AB INITIO CALCULATIONS OF LIGHT NUCLEI USING OPTIMIZED CHIRAL HAMILTONIANS

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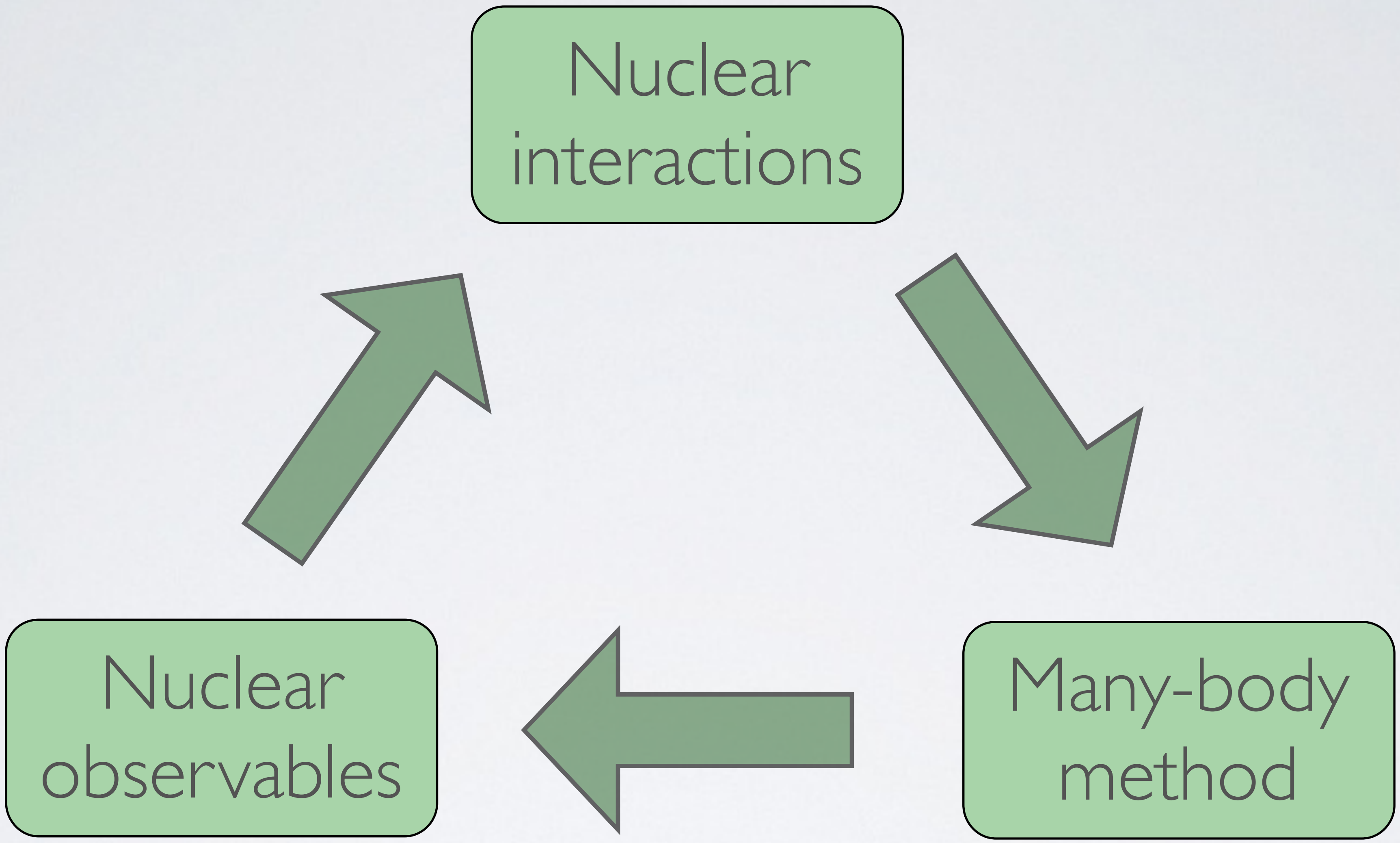
Outline

- ❖ INTRODUCTION
- ❖ PART I: Optimized chiral Hamiltonians
- ❖ PART II: From few to many with uncertainty quantification
- ❖ CONCLUSION

The ab initio nuclear theory approach

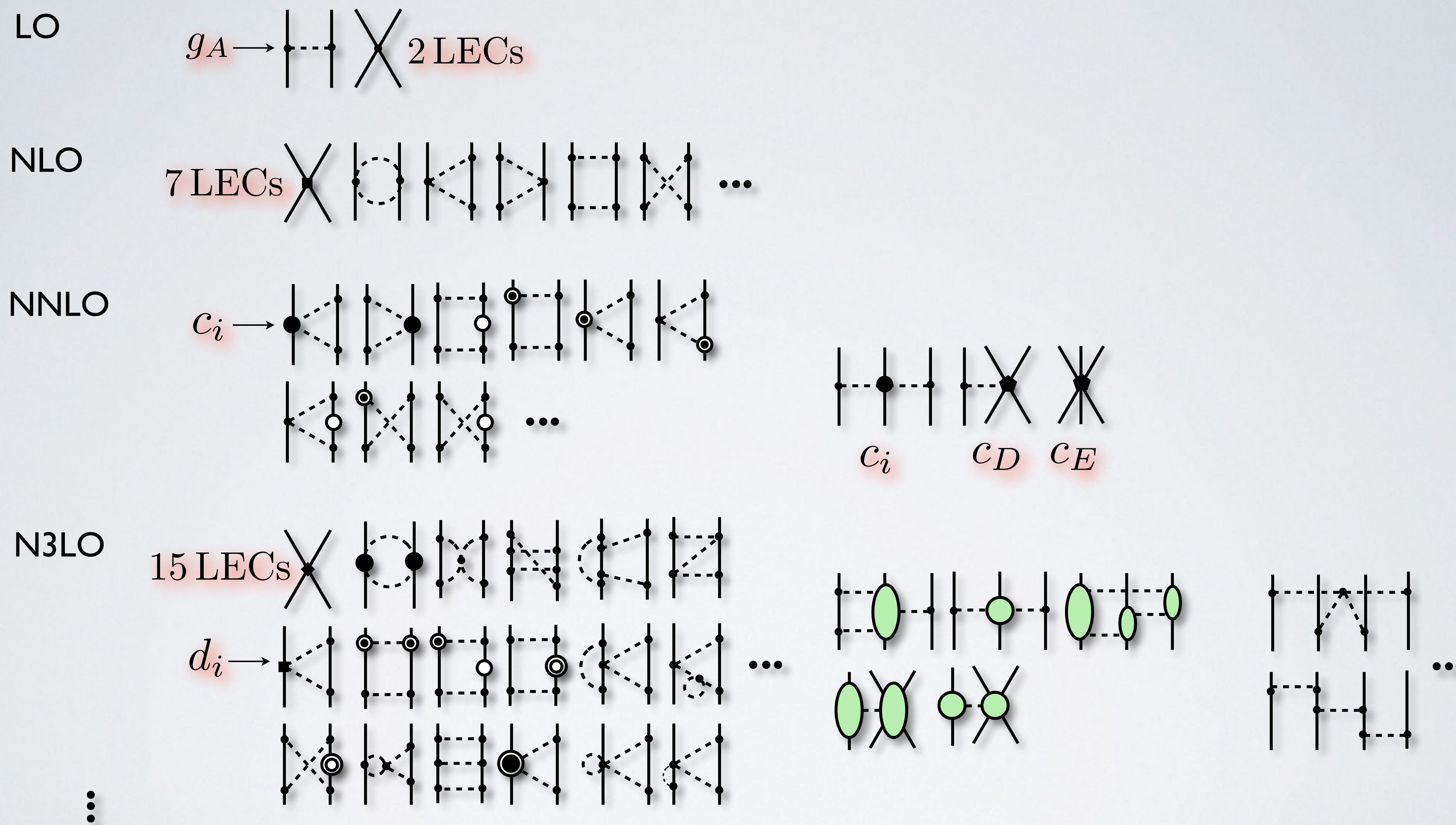


Two sources of uncertainty that can be tracked using *ab initio* methods:

- Nuclear interaction uncertainties
- Many-body calculation uncertainties

OPTIMIZED CHIRAL HAMILTONIANS

Nuclear forces from chiral EFT



E. Epelbaum et al. Rev. Mod. Phys. 81, 1773 (2009)
R. Machleidt et al. Phys. Rep. 503, 1 (2011)

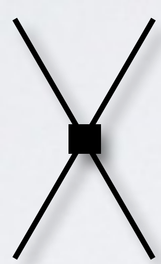
Low-energy constants at NNLO

Optimized chiral NN interaction at NNLO

- A. Ekström, et al., 2013. Phys. Rev. Lett., **110** (2013), 192502.

2 LECs

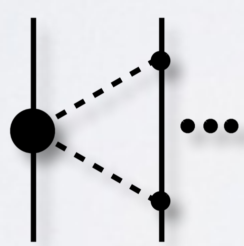
$\tilde{C}^{pp}_{^1S_0}$ $\tilde{C}^{np}_{^1S_0}$ $\tilde{C}^{nn}_{^1S_0}$ $\tilde{C}_{^3S_1}$



7 LECs

$C_{^1S_0}$ $C_{^3P_0}$ $C_{^3P_1}$ $C_{^3P_2}$

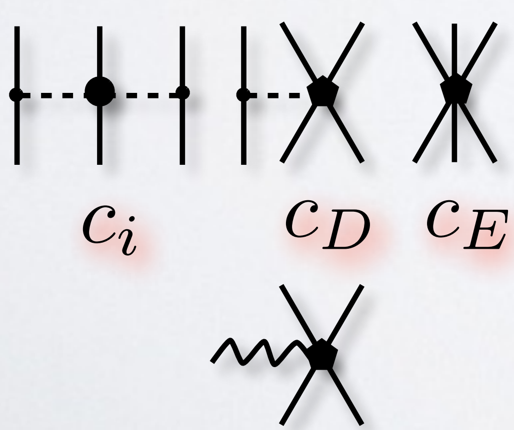
$C_{^1P_1}$ $C_{^3S_1}$ $C_{^3S_1-^3D_1}$



c_i

c_1 c_3 c_4

long-range physics



two new parameters that can be determined from the A>2 systems

Two new optimization strategies

Any "potential model" will contain coupling constants that need to be determined from data one way or the other.

$$\min_{\vec{x}} \left[f(\vec{x}) = \sum_{q=1}^{N} \left(\frac{O(\vec{x})_q - O_q^{\exp}}{w_q} \right)^2 \right]$$

Define an objective function that is relevant for the "objective"

1. **πN LECs determined first** from Pion-Nucleon scattering phase shifts
2. **(NN-only) objective function based on observables only**
   - Nucleon-Nucleon scattering data
   - $^1S_0$ effective range expansion
   - A=2: energy, radius, Q
3. **NNN LECs determined at the end** given the NN part

1. **Expanded (NN+NNN) objective function**
   - Nucleon-Nucleon scattering data
   - Pion-Nucleon scattering phase shifts
   - $^1S_0$ effective range expansion
   - Few-body observables: NCSM 2H/3H/4He Binding energies and radii
   - Energy and saturation momentum of symmetric nuclear matter from MBPT2

πN LECs: overview

	piN-Krebs	piN-BM	NN-PWA	NNLO (Bochum)	N3LO (Idaho)	NNLOopt
c1	[-1.13,-0.75]	**-0.81±0.12**	**-0.76±0.07**	**-0.81**	**-0.81**	**-0.9186**
c3	[-5.51,-4.77]	**-4.70±1.16**	**-4.78±0.10**	**-3.4**	**-3.2**	**-3.8887**
c4	[3.34,3.71]	**3.40±0.04**	**+3.96±0.22**	**+3.40**	**+5.40**	**+4.3103**

piN-Krebs: The most recently published, and to fourth order, analysis of the piN scattering phase shifts up to pLab=150 MeV [GW06,KH86]

piN-BM: Analysis of KA84 piN scattering phase shifts pLab=40-97

NN-PWA: Nijmegen PWA analysis of NN scattering data, with the long range physics described by subleading chiral two-pion exchanges

NNLO (Juelich): pion-nucleon couplings taken from piN-BM, but c3 chosen on the larger side within the uncertainty. This value is consistent with the Entem Machleidt analysis of NN data.

N3LO (Idaho): Guided by fit to NN data

NNLOopt: Guided by fit to NN data

E. Epelbaum *et al.* Rev. Mod. Phys. 81, 1773 (2009)
E. Epelbaum *et al.* Eur. Phys. J. A19, 401 (2004)
R. Machleidt *et al.* Phys. Rep. 503, 1 (2011)
A. Ekström *et al.* Phys. Rev. Lett. 110, 192502 (2013)
H. Krebs *et al.* Phys. Rev. C, 85, 054006 (2012)
M. C. M. Rentmeester *et al.* Phys. Rev. C, 67, 044001 (2003)

πN LECs: new results

	piN-Krebs	piN-BM	NN-PWA	NNLO (Bochum)	N3LO (Idaho)	NNLOopt
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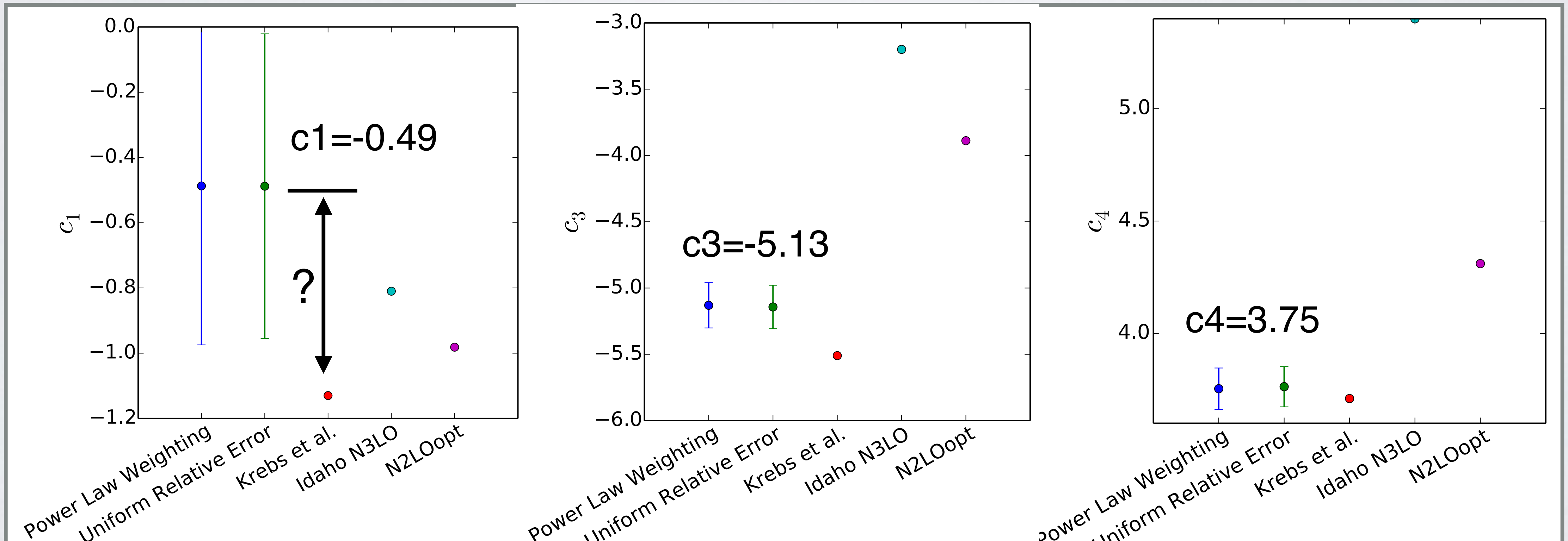


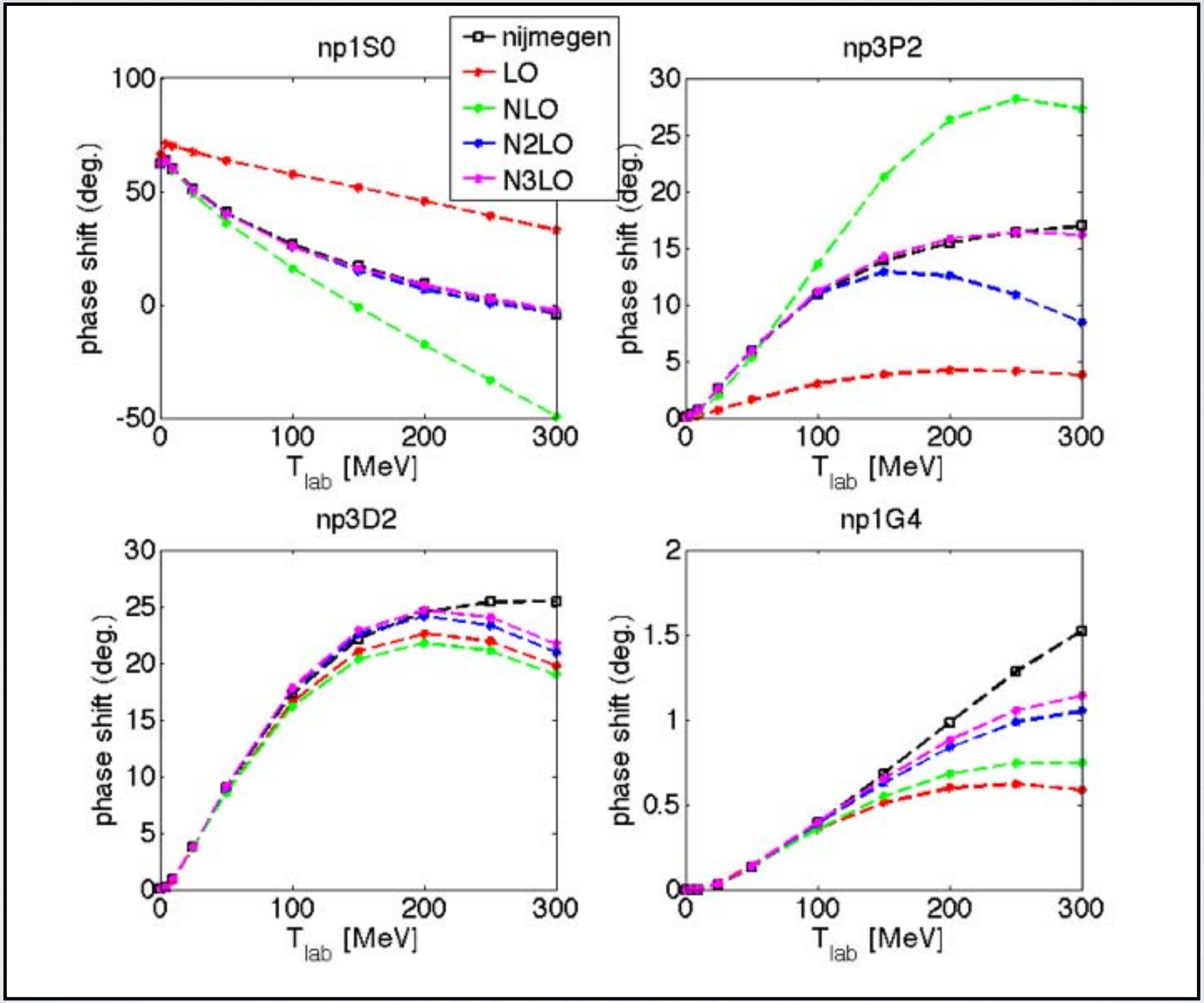
Figures from K. Wendt

order-by-order optimization

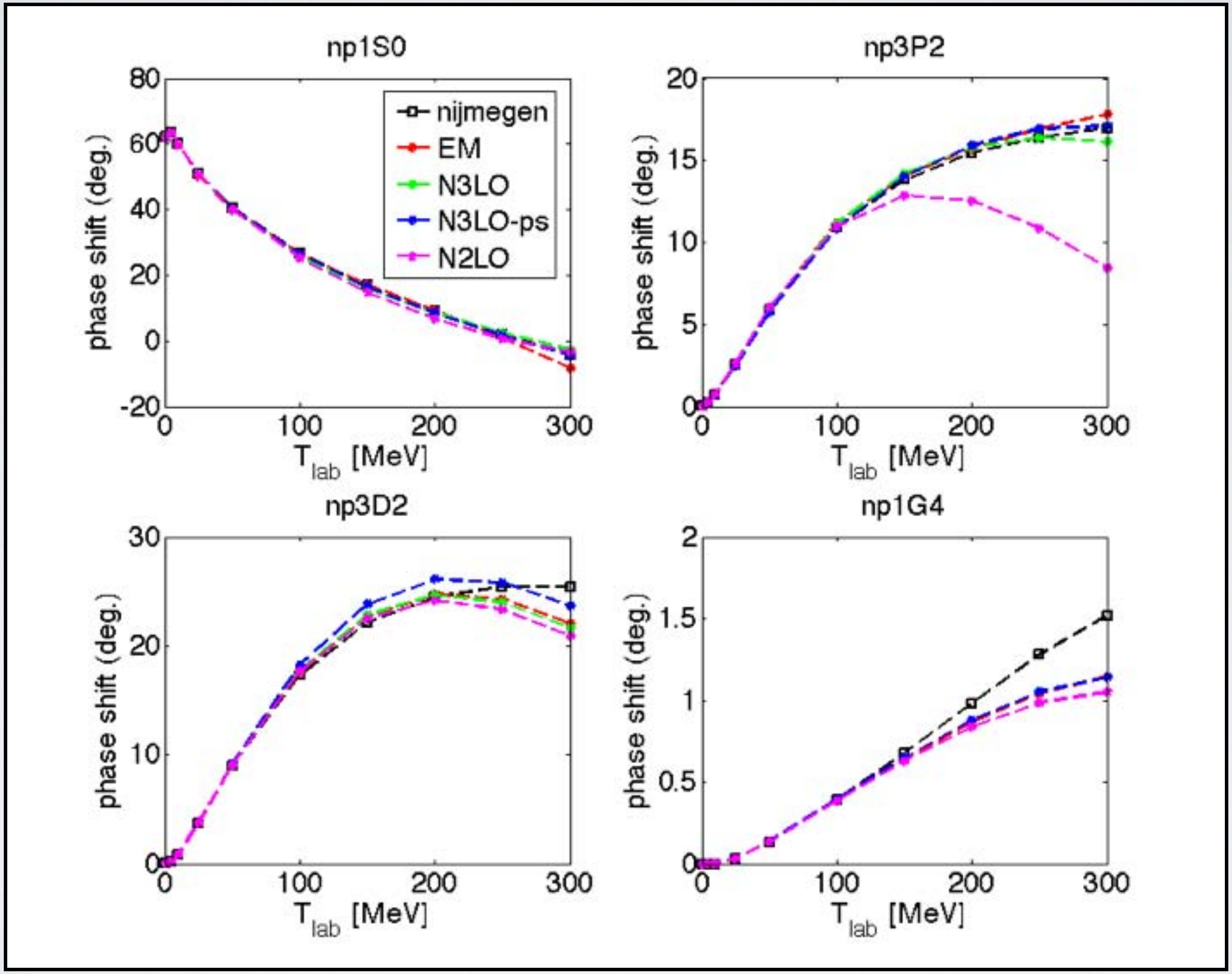
In progress

- LO optimization
  - NN scattering observables ($T_{lab} \leq 0.5$ MeV), $^1S_0$ ERE, A=2 observables
- NLO optimization
  - NN scattering observables ($T_{lab} \leq 75$ MeV, s-waves / p-waves mainly for 0-8 / 8-75 MeV, respectively), $^1S_0$ ERE, A=2 observables
- NNLO optimization
  - Work in progress. The results presented here are with $NNLO_{opt}$
- N3LO optimization
  - NN scattering observables ($T_{lab} \leq 350$ MeV), $^1S_0$ ERE, A=2 observables

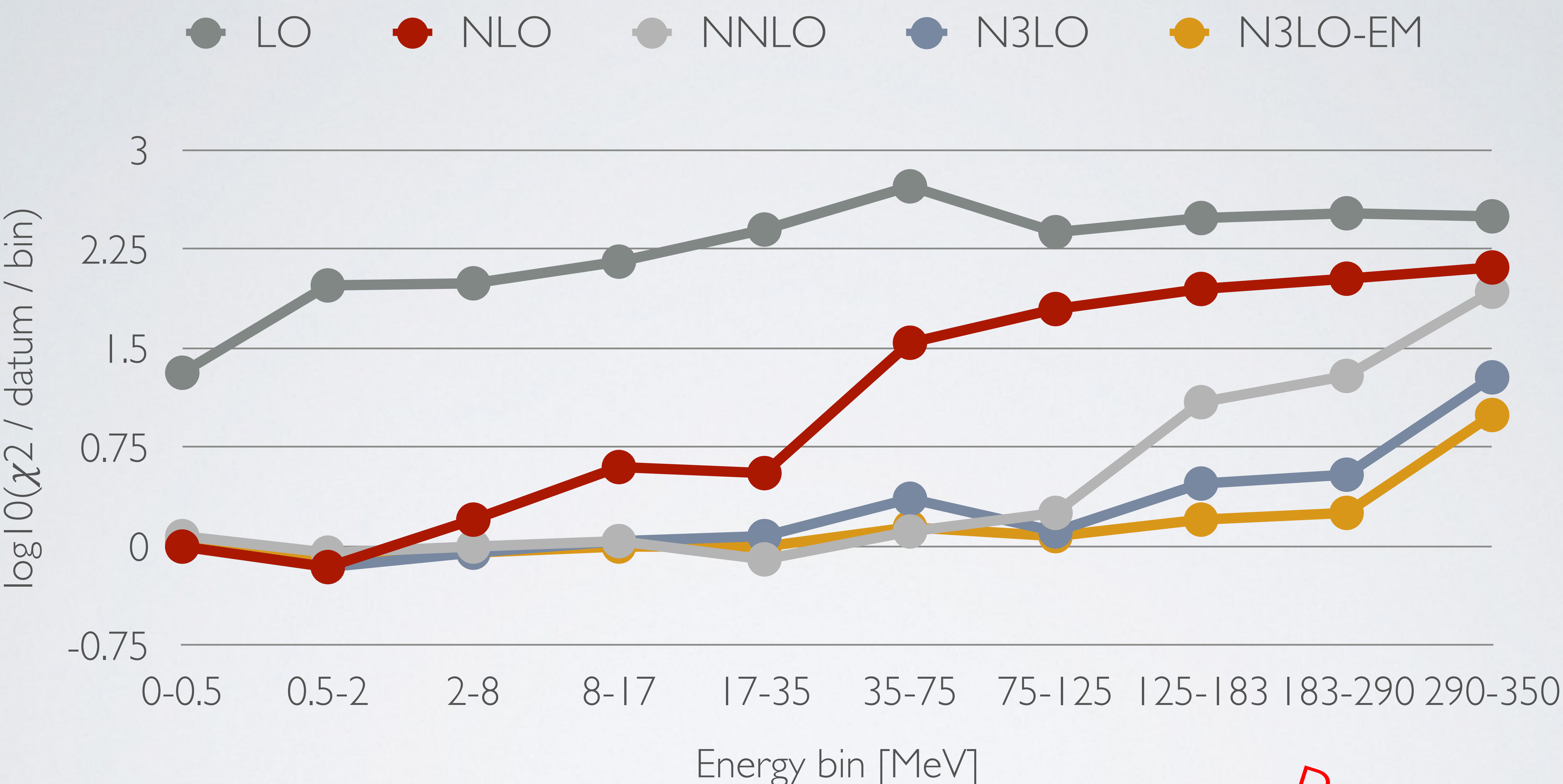
Selected np phase shifts



Selected np phase shifts



χ^2 / datum per energy bin



Preliminary

From few to many

Frontiers of *ab initio* nuclear many-body theory

- The **many-body frontier**
  - Heavier systems, away from closed shells
- The **continuum frontier**
  - Approaching the drip lines
  - Unified theory of structure and reactions
- The **convergence frontier**
  - Uncertainty quantification, error propagation

The No-Core Shell Model

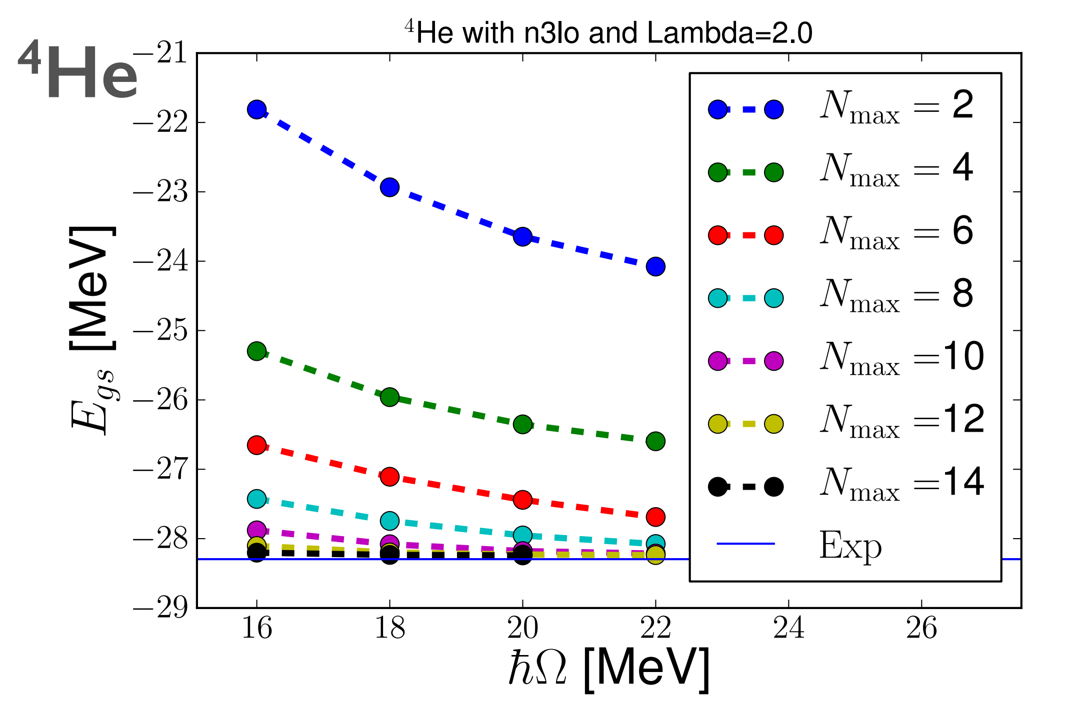
- Many-body Schrödinger equation
  - *A*-nucleon wave function
  - Non-relativistic, point nucleons
- Hamiltonian:

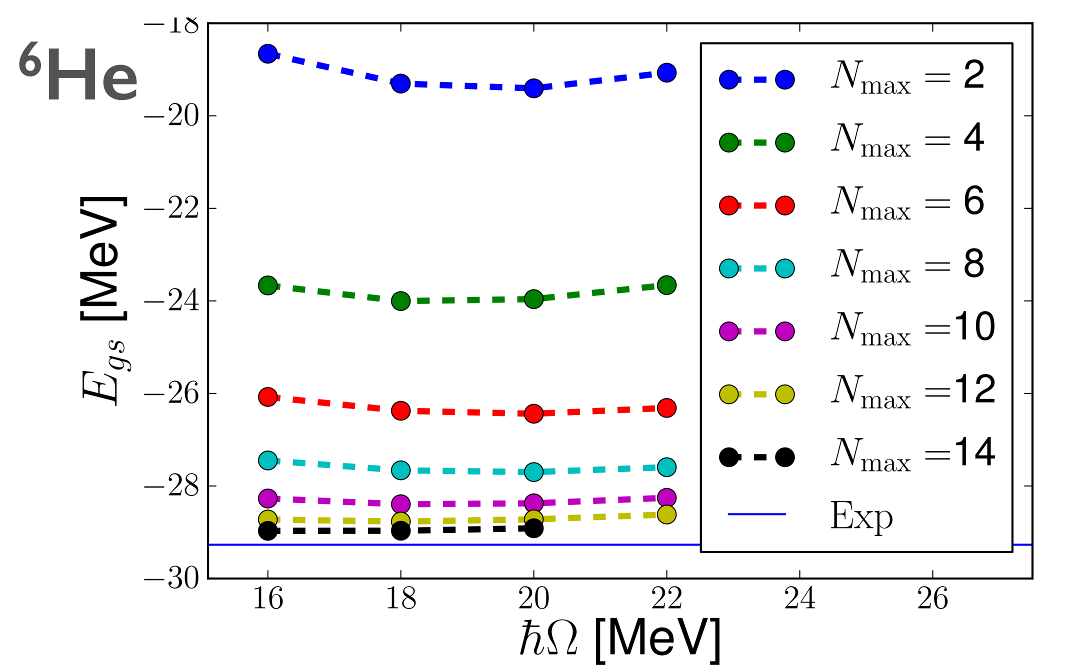
$$H_A = \frac{1}{A} \sum_{i<j}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j}^{A} V_{NN,ij} + \sum_{i<j<k}^{A} V_{NNN,ijk}$$

- Many-body basis: Slater determinants composed of harmonic oscillator single-particle states
- Respects translational invariance and includes full antisymmetrization

NCSM convergence: finite HO space

N^{3}LO, SRG (NN only, Λ = 2.0 fm^{-1})





HO basis cutoff scales

$$\Lambda_{\rm UV} = \sqrt{2(N+3/2)}\hbar/b$$

$$L_{\rm IR} = L_2 \equiv \sqrt{2(N+3/2+2)}b$$

Extrapolations from finite HO basis

- R.J. Furnstahl et al., Phys. Rev. C 86(2012)031301R
- S. Coon et al., Phys. Rev. C 86(2012)054002
- R.J. Furnstahl et al., Phys. Rev. C 87(2013)044326
- R.J. Furnstahl et al., arXiv:1312.6876

Previous work with N_{max} / ħΩ extrapolation

- C. Forssén et al., Phys. Rev. C 77(2008)024301
- P. Maris et al., Phys. Rev. C 79 (2009)014308

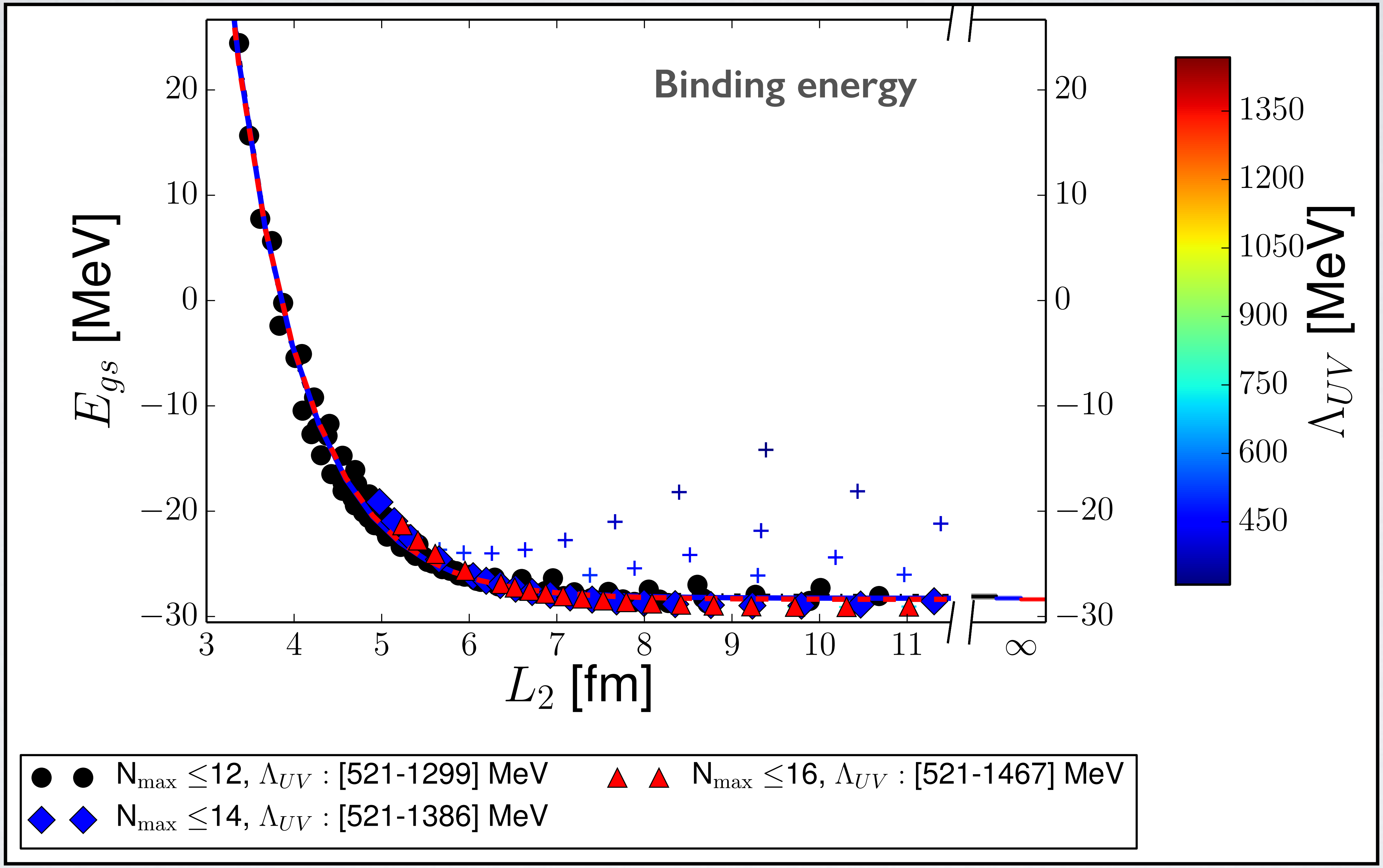
LO correction to the energy due to finite HO space (Dirichlet bc):

$$E_L = E_\infty + \Delta E_L$$

$$\text{with} \Delta\ E_L = a_0 \exp(-2k_\infty L)$$

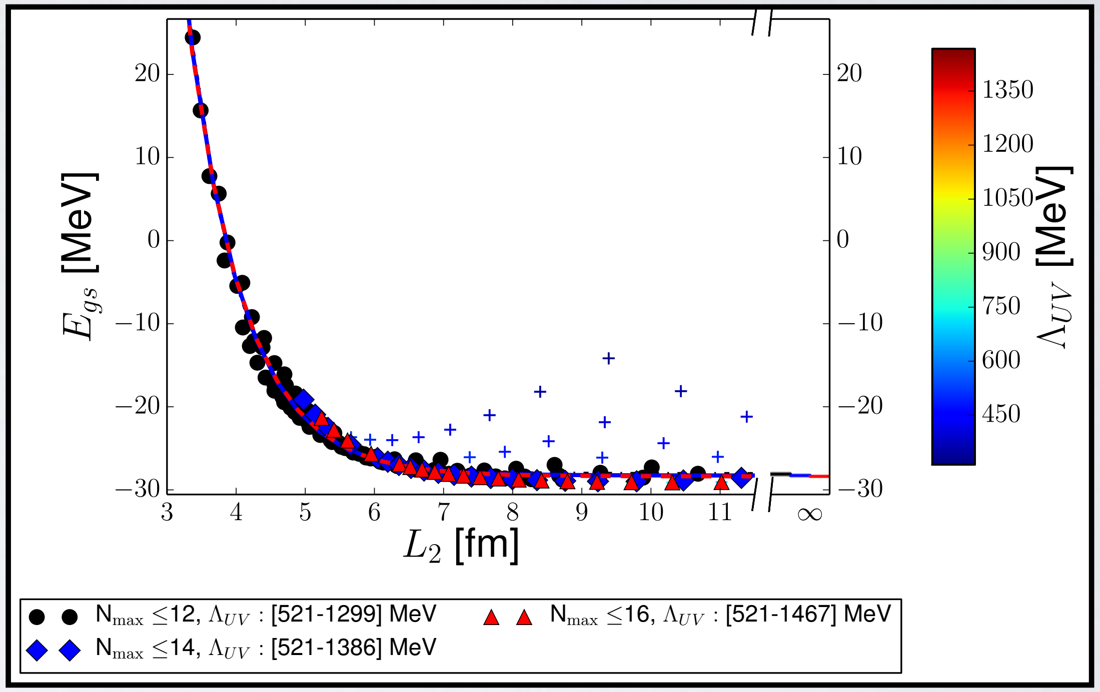
HO basis extrapolation schemes

^{6}He N^{3}LO, SRG (NN only, Λ = 2.0 fm^{-1})



^6He: Ground-State Properties

N^3LO, SRG (NN only, $\Lambda = 2.0\ \mathrm{fm}^{-1}$)



	Exp. [5]	This work			Bacca *et al.* [6]
		$\Lambda_{\mathrm{SRG}} = 1.8$	$\Lambda_{\mathrm{SRG}} = 2.0$	$\Lambda_{\mathrm{SRG}} = 2.2$	$V_{\mathrm{low}-k}$ ($\Lambda = 2.0\ \mathrm{fm}^{-1}$)
E_{gs} [MeV]	29.269	29.42(9)	28.79(6)	28.03(10)	29.47(3)
S_{2n} [MeV]	0.975	0.97(9)	0.54(6)	0.09(11)	0.82(4)
$r_{\mathrm{pt-p}}$ [fm]	1.938(23)	1.786(4)	1.788(3)	1.805(4)	1.804(9)

CONCLUSION

Summary

- Optimization of chiral Hamiltonian up to N3LO
  - POUNDerS shows great promise to deliver state-of-the-art optimized nuclear forces
  - Optimized with respect to scattering data
  - Two different optimization strategies

- No-core shell model for light nuclei
  - Introduction of UV and IR scales gives error estimate

- Outlook
  - Correlated uncertainty estimates
  - Error propagation to nuclear observables
  - Cutoff dependence

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