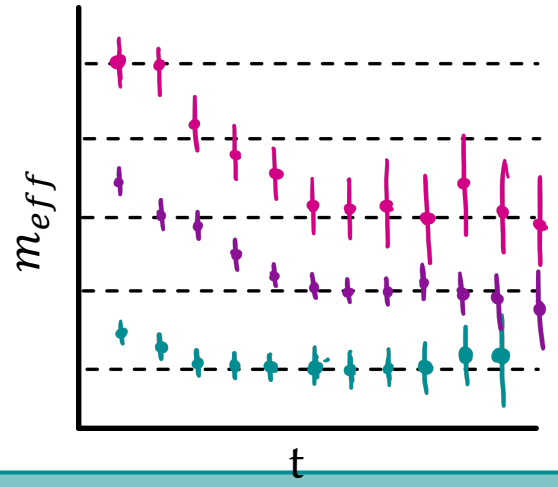

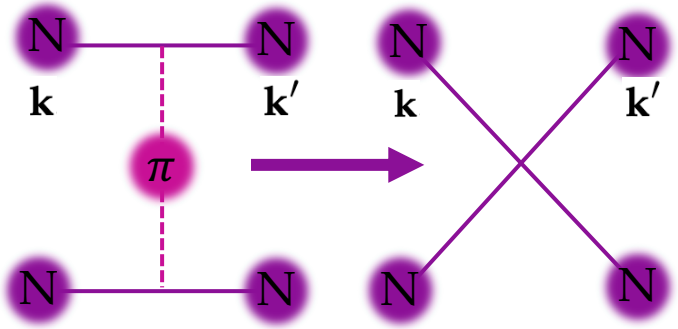

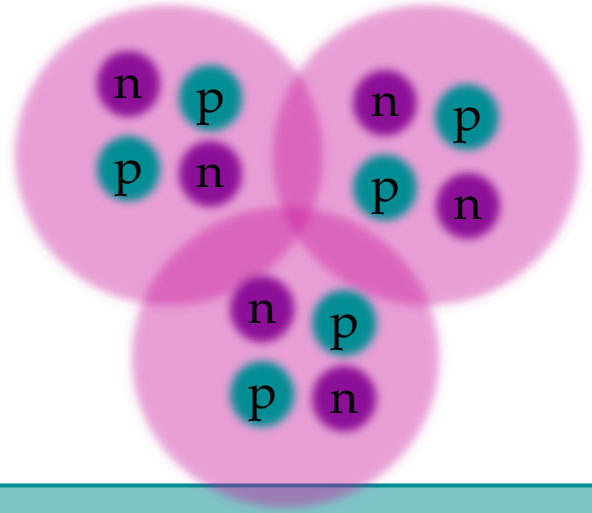

From lattice QCD to *ab initio* nuclear physics via finite-volume pionless EFT

Rosemary Zielinski (rosie_z@mit.edu)

William Detmold[1], Robert Perry[1], Andrew Pochinsky[1], Fernando Romero-López[2], Phiala Shanahan[1]

1. Massachusetts Institute of Technology 2. University of Bern

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

MIT CENTER FOR THEORETICAL PHYSICS – A LEINWEBER INSTITUTE

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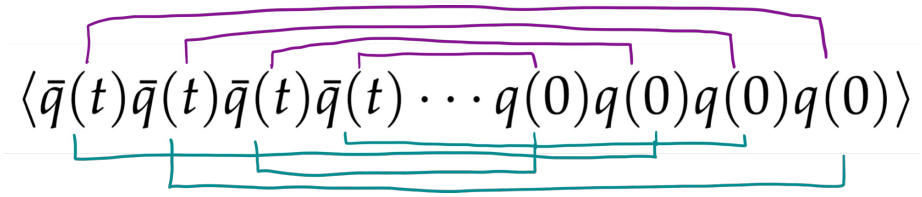
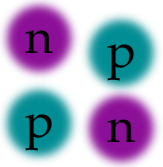
Issue 1: Wick contractions for correlation functions are *factorially* difficult to compute ~ $3A!$ (naïve algorithm)





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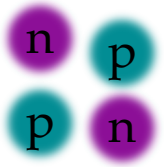

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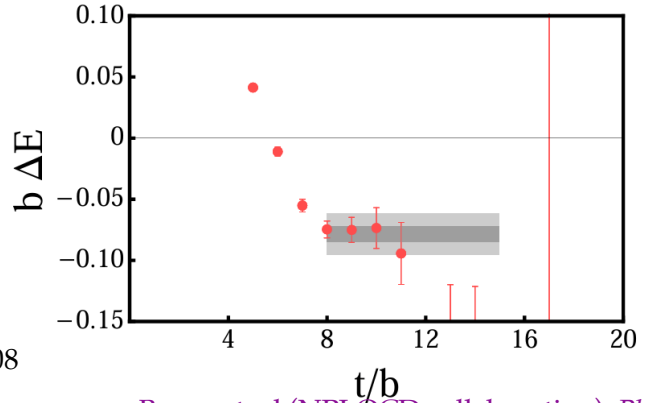

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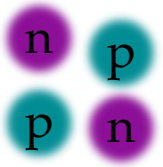

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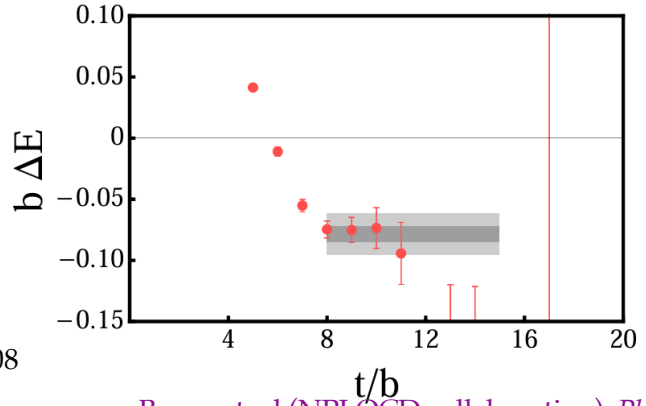

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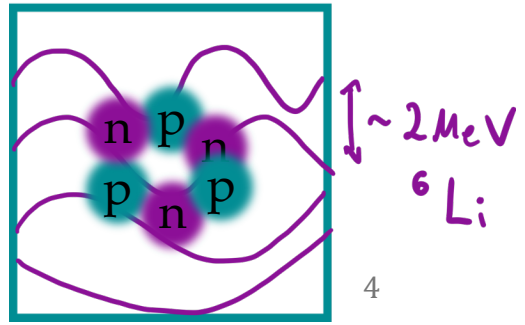
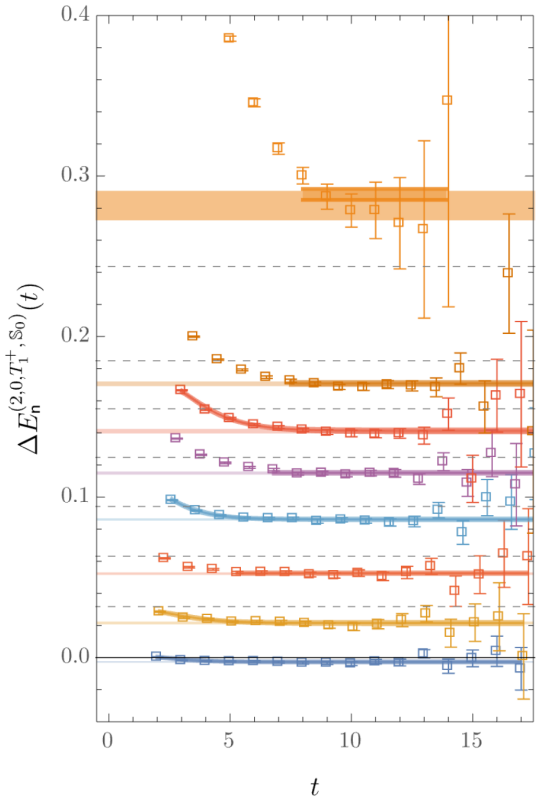
Issue 3: More difficult to extract matrix elements. Excited states densely spaced ~ MeV

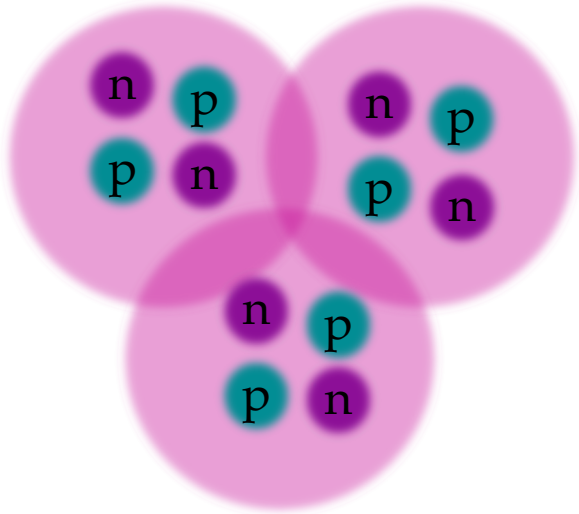
$$p_{min} = \frac{2\pi}{L} \implies L \approx 124 \text{ fm for } \Delta E \approx 10 \text{ MeV}$$



How to relate a two-nucleon energy spectrum computed on the lattice, to binding energy of ^{12}C, ^{208}Pb? Need a principled way!



?



Amarasinghe et al, *Phys. Rev. D.*, 107, 094508 (2023)

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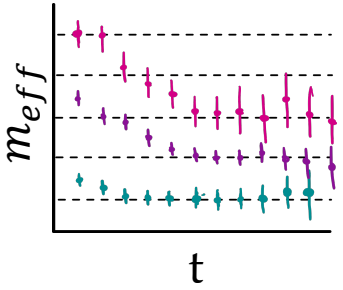

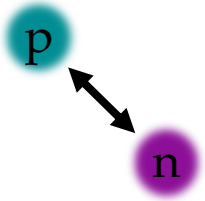

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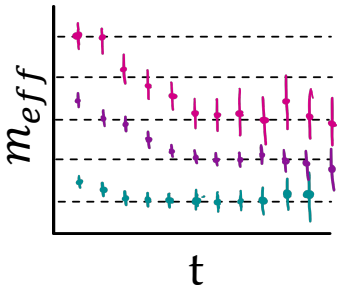

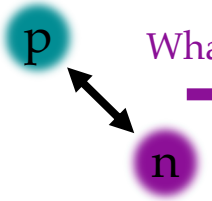

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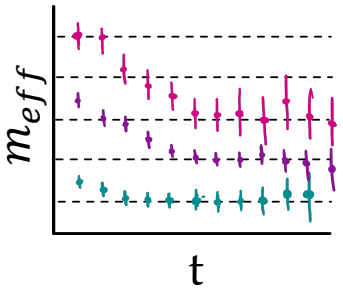

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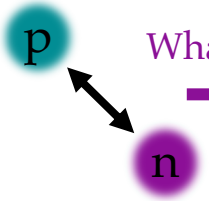

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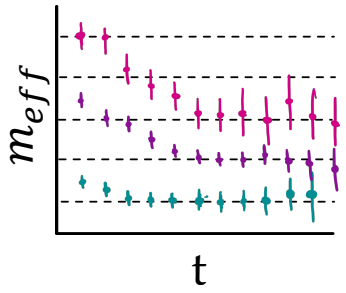

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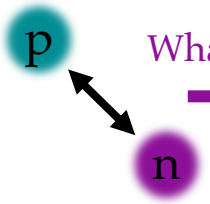

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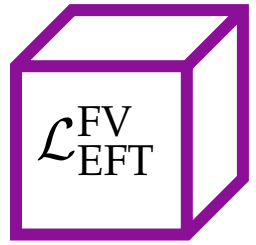

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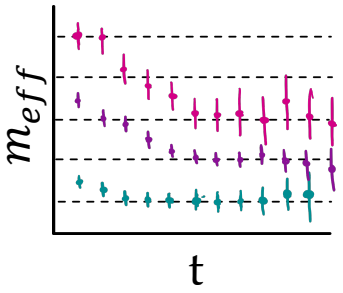

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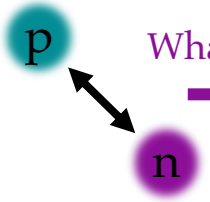

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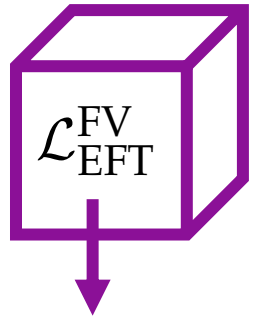

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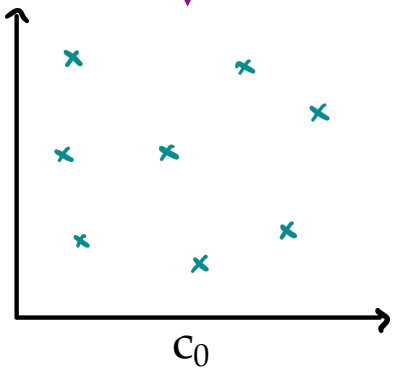

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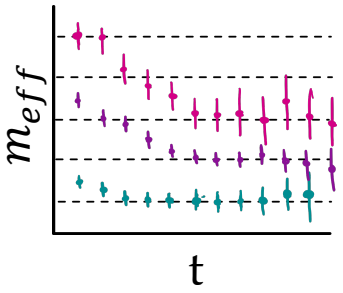

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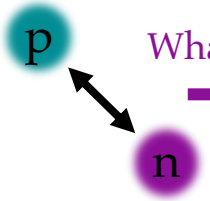

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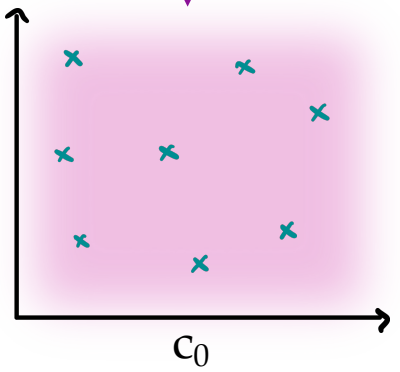

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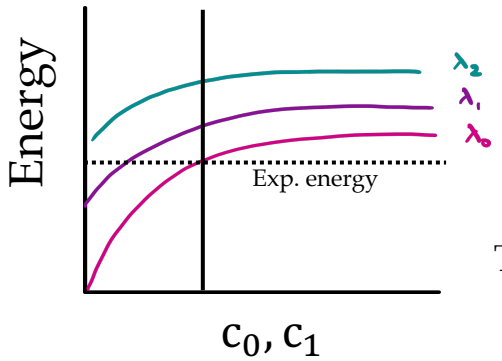

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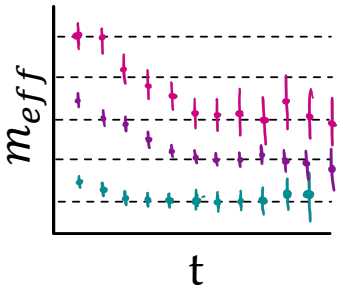

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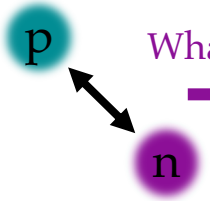

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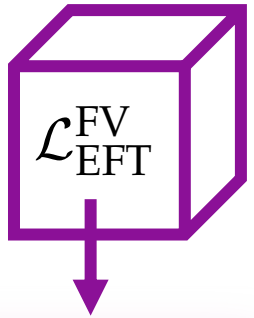

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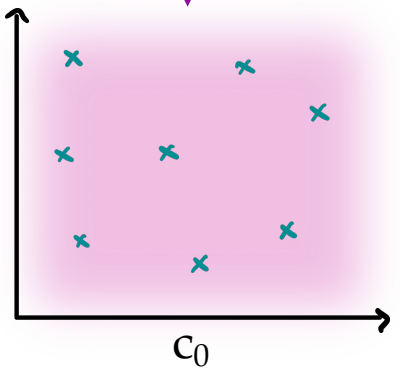

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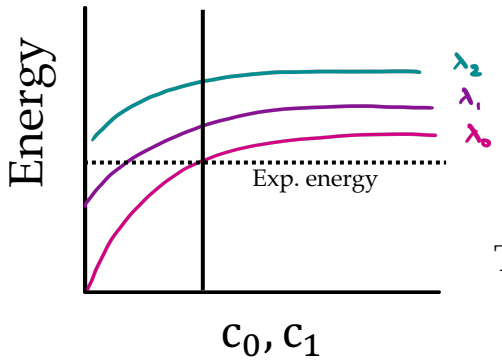

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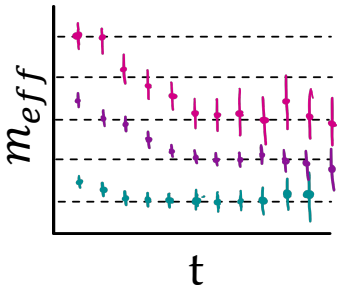

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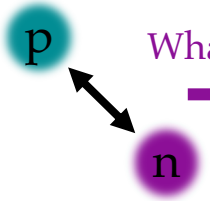

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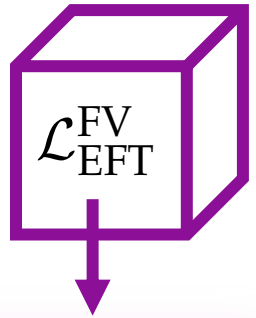

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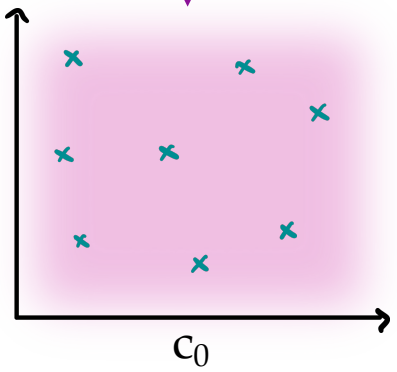

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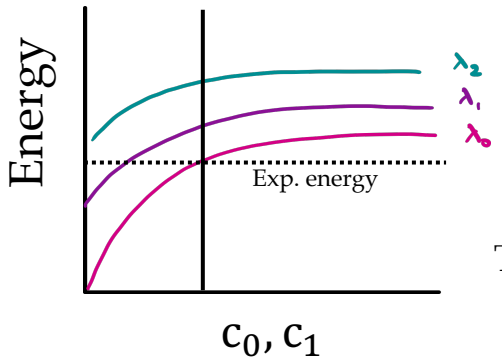

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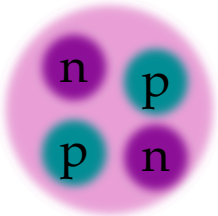
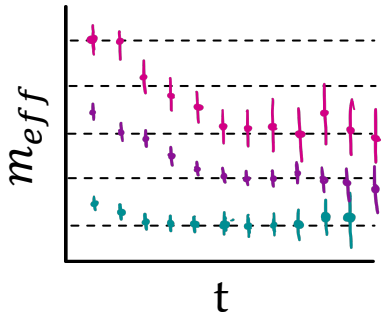
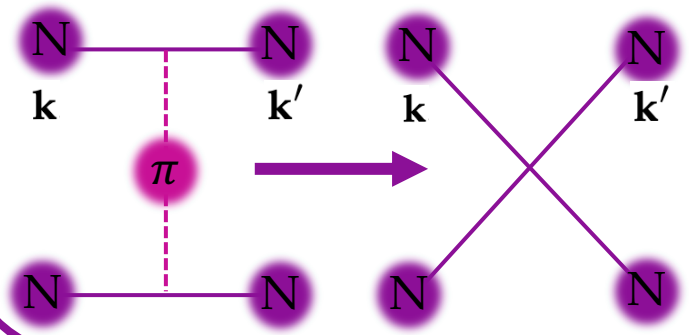


Infinite volume binding energies/other observables!

Past work: EFT matching





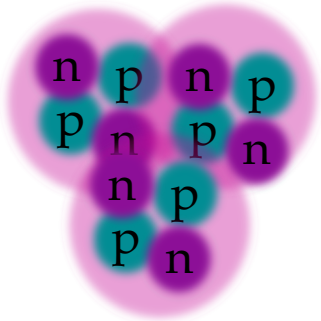
Previous work: Developing FVEFT formalism + proof of principle

1. Contessi et. al, *Phys. Lett. B*, 772, 839-849 (2017)
2. Eliyahu et. al, *Phys. Rev. C. 102*, 044003 (2020)
3. Detmold and Shanahan, *Phys. Rev. D* 103, 074503, 2021
4. Sun et. al, *Phys. Rev. D.* 105, 074508 (2022)
5. Detmold et. al, *Phys. Rev. D.* 108, 034509, (2023)

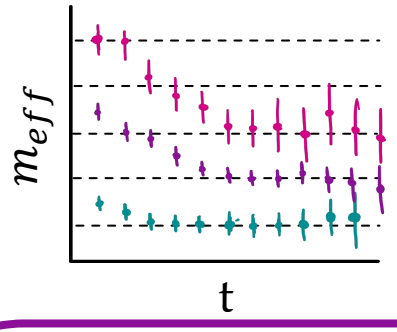
Pionless EFT LO Hamiltonian + NLO Corrections

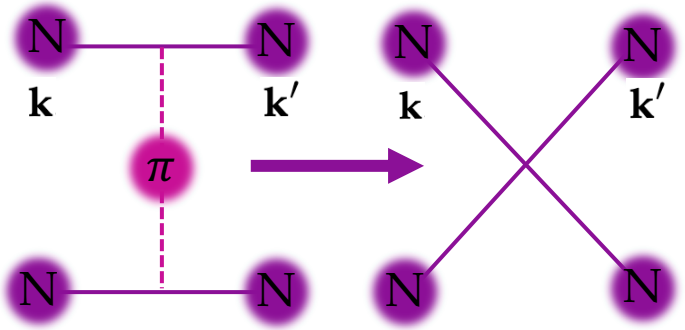
Variational method with N-body correlated Gaussian Ansatz. Differentiable programming to optimize wavefunction.

Match EFT low-energy constants to reproduce 2-body and 3-body **lattice** results

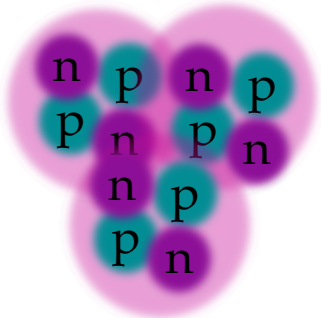


This work: EFT matching





This work: scaling to larger systems, at **physical pion mass** (experimental data), with FVEFT formalism established



$$\mathcal{L}_{\text{EFT}}^{\text{matched}} = c_0^{\text{matched}}\mathcal{L}_0 + c_1^{\text{matched}}\mathcal{L}_1 + \cdots$$

Pionless EFT LO Hamiltonian + NLO Corrections

Variational method with N-body correlated Gaussian Ansatz. Differentiable programming to optimize wavefunction.

Match EFT low-energy constants to reproduce 2-body and 3-body **physical** results

With matched EFT, use variational method to extract energies of larger nuclei $A \leq 12$

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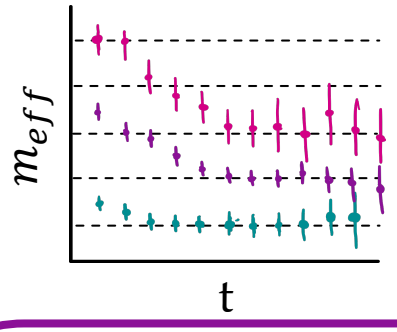
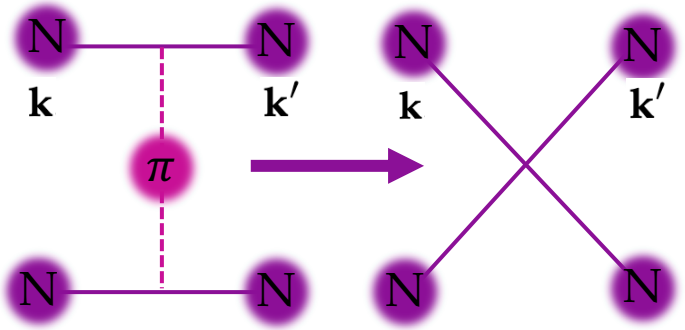


Important: we are *not* using lattice data in this particular work!



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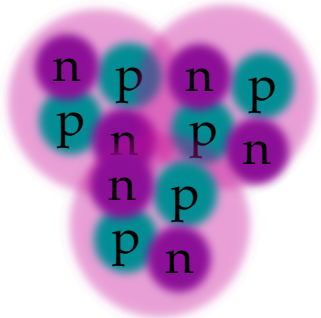

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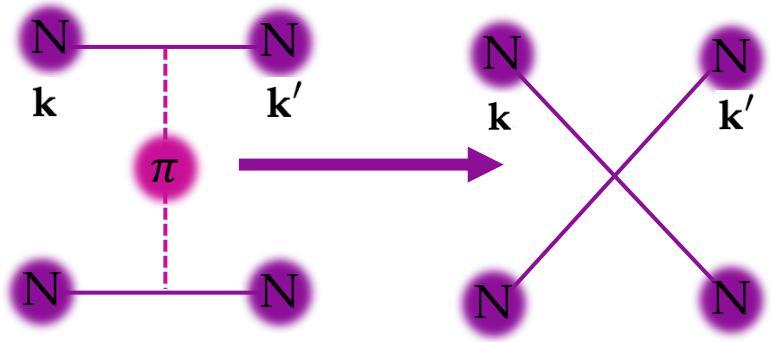
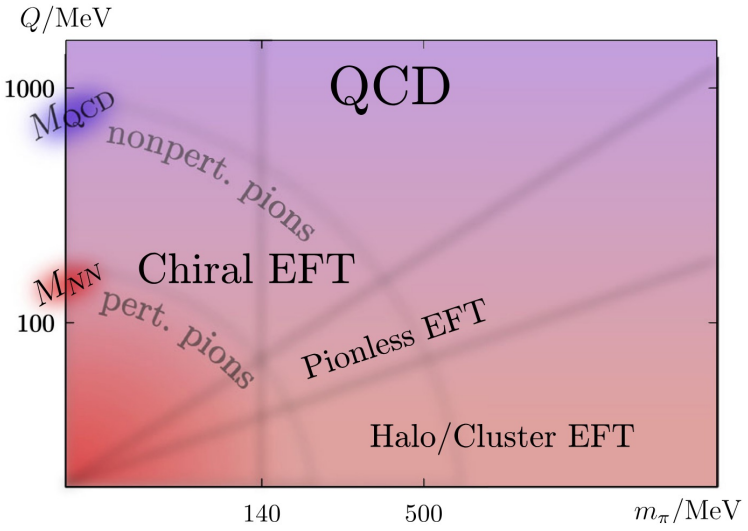
Pionless EFT

- Effective field theory of nucleons with pionic degrees of freedom integrated out [Hammer et. al, *Rev. Mod. Phys.* 92(2) 2020][Bedaque, and van Kolck, *Ann. Rev. Nuc. and Part. Science*. 52:339-396, 2002][Kaplan et. al, *Nuc. Phys. B.*, 534 (1-2) 1998]
  - Power counting in terms of p_N^2 for nucleon momenta below $\frac{m_\pi^2}{4}$ (one pion exchange threshold), $p_N \sim 70$ MeV
  - Predicts α particle properties [Platter, et. al, *Phys. Lett. B*, 607, 254, 2005] and ^{6}Li ground state surprisingly well [Stetcu, et. al, *Phys. Lett. B*, 653, 358–362, (2007)], given power counting arguments



$$\langle \mathbf{k}' \,|\, V_{2N,\pi} \,|\, \mathbf{k} \rangle \propto \frac{1}{\mathbf{q}^2 + m_\pi^2}, \qquad \mathbf{q} = \mathbf{k}' - \mathbf{k}.$$



Three-body coupling

$$\mathcal{L}_{\not\pi} = N^\dagger \left(iD + \frac{\mathbf{D}^2}{2M_N} \right) N - \frac{1}{4} C_0 (N^\dagger N)^2 - \frac{1}{2} C_1 (N^\dagger \sigma N)^2 - \frac{1}{6} D_0 (N^\dagger N)^3 + \cdots$$

Nucleon field

LO spin-dependent interaction

Pionless EFT: Hamiltonian Formulation

- **Goal:** Constrain pionless EFT LECs and optimize many-body nuclear wavefunctions using **variational method** to predict properties of larger nuclei
  - **Hamiltonian formulation more useful!**

$$H = -\frac{1}{2M_N}\sum_i \nabla_i^2 + \sum_{i<j} V_2(r_{ij}) + \sum_{i<j<k} V_3(r_{ij}, r_{jk}).$$

$$\mathcal{E}[\Psi_h] = \frac{\int \Psi_h^*(x)\hat{H}\Psi_h(x)dx}{\int \Psi_h^*(x)\Psi_h(x)dx}$$

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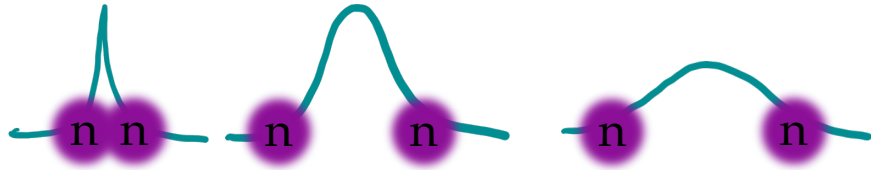

Decreasing Λ smears contact interaction

- EFT is are regulated with a gaussian regulator, cutoff Λ.
  - Physical quantities should be independent of Λ, if renormalizable!

$$V_2^{LO}(r_{ij}) = \left(C_0 + C_1\,\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j\right) g_\Lambda(r_{ij}).$$

Gaussian regulator

$$V_2^{\mathrm{NLO}}(r_{ij}) = \frac{1}{2}\left(C_0^{(2)} + C_1^{(2)}\,\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j\right)\left[g_\Lambda(r_{ij})(\nabla_i - \nabla_j)^2 + (\overleftarrow{\nabla}_i - \overleftarrow{\nabla}_j)^2 g_\Lambda(r_{ij})\right].$$

Wavefunction Optimization

- **Correlated Gaussian Basis**
  - Allows analytic, rapid, calculation of Hamiltonian matrix elements [Yin and Blume, *Phys. Rev. A.* **87**, 063609 (2013)] [Sun et. al, *Phys. Rev. D.* **105**, 074508, 2022] [Mitroy et. al Rev. Mod. Phys. **85**, 693, 2013] [Detmold and Shanahan, *Phys. Rev. D* 103, 074503, 2021]
  - No Monte Carlo integration needed for wavefunction → this is what makes A=12 calculation feasible!
  - Expressive enough to include spatial entanglement
  - Assume spin and flavor factorize from spatial wavefunction

N-dimensional shift vector

$$\Psi^{(\alpha)}\left(A^{(\alpha)}, B^{(\alpha)}, \mathbf{d}^{(\alpha)}, \mathbf{x}^{(\alpha)}\right) = \exp\left[-\frac{1}{2}\mathbf{x}^{(\alpha)T} A^{(\alpha)} \mathbf{x}^{(\alpha)} - \frac{1}{2}\left(\mathbf{x}^{(\alpha)} - \mathbf{d}^{(\alpha)}\right)^{T} B^{(\alpha)} \left(\mathbf{x}^{(\alpha)} - \mathbf{d}^{(\alpha)}\right)\right]$$

Determines particle correlations ($N\times N$) symmetric matrix

Determines Gaussian width ($N\times N$) diagonal matrix

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Determines Gaussian width ($N\times N$) diagonal matrix

$$|\Psi\rangle = \left(\sum_{i}^{i=N_G} c_i \prod_{\alpha\in\{x,y,z\}} |\Psi_i^{(\alpha)}\rangle\right) \otimes |\sigma\rangle \otimes |\tau\rangle.$$

Spatial DOF

Spin/flavor

Free parameters in one optimization: $\frac{N(N+3)}{2}\times N_G \times N_D + N_G$

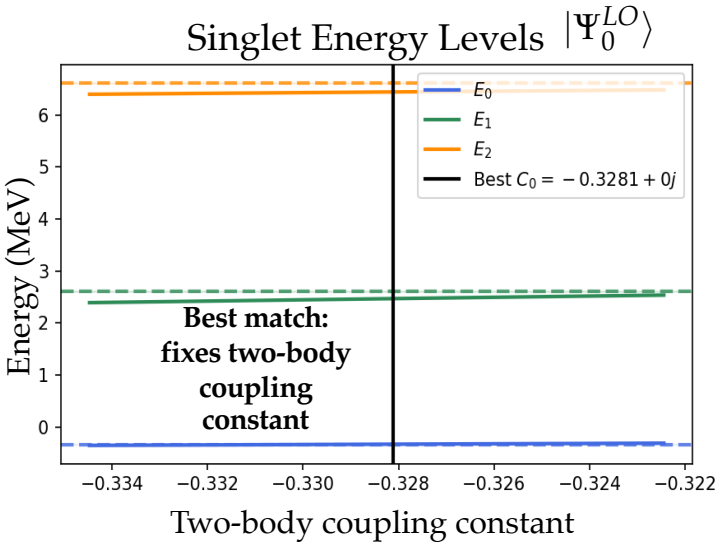
E.g. N=4 nucleons, $N_G = 8$ Gaussians, 3 dimensions → 344 parameters

LEC Determination

Optimize with LO **two-body** Hamiltonian

Inputs: Physical singlet and triplet np scattering lengths

	$^1S_0$	$^3S_1$
a [fm]	-23.74	5.42
r [fm]	2.75	1.76



Outputs: matched 2-body EFT

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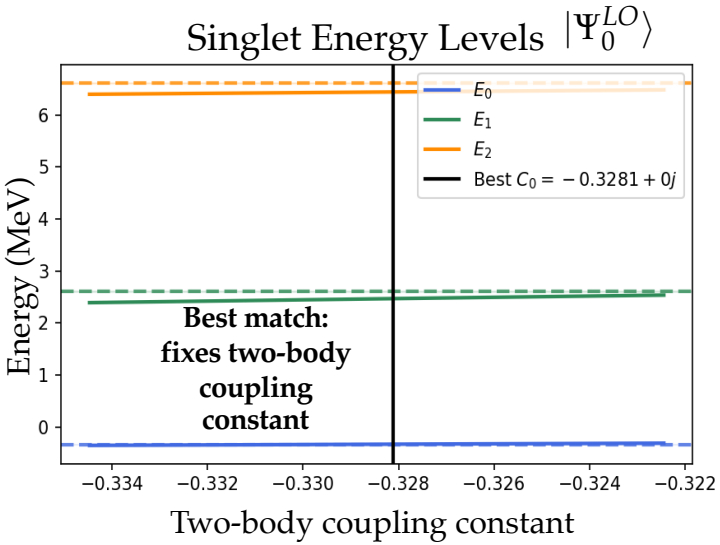

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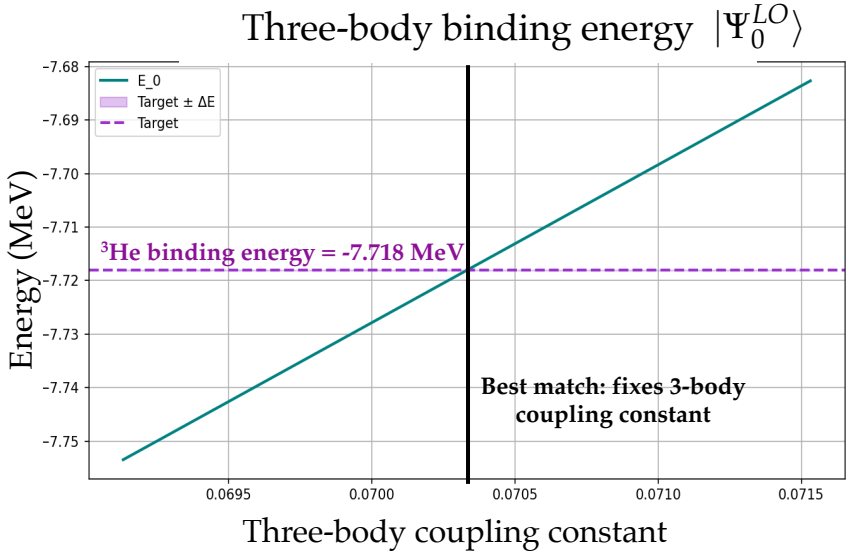
Optimize with LO **three-body** Hamiltonian

Inputs: Physical ^{3}He binding energy



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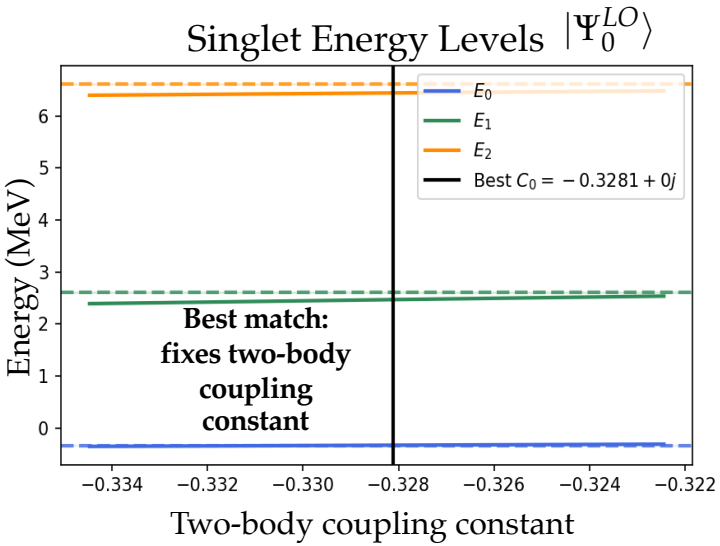

Outputs: matched 2-body EFT

Optimize with LO **three-body** Hamiltonian

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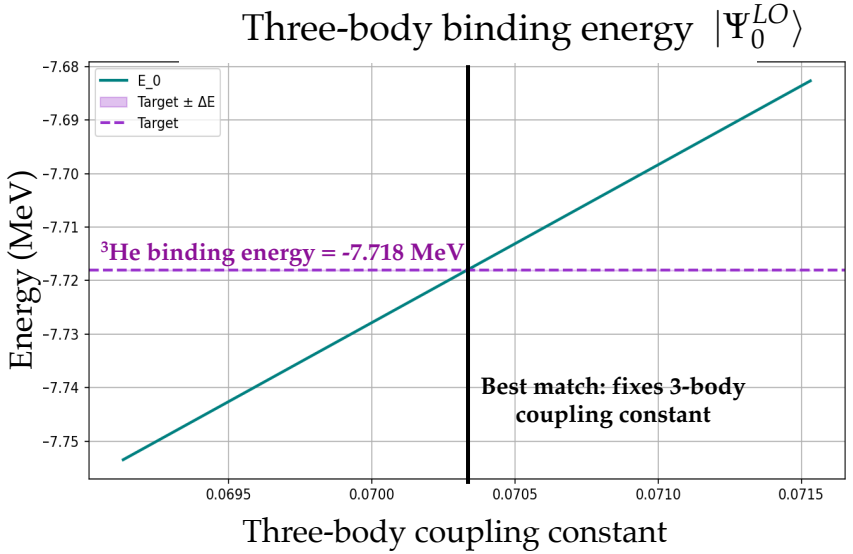


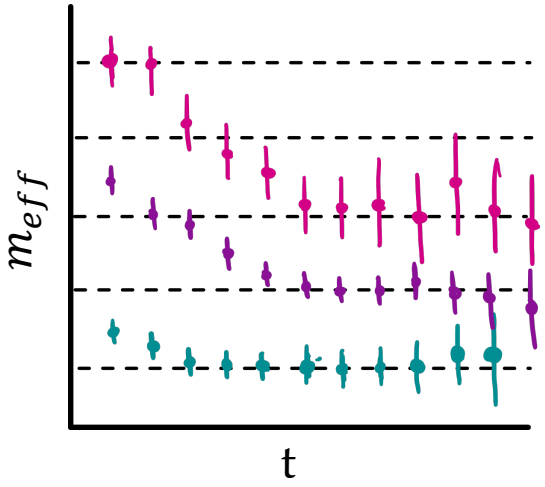
Outputs: matched 3-body EFT

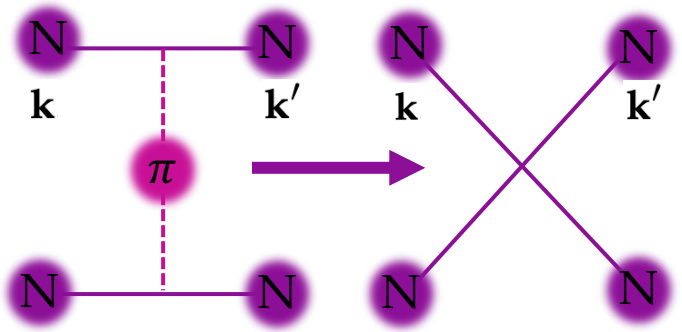
Perturbative NLO treatment with optimized LO wavefunctions

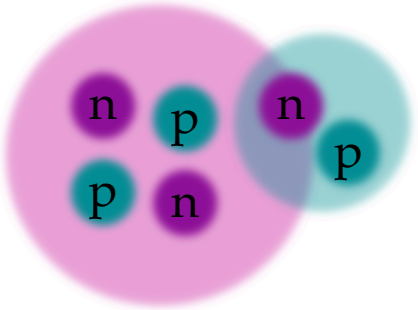
$$\langle \Psi_0^{LO} | V_2^{NLO} | \Psi_0^{LO} \rangle = \Delta E_0$$

$$H = -\frac{1}{2M_N}\sum_i \nabla_i^2 + \sum_{i<j} V_2(r_{ij}) + \sum_{i<j<k} V_3(r_{ij}, r_{jk}).$$

Completely determined pionless LO + NLO EFT Hamiltonian for use in $A \geq 3$ sector



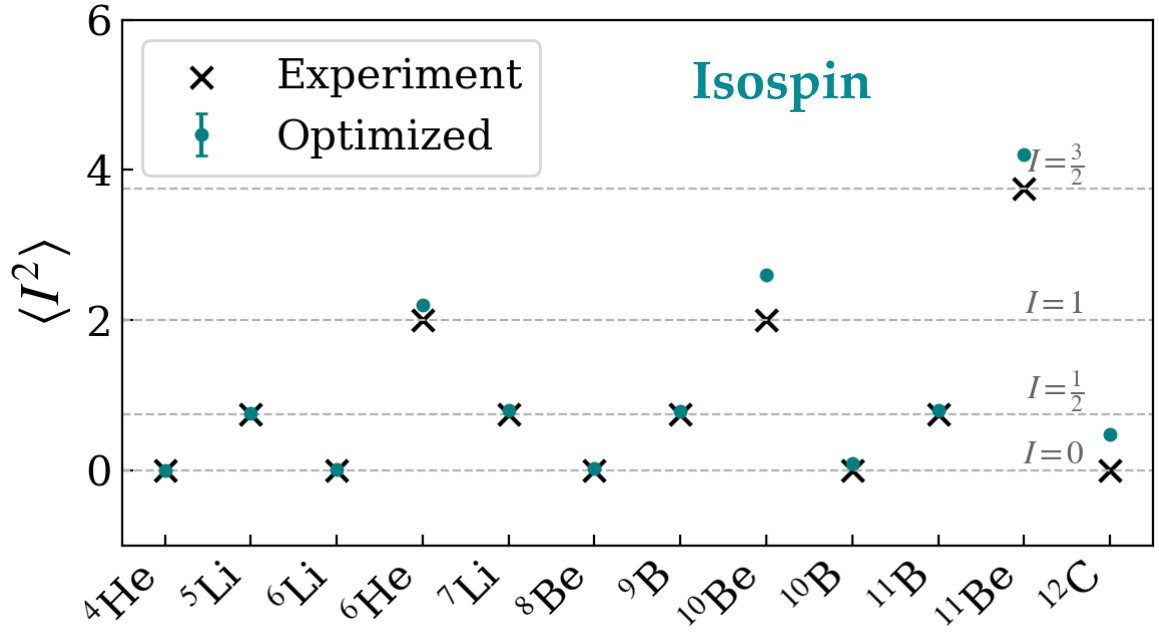


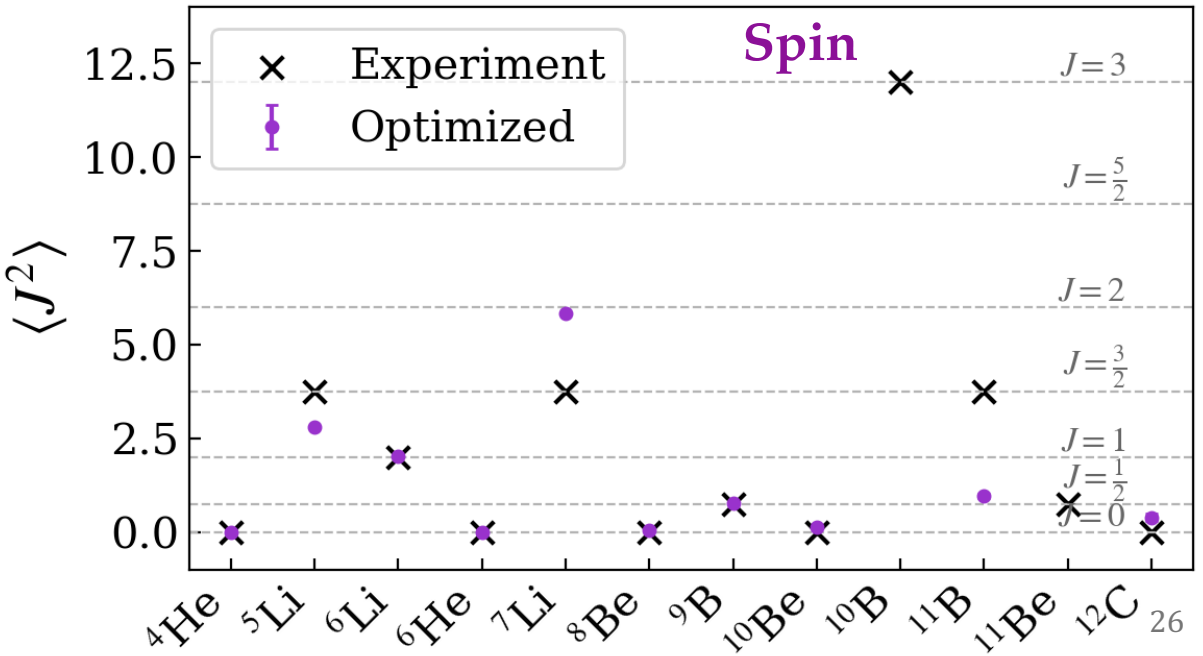


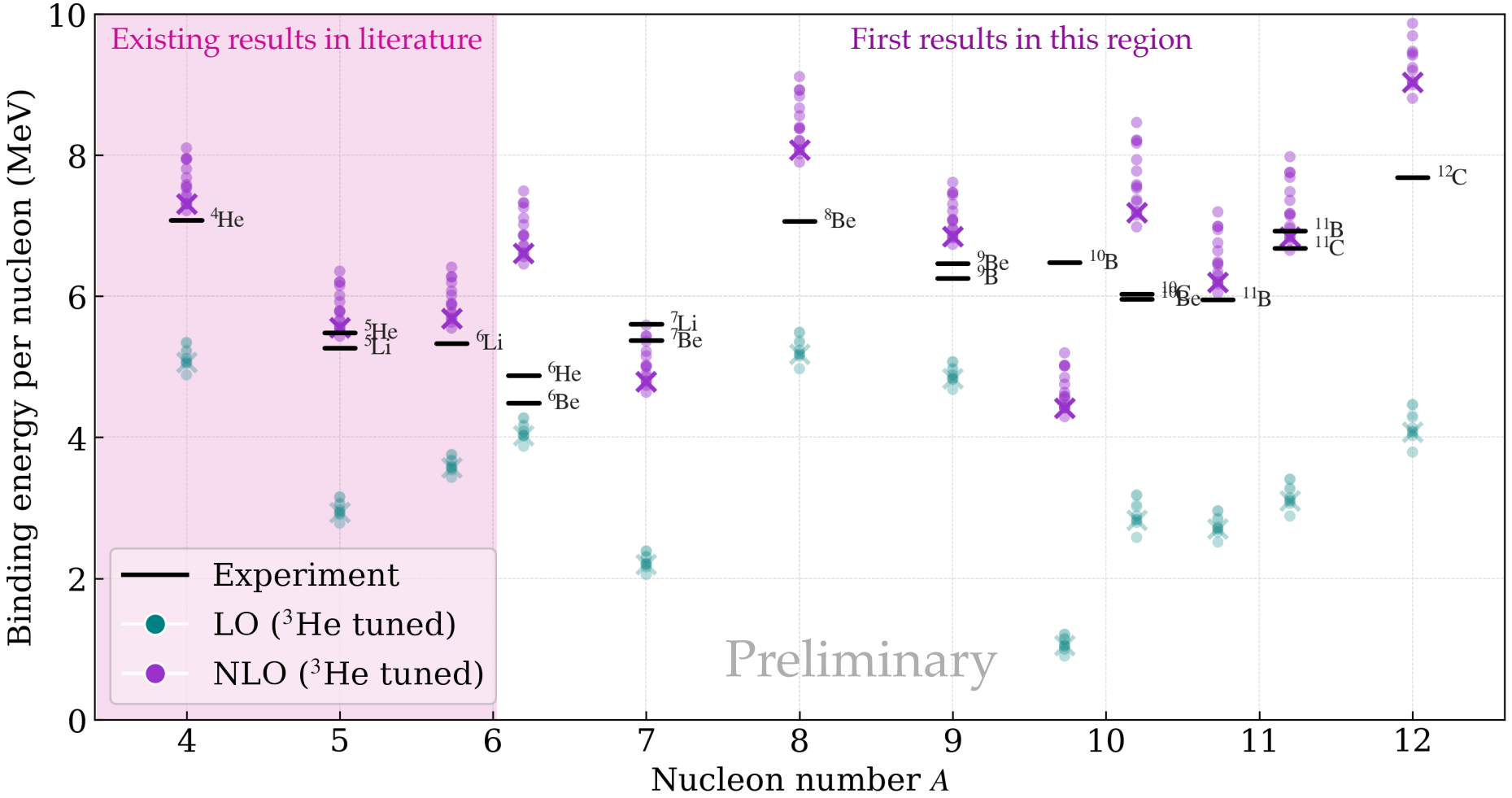
Numerical Results

Spin-Isospin sectors

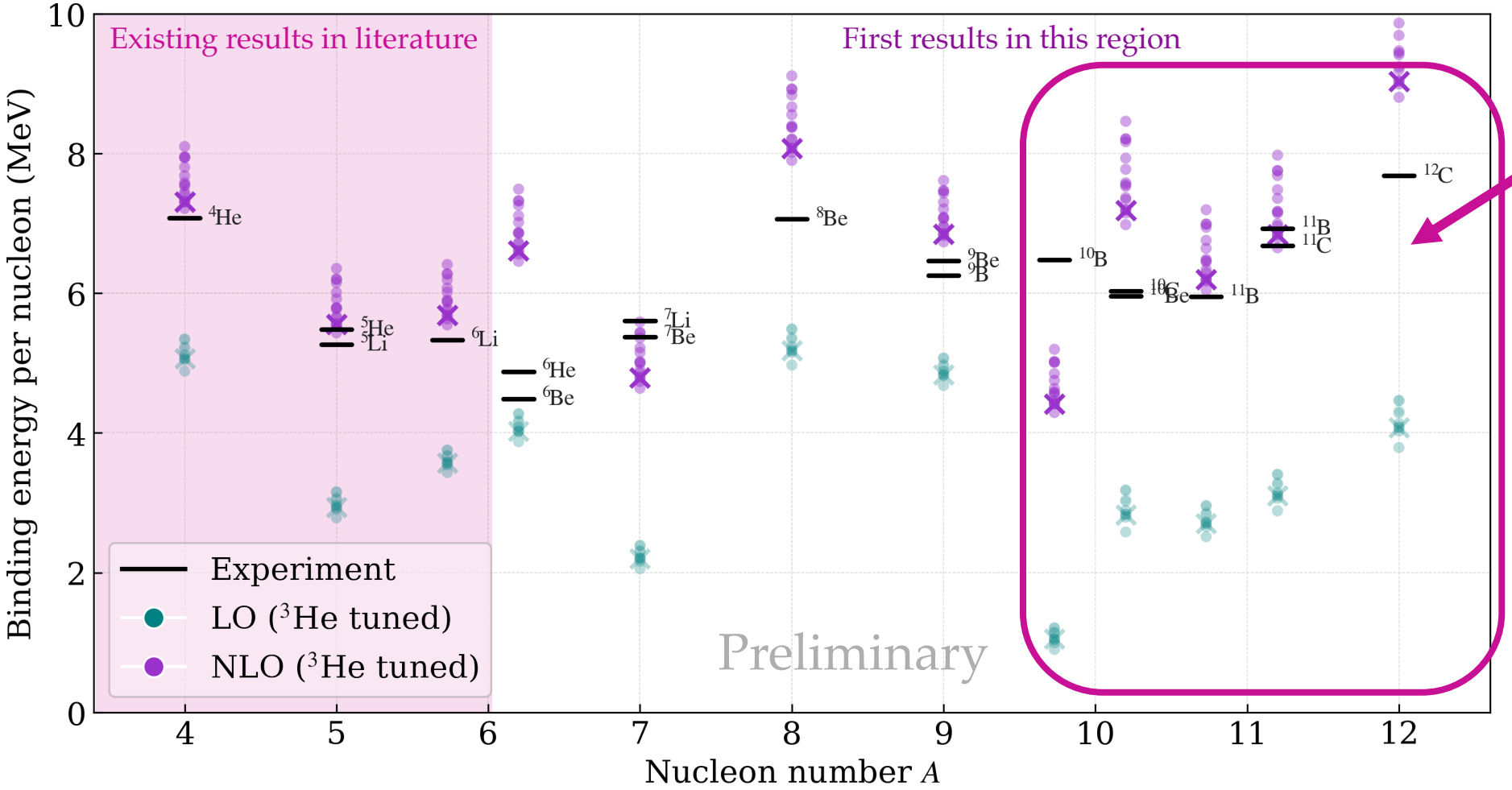
- **Recall:** Spin/isospin are not fixed in optimization
- Nuclei identified by isospin quantum number
- **Variational procedure mostly reproduces the correct spin/isospin spectrum for low A**
- Less well-reproduced for larger nuclei







- Each point represents a choice of scattering length/effective range to fit (systematic spread)
- **First pionless EFT calculation of binding energies for $7 \leq A \leq 12$**
- LO results systematically underbind
- NLO perturbative correction always positive, due to smaller three-body coupling



Large NLO corrections. Is pionless EFT applicable here?

Some power counting arguments suggest LO uncertainty should be ~ 0.8

Limitation: Results calculated for *single* $\Lambda = 310$ MeV cut-off.

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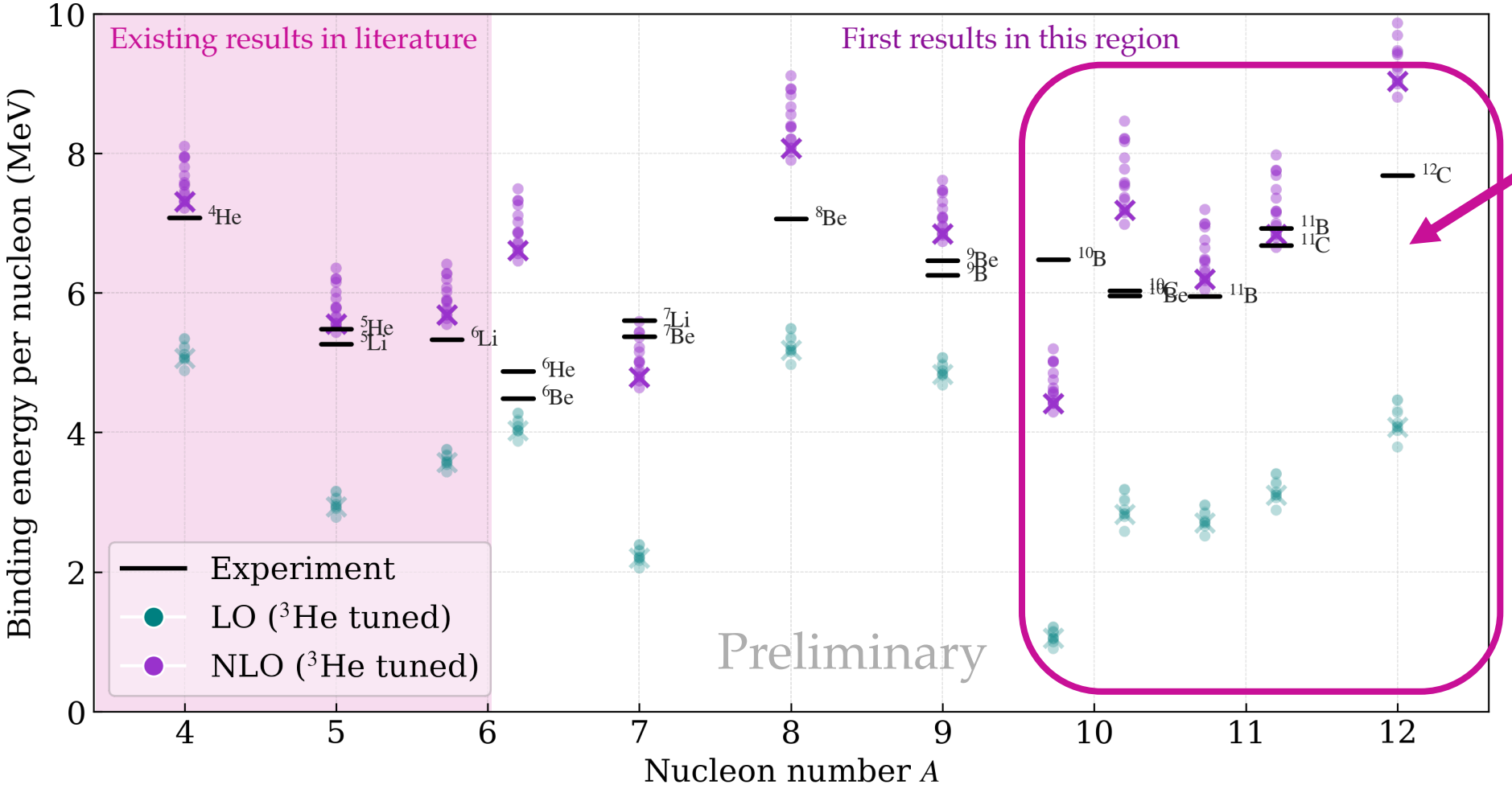

Large NLO corrections. Is pionless EFT applicable here?

Some power counting arguments suggest LO uncertainty should be ~ 0.8

Limitation: Results calculated for *single* $\Lambda = 310$ MeV cut-off.

Can in principle, using identical methods, implement another EFT at the physical point!

Still a robust proof-of-concept of scalability of EFT matching approach

- Each point represents a choice of scattering length/effective range to fit (systematic spread)
- **First pionless EFT calculation of binding energies for $7 \leq A \leq 12$**
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Summary and Outlook

Approach

1. Pionless EFT in finite volume + variational method to optimized correlated Gaussian wavefunctions
2. EFT in finite volume extrapolated the *infinite volume* to compute $A \leq 12$ systems

Contribution

1. **First ab-initio calculation of binding energies, spins, and isospins of $7 \leq A \leq 12$ systems with pionless EFT with NLO corrections**
2. **Demonstration of feasibility of LQCD finite volume data → many body predictions**

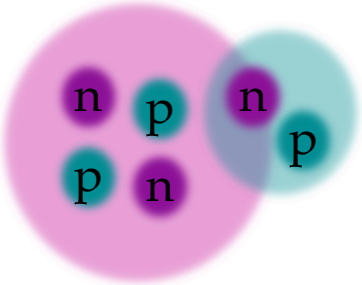
Outlook

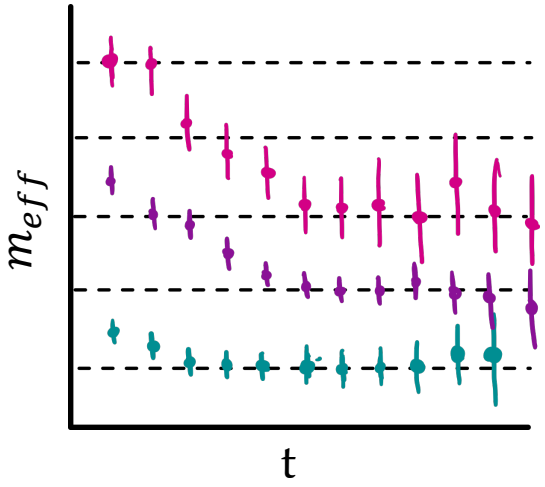
1. Method extends beyond pionless EFT to EFT of choice!
2. Validation of approach with cut-off dependence investigated + Matter radii, charge radii, nuclear magnetic moment comparisons

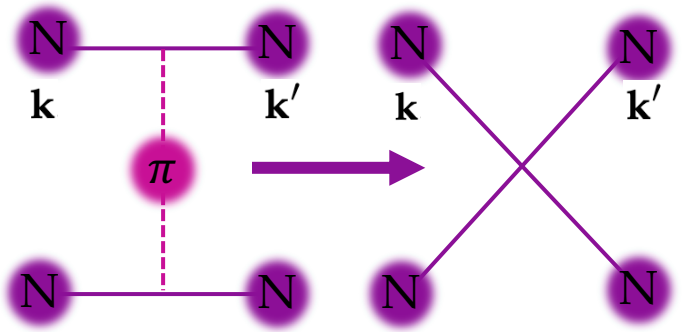
$$\mathcal{E}[\Psi_h] = \frac{\int \Psi_h^*(x)\hat{H}\Psi_h(x)dx}{\int \Psi_h^*(x)\Psi_h(x)dx}$$

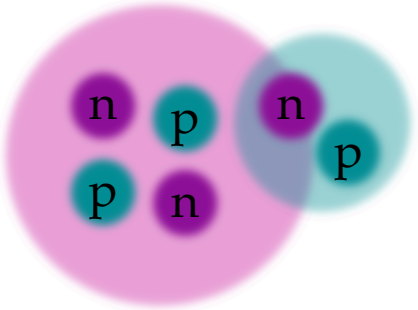
Upshot

We can take *finite volume* data from few-body lattice calculations and give an *infinite volume* many-body observable!









Back up

Single wavefunction optimization procedure

Initial parameters of wavefunction: $\theta = \{A_i, B_i, d_i, c_i\}, i \in N_G$
Trainable parameters: $\frac{N(N+3)}{2} \times N_G \times N_D + \mathrm{N_G}$

Set of LECs $\{C_0, C_1, D_0\}$

$|\Psi_h\rangle$

Cost function $\mathcal{E}[\Psi_h] = \frac{\int \Psi_h^*(x)\hat{H}\Psi_h(x)dx}{\int \Psi_h^*(x)\Psi_h(x)dx}$

Automatic differentiation $\theta' = \theta - \eta \nabla_\theta \mathcal{E}[\Psi_h]$

New wavefunction $|\Psi_h'\rangle = \sum_i^{i=N_G} c_i' \prod_{\alpha \in \{x,y,z\}} |\Psi_i'^{(\alpha)}\rangle$

$|\Psi_h'\rangle$

Optimized wavefunction parameters $\{A'_i, B'_i, d'_i, c'_i\}, i \in N_G$

GEVP procedure

Optimized wavefunction parameters $\{A'_i, B'_i, d'_i, c'_i\}, i \in N_G$

Set of LECs $\{C_0, C_1, D_0\}$

$\Psi_2(A_i, B_i, d_i)$ LECs: $\{C_0^2, C_1^2, D_0^2\}$

$\Psi_1(A_i, B_i, d_i)$ LECs: $\{C_0^1, C_1^1, D_0^1\}$

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$(\Psi_\alpha(A_i, B_i, d_i)$ LECs: $\{C_0^\alpha, C_1^\alpha, D_0^\alpha\}$

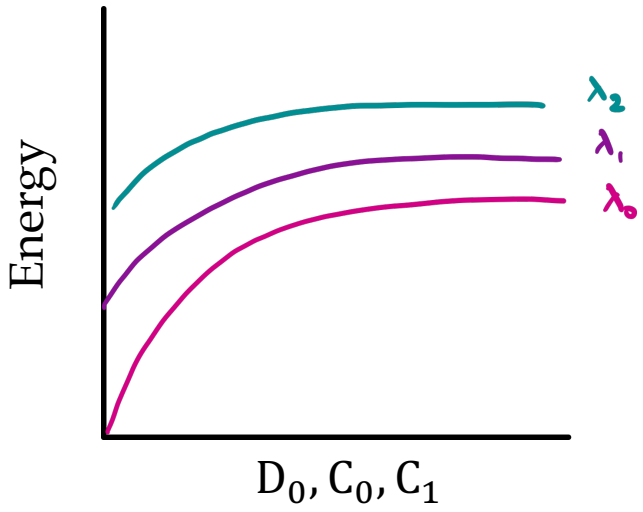
$\Psi_2(A_i, B_i, d_i)$ LECs: $\{C_0^2, C_1^2, D_0^2\}$

$$\mathbb{H}^{\{C_0, C_1, D_0\}} \vec{c} = \lambda \mathbb{N} \vec{c}$$

Solve GEVP with α sets of optimized wavefunctions, for a range of LECs, for ground state + excited states

$$\mathrm{E}^{\{C_0, C_1, D_0\}} = \lambda_0$$

Scan over LEC values



Binding energies

- **First pionless EFT calculation of binding energies for $7 \leq A \leq 12$**
- Systematic spread ~ 20% for each binding energy
- Results calculated for *single* 310 MeV cut-off

Nucleus	E_{LO} (MeV)	E_{NLO} (MeV)	E_{exp} (MeV)	$\delta_{\mathrm{LO}\to\mathrm{NLO}}$ (%)
^{4}He	20 (2)	29 (4)	28.30	45%
^{5}Li/^{5}He	15 (2)	28 (5)	26.33/27.41	87%
^{6}Li	21 (2)	34 (5)	31.99	62%
^{6}He/^{6}Be	24 (2)	40 (6)	29.27/26.92	67%
^{7}Li/^{7}Be	15 (2)	34 (7)	39.24/37.60	127%
^{8}Be	40 (4)	65 (10)	56.50	62%
^{9}Be/^{9}B	43 (4)	62 (8)	58.16/56.31	44%
^{10}C	28 (6)	72 (15)	60.32	157%
^{10}B	10 (3)	44 (9)	64.75	340%
^{11}B/^{11}C	34 (6)	75 (15)	76.20/73.44	121%
^{11}Be	30 (6)	76 (14)	65.48	153%
^{12}C	49 (8)	108 (20)	92.16	120%

Binding energies

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- Systematic spread ~ 20% for each binding energy
- Results calculated for *single* 310 MeV cut-off
- Convergence parameter, $\frac{Q_A}{m_\pi} \approx \sqrt{\frac{2m_N B_A}{Am_\pi^2}} \approx 0.8$ at physical pion mass
- NLO correction within this range for lighter nuclei, larger nuclei do not appear to converge

Corrections consistent with expected power-counting

Nucleus	E_{LO} (MeV)	E_{NLO} (MeV)	E_{exp} (MeV)	$\delta_{\mathrm{LO}\to\mathrm{NLO}}$ (%)
^{4}He	20 (2)	29 (4)	28.30	45%
^{5}Li/^{5}He	15 (2)	28 (5)	26.33/27.41	87%
^{6}Li	21 (2)	34 (5)	31.99	62%
^{6}He/^{6}Be	24 (2)	40 (6)	29.27/26.92	67%
^{7}Li/^{7}Be	15 (2)	34 (7)	39.24/37.60	127%
^{8}Be	40 (4)	65 (10)	56.50	62%
^{9}Be/^{9}B	43 (4)	62 (8)	58.16/56.31	44%
^{10}C	28 (6)	72 (15)	60.32	157%
^{10}B	10 (3)	44 (9)	64.75	340%
^{11}B/^{11}C	34 (6)	75 (15)	76.20/73.44	121%
^{11}Be	30 (6)	76 (14)	65.48	153%
^{12}C	49 (8)	108 (20)	92.16	120%

Corrections *larger* than expected power counting

LEC Determination: two body sector

Optimize with LO two-body Hamiltonian

$$H = -\frac{1}{2M_N}\sum_i \nabla_i^2 + \sum_{i<j} V_2(r_{ij})$$

→ DP +GEVP at different couplings → $|\Psi_0^{LO}\rangle$

Extract FV energy levels via Lüscher formalism

Match C_0 C_1 to np scattering lengths + effective ranges

Include V_2^{NLO} correction perturbatively using ground state LO wavefunction Ψ^{LO}

LEC Determination: two body sector

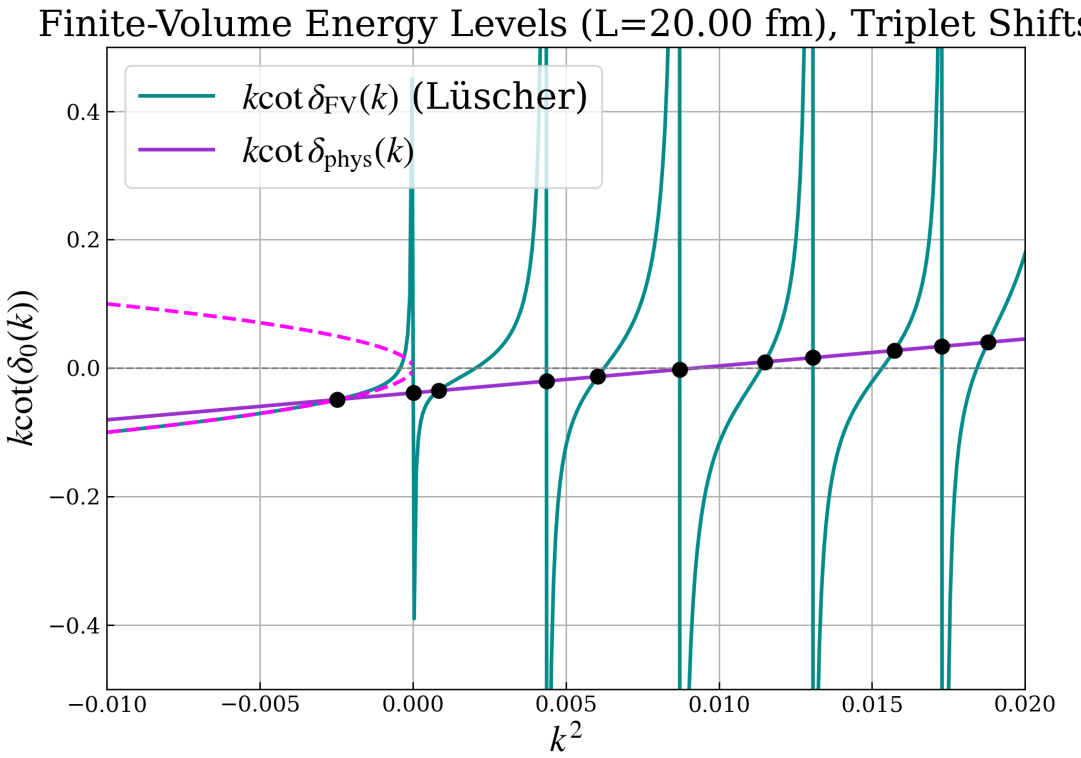
In principle can choose *nn*, *pp*, scattering lengths to investigate systematic spread

Optimize with LO two-body Hamiltonian

Extract FV energy levels via Lüscher formalism

Match C_0 C_1 to *np* scattering lengths + effective ranges

Include V_2^{NLO} correction perturbatively using ground state LO wavefunction Ψ^{LO}



	$^1S_0$	$^3S_1$
a [fm]	−23.74	5.42
r [fm]	2.75	1.76
E_1 [MeV]	−0.340	−2.326
E_2 [MeV]	2.600	0.787
E_3 [MeV]	6.612	5.686

$$k\cot\delta_0(k) = -\frac{1}{a} + \frac{1}{2}rk^2 + \mathcal{O}(k^4)$$

$$k\cot\delta_0(k) = \frac{1}{\pi L}\mathcal{Z}\left(\left(\frac{kL}{2\pi}\right)^2\right)$$

LEC Determination: two body sector

Optimize with LO two-body Hamiltonian

Extract FV energy levels via Lüscher formalism

Match C_0 C_1 to np scattering lengths + effective ranges

Include V_2^{NLO} correction perturbatively using ground state LO wavefunction Ψ^{LO}

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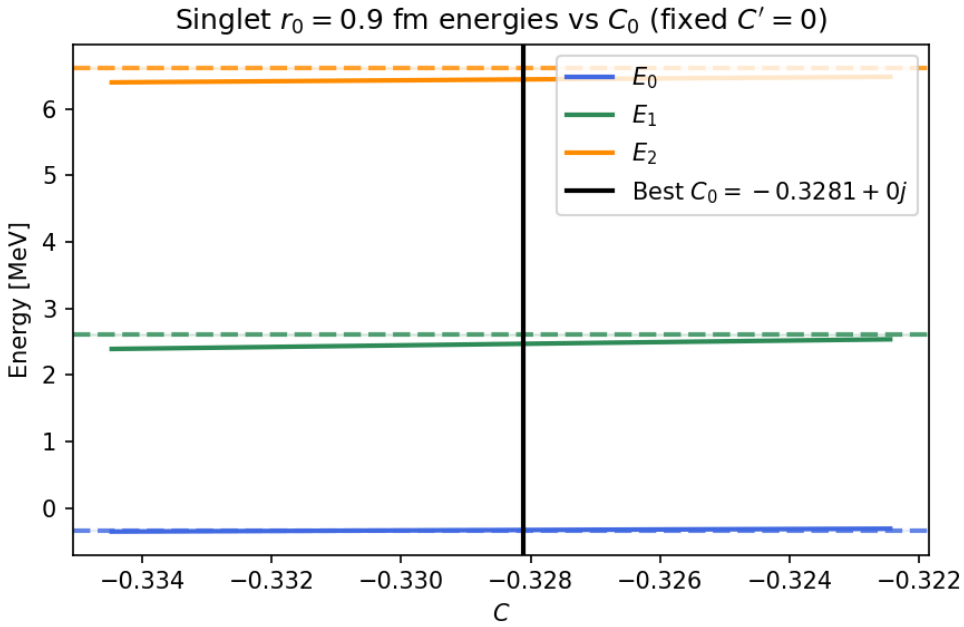
LO fit to two levels



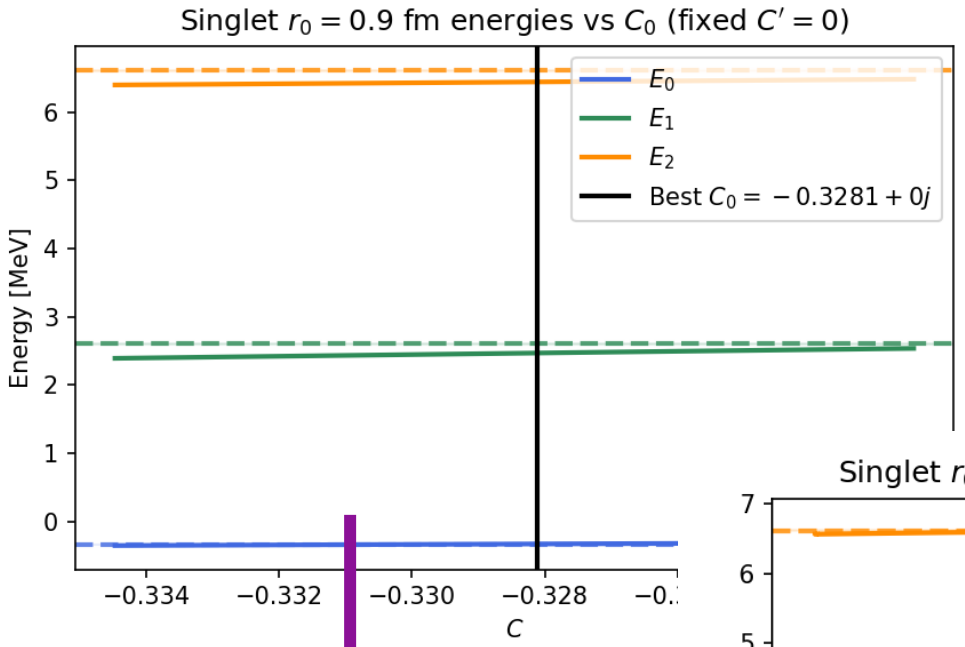
LEC Determination: two body sector

Optimize with LO two-body Hamiltonian

Extract FV energy levels via Lüscher formalism

Match C_0 C_1 to np scattering lengths + effective ranges

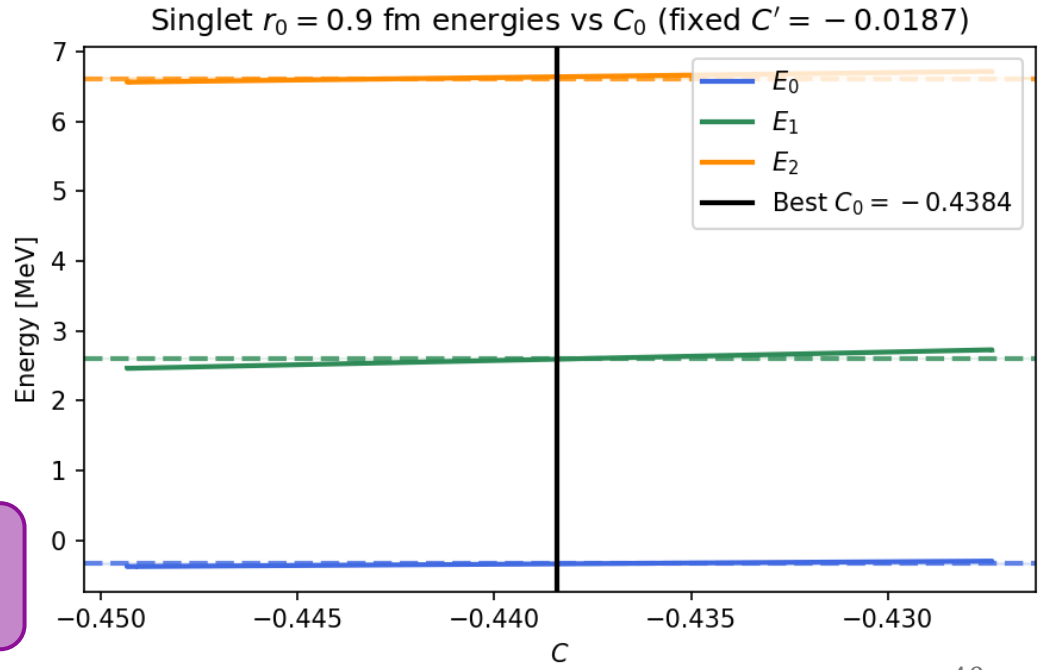
Include V_2^{NLO} correction perturbatively using ground state LO wavefunction Ψ^{LO}



$$\langle \Psi_0^{LO} | V_2^{NLO} | \Psi_0^{LO} \rangle = \Delta E_0$$

NLO fit to three levels to determine C′

In principle can choose to fit to 2 or 3 levels!



LEC Determination: three body sector

- **Three body sector:** Inputs are infinite volume ^{3}He binding energy

Optimize with *fixed* LO two-body + 3 body H

Match D_0^{LO} to ^{3}He binding energy

Match D_0^{NLO} perturbatively using LO ground state wavefunctions with *fixed* two-body NLO couplings