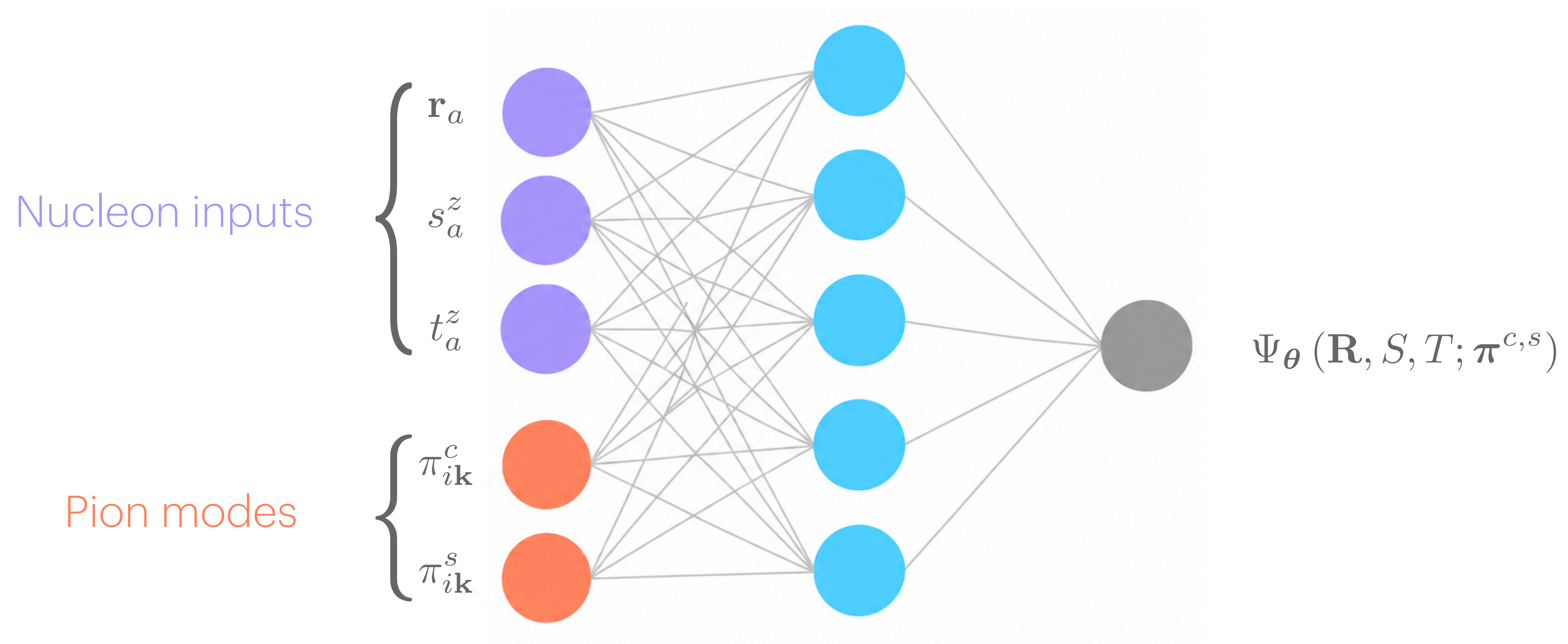
$$\mathbf{B}_{\mathbf{k}}^c \equiv \sqrt{\frac{2}{L^3}} \frac{g_A}{f_\pi} \sum_{a=1}^A \boldsymbol{\tau}_a \sin(\mathbf{k} \cdot \mathbf{r}_a) (\boldsymbol{\sigma}_a \cdot \mathbf{k}) \quad ; \quad \mathbf{B}_{\mathbf{k}}^s \equiv -\sqrt{\frac{2}{L^3}} \frac{g_A}{f_\pi} \sum_{a=1}^A \boldsymbol{\tau}_a \cos(\mathbf{k} \cdot \mathbf{r}_a) (\boldsymbol{\sigma}_a \cdot \mathbf{k})$$

- Exact ground state is obtained by means of imaginary-time projection

$$|\Psi_0\rangle \propto \lim_{\tau \rightarrow \infty} \exp[-(H - E_T)\tau] |\Psi_T\rangle$$

Solve the many-body problem (“NQS” way)

- We represent the quantum many-body wave function with artificial neural networks



$$\Psi_{\theta}(\mathbf{R}, S, T; \boldsymbol{\pi}^{c,s}) = \exp \left[-\frac{1}{2} \sum_{\mathbf{k} \in \mathcal{S}_+} \omega_{\mathbf{k}} \left(|\boldsymbol{\pi}_{\mathbf{k}}^c|^2 + |\boldsymbol{\pi}_{\mathbf{k}}^s|^2 \right) + A_{\theta}(\mathcal{L}) + i\Phi_{\theta}(\mathcal{L}) \right] \text{Pf}[\varphi_{\theta}(\mathcal{X})]$$

Mass renormalization

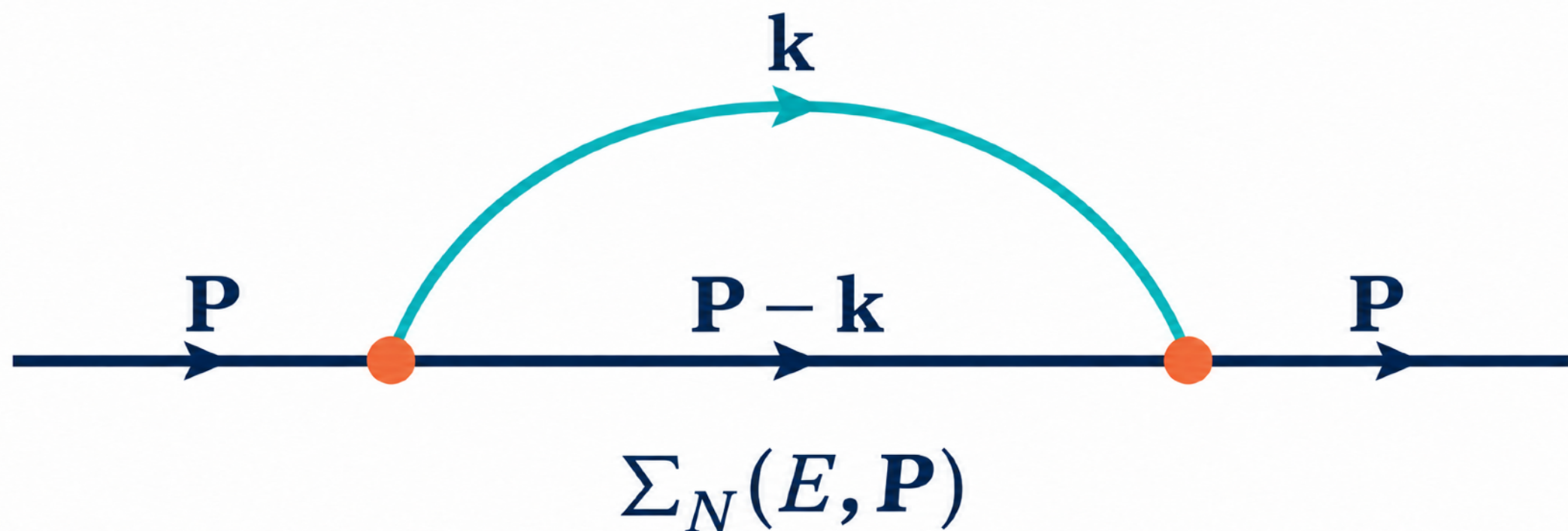
- The momentum cutoff is not Lorentz invariant $\longrightarrow \delta M$ and β_K must be fixed independently

$$E_N(\mathbf{P}) = M_P + \delta M + \left(\frac{1}{2M_P} + \beta_K \right) \mathbf{P}^2 + \Sigma_N(E_N(\mathbf{P}), \mathbf{P})$$

- The renormalization conditions are

$$E_N(\mathbf{0}) = M_P, \quad \left. \frac{\partial E_N(\mathbf{P})}{\partial \mathbf{P}^2} \right|_{\mathbf{P}=\mathbf{0}} = \frac{1}{2M_P}. \quad \longrightarrow \quad E_N(\mathbf{P}) = M_P + \frac{\mathbf{P}^2}{2M_P} + \mathcal{O}(\mathbf{P}^4)$$

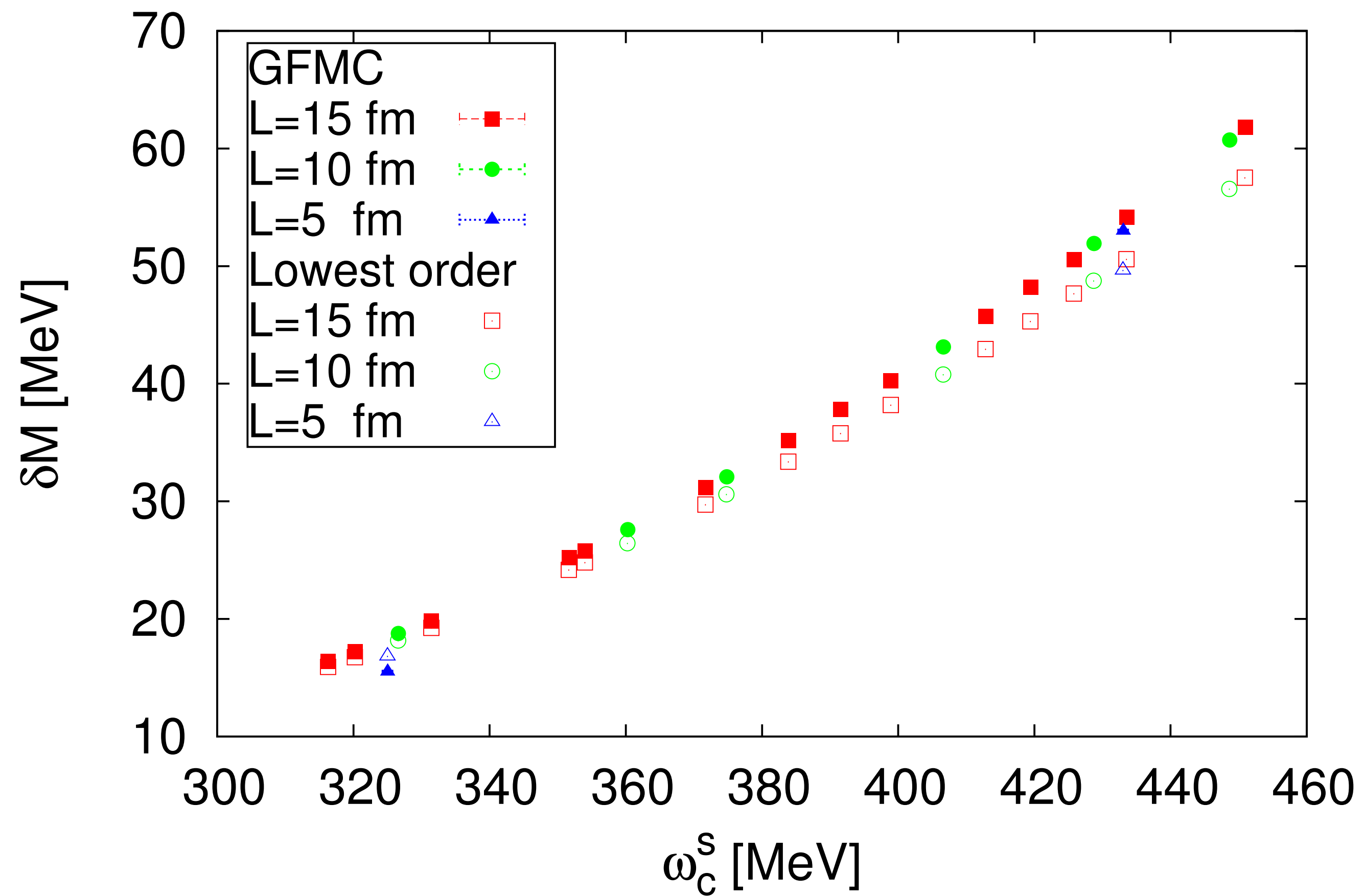
- At one-loop level:



$$\Sigma_N(E, \mathbf{P}) = \frac{3}{2} \left(\frac{g_A}{2f_\pi} \right)^2 \frac{1}{L^3} \sum_{\mathbf{k}}^{(\Lambda)} \frac{\mathbf{k}^2}{\omega_{\mathbf{k}}} \frac{1}{E - E_{N\pi}^{(0)}(\mathbf{P}, \mathbf{k}) + i0}.$$

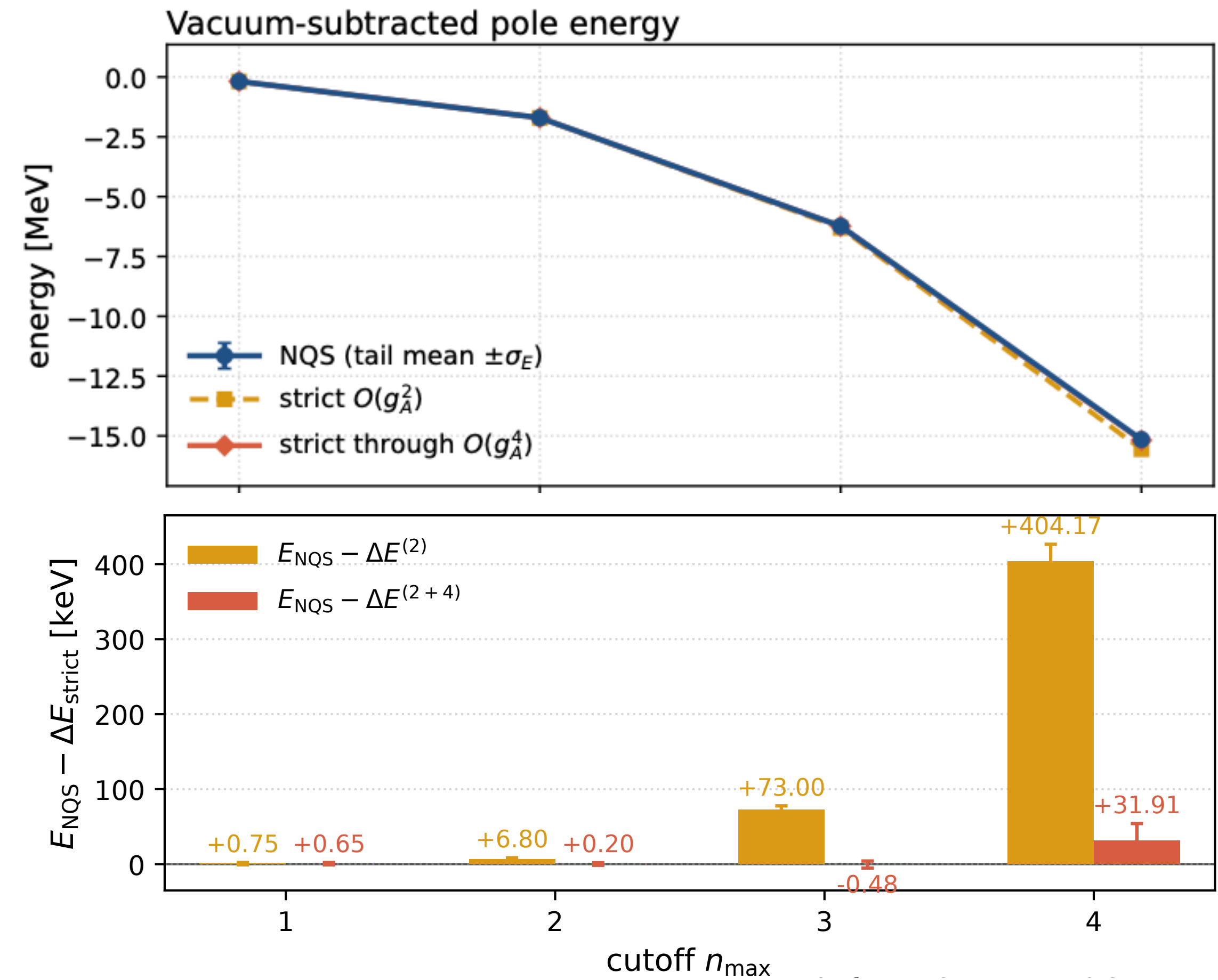
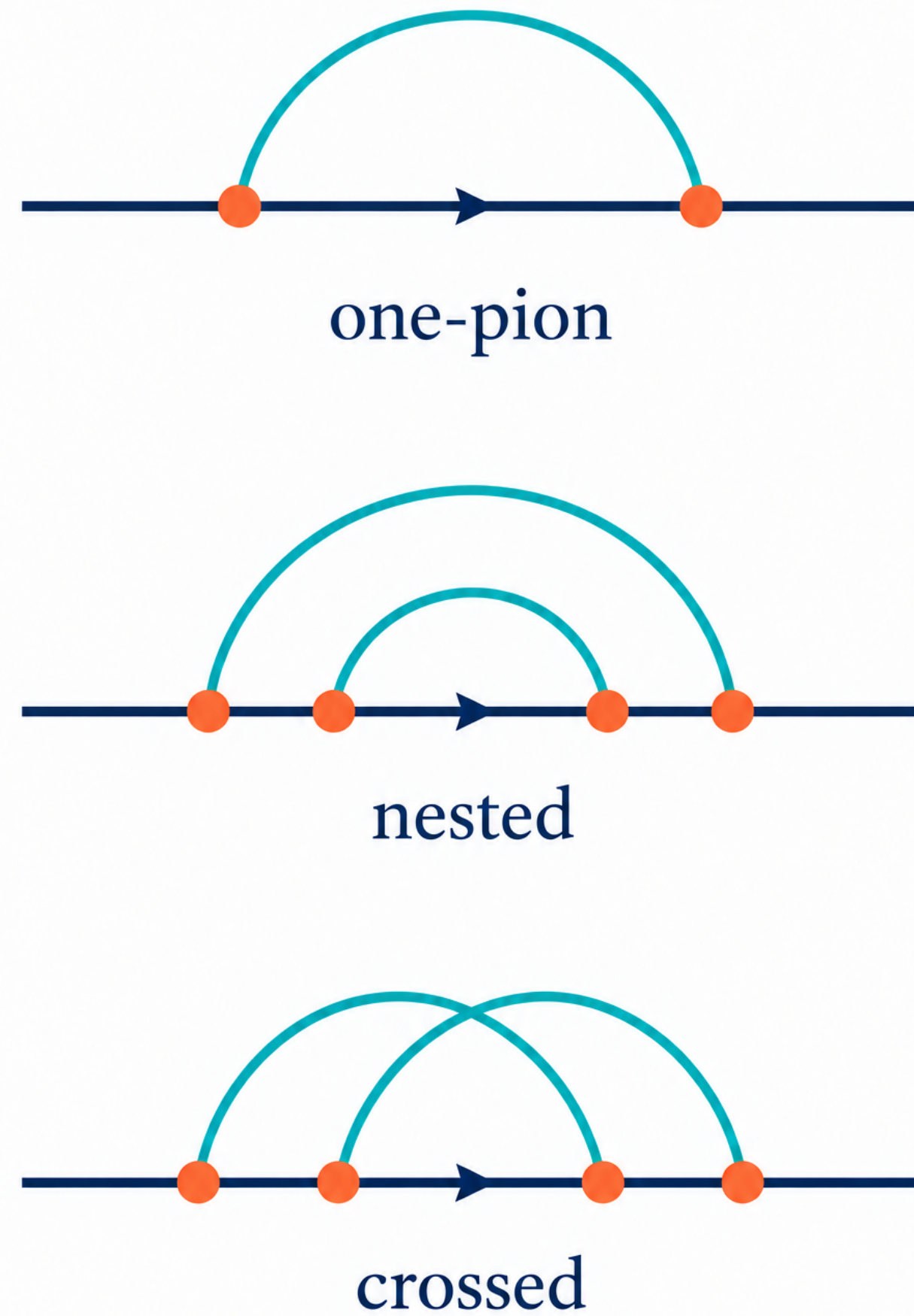
Mass renormalization

- Total energy of a single nucleon is equal to the physical mass of the nucleon



Mass renormalization

- Including fourth-order irreducible contributions largely accounts for the difference from the NQS result.



The pion cloud

- Define the pion annihilation field in the Cartesian isospin basis

$$\psi_i(\mathbf{x}) = \frac{1}{\sqrt{L^3}} \sum_{\mathbf{k}} a_{i\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}$$

- The corresponding isospin fields are given by

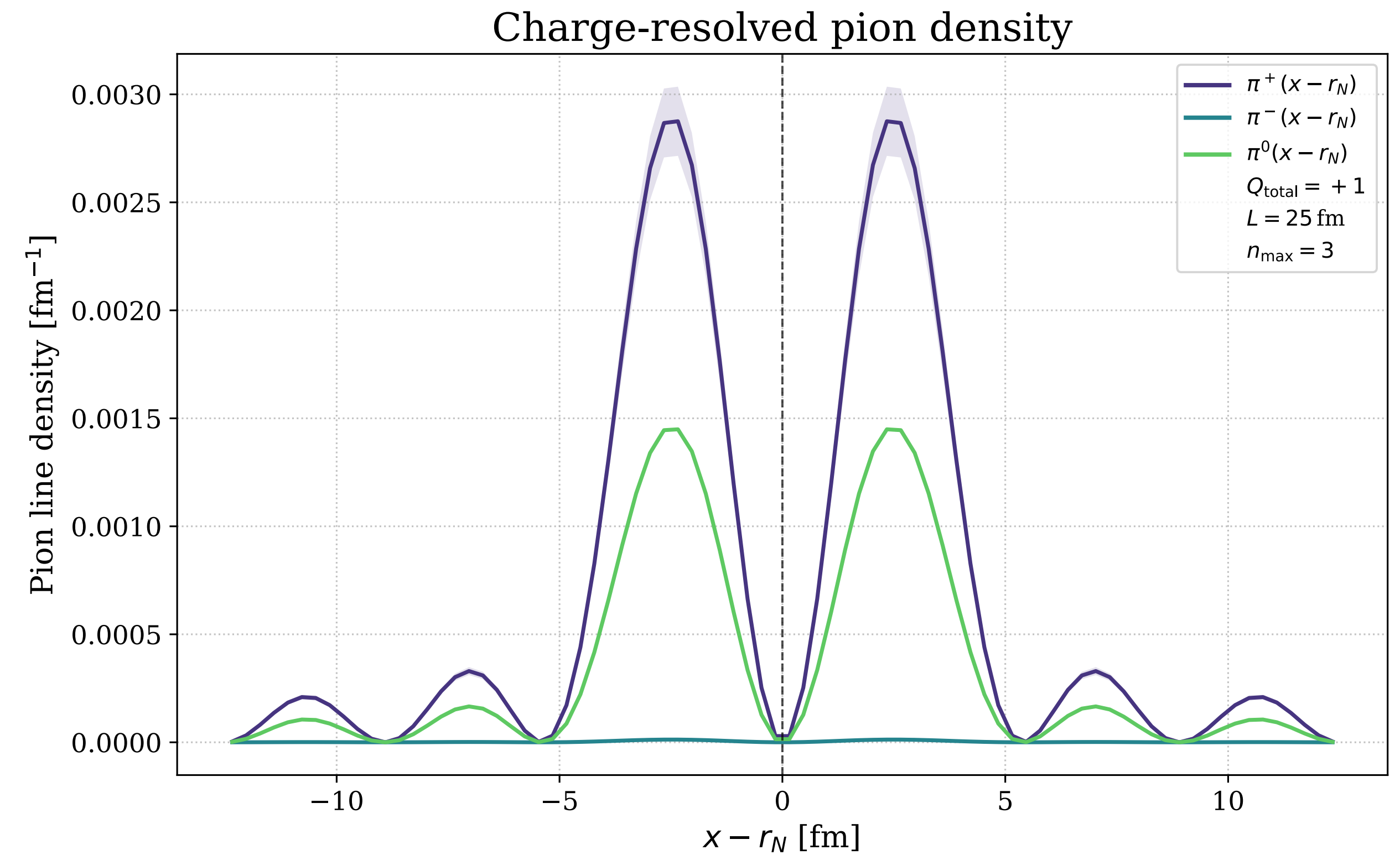
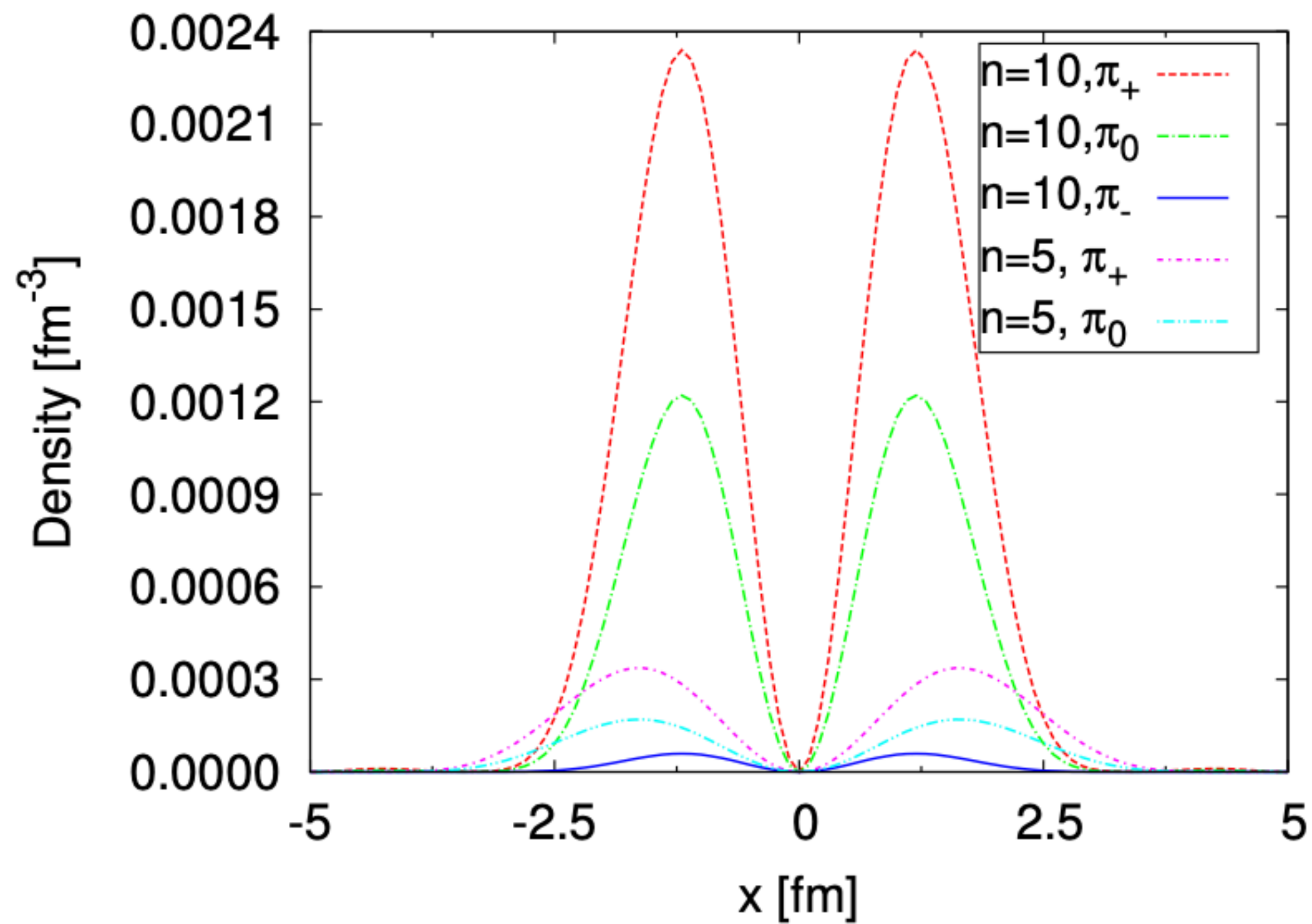
$$\psi_{\pi^\pm}(\mathbf{x}) = \frac{\psi_x(\mathbf{x}) \pm i \psi_y(\mathbf{x})}{\sqrt{2}}, \quad \psi_{\pi^0}(\mathbf{x}) = \psi_z(\mathbf{x})$$

- So that the pion clouds can be expressed as

$$\rho_{\pi^\alpha}(\mathbf{x}) = \left\langle \Psi \left| \psi_{\pi^\alpha}^\dagger(\mathbf{x}) \psi_{\pi^\alpha}(\mathbf{x}) \right| \Psi \right\rangle, \quad \alpha = +, -, 0$$

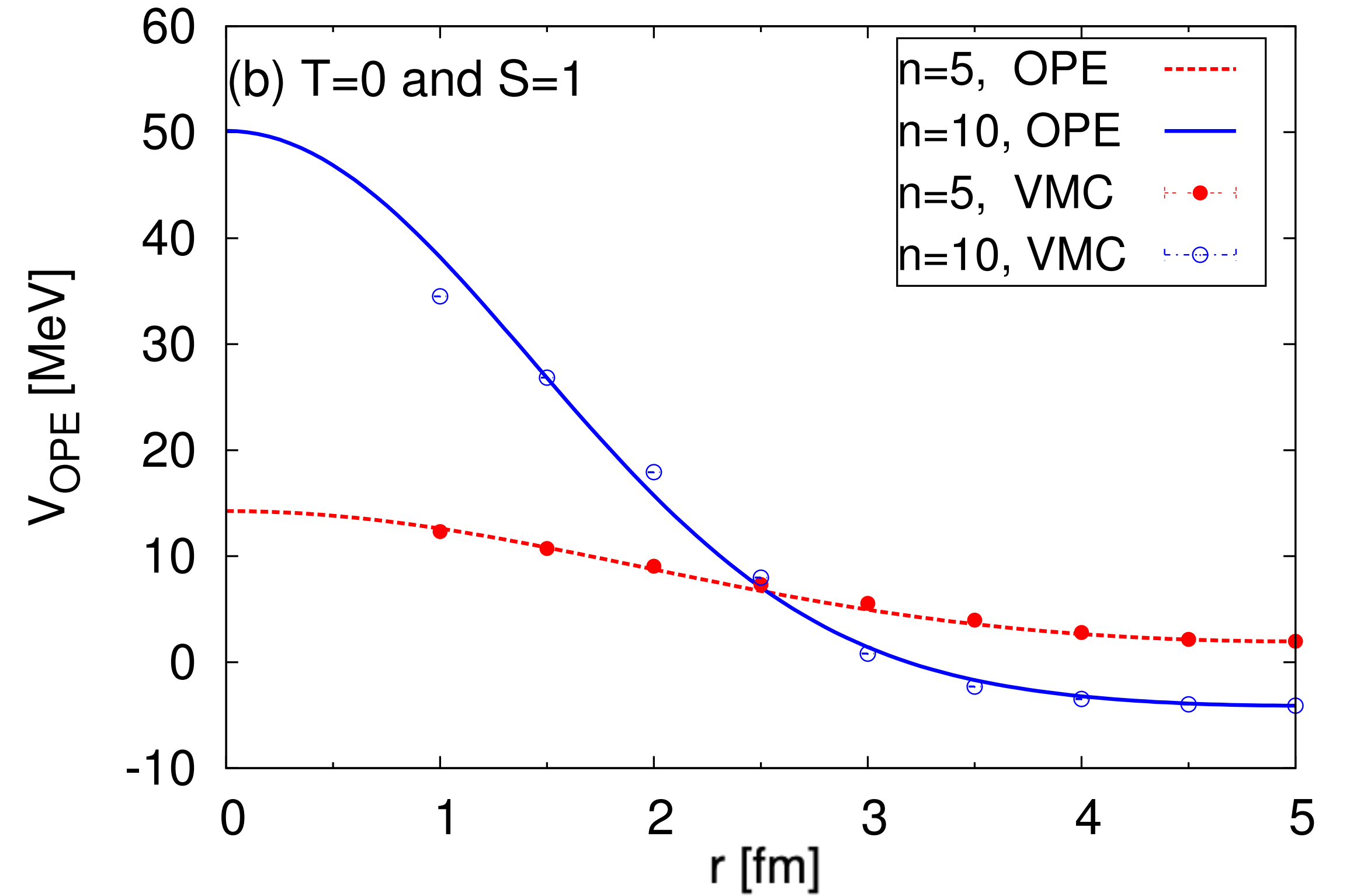
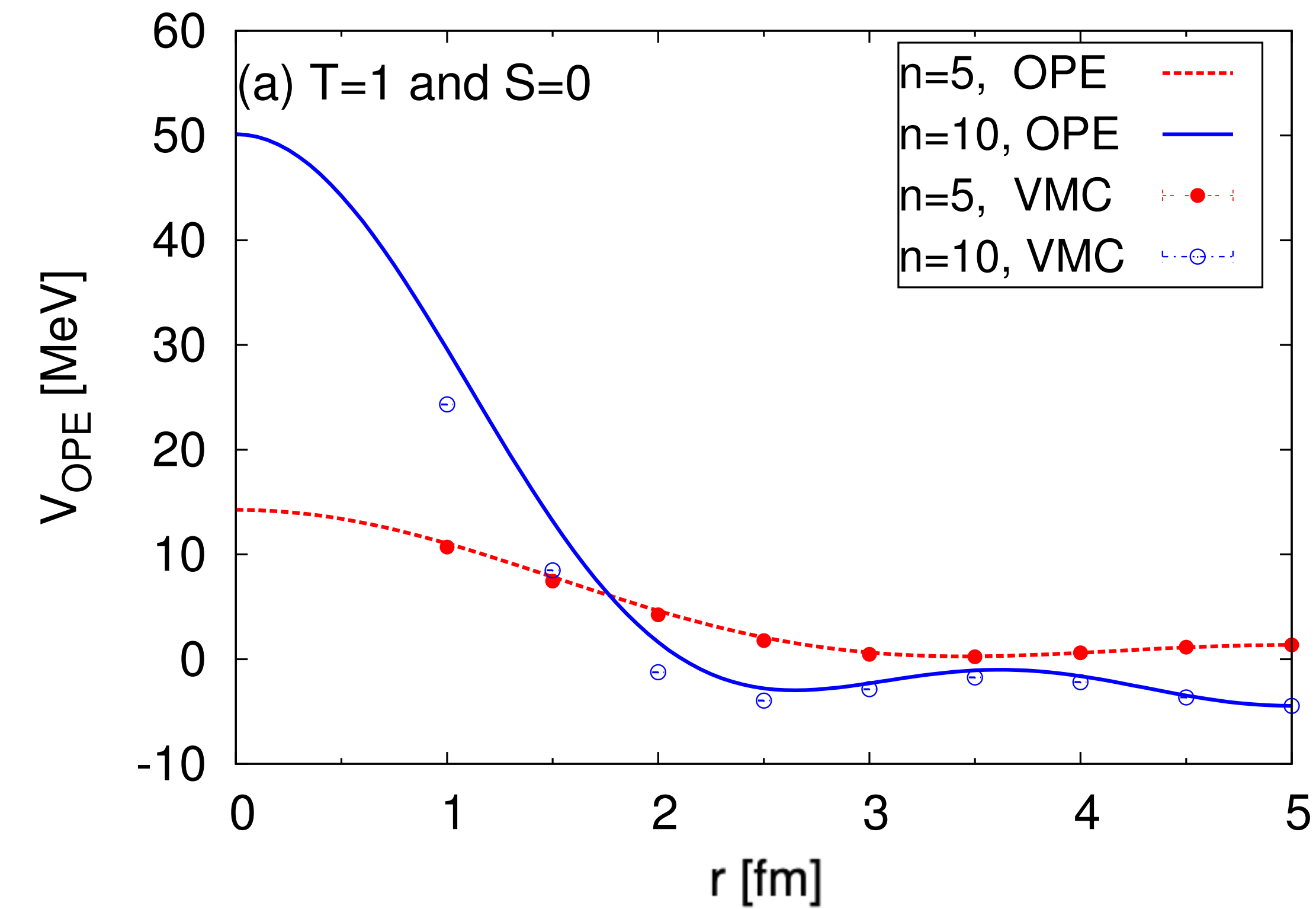
The pion cloud

- Compute the densities at a proton sitting at the center of the simulation box



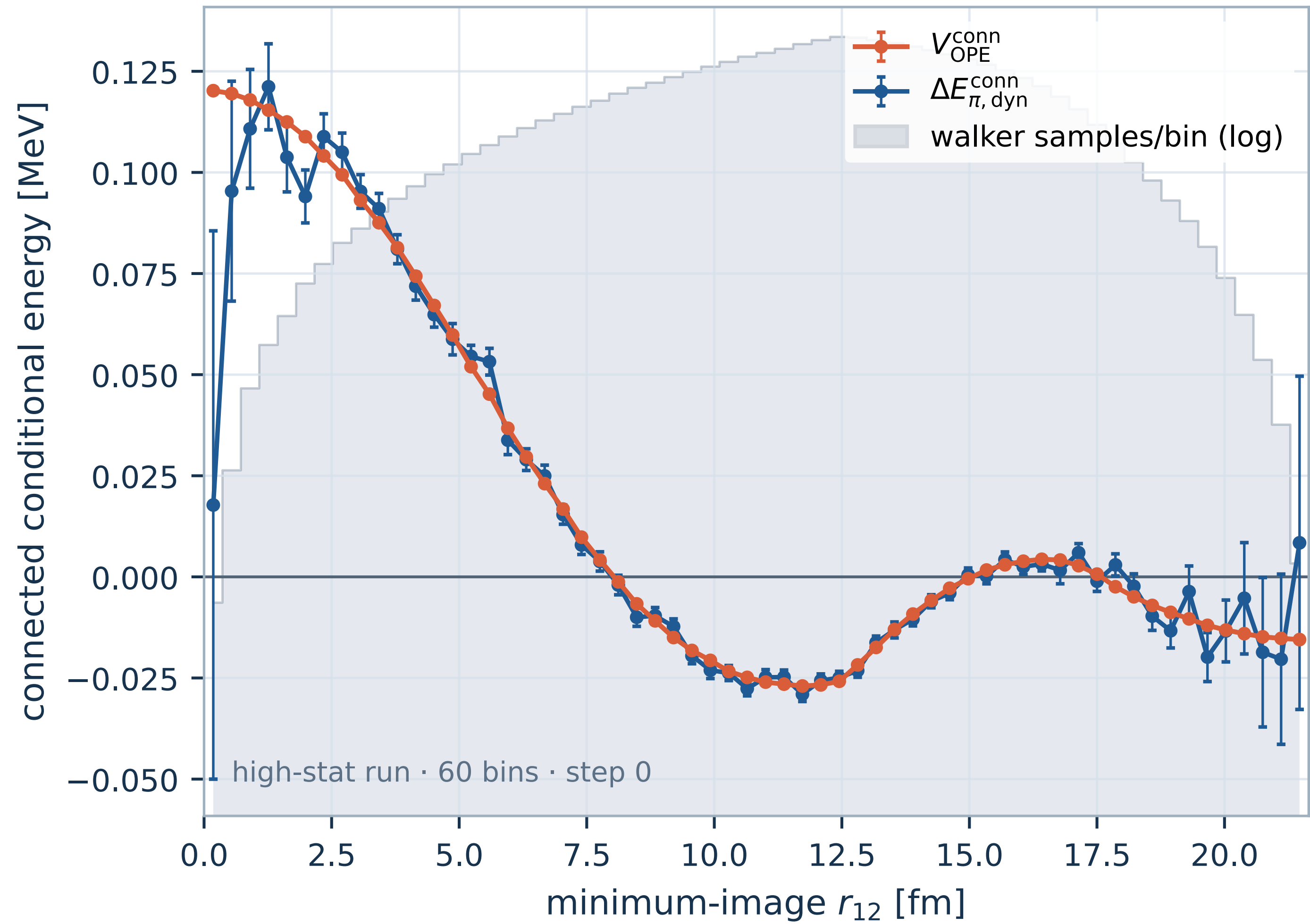
Two-nucleon case

- Minimize the energy of two nucleons fixed at relative distance r



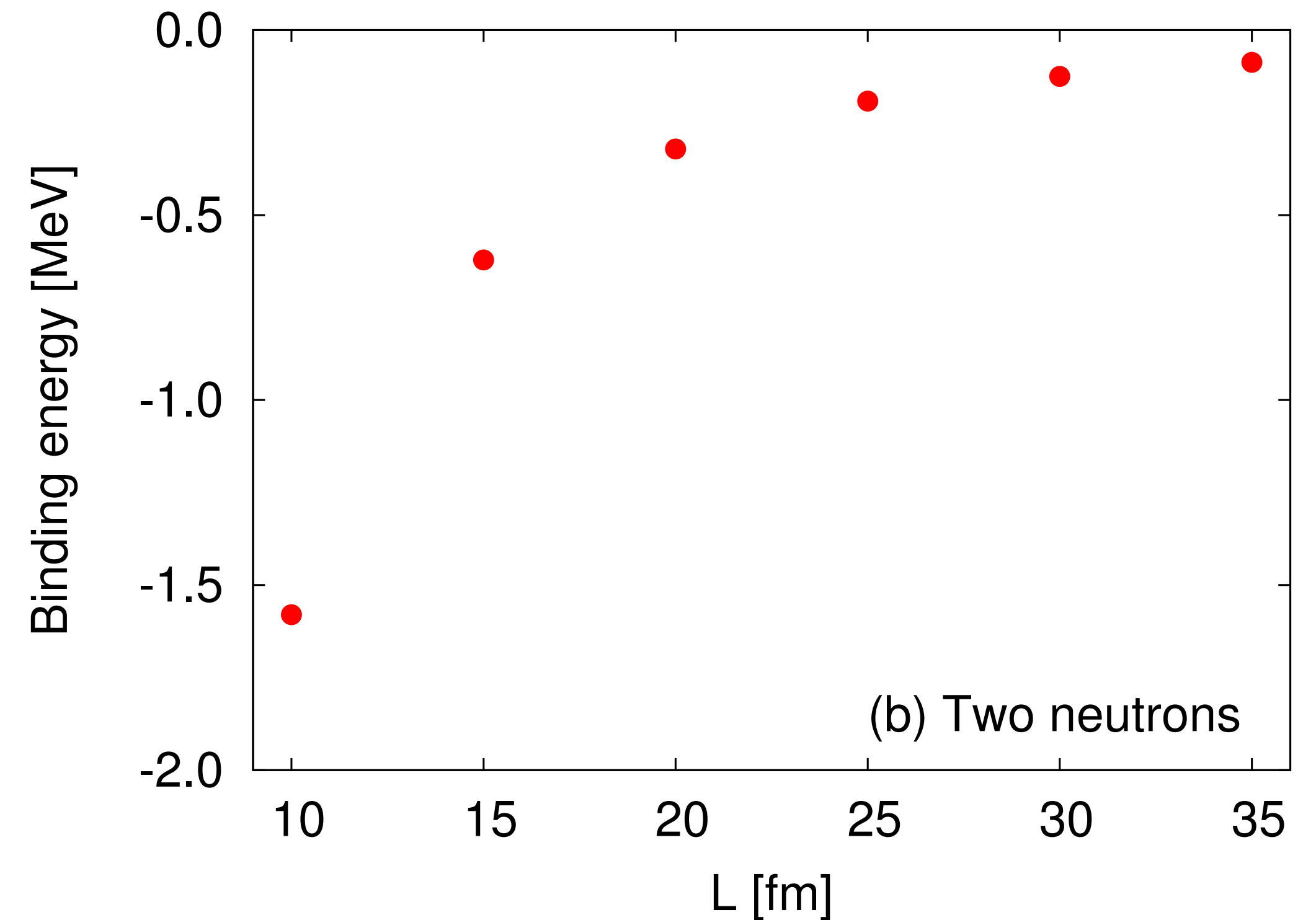
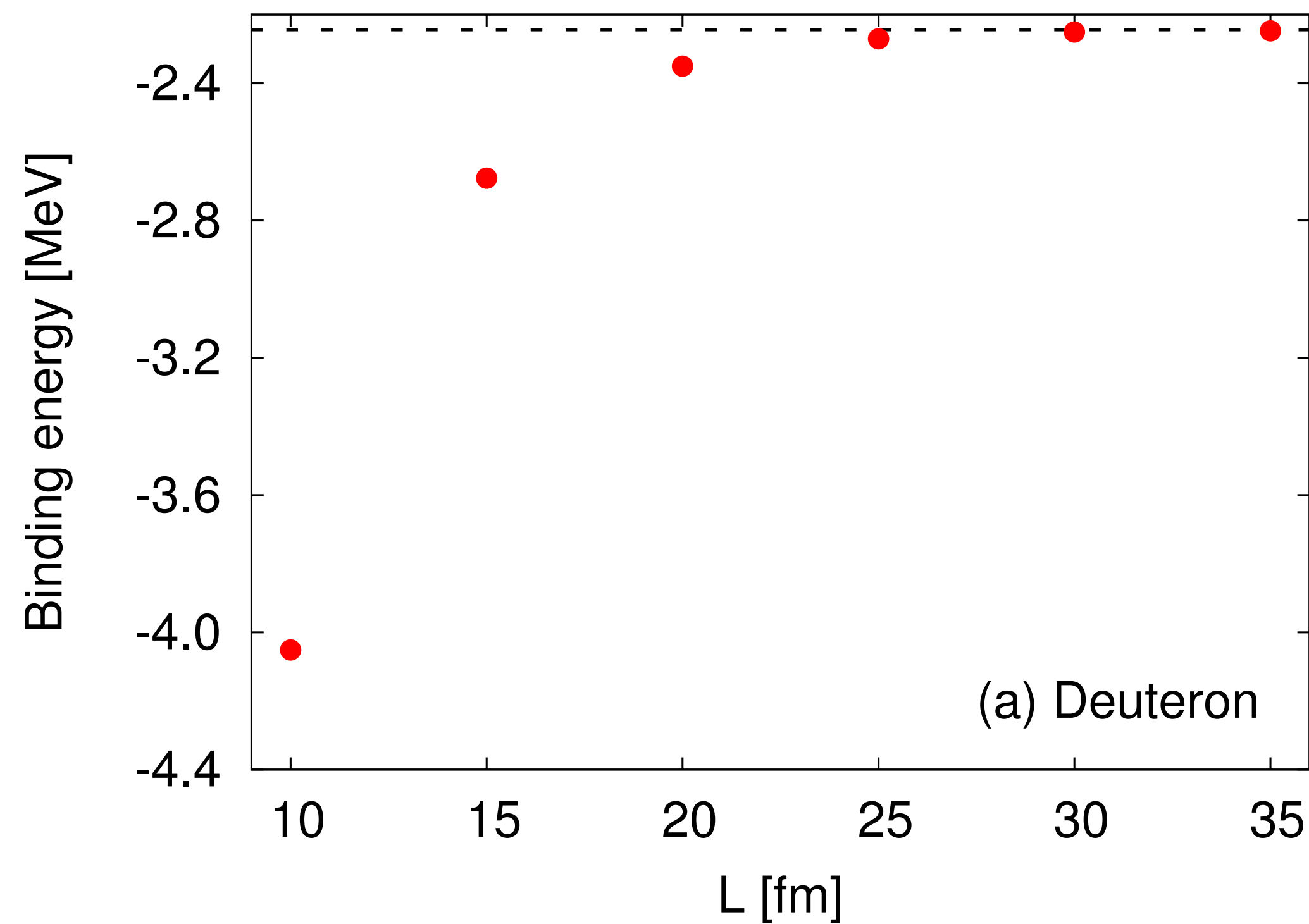
Two-nucleon case

L = 25 fm



Fix the contacts

- Fix the NN LECs to reproduce the deuteron and the two-neutron state in a box



Conclusions

- Dynamical pion modes can be included directly in continuum nuclear wave functions.
 - ▶ Renormalization tested against explicit self-energy calculations
 - ▶ Two-nucleon sector validated against explicit OPE calculation
- NQS reproduce one-nucleon self-energy and two-nucleon OPE benchmarks, including higher-order pion effects.
- Two-body LECs fixed against deuteron and two-neutron state in a box

Perspectives

- Compute pion-cloud contributions to the nucleon electromagnetic and axial form factors.
- Study pion production on the single nucleon
- Extend the framework to calibrated few- and many-nucleon calculations.
- Include NLO terms in the Hamiltonian and study the convergence against conventional EFT

Thank you

Solve the many-body problem (“old” way)

- The exact ground state is obtained by means of imaginary-time projection techniques

$$|\Psi_0\rangle \propto \lim_{\tau \rightarrow \infty} \exp[-(H - E_T)\tau] |\Psi_T\rangle$$

- Compared to “conventional” QMC:
 - ▶ Extra a set of boson field amplitudes (i.e. harmonic oscillators) to diffuse
 - ▶ The nucleonic charge is not conserved separately; the total nucleon-plus-pion charge is conserved.
- Very accurate approach, but limited to light nuclei (exponential scaling)