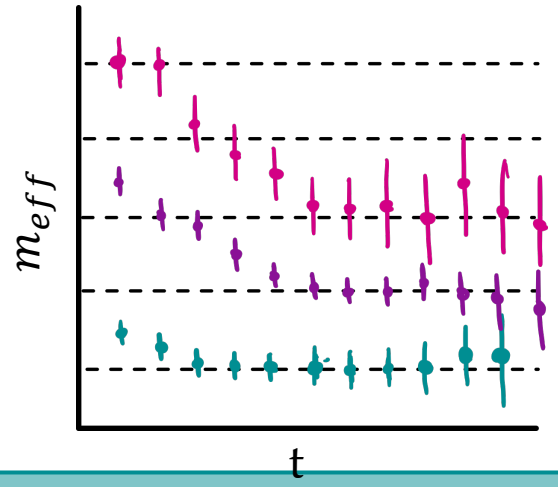

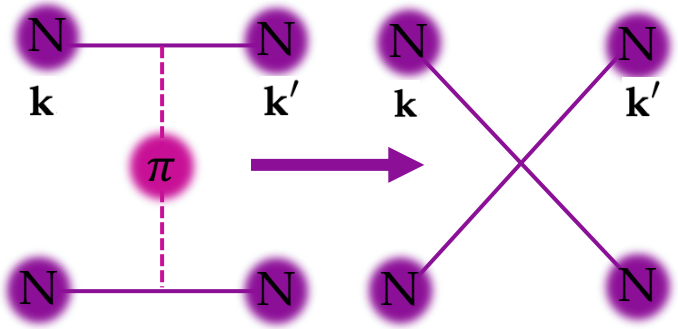

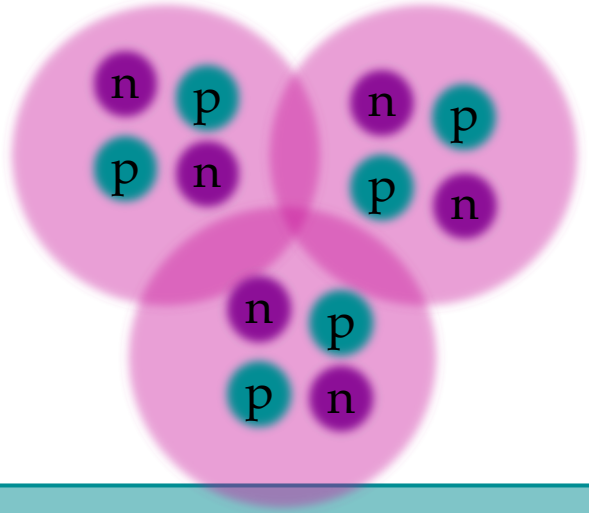

From lattice QCD to *ab initio* nuclear physics via finite-volume pionless EFT

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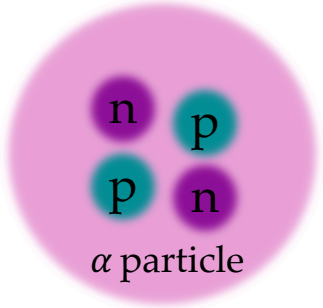
MIT CENTER FOR THEORETICAL PHYSICS – A LEINWEBER INSTITUTE

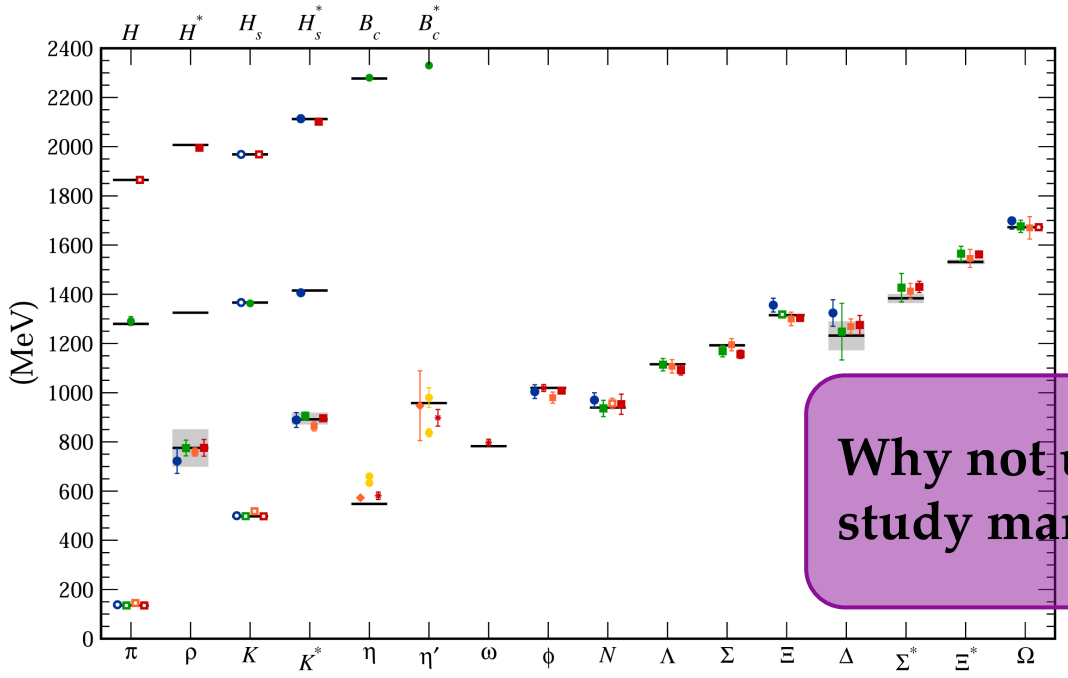
Lattice QCD to nuclear physics

- In principle, QCD should underpin nuclear physics
  - QCD degrees of freedom are quarks and gluons, while hadrons are the natural degrees of freedom in nuclear theory
- Lattice QCD is the *only* systematically improvable way to study QCD with a *non-perturbative* regulator
  - Remarkable post-diction for the QCD meson and low-lying hadron spectrum!

Proton



α particle



Why not use LQCD to directly study many-nucleon systems?

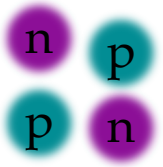
[Kronfeld *Annu. Rev. Nucl. Part. Sci.* 62, 2012]

Lattice QCD to nuclear physics

- Why not use LQCD directly?

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

$$\langle \bar{q}(t)\bar{q}(t)\bar{q}(t)\bar{q}(t)\cdots q(0)q(0)q(0)q(0)\rangle$$

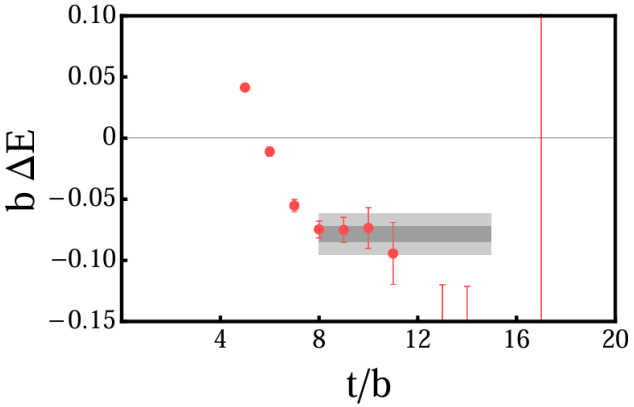


^{4}He ~ 479 million contractions!

Issue 2: Signal-to-noise ratio of correlation functions *exponentially* degrades

$$\lim_{t\to\infty} \frac{\langle C_A(t)\rangle}{\sqrt{\langle |C_A(t)|^2\rangle}} \sim e^{-(AM_N - \frac{3A}{2}m_\pi)t}$$

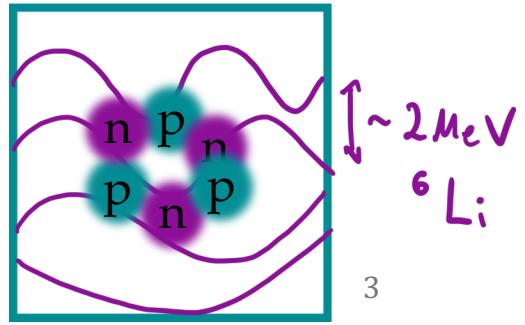
[Wagman and Savage (NPLQCD collaboration) *Phys. Rev. D* 96, 114508 2017, G. Parisi, *Phys. Rep.* 103, 203 (1984)]



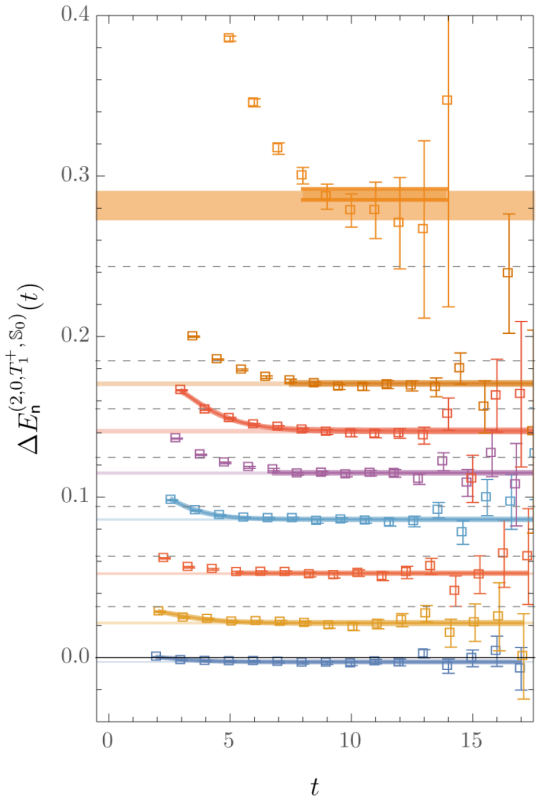
arXiv:1206.5219v2

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

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

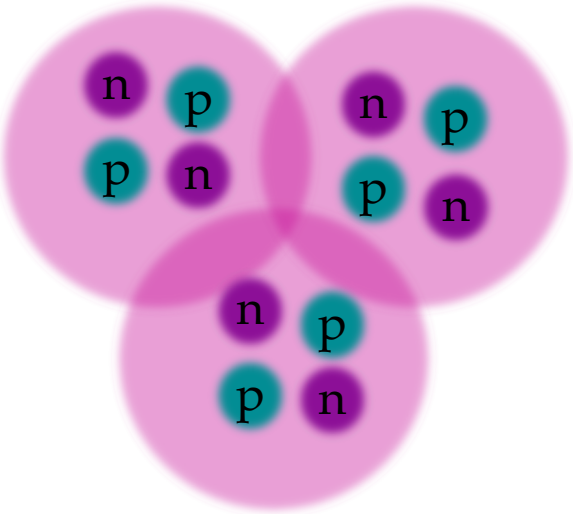


How to relate a two-nucleon energy spectrum computed on the lattice, to binding energy of ^{12}C, ^{208}Pb?

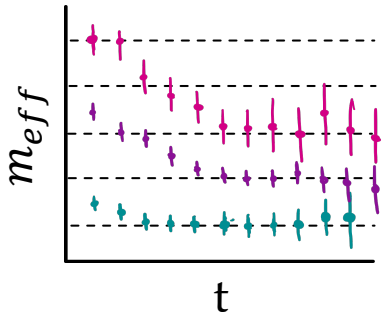


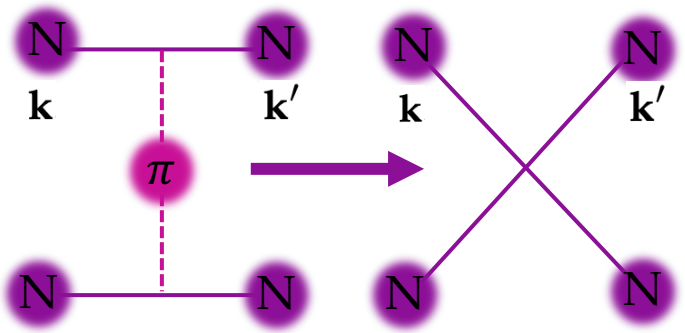
[Amarasinghe et al, *Phys. Rev. D.*, 107, 094508 (2023)]

?



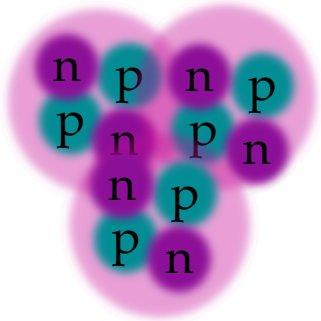
This work





Previous work: Developing FVEFT formalism + proof of principle

1. Finite-volume pionless effective field theory for few-nucleon systems with differentiable programming [Sun et. al, *Phys. Rev. D.* 105, 074508 (2022)]
2. Constraint of pionless EFT using two-nucleon spectra from lattice QCD [Detmold et. al, *Phys. Rev. D.* 108, 034509, 2023]
3. Few-nucleon matrix elements in pionless effective field theory in a finite volume [Detmold and Shanahan, *Phys. Rev. D* 103, 074503, 2021]



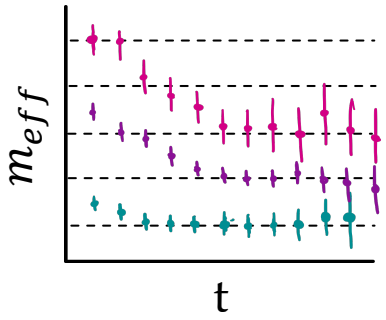
1. Pionless EFT LO Hamiltonian + NLO Corrections

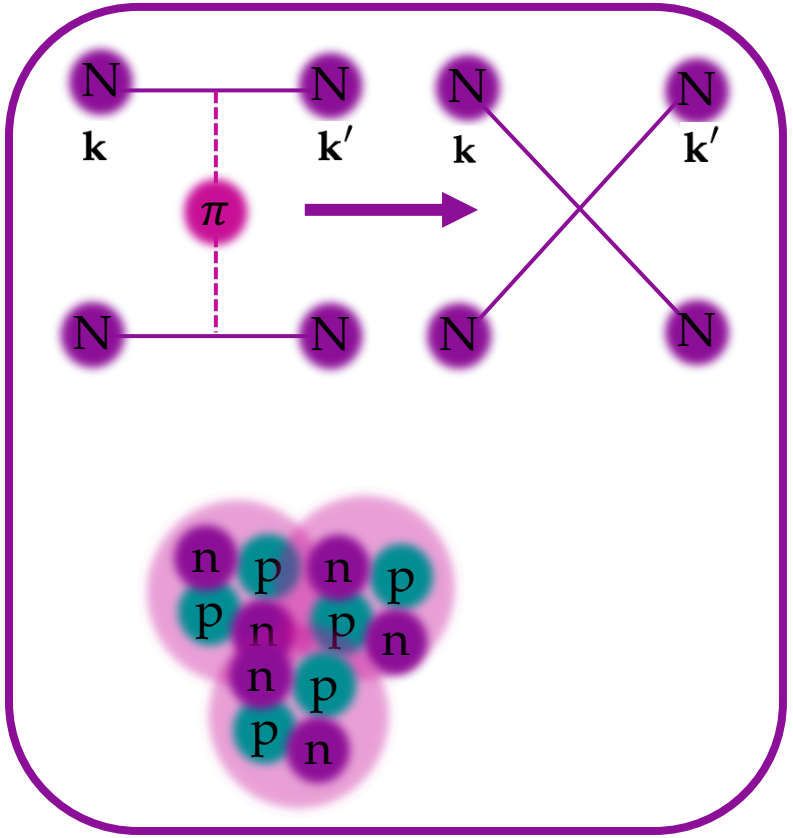
2. Variational Method with N-body correlated Gaussian Ansatz. Differentiable programming to optimize wavefunction.

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

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

This work





This work: Pushing to larger systems, at physical pion mass, with FVEFT formalism established

1. Pionless EFT LO Hamiltonian + NLO Corrections

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

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

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

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 $\{C_0, C_1, D_0\}$

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

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

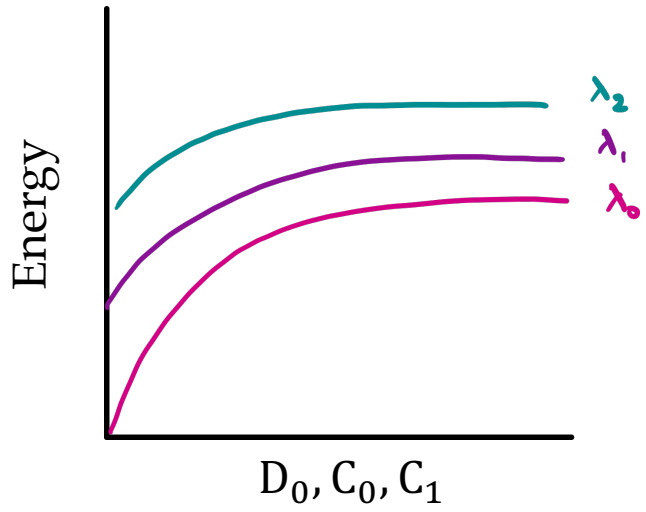
$(\Psi_\alpha(A_i, B_i, d_i)$ LECs: $\{C_0^\alpha, C_1^\alpha, D_0^\alpha\}$

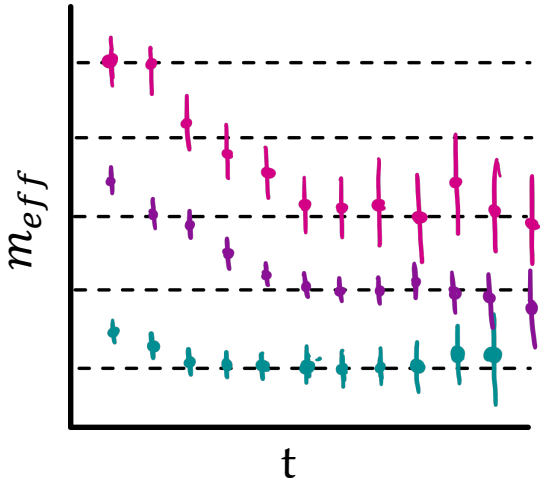
$$\mathbb{H}^{\{C_0, C_1, D_0\}}\vec{c} = \lambda \mathbb{N}\vec{c}$$

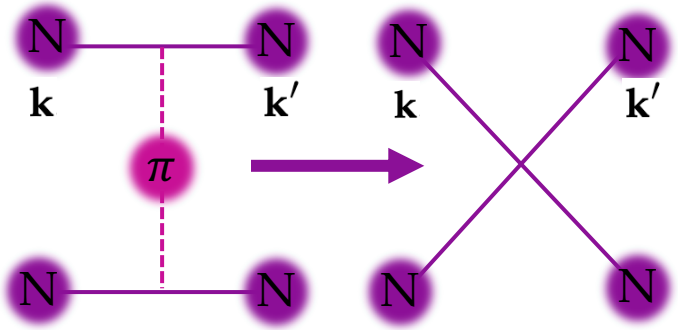
Solve GEVP with α sets of optimized wavefunctions, for a range of LECs, for ground state + excited states

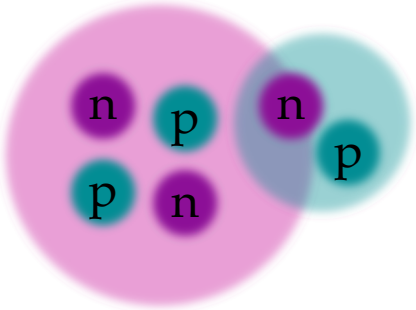
$$\mathrm{E}^{\{C_0, C_1, D_0\}} = \lambda_0$$

Scan over LEC values

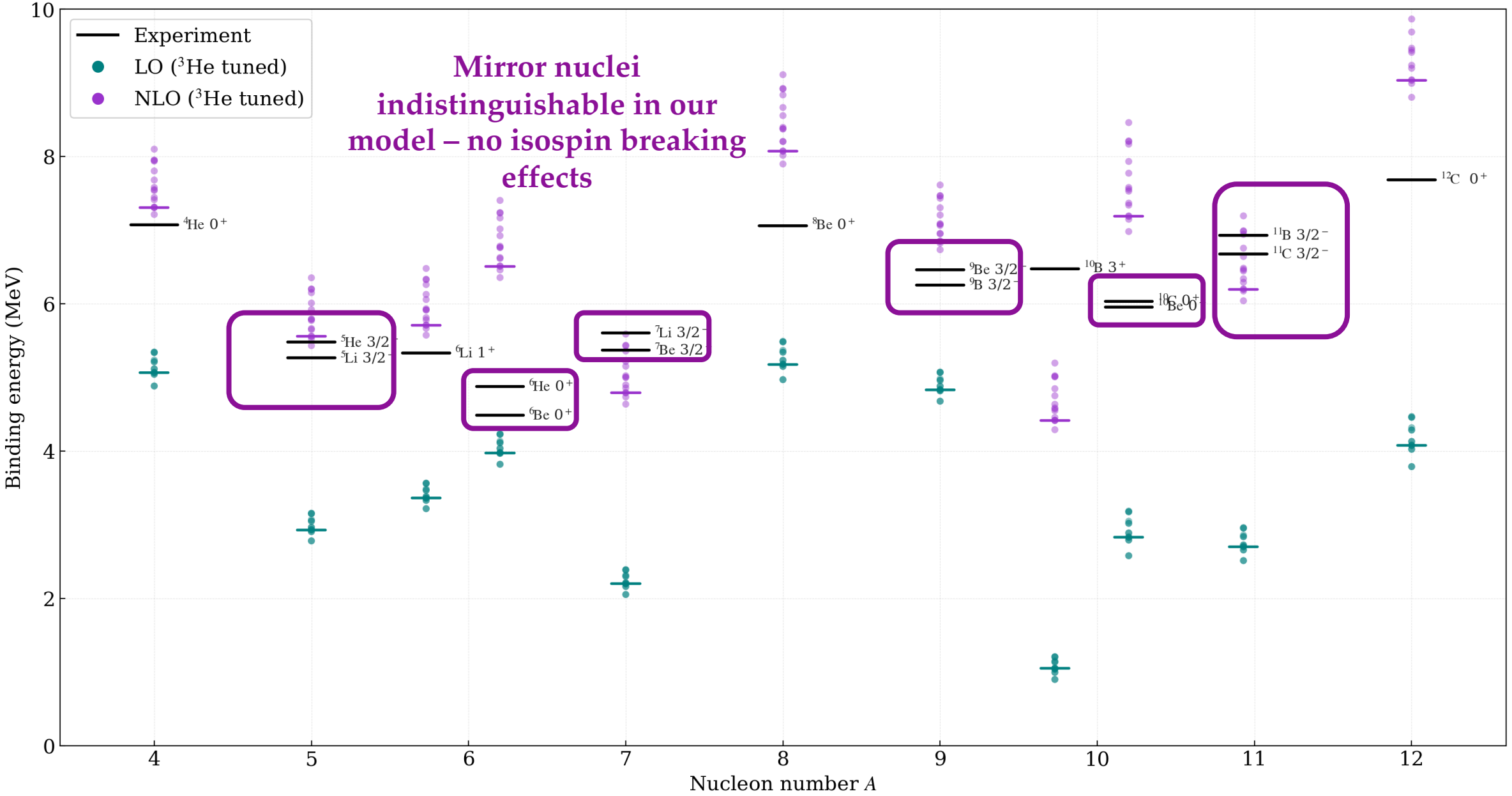


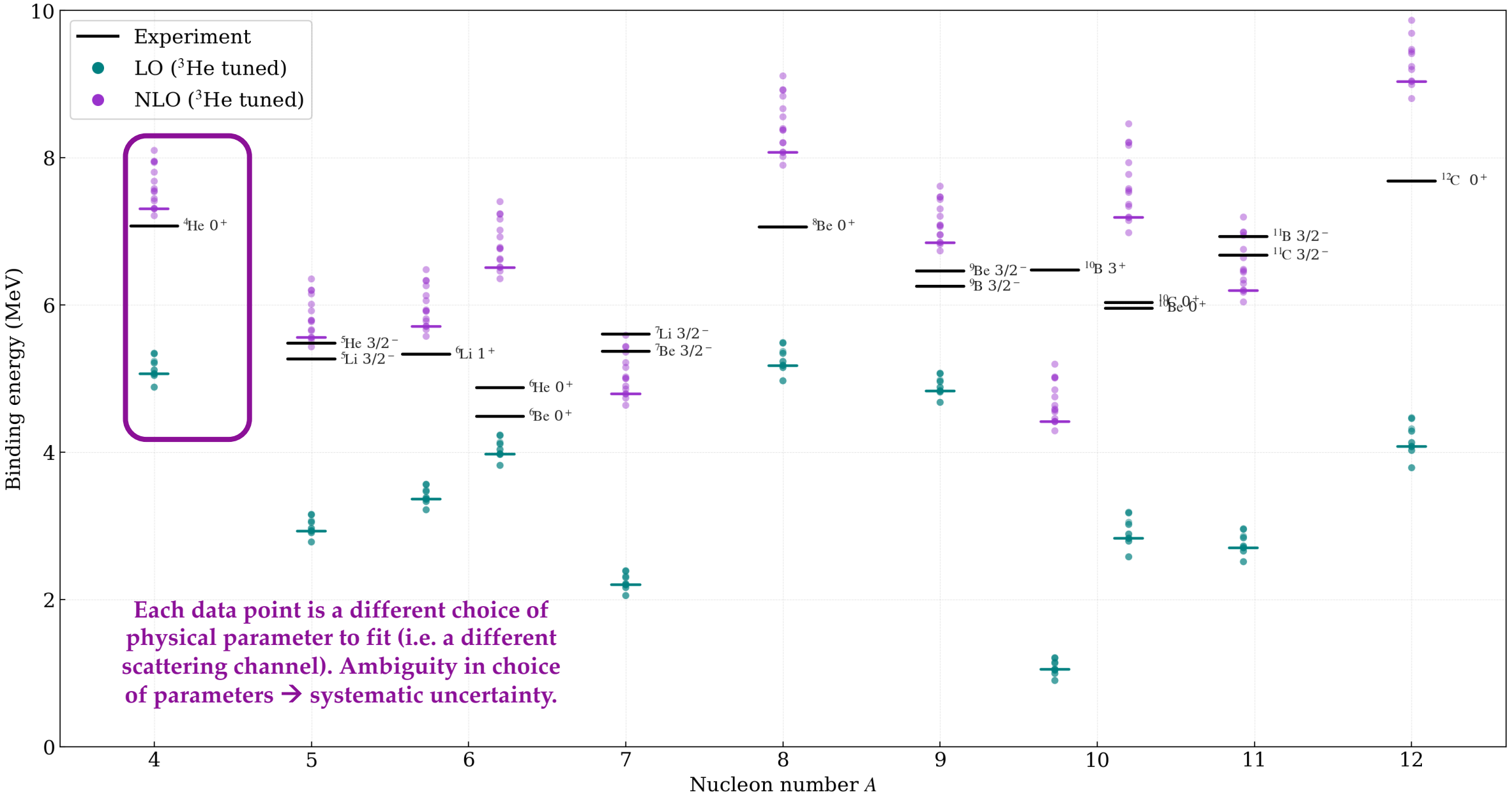


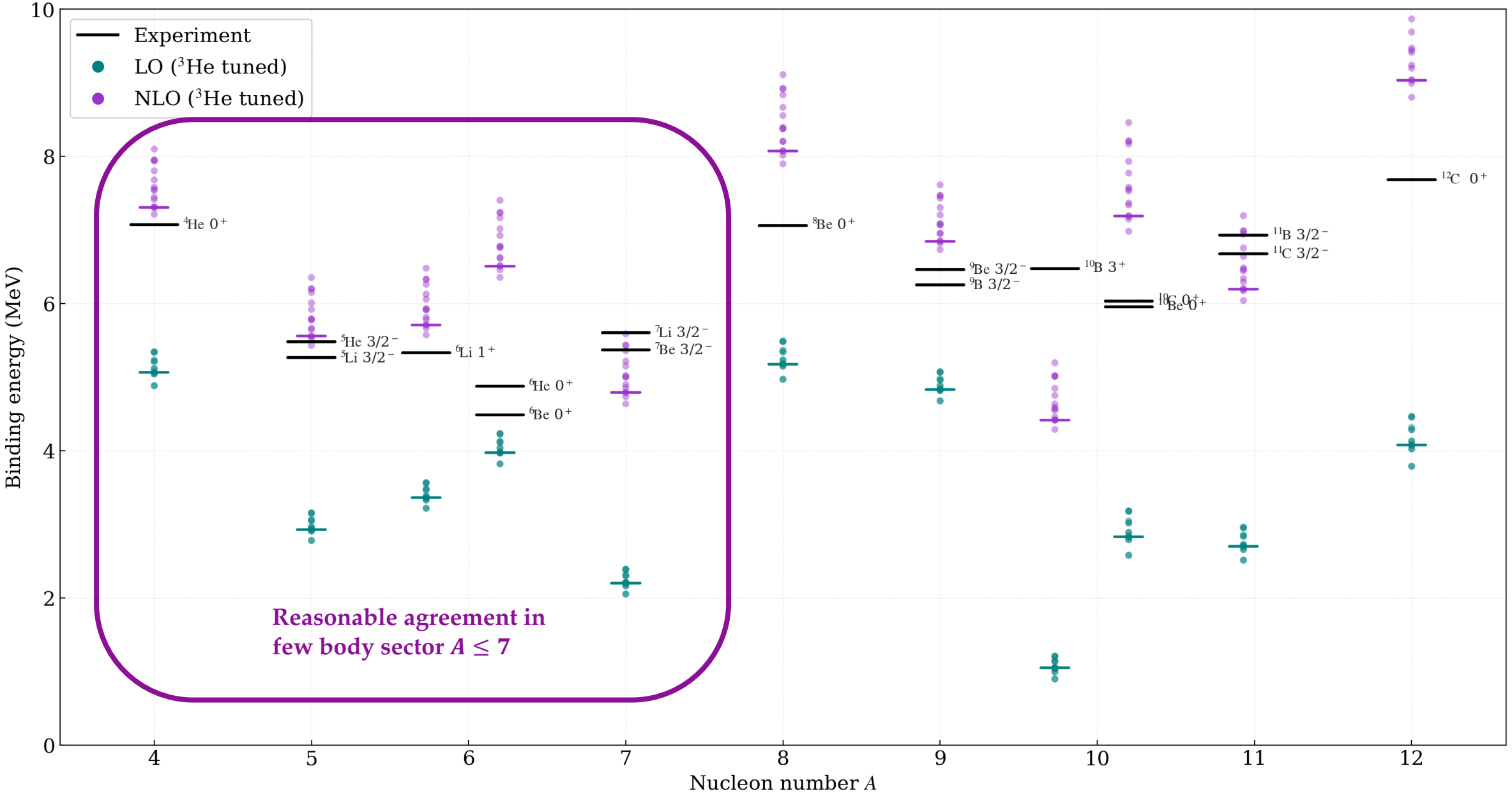


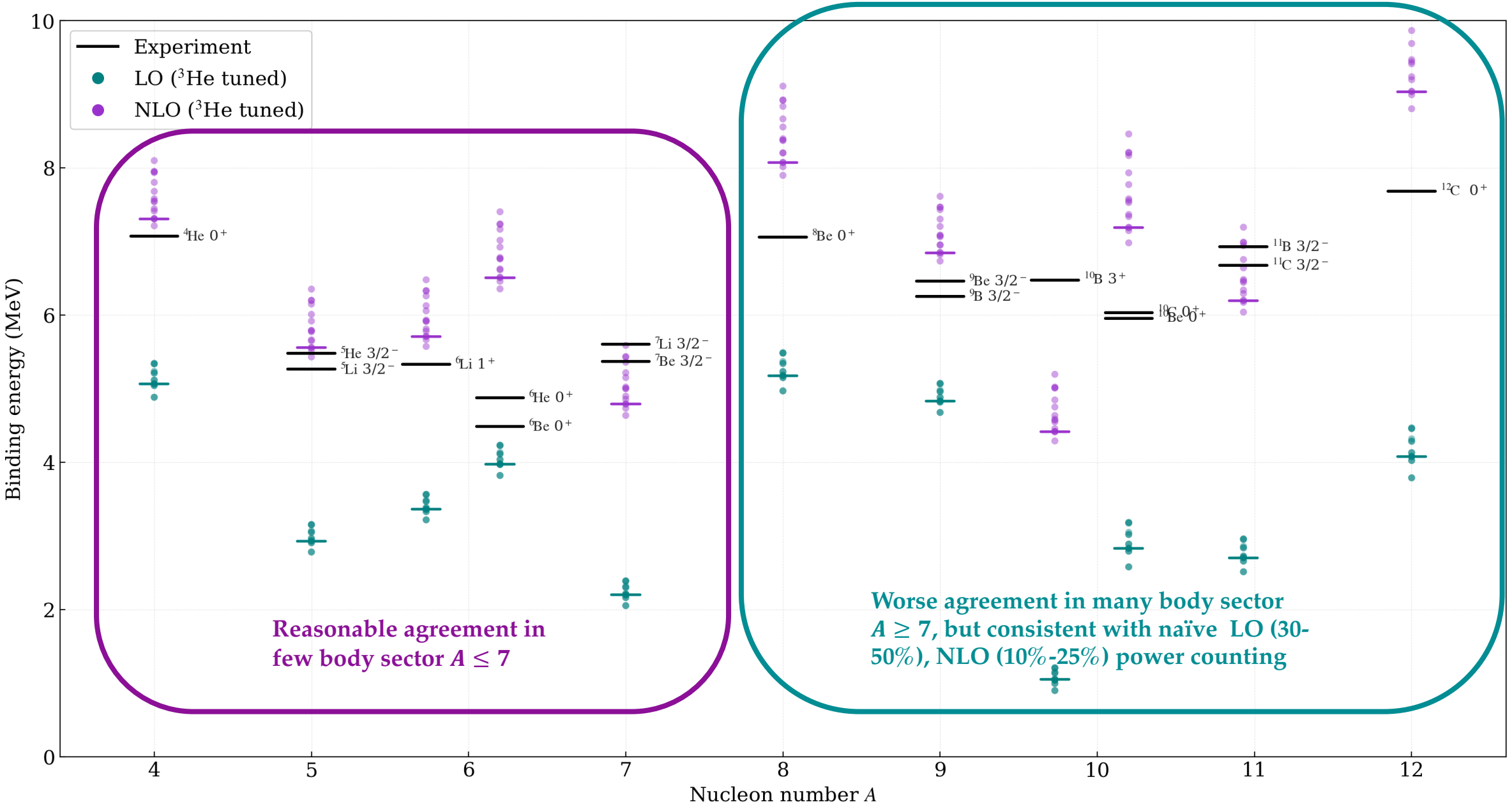


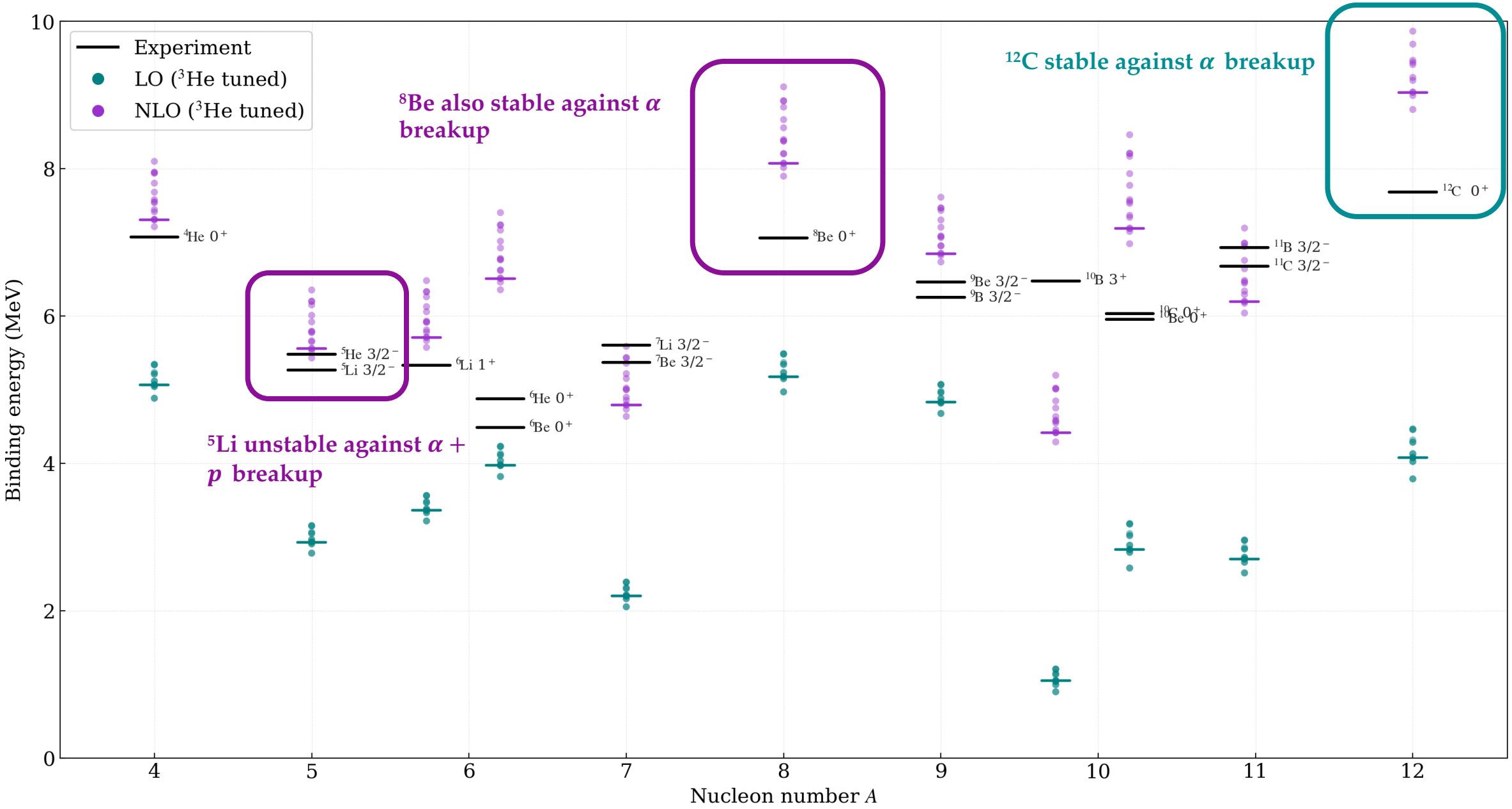
Numerical Results


Experiment
LO (^{3}He tuned)
NLO (^{3}He tuned)
Mirror nuclei indistinguishable in our model – no isospin breaking effects
Binding energy (MeV)
Nucleon number A
^{4}He 0$^+$
^{5}He 3/2$^-$
^{5}Li 3/2$^-$
^{6}Li 1$^+$
^{6}He 0$^+$
^{6}Be 0$^+$
^{7}Li 3/2$^-$
^{7}Be 3/2$^-$
^{8}Be 0$^+$
^{9}Be 3/2$^-$
^{9}B 3/2$^-$
^{10}B 3$^+$
^{10}C 0$^+$
^{10}Be 0$^+$
^{11}B 3/2$^-$
^{11}C 3/2$^-$
^{12}C 0$^+$


Experiment
LO (^{3}He tuned)
NLO (^{3}He tuned)
^{4}He 0$^+$
^{5}He 3/2$^-$
^{5}Li 3/2$^-$
^{6}Li 1$^+$
^{6}He 0$^+$
^{6}Be 0$^+$
^{7}Li 3/2$^-$
^{7}Be 3/2$^-$
^{8}Be 0$^+$
^{9}Be 3/2$^-$
^{9}B 3/2$^-$
^{10}B 3$^+$
^{10}C 0$^+$
^{10}Be 0$^+$
^{11}B 3/2$^-$
^{11}C 3/2$^-$
^{12}C 0$^+$
Each data point is a different choice of physical parameter to fit (i.e. a different scattering channel). Ambiguity in choice of parameters → systematic uncertainty.
Binding energy (MeV)
Nucleon number A
0
2
4
6
8
10
4
5
6
7
8
9
10
11
12


Experiment
LO (^{3}He tuned)
NLO (^{3}He tuned)
Binding energy (MeV)
Nucleon number A
^{4}He 0$^+$
^{5}He 3/2$^-$
^{5}Li 3/2$^-$
^{6}Li 1$^+$
^{6}He 0$^+$
^{6}Be 0$^+$
^{7}Li 3/2$^-$
^{7}Be 3/2$^-$
^{8}Be 0$^+$
^{9}Be 3/2$^-$
^{9}B 3/2$^-$
^{10}B 3$^+$
^{10}C 0$^+$
^{10}Be 0$^+$
^{11}B 3/2$^-$
^{11}C 3/2$^-$
^{12}C 0$^+$
Reasonable agreement in
few body sector $A \leq 7$


Experiment
LO (^{3}He tuned)
NLO (^{3}He tuned)
Binding energy (MeV)
Nucleon number A
^{4}He 0$^+$
^{5}He 3/2$^-$
^{5}Li 3/2$^-$
^{6}Li 1$^+$
^{6}He 0$^+$
^{6}Be 0$^+$
^{7}Li 3/2$^-$
^{7}Be 3/2$^-$
^{8}Be 0$^+$
^{9}Be 3/2$^-$
^{9}B 3/2$^-$
^{10}B 3$^+$
^{10}C 0$^+$
^{10}Be 0$^+$
^{11}B 3/2$^-$
^{11}C 3/2$^-$
^{12}C 0$^+$
Reasonable agreement in few body sector $A \leq 7$
Worse agreement in many body sector $A \geq 7$, but consistent with naïve LO (30-50%), NLO (10%-25%) power counting


Experiment
LO (^{3}He tuned)
NLO (^{3}He tuned)
^{8}Be also stable against α breakup
^{12}C stable against α breakup
^{5}Li unstable against α + p breakup
^{4}He 0$^+$
^{5}He 3/2$^-$
^{5}Li 3/2$^-$
^{6}Li 1$^+$
^{6}He 0$^+$
^{6}Be 0$^+$
^{7}Li 3/2$^-$
^{7}Be 3/2$^-$
^{8}Be 0$^+$
^{9}Be 3/2$^-$
^{9}B 3/2$^-$
^{10}B 3$^+$
^{10}C 0$^+$
^{10}Be 0$^+$
^{11}B 3/2$^-$
^{11}C 3/2$^-$
^{12}C 0$^+$
Binding energy (MeV)
Nucleon number A

Binding energies

- **First pionless EFT calculation of binding energies for $7 \leq A \leq 12$**
- ^{3}H matching produces overbinding due to smaller three-body interaction
- Systematic spread ~ 20% for each binding energy
- Results calculated for *single* 310 MeV cut-off
- NLO correction always positive, due to smaller three-body coupling
- NLO calculation is *not* a variational calculation

Nucleus	J^π	Tuning	E_{LO} (MeV)	E_{NLO} (MeV)	$\langle T^2 \rangle$	$\langle S^2 \rangle$	$\delta_{\mathrm{sys}}/2$ (MeV)	E_{exp} (MeV)
^{4}He	0^+	^{3}He	20.26	**29.24**	0.0025	0.0039	1.77	28.30
	0^+	^{3}H	24.21	34.49	0.0022	0.0044	2.00	
^{5}Li / ^{5}He	$3/2^-$	^{3}He	14.66	**27.78**	0.7667	0.7617	2.30	26.33 / 27.41
	$3/2^-$	^{3}H	18.85	34.31	0.7672	0.7615	2.76	
^{6}Li	1^+	^{3}He	20.17	**34.25**	0.0226	2.0224	2.72	31.99
	1^+	^{3}H	25.14	42.31	0.0208	2.0199	3.41	
^{6}He / ^{6}Be	0^+	^{3}He	23.87	**39.06**	2.0255	0.0083	3.14	29.27 / 26.92
	0^+	^{3}H	28.97	47.38	2.0256	0.0109	3.49	
^{7}Li / ^{7}Be	$3/2^-$	^{3}He	15.39	**33.53**	0.8042	3.7729	3.33	39.24 / 37.60
	$3/2^-$	^{3}H	20.76	42.68	0.8038	3.7700	3.67	
^{8}Be	0^+	^{3}He	41.43	**64.56**	0.0242	0.0086	4.85	56.50
	0^+	^{3}H	49.80	77.98	0.0269	0.0093	5.94	
^{9}Be / ^{9}B	$3/2^-$	^{3}He	43.50	**61.63**	0.7937	0.7690	3.95	58.16 / 56.31
	$3/2^-$	^{3}H	50.92	72.43	0.7928	0.7821	4.28	
^{10}C	0^+	^{3}He	28.30	**71.86**	2.5979	0.0618	7.39	60.32
	0^+	^{3}H	39.22	89.12	2.6259	0.0619	7.42	
^{10}B	3^+	^{3}He	10.53	**44.15**	0.0951	12.0311	4.52	64.75
	3^+	^{3}H	17.67	55.32	0.0930	12.0287	4.54	
^{11}B / ^{11}C	$3/2^-$	^{3}He	29.73	**68.16**	0.8030	3.7748	6.34	76.20 / 73.44
	$3/2^-$	^{3}H	40.11	84.55	0.7938	3.7693	7.37	
^{12}C	0^+	^{3}He	48.92	**108.40**	0.4894	0.2662	9.97	92.16
	0^+	^{3}H	63.41	131.65	0.4644	0.2986	10.54	

Compare bolded and unbolded values (^{3}He and ^{3}H fitting)

Summary and Outlook

Approach

1. Pionless EFT LO Hamiltonian + NLO Corrections
2. Differentiable programming to optimize wavefunction.
3. 3. Match EFT low-energy constants to reproduce 2-body and 3-body physical results.
4. With matched EFT, use variational method to extract energies of larger nuclei $A \leq 12$

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. Reasonable agreement in few body sector $A \leq 7$
3. Results consistent with naïve LO (30%-50%), NLO (10%-25%) power counting
4. Demonstration of feasibility of LQCD → many body systems

Outlook

1. Systematic investigation for range of Λ
2. Matter radii, charge radii, nuclear magnetic moment comparisons
3. Is pionless EFT justified for $A \geq 4$ systems?
4. Are 4-body interactions needed for renormalization?
5. Do other EFTs show more promise? (chiral, cluster, etc)

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

Nucleus	$E_{\mathrm{NLO}}(\delta_{\mathrm{sys}})$ (MeV)	E_{exp} (MeV)
^{4}He	29.24(3.54)	28.30
^{5}Li / ^{5}He	27.78(4.60)	26.33 / 27.41
^{6}Li	34.25(5.44)	31.99
^{6}He / ^{6}Be	39.06(6.38)	29.27 / 26.92
^{7}Li / ^{7}Be	33.53(6.66)	39.24 / 37.60
^{8}Be	64.56(9.70)	56.50
^{9}Be / ^{9}B	61.63(7.90)	58.16 / 56.31
^{10}C	71.86(14.78)	60.32
^{10}B	44.15(9.04)	64.75
^{11}B / ^{11}C	68.16(12.68)	76.20 / 73.44
^{12}C	108.40(19.94)	92.16