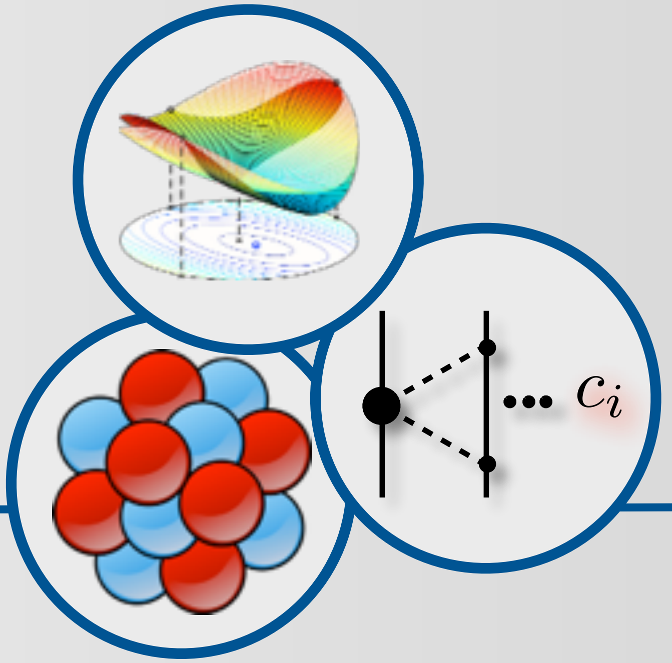
Optimized chiral hamiltonians for practical use:

- current status and perspectives



***Andreas Ekström** (Oslo University, Norway and Chalmers University of Technology, Sweden)*

Collaborators:

Gustav Baardsen (UiO)
Boris Carlsson (UiO/Chalmers)
Christian Forssen(Chalmers)
Gaute Hagen(ORNL)
Morten Hjorth-Jensen(UiO/MSU)
Gustav Jansen(UT/ORNL)
Ruprecht Machleidt(UI)
Witold Nazarewicz(UT/ORNL)
Thomas Papenbrock(UT/ORNL)
Jason Sarich(ANL)
Kyle Wendt(UT/ORNL)
Stefan Wild(ANL)

TRIUMF Workshop
"Nuclear Structure & Reactions : Experimental and Ab Initio Theoretical Perspectives"
February 18-21, 2014, TRIUMF, Vancouver.

contents

Introduction

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"

<u>"a well-founded and quantitative Hamiltonian for practical use"</u>

Introduction

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

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

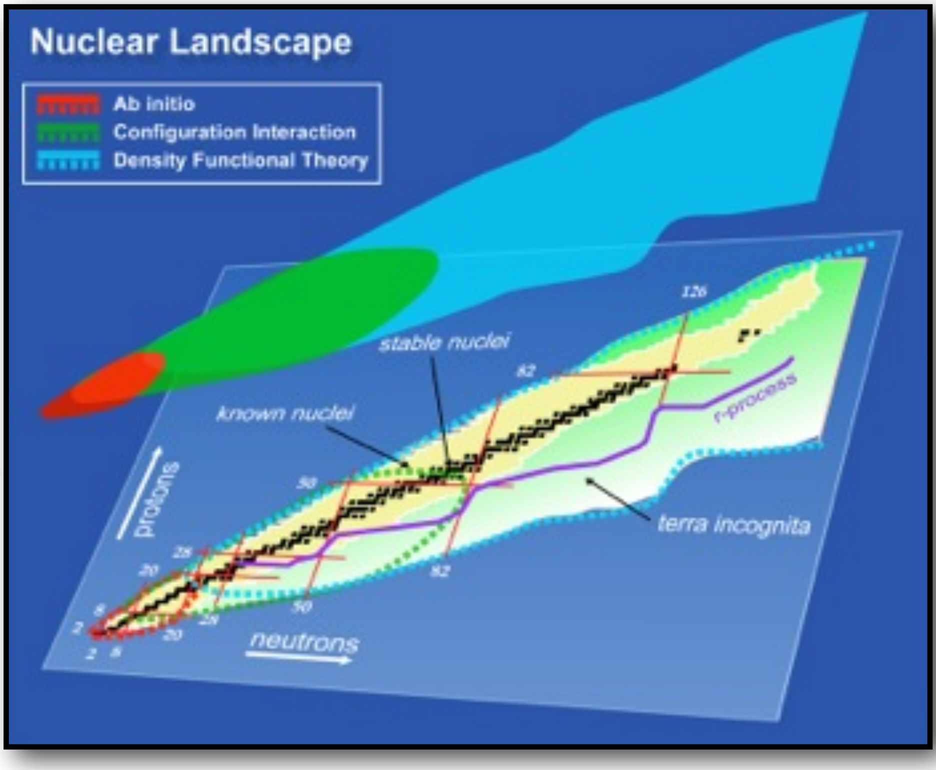
Define an objective function that is relevant for the "objective"
"a well-founded and quantitative Hamiltonian for practical use"

Several **high-precision** potentials on the market:

CD-Bonn, AV18, Idaho-N3LO, Nijmegen

Tlab (MeV)	**N3LO (Idaho)**	AV18
0-100	**1.06**	0.95
100-190	**1.08**	1.1
190-290	**1.15**	1.11
0-290	**1.1**	1.04

Chi Square



Chiral forces: current status

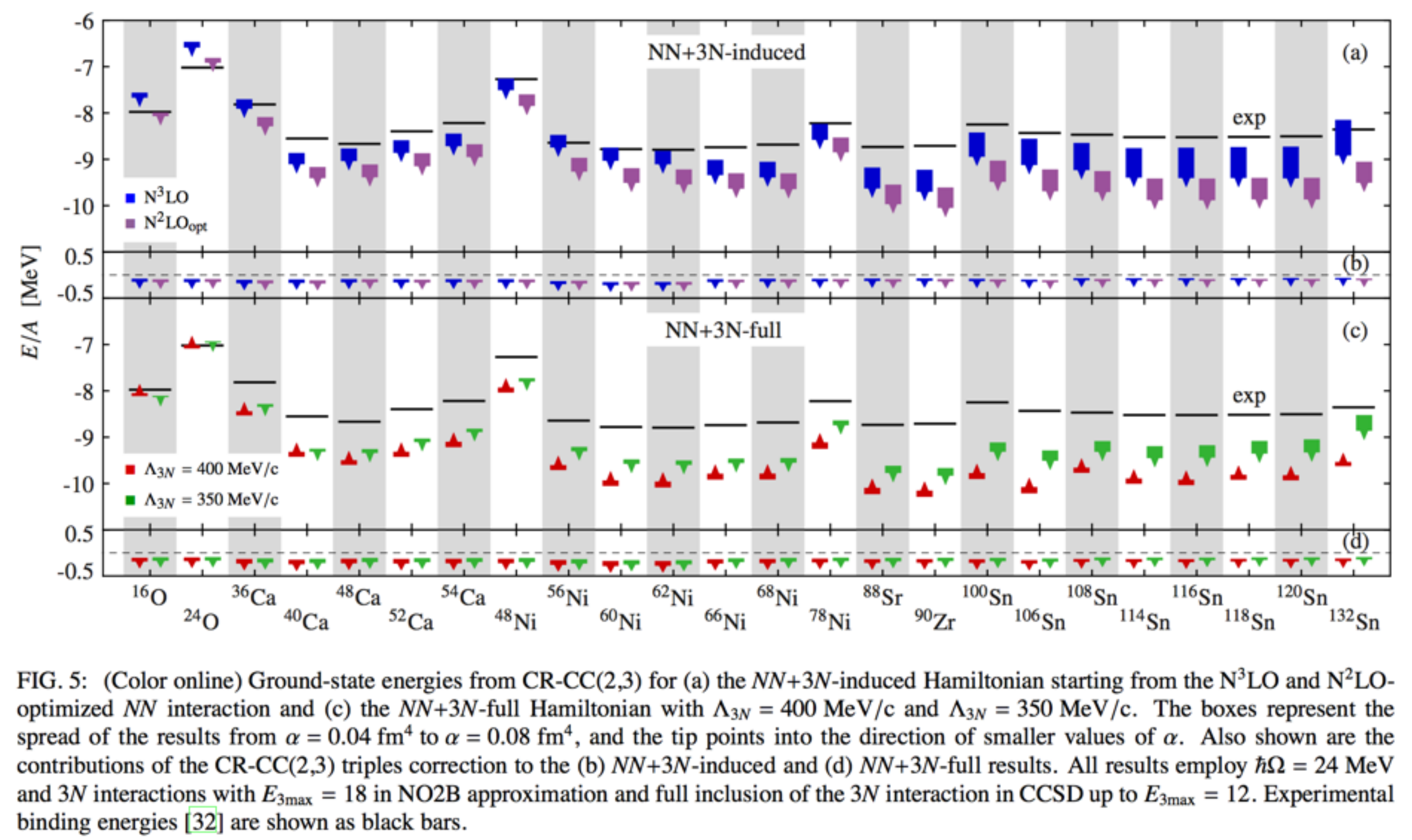


FIG. 5: (Color online) Ground-state energies from CR-CC(2,3) for (a) the *NN*+3*N*-induced Hamiltonian starting from the N^{3}LO and N^{2}LO-optimized *NN* interaction and (c) the *NN*+3*N*-full Hamiltonian with Λ_{3N} = 400 MeV/c and Λ_{3N} = 350 MeV/c. The boxes represent the spread of the results from $\alpha = 0.04$ fm^4 to $\alpha = 0.08$ fm^4, and the tip points into the direction of smaller values of α. Also shown are the contributions of the CR-CC(2,3) triples correction to the (b) *NN*+3*N*-induced and (d) *NN*+3*N*-full results. All results employ $\hbar\Omega = 24$ MeV and 3*N* interactions with $E_{3\max} = 18$ in NO2B approximation and full inclusion of the 3*N* interaction in CCSD up to $E_{3\max} = 12$. Experimental binding energies [32] are shown as black bars.

Chiral interactions are qualitatively OK, but systematically overbinds and generates too small charge radii. The discrepancies increase with mass number.

Figure from S. Binder *et al.*, arXiv 1312.5685 (2013)

Current Work: Expanded objective function

$$\min_{\vec{x}} \left[f(\vec{x}) = \sum_{d} \frac{1}{w_d} \sum_{q} \left(\frac{O(\vec{x})_{d,q} - O^{\exp}_{d,q}}{w_q} \right)^2 \right]$$

Terms included in the objective function

potential: ***NN + 3NF(local or non-local) at NNLO***

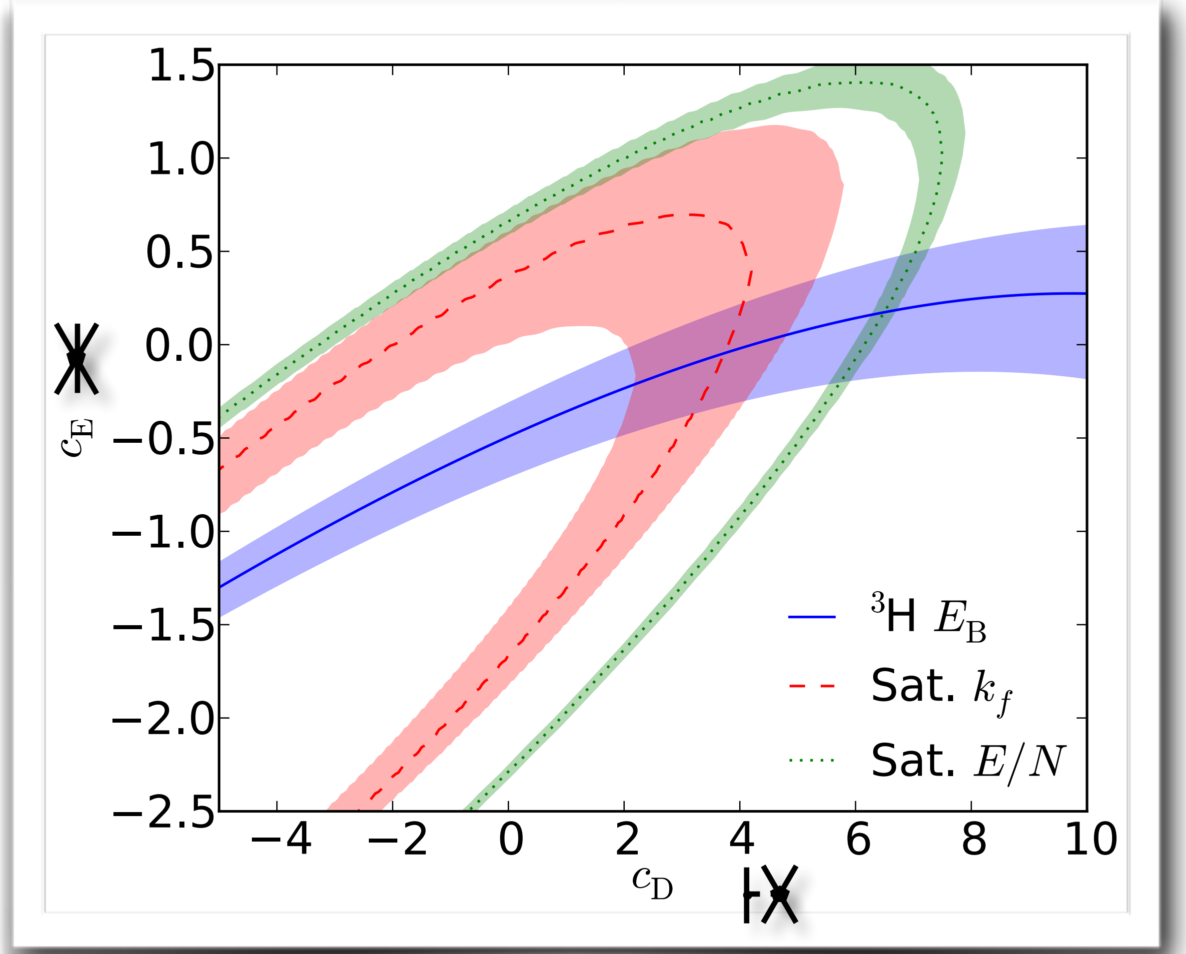
Nucleon-Nucleon scattering data

1S0 effective range expansion

Pion-Nucleon scattering phase shifts

Few-body observables:
NCSM 2H/3H/4He Binding energies and radii

Energy and saturation momentum
of symmetric nuclear matter from
MBPT2



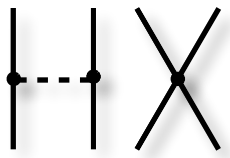
G. Hagen et al. Phys. Rev. C ***89****, 014319 (2014)*

Nuclear forces from chiral EFT

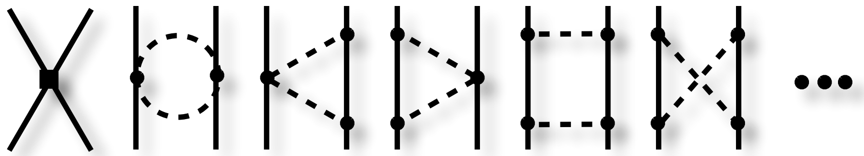
$$
\begin{aligned}
\widehat{\mathcal{L}}^{\Delta=0} &= \frac{1}{2}\partial_\mu \boldsymbol{\pi}\cdot\partial^\mu\boldsymbol{\pi} - \frac{1}{2}m_\pi^2 \boldsymbol{\pi}^2 + \frac{1-4\alpha}{2f_\pi^2}(\boldsymbol{\pi}\cdot\partial_\mu\boldsymbol{\pi})(\boldsymbol{\pi}\cdot\partial^\mu\boldsymbol{\pi}) - \frac{\alpha}{f_\pi^2}\boldsymbol{\pi}^2\partial_\mu\boldsymbol{\pi}\cdot\partial^\mu\boldsymbol{\pi} + \frac{8\alpha-1}{8f_\pi^2}m_\pi^2\boldsymbol{\pi}^4 \\
&\quad + \bar{N}\left[i\partial_0 - \frac{g_A}{2f_\pi}\,\boldsymbol{\tau}\cdot(\vec{\sigma}\cdot\vec{\nabla})\boldsymbol{\pi} - \frac{1}{4f_\pi^2}\,\boldsymbol{\tau}\cdot(\boldsymbol{\pi}\times\partial_0\boldsymbol{\pi})\right] N \\
&\quad + \bar{N}\left\{ \frac{g_A(4\alpha-1)}{4f_\pi^3}\,(\boldsymbol{\tau}\cdot\boldsymbol{\pi})\left[\boldsymbol{\pi}\cdot(\vec{\sigma}\cdot\vec{\nabla})\boldsymbol{\pi}\right] + \frac{g_A\alpha}{2f_\pi^3}\,\boldsymbol{\pi}^2\left[\boldsymbol{\tau}\cdot(\vec{\sigma}\cdot\vec{\nabla})\boldsymbol{\pi}\right]\right\} N \\
&\quad - \frac{1}{2}C_S\bar{N}N\bar{N}N - \frac{1}{2}C_T(\bar{N}\vec{\sigma}N)\cdot(\bar{N}\vec{\sigma}N) + \cdots, \\
\widehat{\mathcal{L}}^{\Delta=1} &= \bar{N}\left\{ \frac{\vec{\nabla}^2}{2M_N} - \frac{ig_A}{4M_Nf_\pi}\boldsymbol{\tau}\cdot\left[\vec{\sigma}\cdot\left(\overleftarrow{\nabla}\,\partial_0\boldsymbol{\pi} - \partial_0\boldsymbol{\pi}\,\overrightarrow{\nabla}\right)\right] - \frac{i}{8M_Nf_\pi^2}\boldsymbol{\tau}\cdot\left[\overleftarrow{\nabla}\cdot(\boldsymbol{\pi}\times\vec{\nabla}\boldsymbol{\pi}) - (\boldsymbol{\pi}\times\vec{\nabla}\boldsymbol{\pi})\cdot\overrightarrow{\nabla}\right]\right\} N \\
&\quad + \bar{N}\left[4c_1m_\pi^2 - \frac{2c_1}{f_\pi^2}\,m_\pi^2\,\boldsymbol{\pi}^2 + \left(c_2 - \frac{g_A^2}{8M_N}\right)\frac{1}{f_\pi^2}(\partial_0\boldsymbol{\pi}\cdot\partial_0\boldsymbol{\pi}) \right. \\
&\quad \left. + \frac{c_3}{f_\pi^2}\,(\partial_\mu\boldsymbol{\pi}\cdot\partial^\mu\boldsymbol{\pi}) - \left(c_4 + \frac{1}{4M_N}\right)\frac{1}{2f_\pi^2}\epsilon^{ijk}\epsilon^{abc}\sigma^i\tau^a(\partial^j\pi^b)(\partial^k\pi^c)\right] N \\
&\quad - \frac{D}{4f_\pi}(\bar{N}N)\bar{N}\left[\boldsymbol{\tau}\cdot(\vec{\sigma}\cdot\vec{\nabla})\boldsymbol{\pi}\right]N - \frac{1}{2}E(\bar{N}N)(\bar{N}\boldsymbol{\tau}N)\cdot(\bar{N}\boldsymbol{\tau}N) + \cdots, \\
\widehat{\mathcal{L}}^{\Delta=2} &= \mathcal{L}_{\pi\pi}^{(4)} + \widehat{\mathcal{L}}_{\pi N}^{(3)} + \widehat{\mathcal{L}}_{NN}^{(2)} + \cdots, \\
\widehat{\mathcal{L}}^{\Delta=4} &= \widehat{\mathcal{L}}_{NN}^{(4)} + \cdots,
\end{aligned}
$$

Nuclear forces from chiral EFT

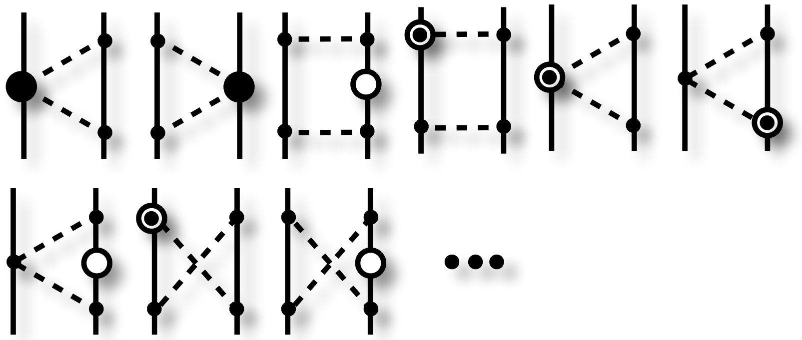
LO



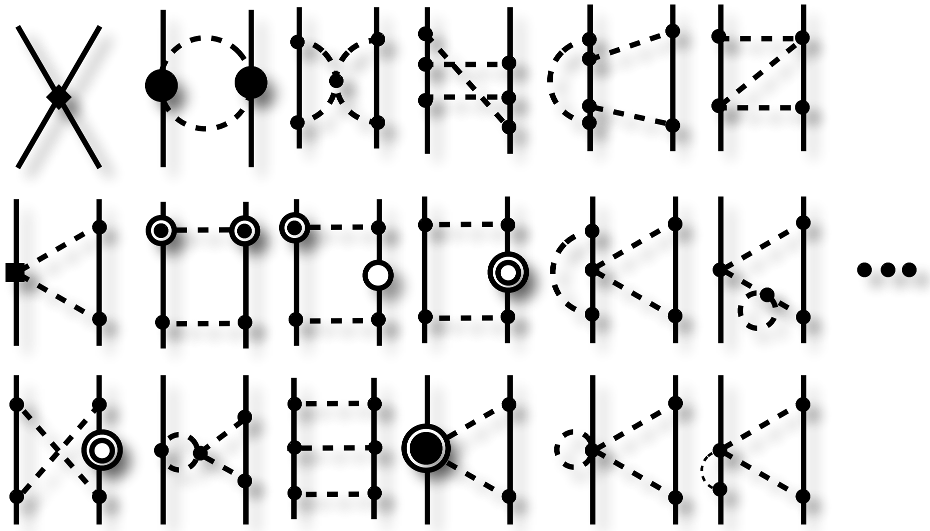
NLO



NNLO

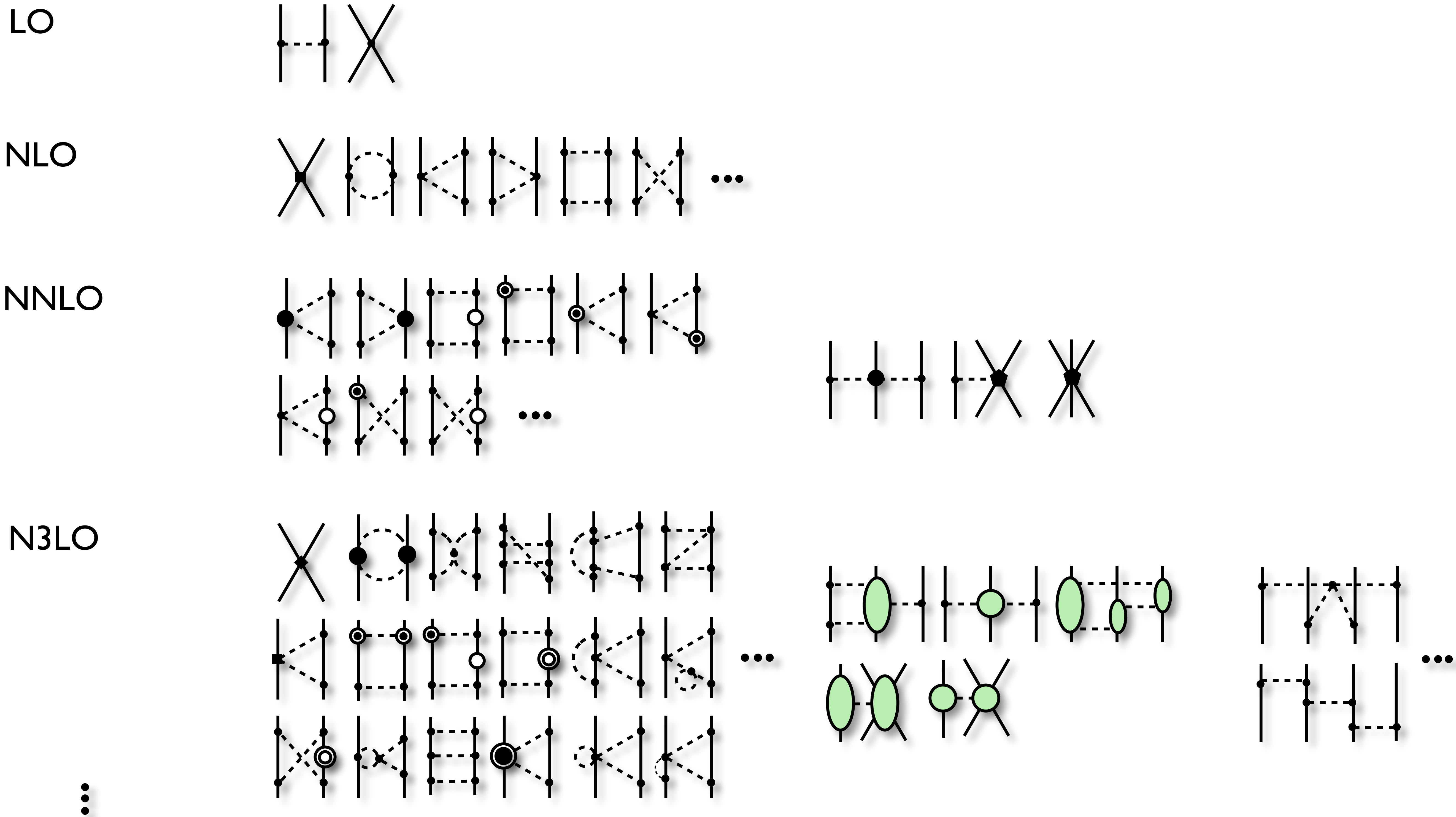


N3LO



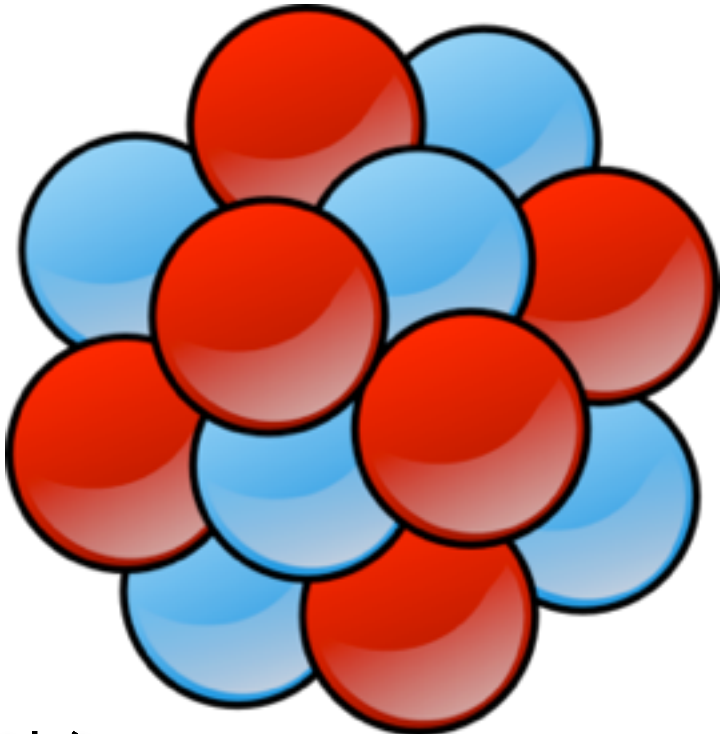
⋮

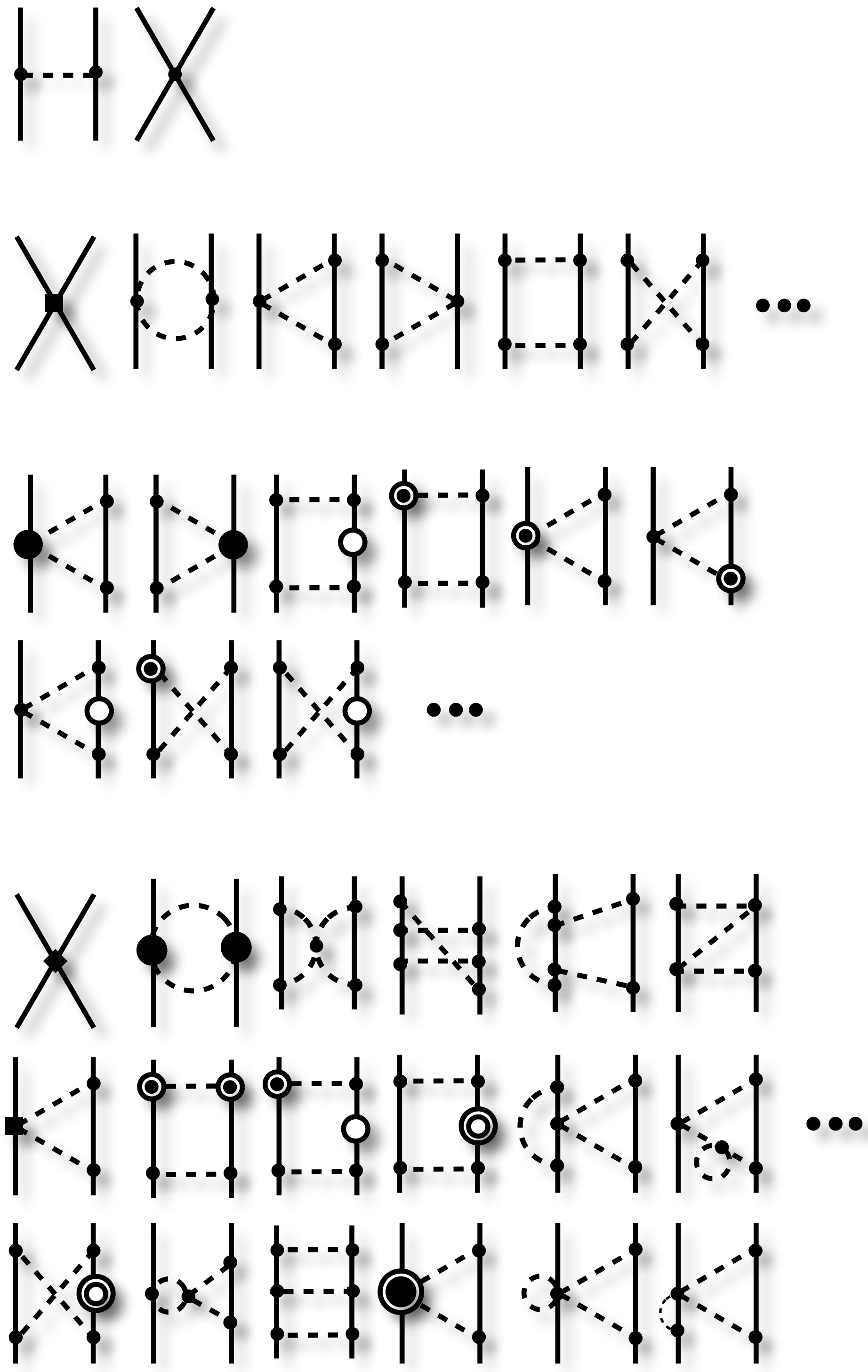
Nuclear forces from chiral EFT



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

Nuclear forces from chiral EFT





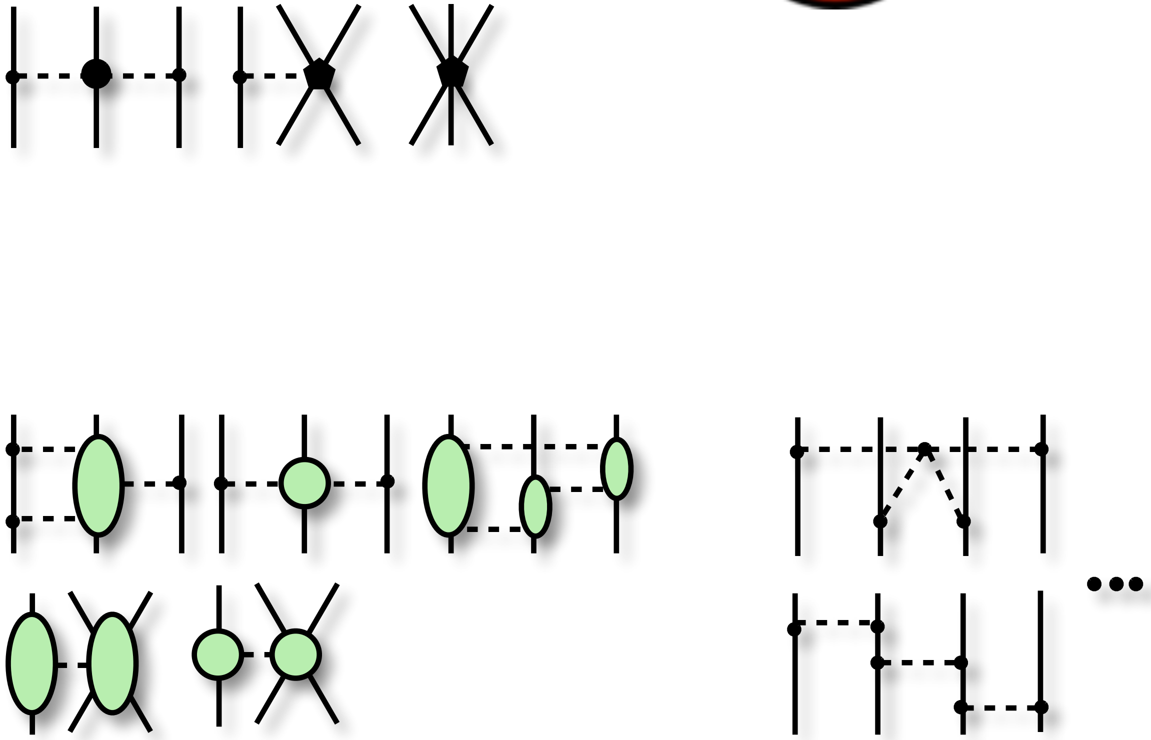
LO

NLO

NNLO

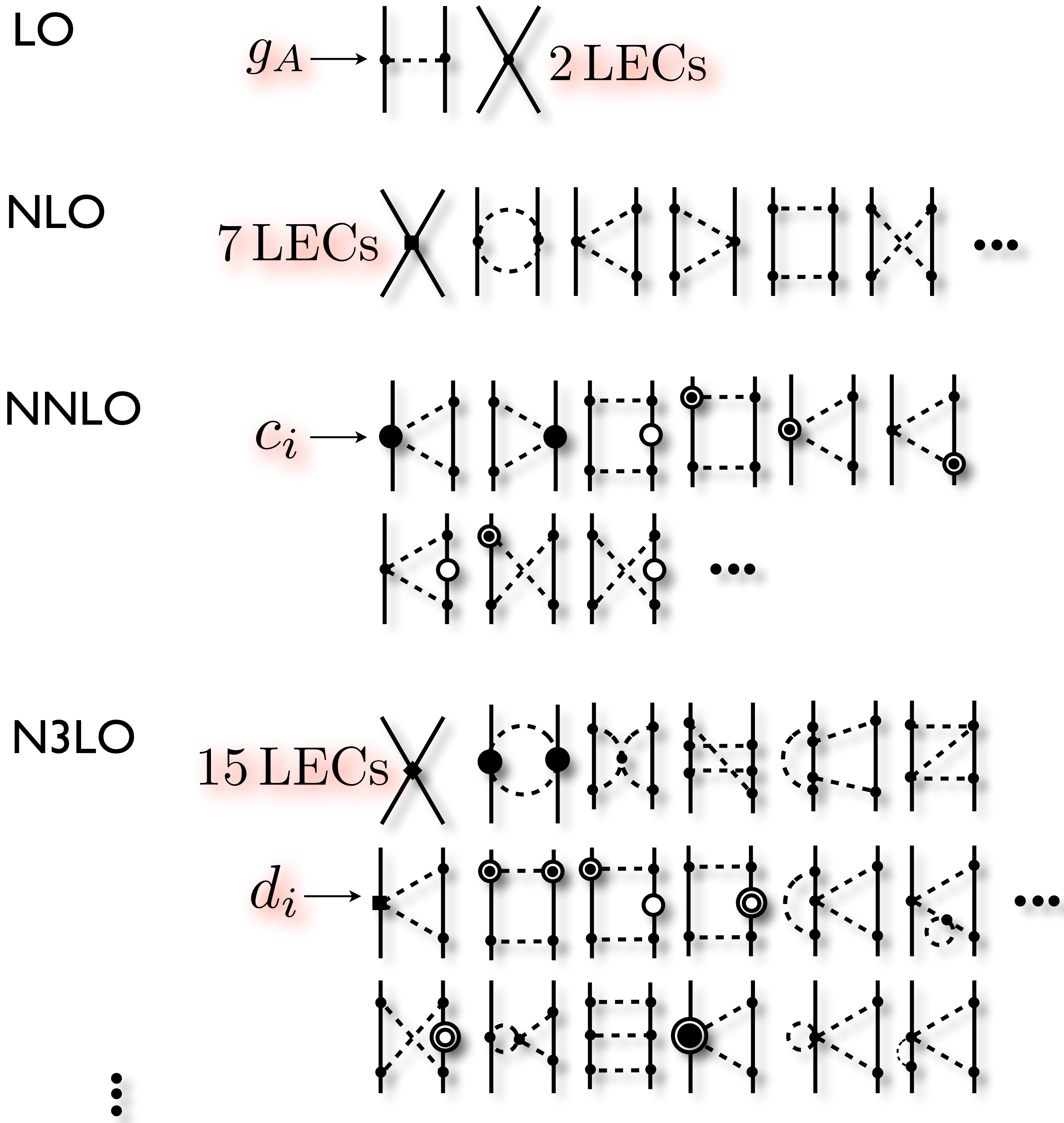
N3LO

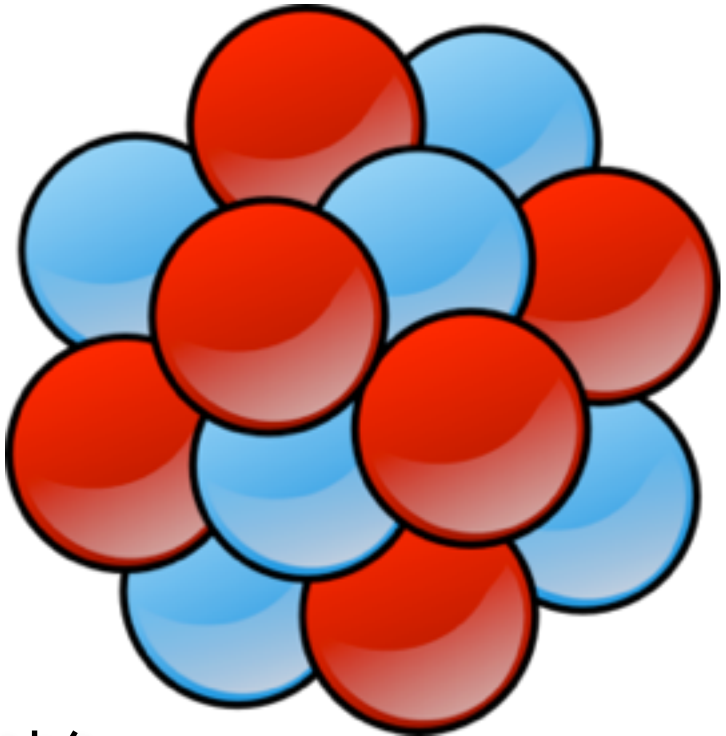
⋮

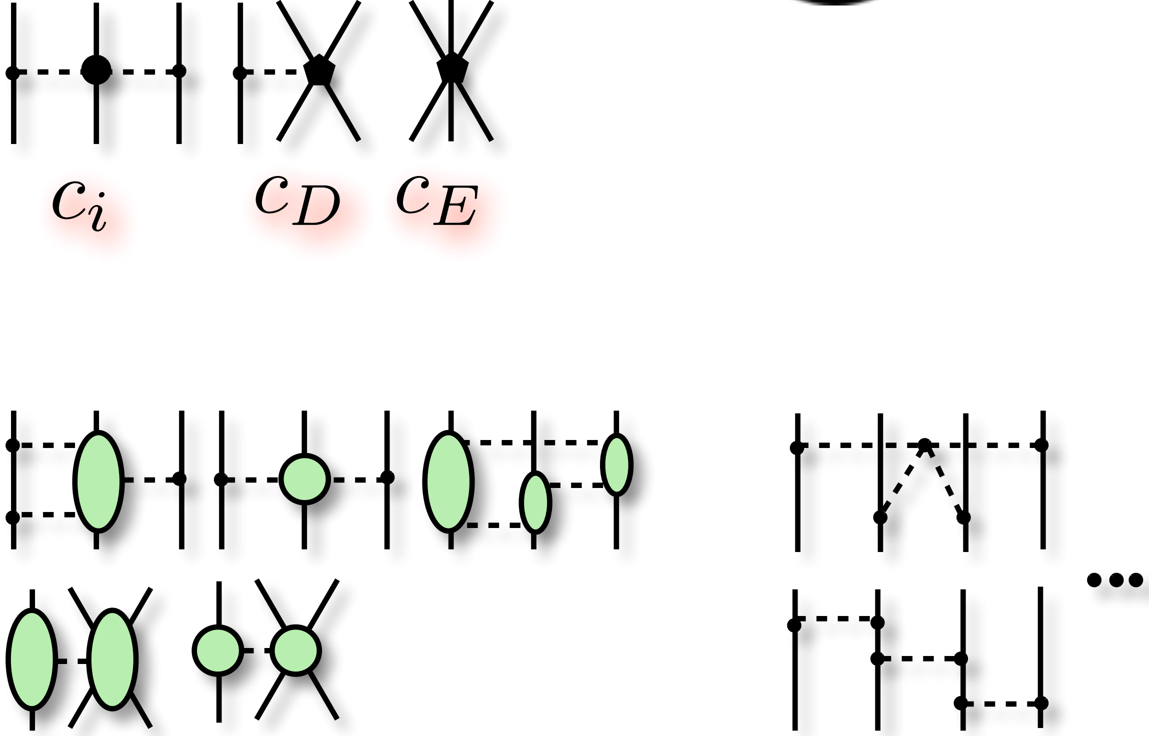


E. Epelbaum et al. Rev. Mod. Phys. 81, 1773 (2009)
R. Machleidt et al. Phys. Rep. 503, 1 (2011)

Nuclear forces from chiral EFT

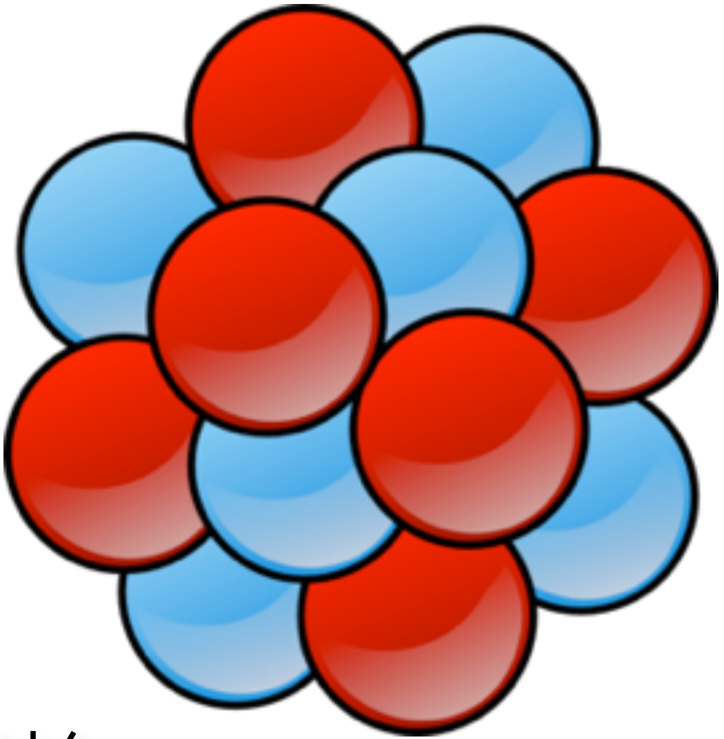




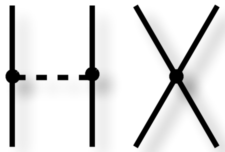


E. Epelbaum et al. Rev. Mod. Phys. 81, 1773 (2009)
R. Machleidt et al. Phys. Rep. 503, 1 (2011)

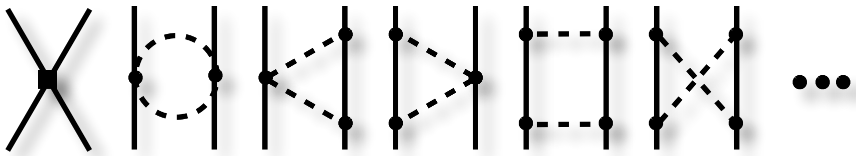
Nuclear forces from chiral EFT



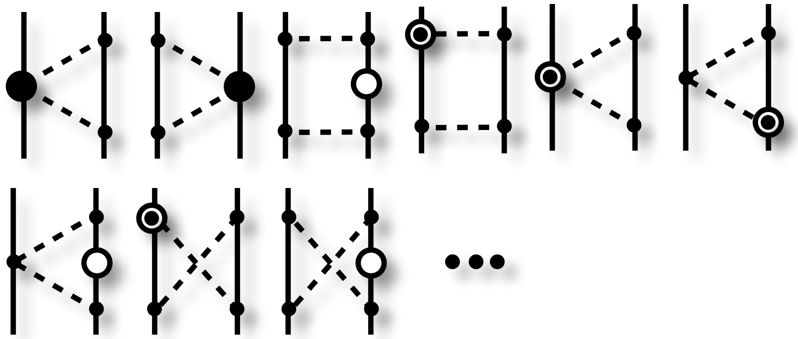
LO

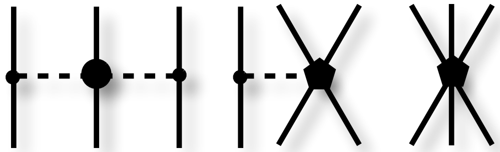


NLO



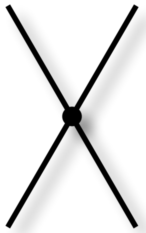
NNLO





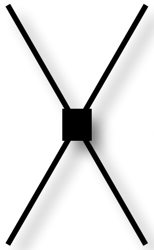
E. Epelbaum et al. Rev. Mod. Phys. 81, 1773 (2009)
R. Machleidt et al. Phys. Rep. 503, 1 (2011)

Low-energy constants at NNLO



2 LECs

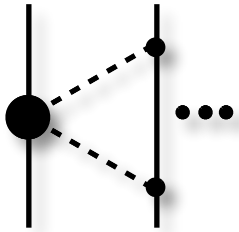
$\tilde{C}^{pp}_{^1S_0}\ \tilde{C}^{np}_{^1S_0}\ \tilde{C}^{nn}_{^1S_0}\ \tilde{C}_{^3S_1}$



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

$c_1 \quad c_3 \quad c_4$

long-range physics

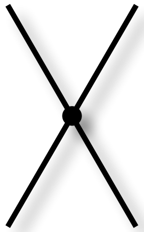
The contact potential

parametrizes the unresolved shortrange nuclear interaction.

In conventional meson theory, the short range force is described by heavy-meson exchange. The heavy mesons can't be resolved in ChPT.

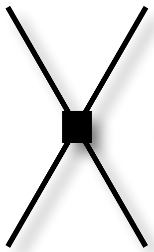
$$\frac{1}{m_{\rho^2+Q^2}} \approx \frac{1}{m_\rho^2}\left(1 - \frac{Q^2}{m_\rho^2} + \frac{Q^4}{m_\rho^4} - \ldots\right)$$

Low-energy constants at NNLO



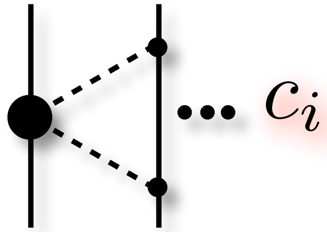
2 LECs

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



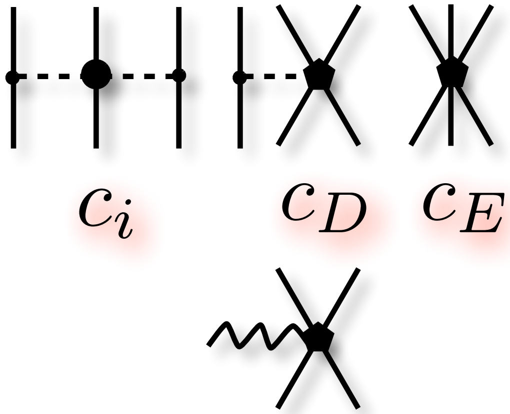
7 LECs

$$C_{{}^1S_0}\ C_{{}^3P_0}\ C_{{}^3P_1}\ C_{{}^3P_2}$$
$$C_{{}^1P_1}\ C_{{}^3S_1}\ C_{{}^3S_1-{}^3D_1}$$



$$c_1 \quad c_3 \quad c_4$$

long-range physics



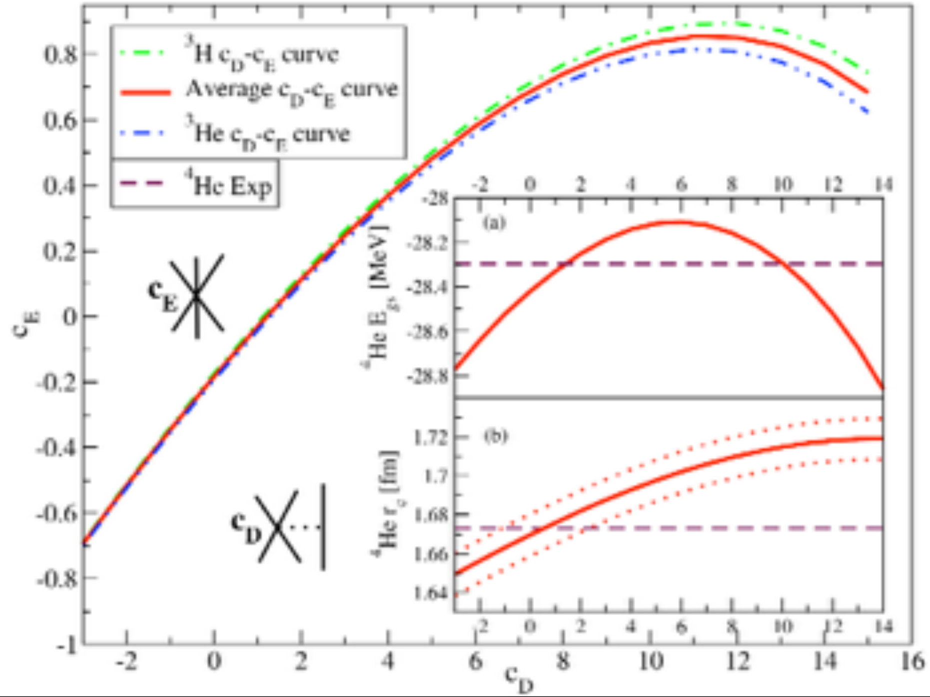
two new parameters that can be determined from the A>2 systems

The contact potential

parametrizes the unresolved shortrange nuclear interaction.

In conventional meson theory, the short range force is described by heavy-meson exchange. The heavy mesons can't be resolved in ChPT.

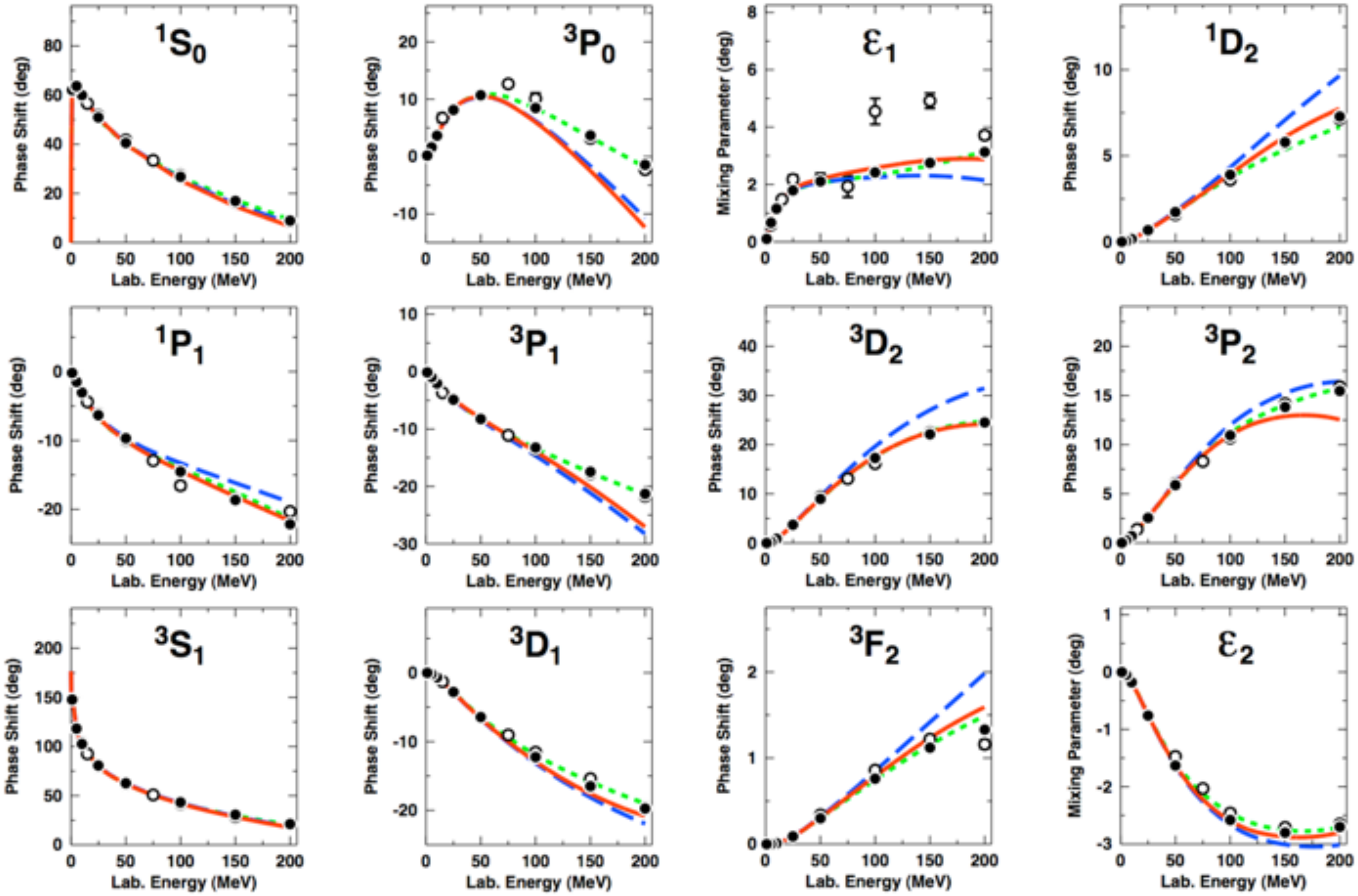
$$\frac{1}{m_{\rho^2+Q^2}} \approx \frac{1}{m_\rho^2}\left(1 - \frac{Q^2}{m_\rho^2} + \frac{Q^4}{m_\rho^4} - \dots\right)$$



NNLOopt

Tlab (MeV)	NNLOopt(np)
0-35	0.85
35-125	1.17
125-183	1.87
183-290	6.09
0-290	2.95

Tlab (MeV)	NNLOopt(pp)
0-35	1.11
35-125	1.56
125-183	23.95 (4.35)
183-290	29.26
0-290	17.10 (14.03)



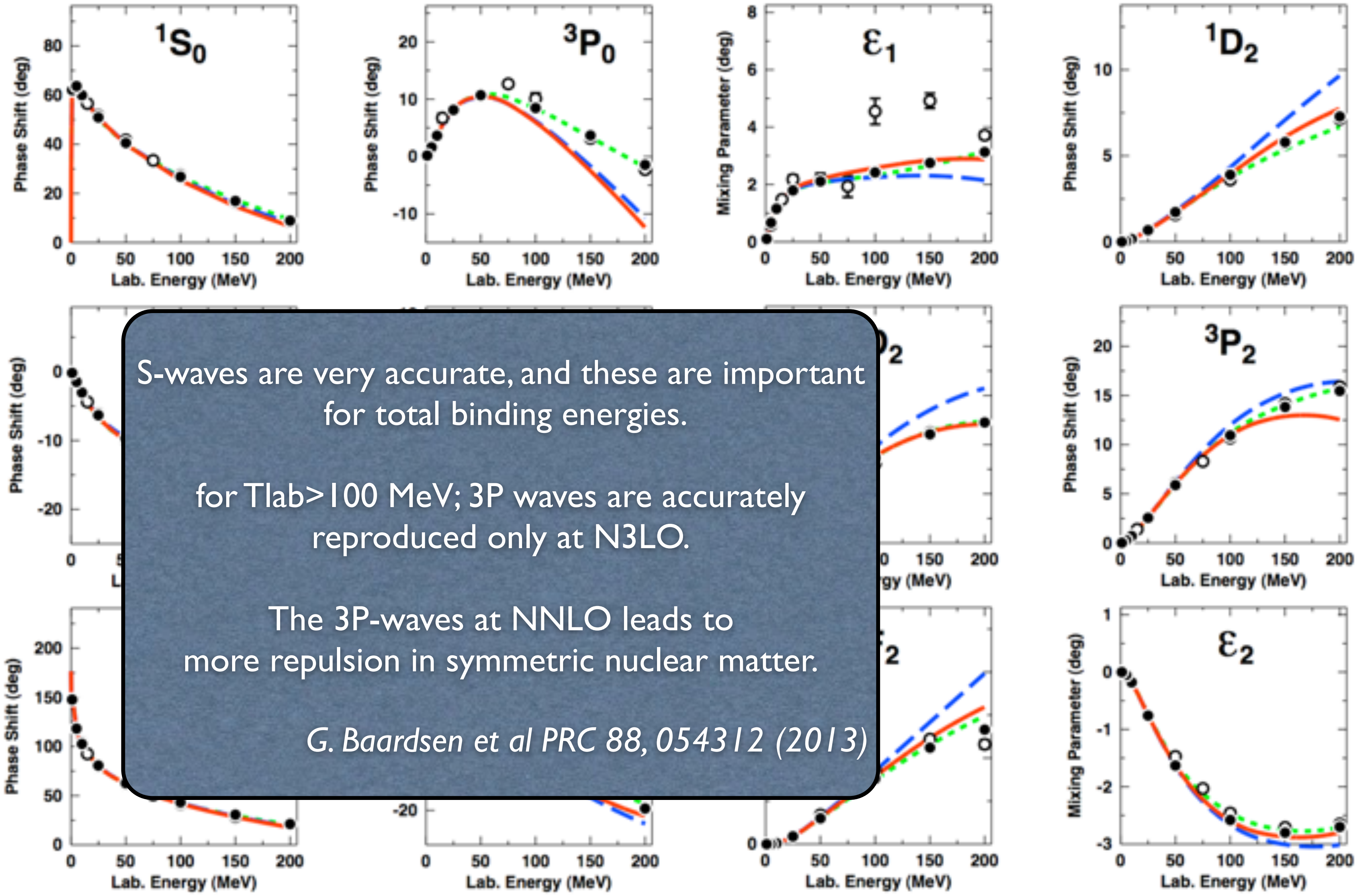
Our first study, at next-to-next-to-leading order (NNLO), shows that **there is room for improvement.** Chi2 drops from ~10-20 to 3. Optimization has an impact on nuclear structure!

A. Ekström et al.PRL 110, 192502 (2013)

NNLOopt

Tlab (MeV)	NNLOopt(np)
0-35	0.85
35-125	1.17
125-183	1.87
183-290	6.09
0-290	2.95

Tlab (MeV)	NNLOopt(pp)
0-35	1.11
35-125	1.56
125-183	23.95 (4.35)
183-290	29.26
0-290	17.10 (14.03)



S-waves are very accurate, and these are important for total binding energies.

for Tlab>100 MeV; 3P waves are accurately reproduced only at N3LO.

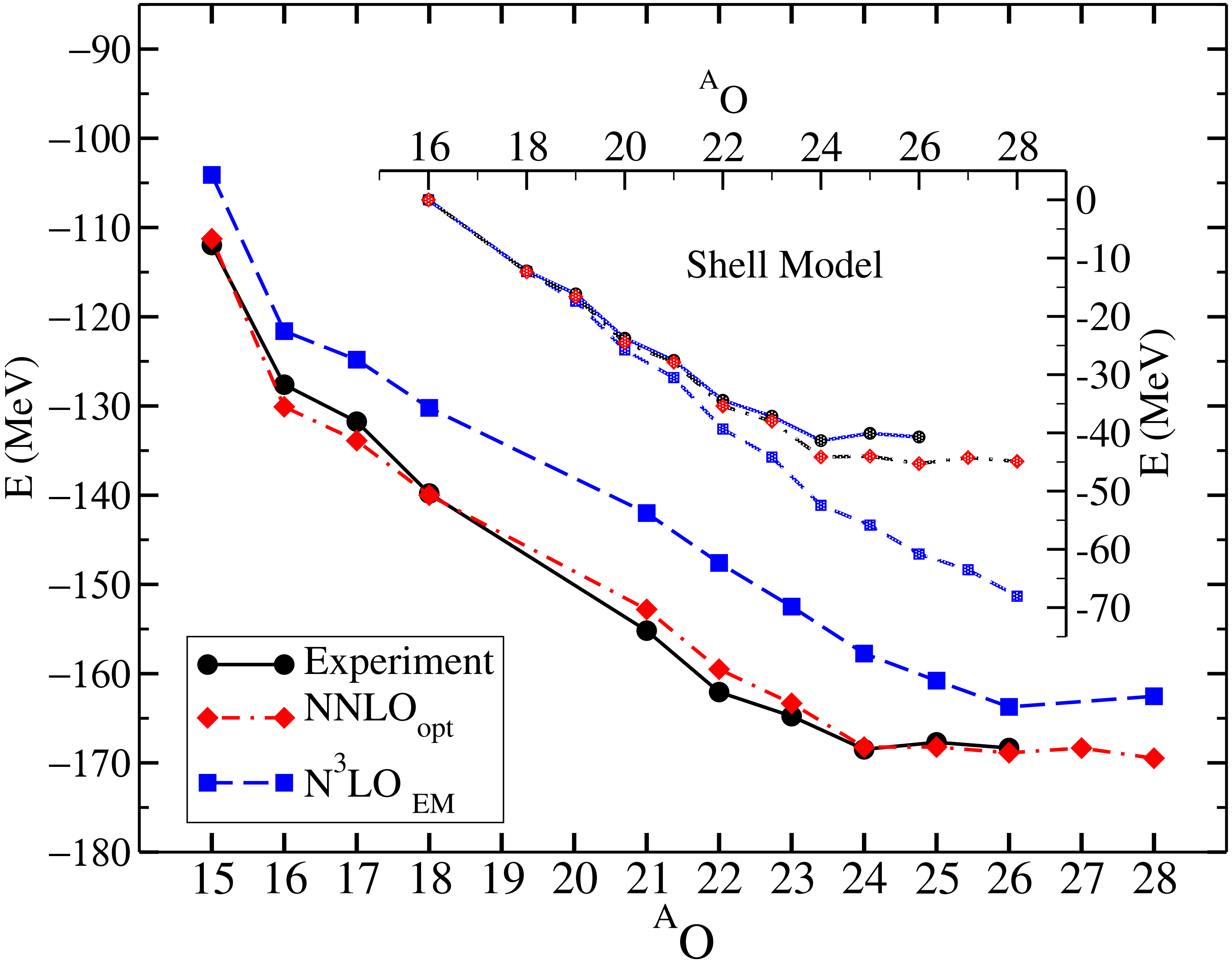
The 3P-waves at NNLO leads to more repulsion in symmetric nuclear matter.

G. Baardsen et al PRC 88, 054312 (2013)

Our first study, at next-to-next-to-leading order (NNLO), shows that **there is room for improvement**. Chi2 drops from ~10-20 to 3. Optimization has an impact on nuclear structure!

A. Ekström et al.PRL 110, 192502 (2013)

Oxygen isotopes



	16O	22O	24O
NNLOopt	-130.28	-159.76	-168.45
NNLO(EGM 450/500)	-156.76	-208.85	-225.65
Experiment	-127.62	-162.06	-168.48

1970: *last stable oxygen isotope 24O*

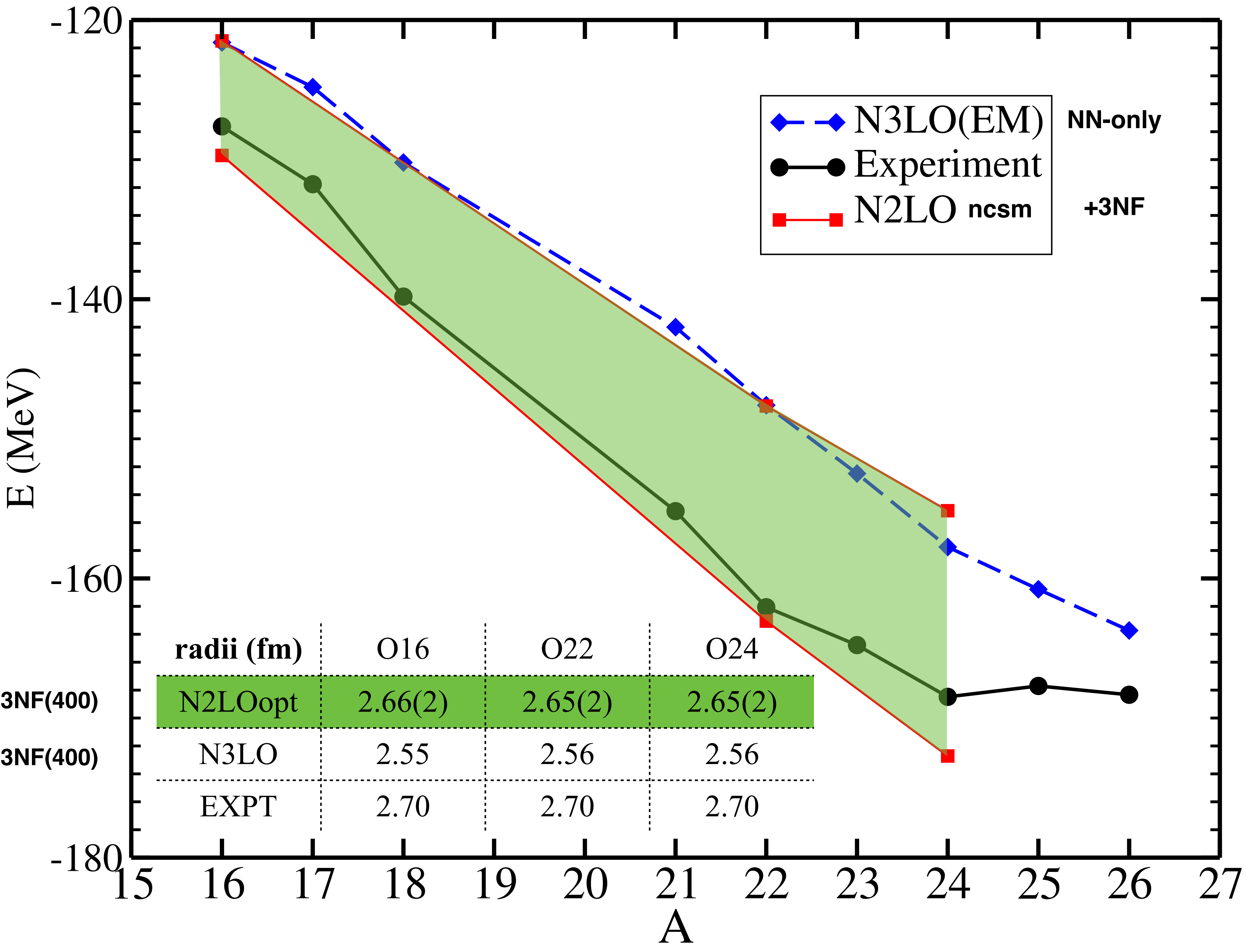
2012/2013: *26O unstable (MSU, GSI, RIKEN)*

sd-shell model
effective interaction from
g-matrix and MBPT(3)
s.p.e. from exp 17O spectrum.

Λ-CCSD(T), HF-basis
Nmax=15 $\hbar\omega$=20 MeV

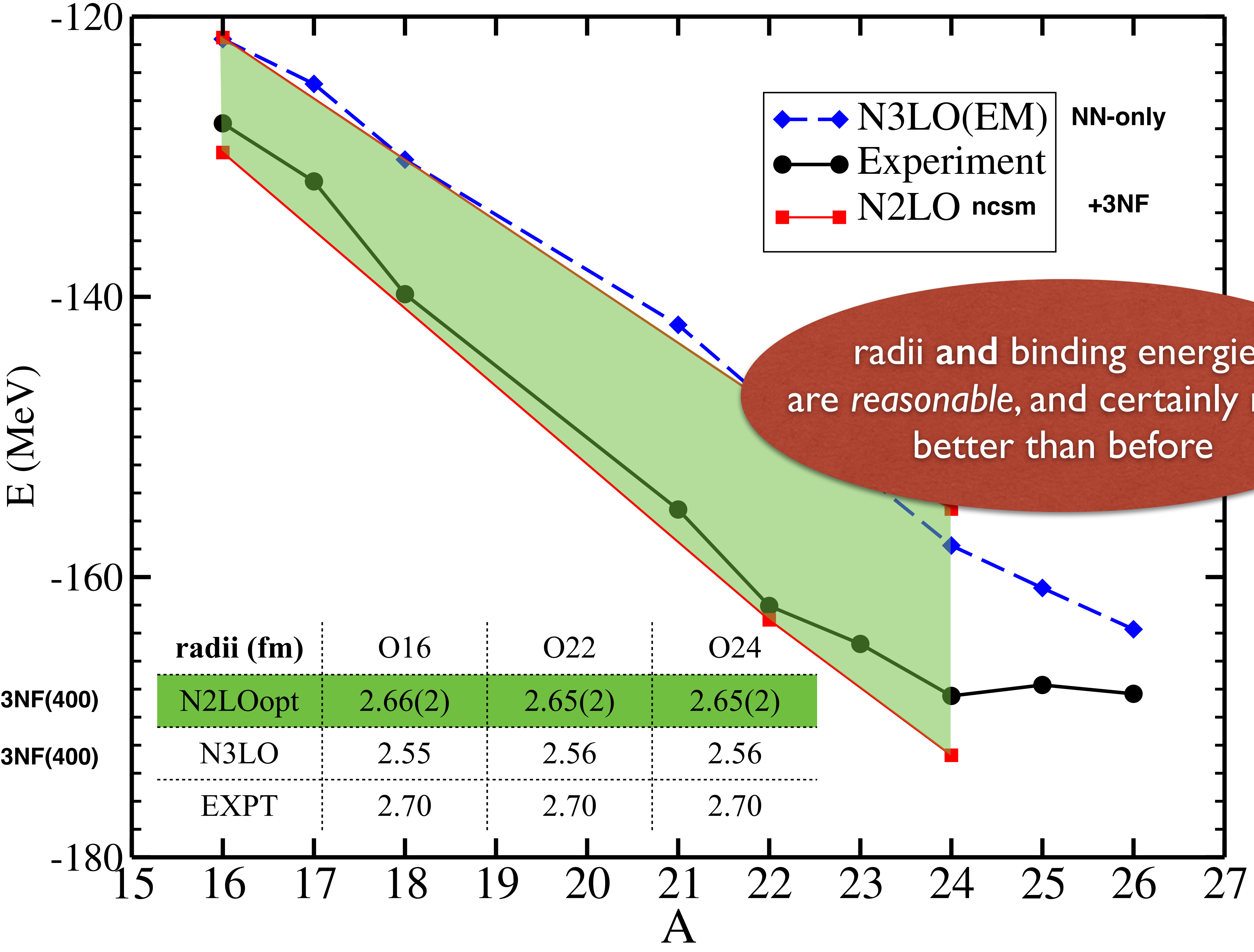
Oxygen dripline at A=24 with optimized 2-body force!

Preliminary: Oxygen from NCSM-objective function



	radii (fm)	O16	O22	O24
+local-3NF(400)	N2LOopt	2.66(2)	2.65(2)	2.65(2)
+local-3NF(400)	N3LO	2.55	2.56	2.56
	EXPT	2.70	2.70	2.70

Preliminary: Oxygen from NCSM-objective function



	radii (fm)	O16	O22	O24
+local-3NF(400)	N2LOopt	2.66(2)	2.65(2)	2.65(2)
+local-3NF(400)	N3LO	2.55	2.56	2.56
	EXPT	2.70	2.70	2.70

radii **and** binding energies are *reasonable*, and certainly much better than before

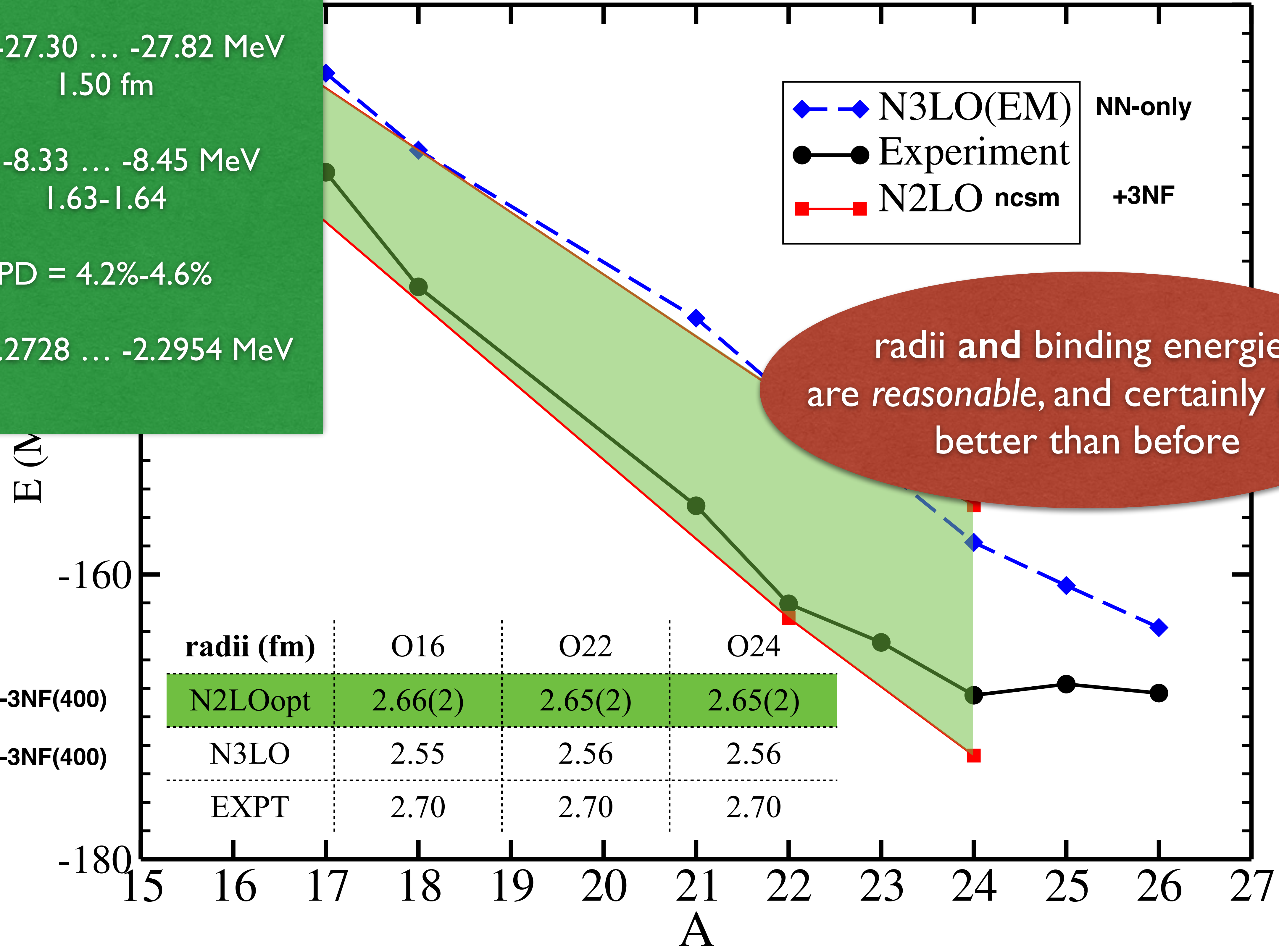
Preliminary: Oxygen from NCSM-objective function

He4: -27.30 … -27.82 MeV
1.50 fm

H3: -8.33 … -8.45 MeV
1.63-1.64

PD = 4.2%-4.6%

H2: -2.2728 … -2.2954 MeV



radii and binding energies are *reasonable*, and certainly much better than before

radii (fm)	O16	O22	O24
N2LOopt	2.66(2)	2.65(2)	2.65(2)
N3LO	2.55	2.56	2.56
EXPT	2.70	2.70	2.70

+local-3NF(400)

+local-3NF(400)

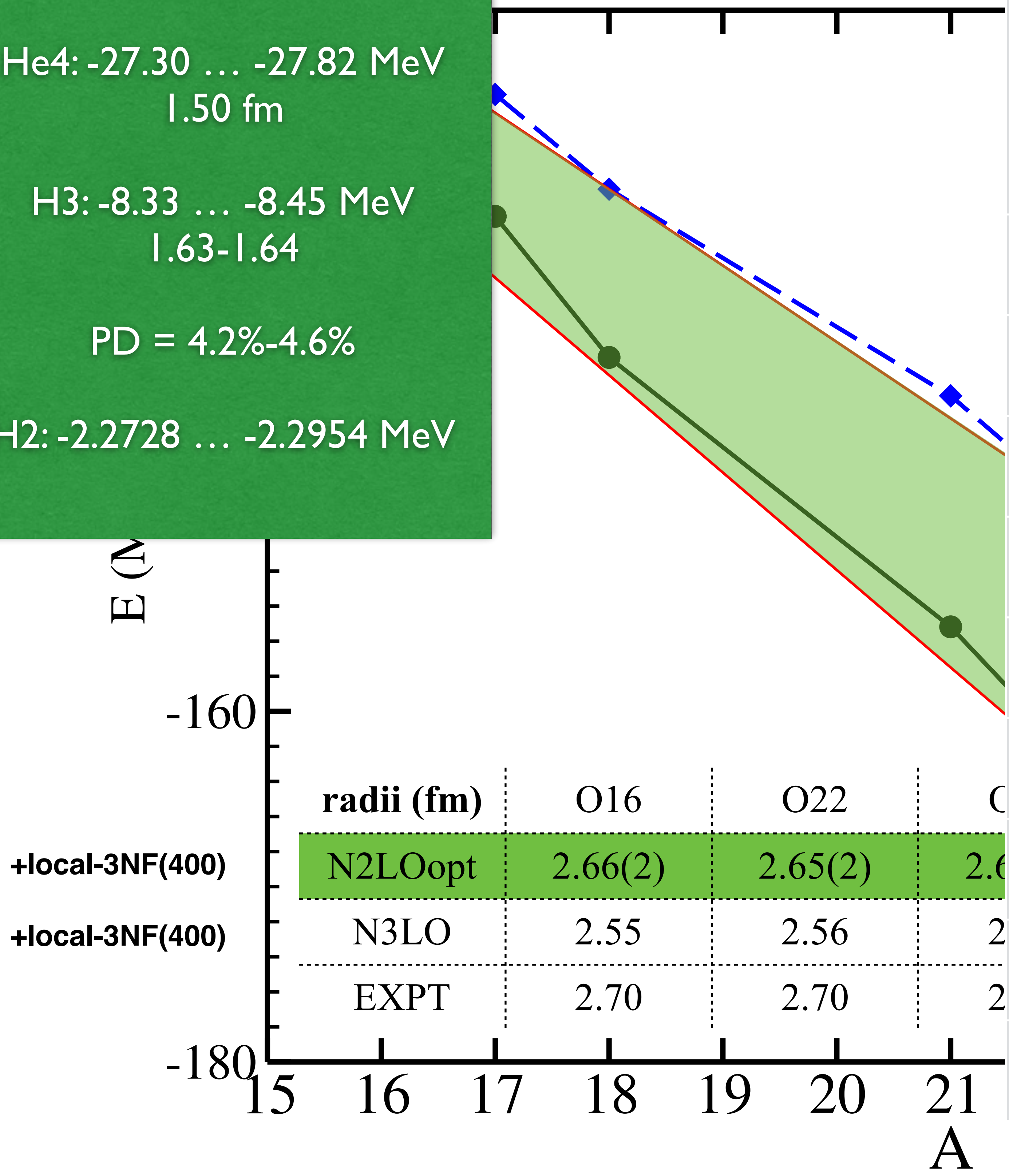
Preliminary: Oxygen from NCSM-objective function

He4: -27.30 … -27.82 MeV
1.50 fm

H3: -8.33 … -8.45 MeV
1.63-1.64

PD = 4.2%-4.6%

H2: -2.2728 … -2.2954 MeV



radii (fm)	O16	O22	O
N2LOopt	2.66(2)	2.65(2)	2.6
N3LO	2.55	2.56	2
EXPT	2.70	2.70	2

Tlab (MeV)	chi2/datum “NNLO NCSM”	chi2/datum NNLOopt
0.5	2.66-8.94	1.27
2	0.67-0.81	0.86
8	2.03-2.93	1.06
17	1.11-1.34	1.08
35	0.99-1.52	0.86
75	3.23-9.15	1.24
125	2.72-3.77	1.35
183	18.22-38.35	14.38
290	29.78-33.41	12.56

πN LECs: overview

	piN-Krebs	piN-BM	NN-PWA	NNLO (Juelich)	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

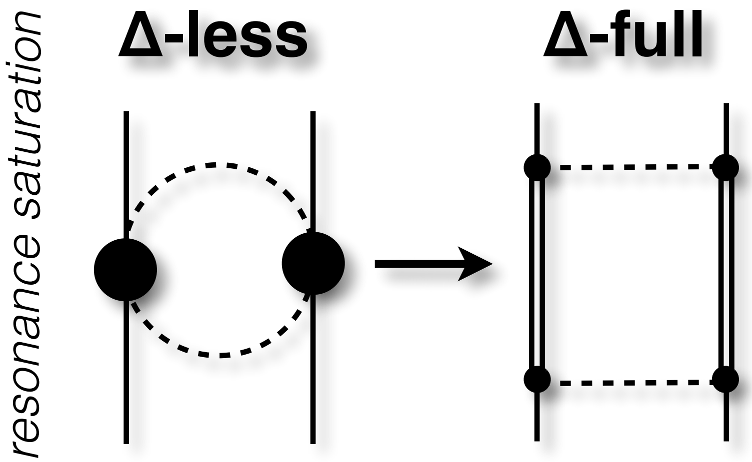
NN-PWA: Nijmegen PWA analysis of NN scattering data, with the long range physics described by subleading chiral two-pion exchanges

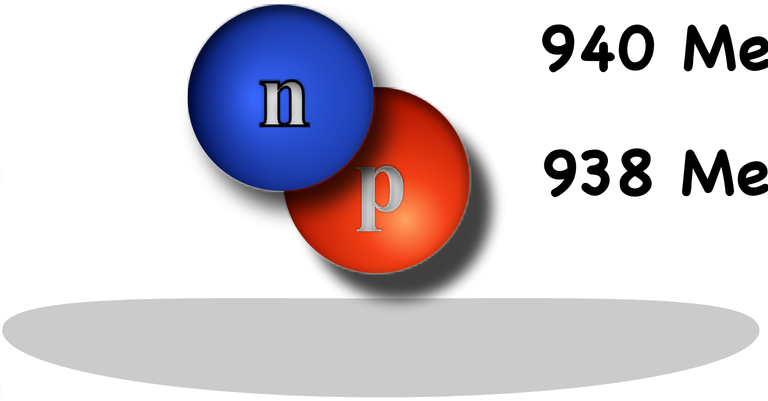
NNLO (Juelich): pion-nucleon couplings taken from piN-BM, but c3 chosen on the larger side within the uncertainty. This value is consistent with the Entem Machleidt analysis of NN data.

N3LO (Idaho): Guided by fit to NN data

NNLOopt: Guided by fit to NN data

1232 MeV





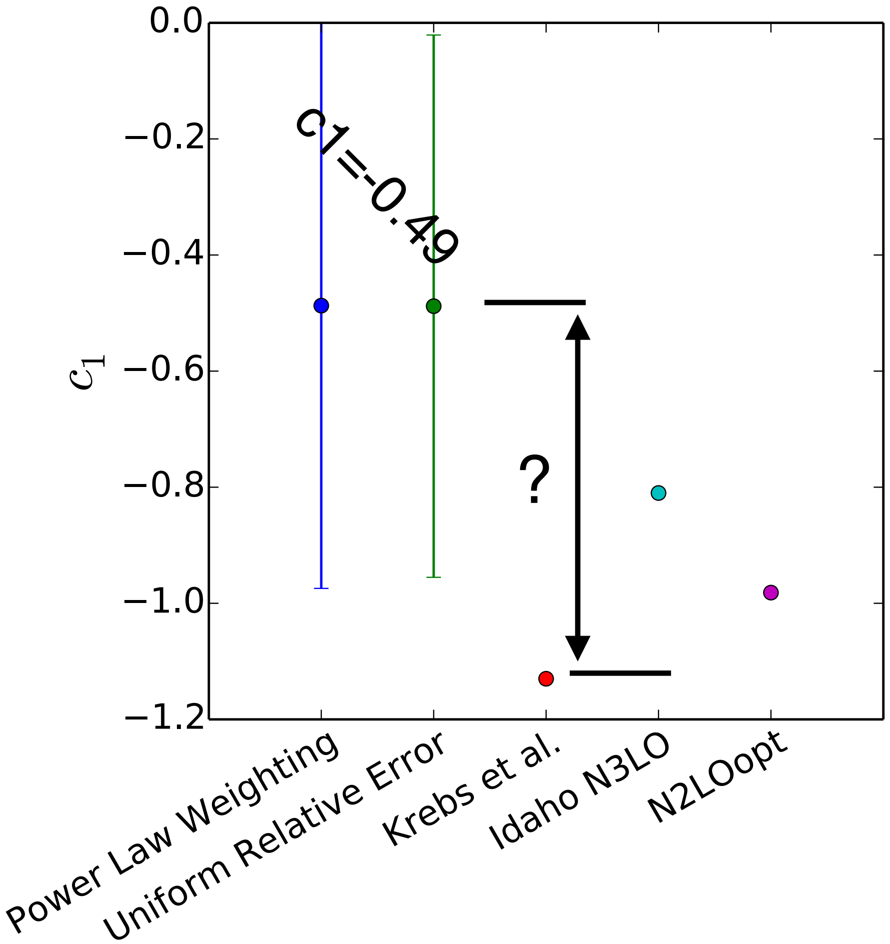
940 MeV

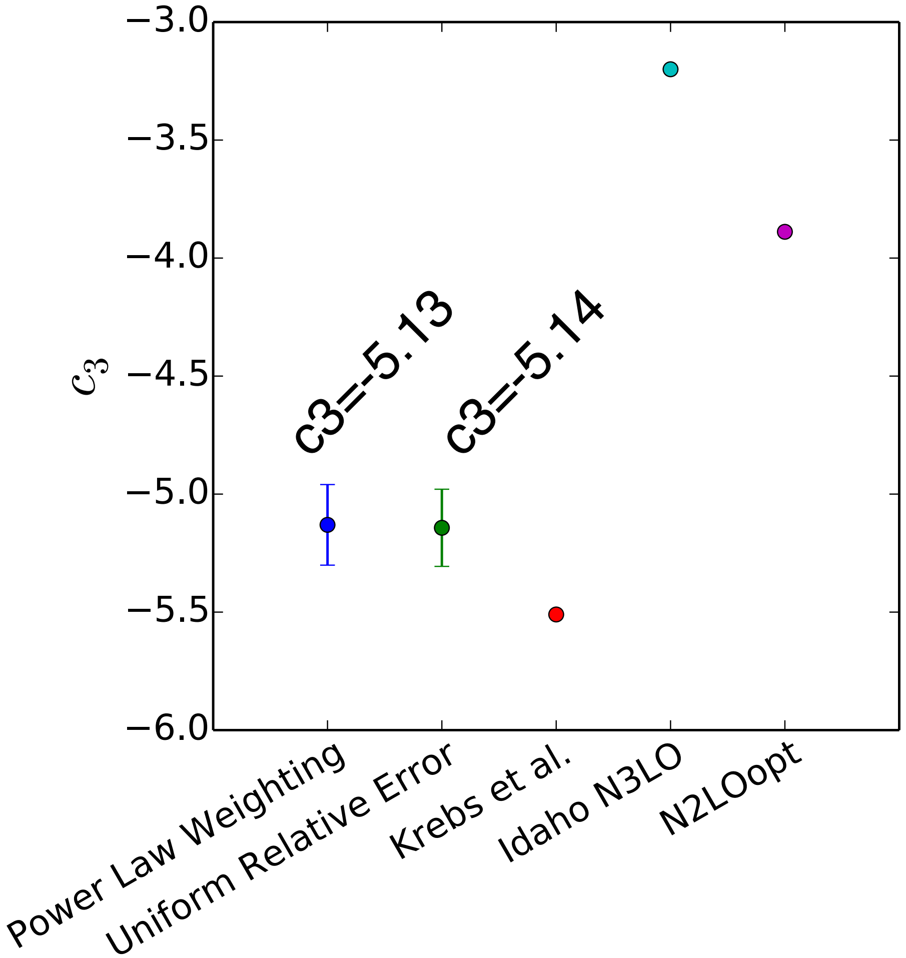
938 MeV

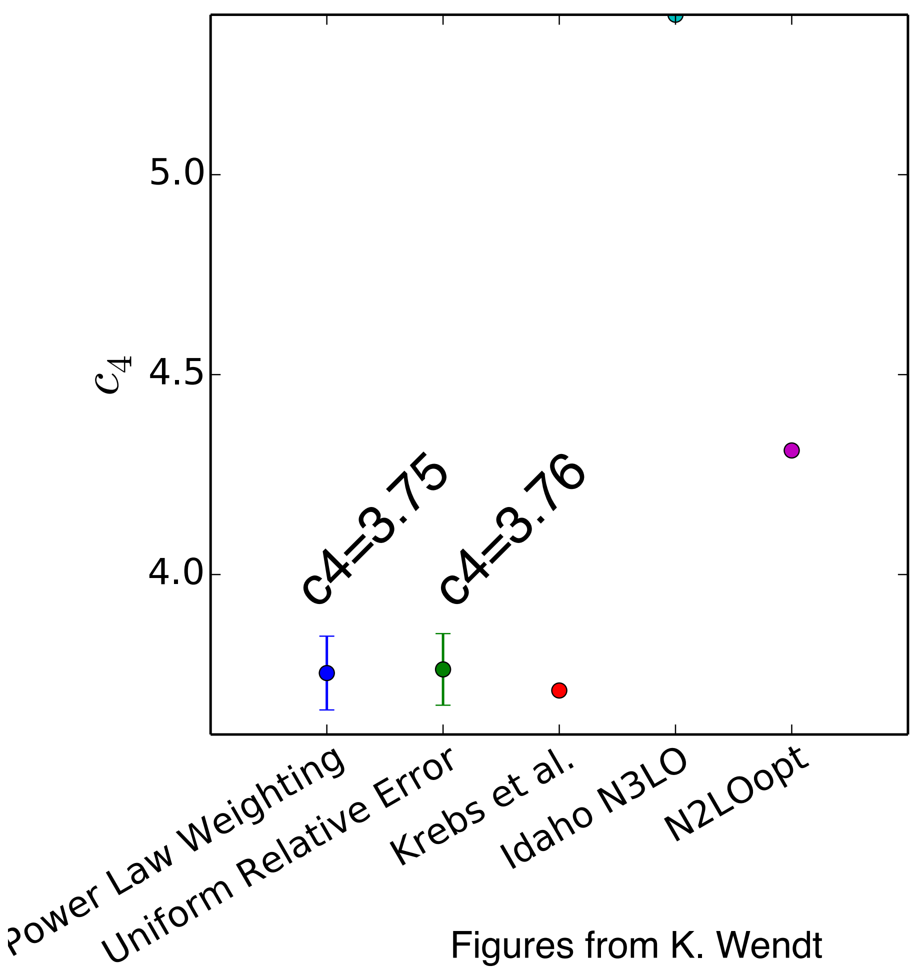
E. Epelbaum *et al.* Rev. Mod. Phys. 81, 1773 (2009)
E. Epelbaum *et al.* Eur. Phys. J. A19, 401 (2004)
R. Machleidt *et al.* Phys. Rep. 503, 1 (2011)
A. Ekström *et al.* Phys. Rev. Lett. 110, 192502 (2013)
H. Krebs *et al.* Phys. Rev. C, 85, 054006 (2012
M. C. M. Rentmeester *et al.* Phys. Rev. C, 67,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

πN LECs: our results

	piN-Krebs	piN-BM	NN-PWA	NNLO (Juelich)	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**







Figures from K. Wendt

πN LECs: our results

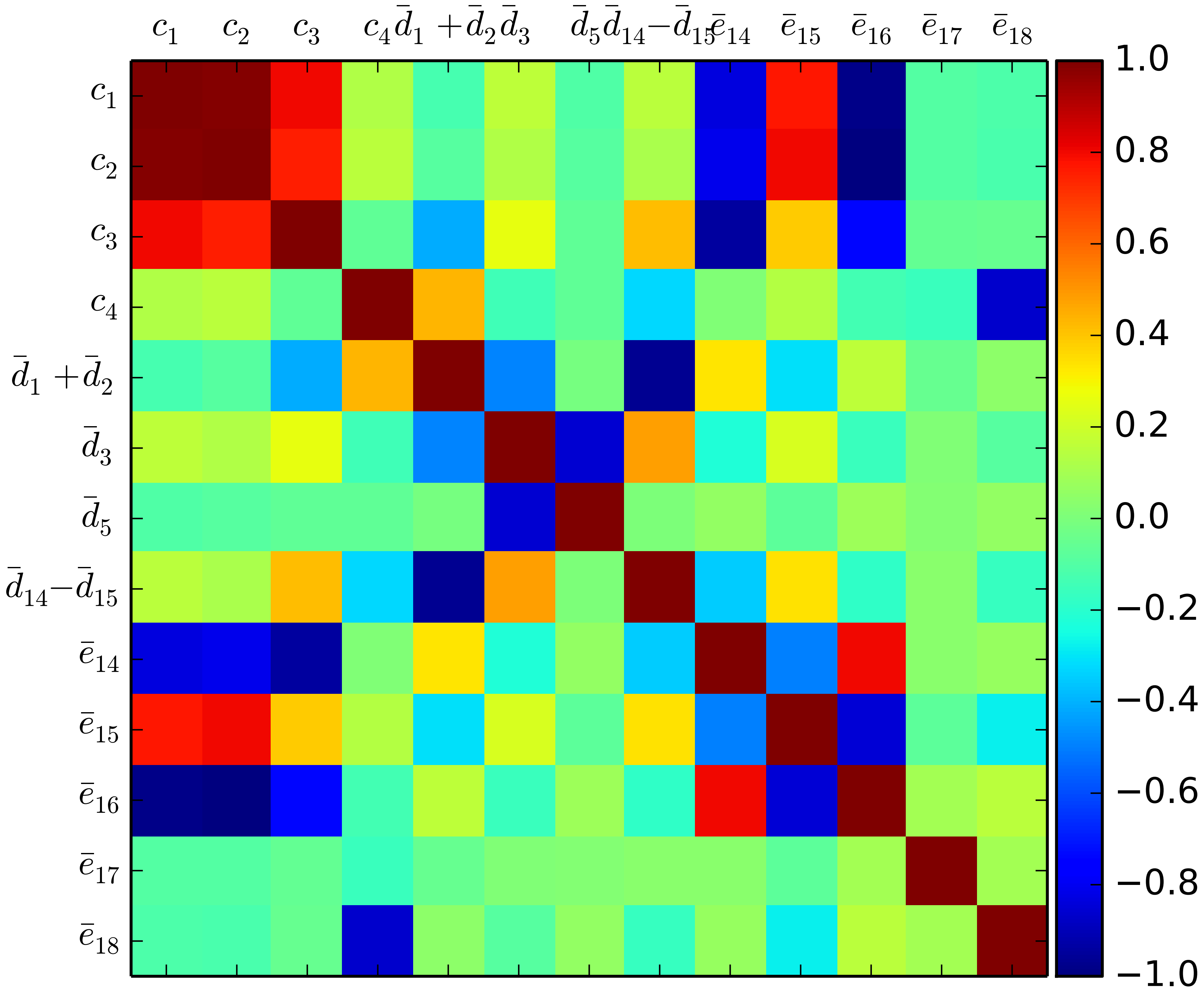


Figure from K. Wendt

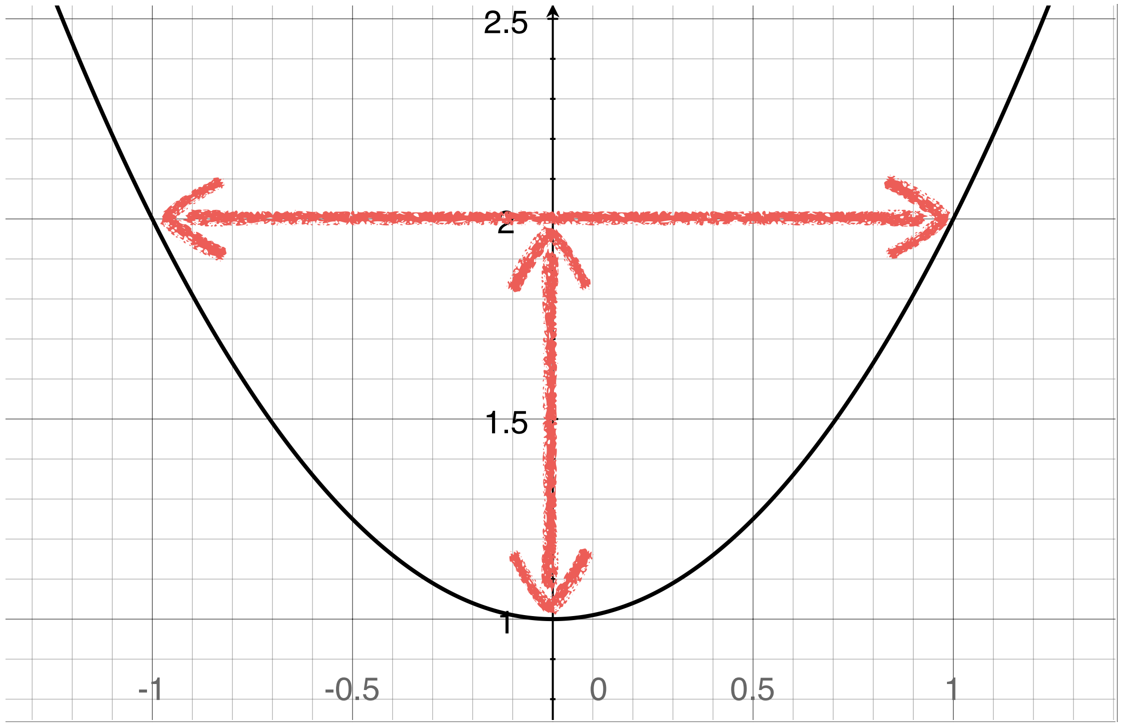
NNLOopt uncertainty estimates (ongoing)

SIMPLE ESTIMATES of the statistical uncertainties of the LECs that come from the experimental cross section errors.

Pros: fast and gives a first hint on the uncertainty and sensitivity of the potential with respect to variations in the parameter values

Cons: neglects all parameter correlations.

(Only OK in the gaussian limit, i.e. where the chi2 curve is parabolic)



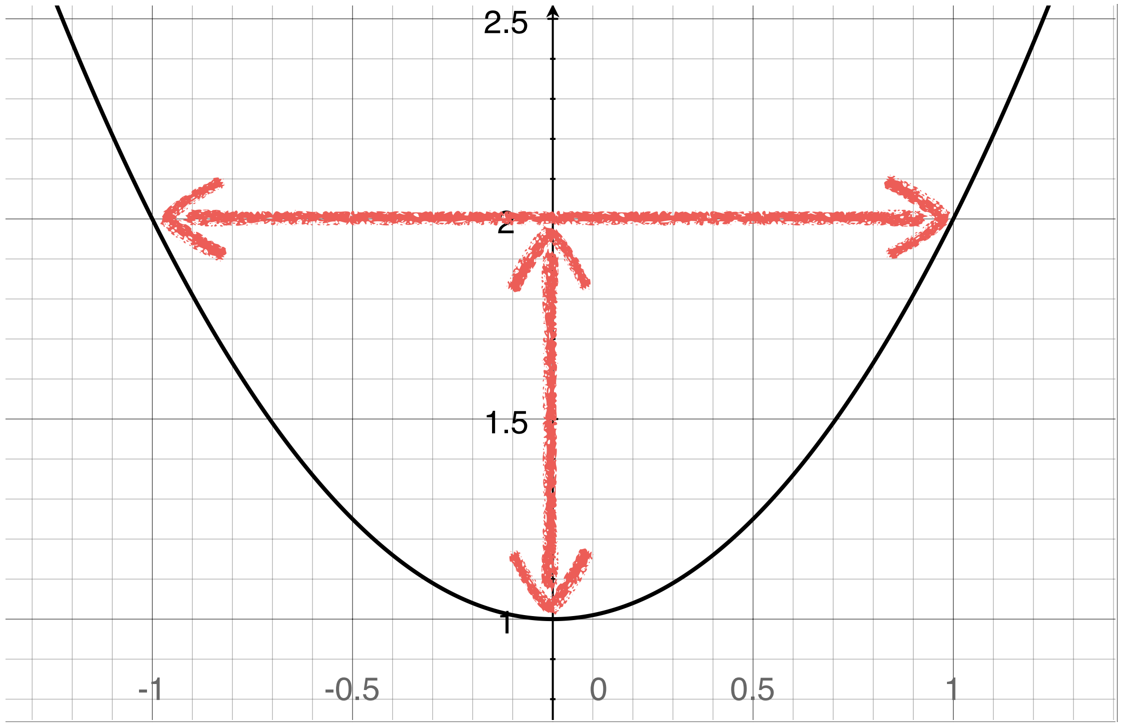
NNLOopt uncertainty estimates (ongoing)

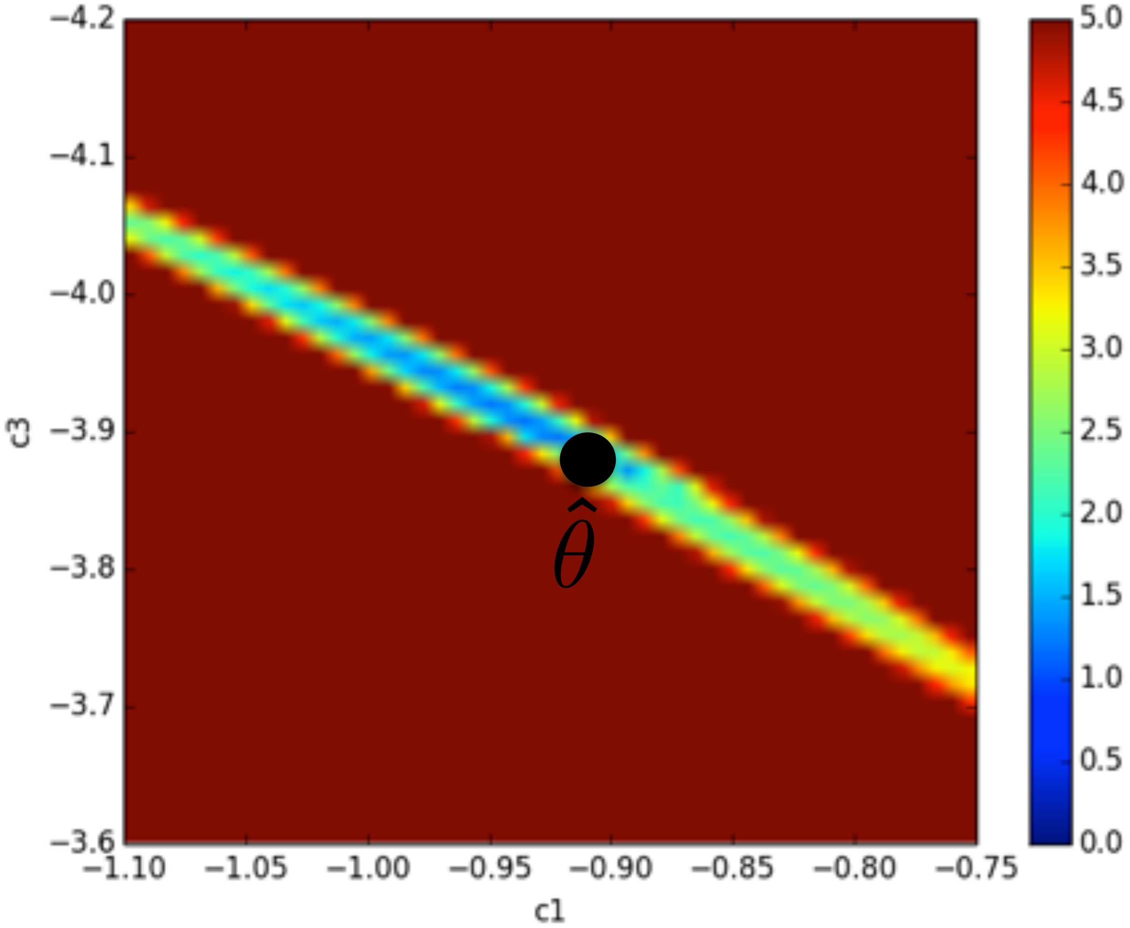
SIMPLE ESTIMATES of the statistical uncertainties of the LECs that come from the experimental cross section errors.

Pros: fast and gives a first hint on the uncertainty and sensitivity of the potential with respect to variations in the parameter values

Cons: neglects all parameter correlations.

(Only OK in the gaussian limit, i.e. where the chi2 curve is parabolic)





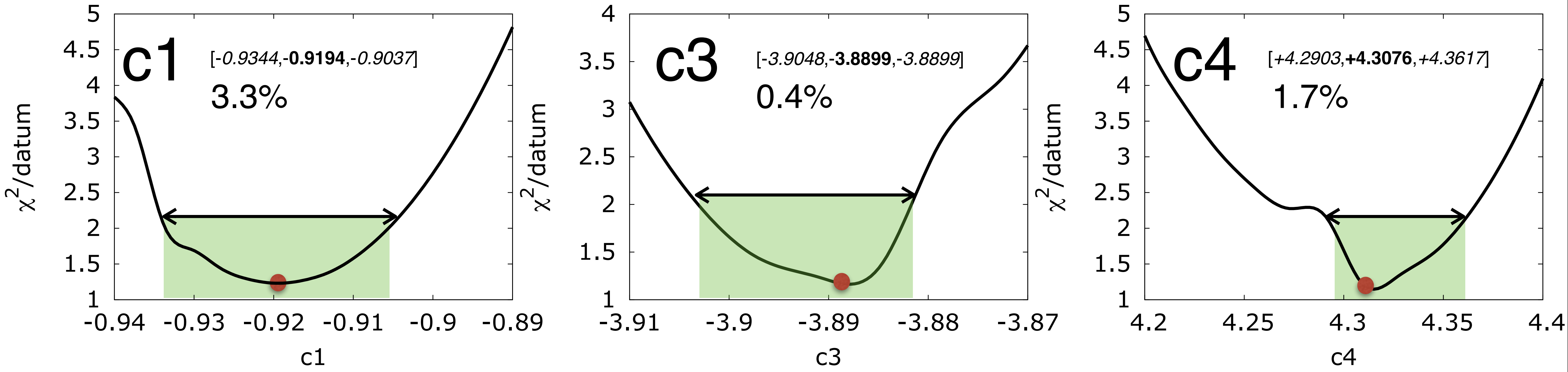
Compute Hessian of Chi2

$$\min_{\vec{x}} \left[f(\vec{x}) = \sum_{d} \sum_{q} \left(\frac{O(\vec{x})_{d,q} - O^{\exp}_{d,q}}{w_q} \right)^2 \right]$$

$$\mathbf{cov}(p_i, p_j) \approx \frac{\chi^2}{N} H(\hat{\theta})^{-1}$$

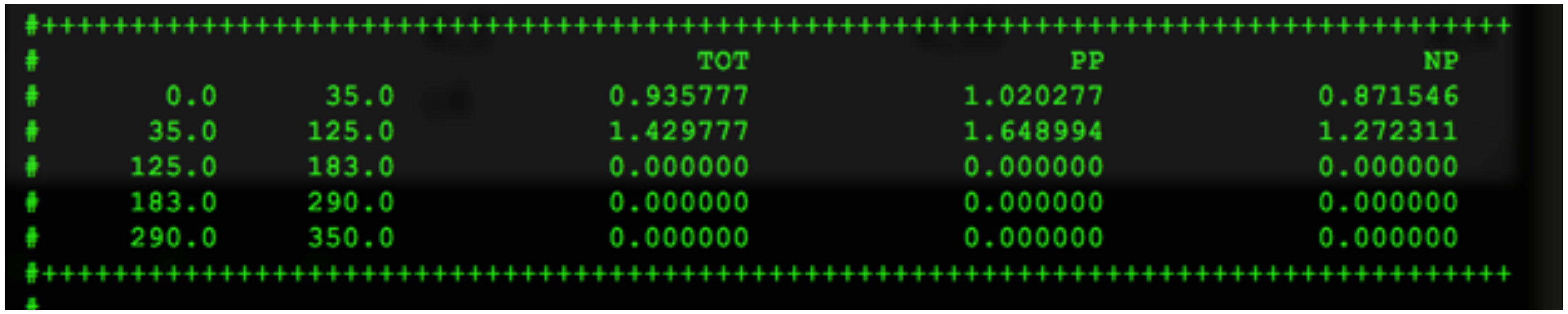
Janet R. Donaldson and Robert B. Schnabel, Technometrics, February 1987 , Vol. 29 , No. 1

NNLOopt (Tlab<125) uncertainty *estimates*



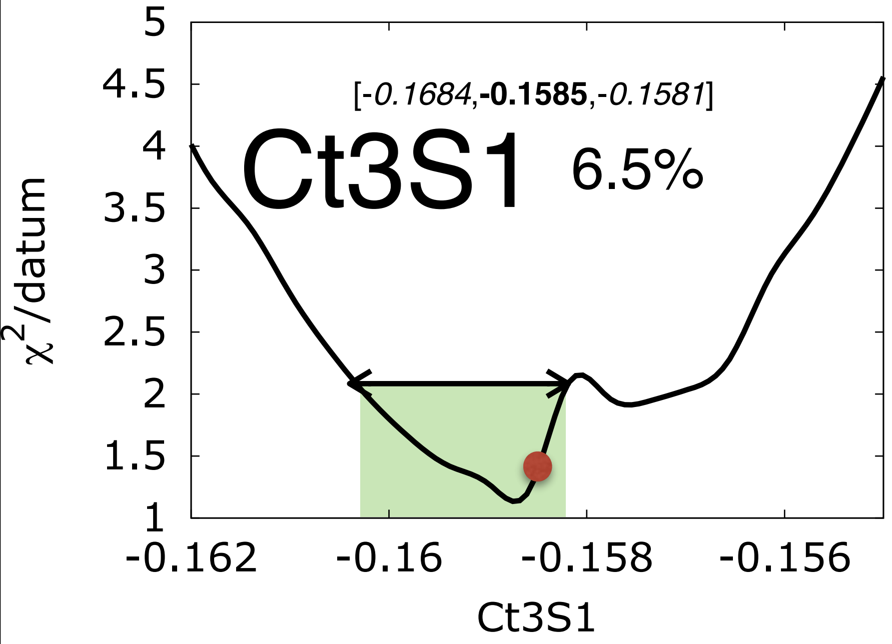
POTENTIAL: NNLOopt, further optimized wrt scattering data below Tlab=125.0 MeV

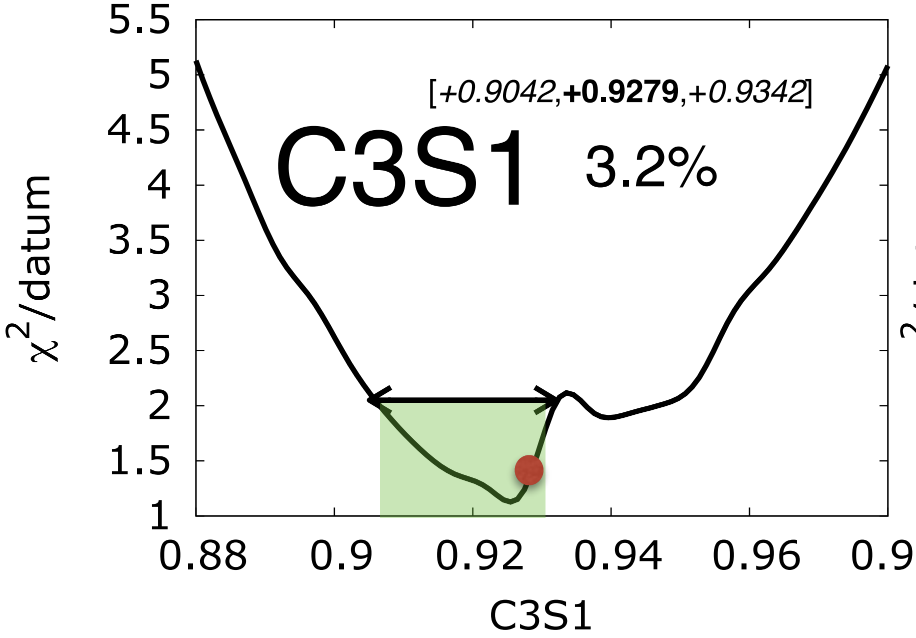
par.c1 = -0.9194168473672011
par.c3 = -3.8898982574932761
par.c4 = 4.3075828920511565
par.Ct_1S0np = -0.1521600767237906
par.Ct_1S0pp = -0.1513601095572962
par.Ct_3S1 = -0.1584760219635368
par.C_1S0 = 2.4042363751110987
par.C_3P0 = 1.2657410632596040
par.C_1P1 = 0.4147958250829769
par.C_3P1 = -0.7799477809574415
par.C_3S1 = 0.9278867972024134
par.C_3S1-3D1 = 0.6185795556481742
par.C_3P2 = -0.6735011268948335

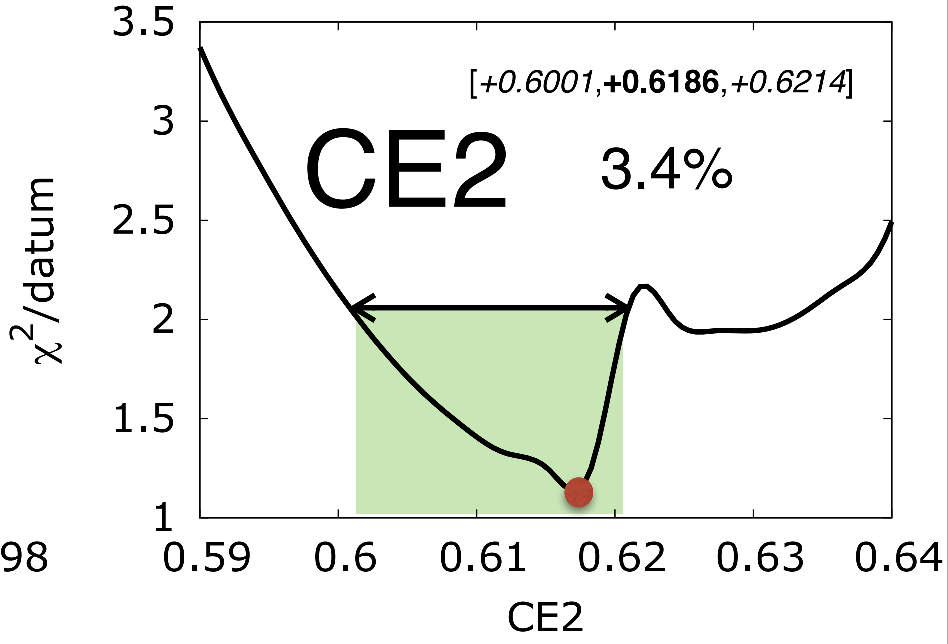


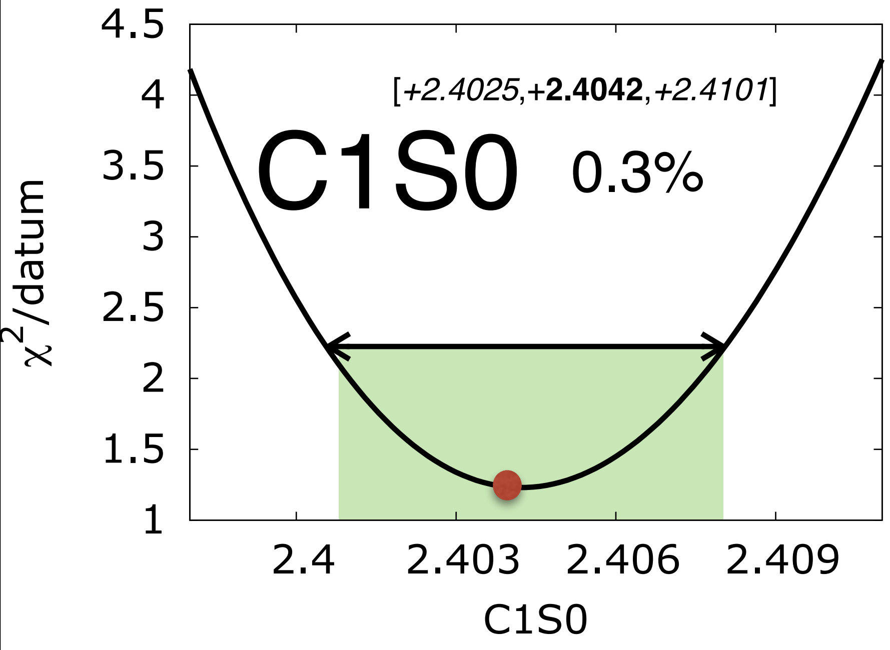
```
#++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
#                                       TOT                     PP                      NP
#      0.0       35.0            0.935777               1.020277               0.871546
#     35.0      125.0            1.429777               1.648994               1.272311
#    125.0      183.0            0.000000               0.000000               0.000000
#    183.0      290.0            0.000000               0.000000               0.000000
#    290.0      350.0            0.000000               0.000000               0.000000
#++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
#
```

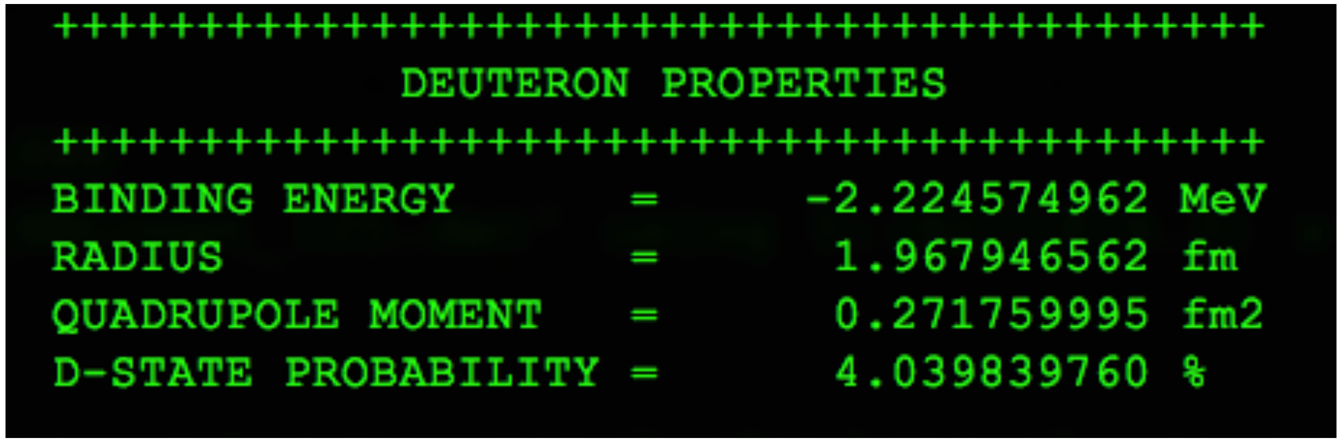
NNLOopt (Tlab<125) uncertainty *estimates*







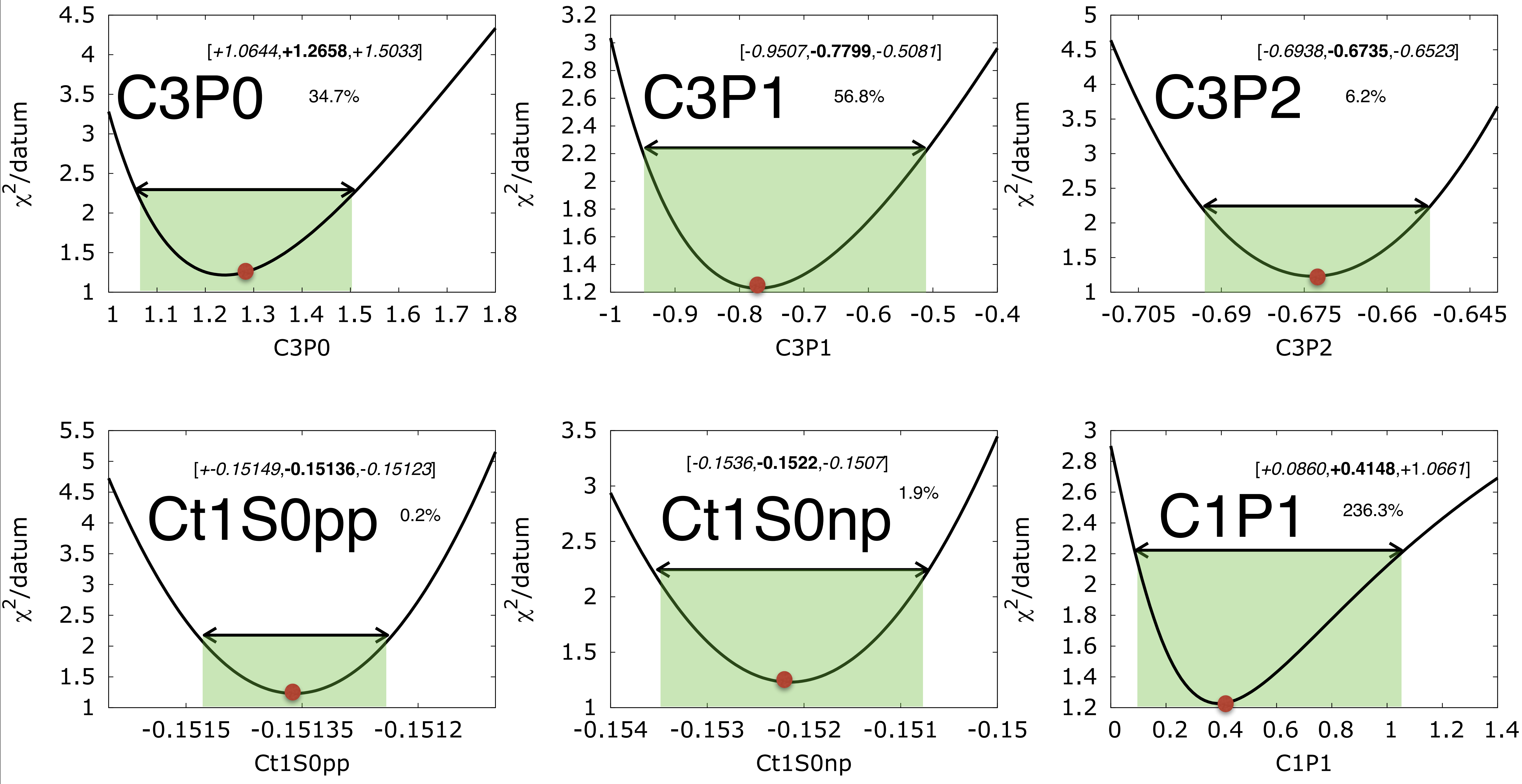




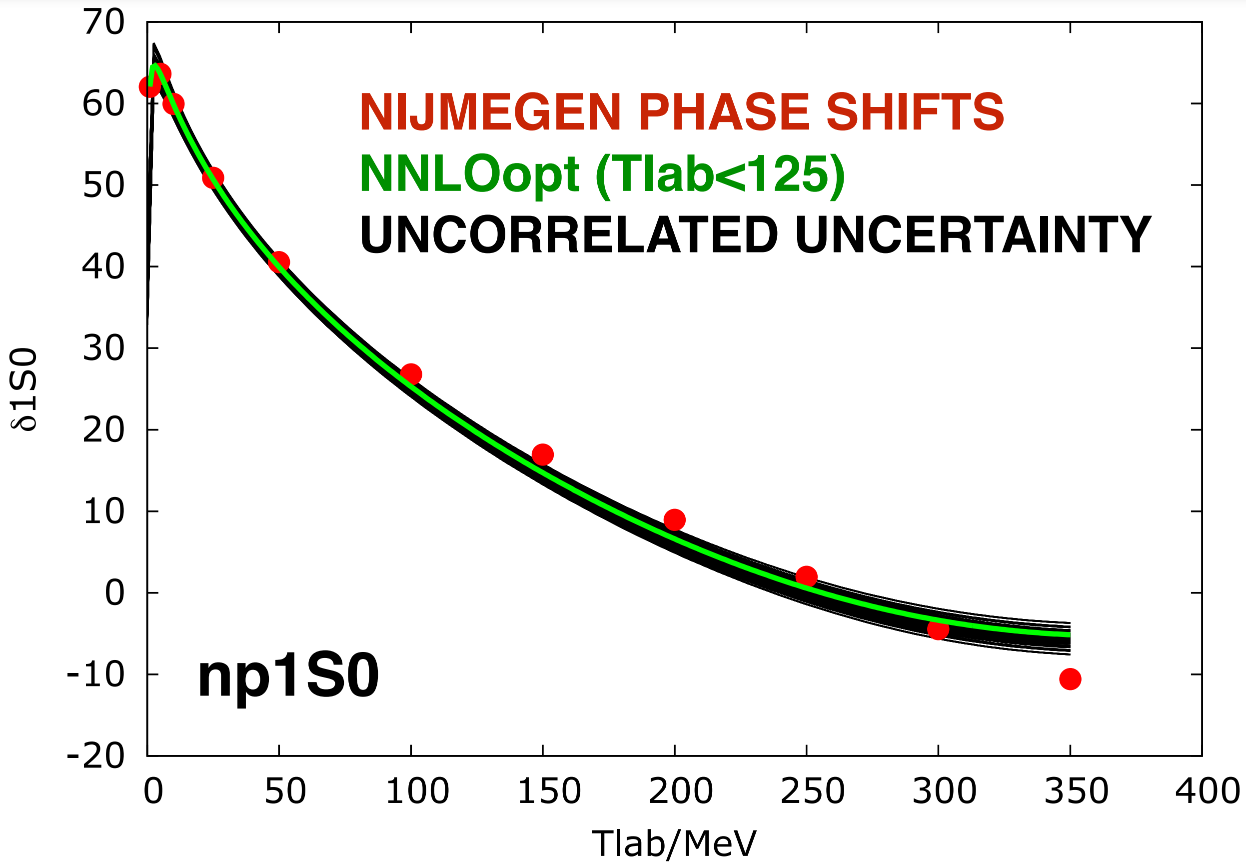
```
+++++++++++++++++++++++++++++++++++++++++
            DEUTERON PROPERTIES
+++++++++++++++++++++++++++++++++++++++++
BINDING ENERGY        =     -2.224574962 MeV
RADIUS                =      1.967946562 fm
QUADRUPOLE MOMENT     =      0.271759995 fm2
D-STATE PROBABILITY   =      4.039839760 %
```

At NNLO(500): The point in parameter space that reproduces the deuteron properties is within the uncertainty estimate. The optimum is slightly less bound.

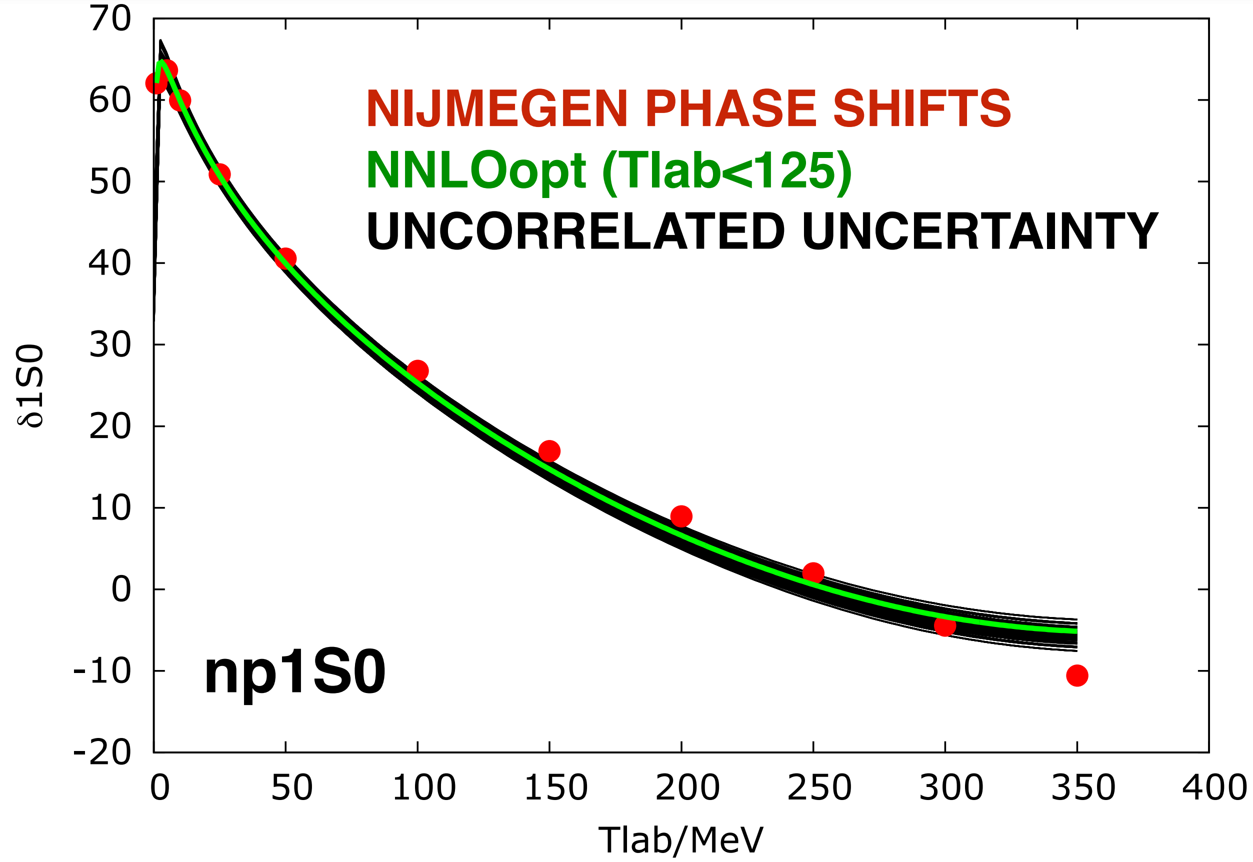
NNLOopt (Tlab<125) uncertainty *estimates*

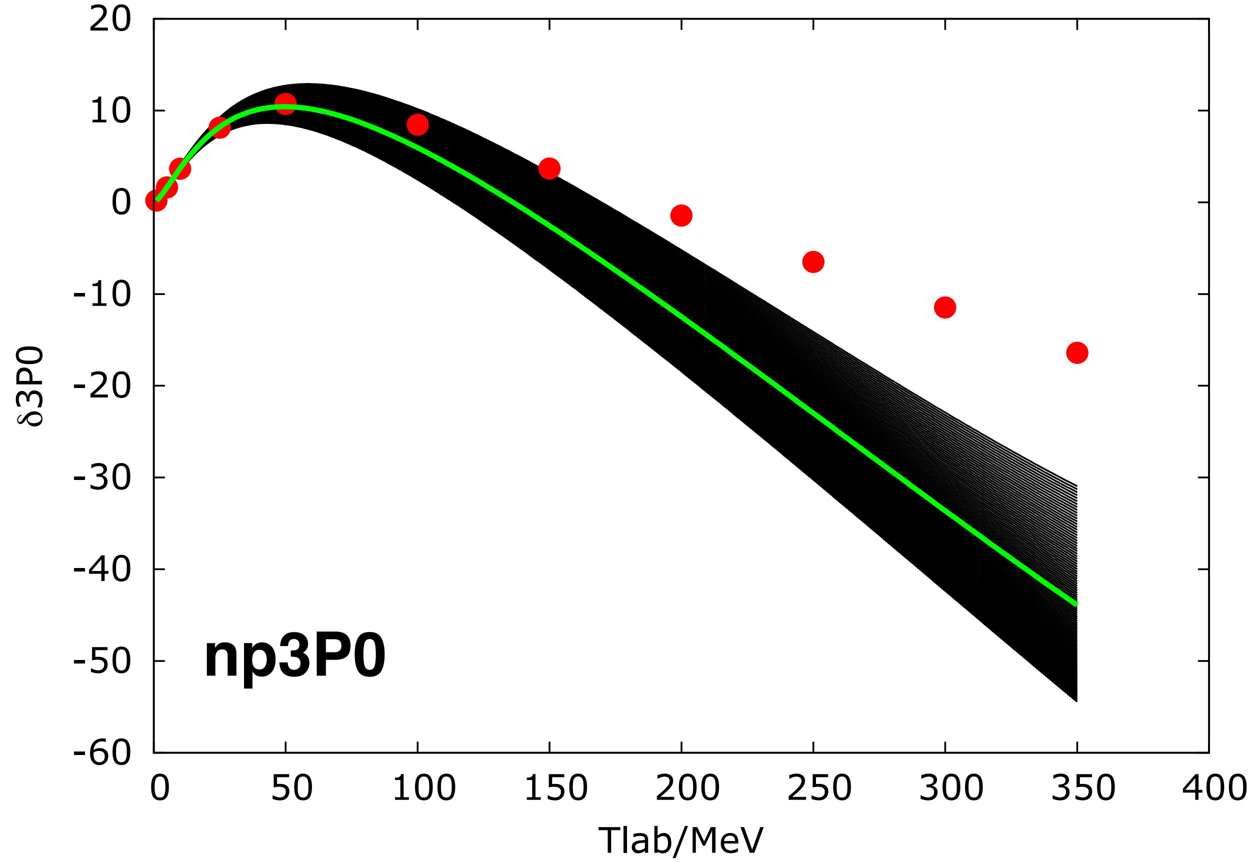


Phase shift sensitivity

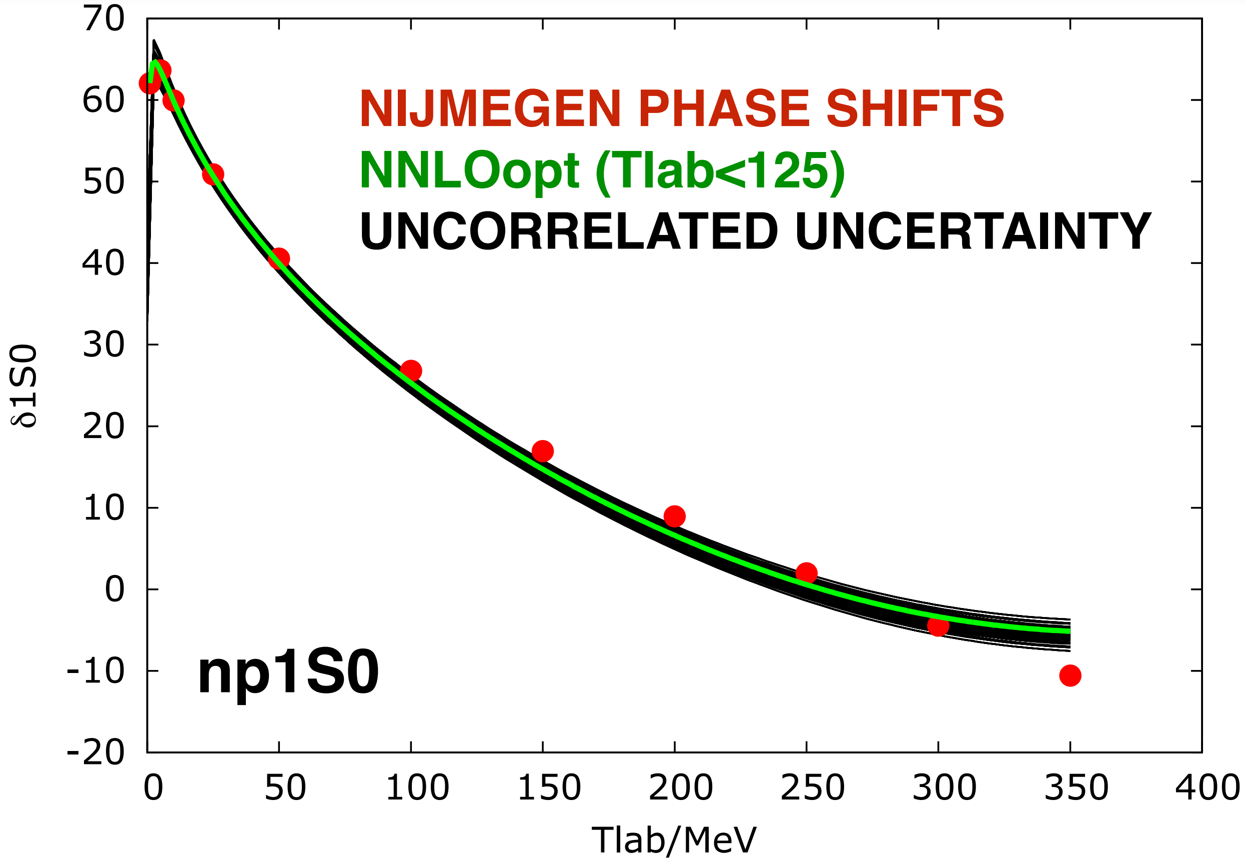


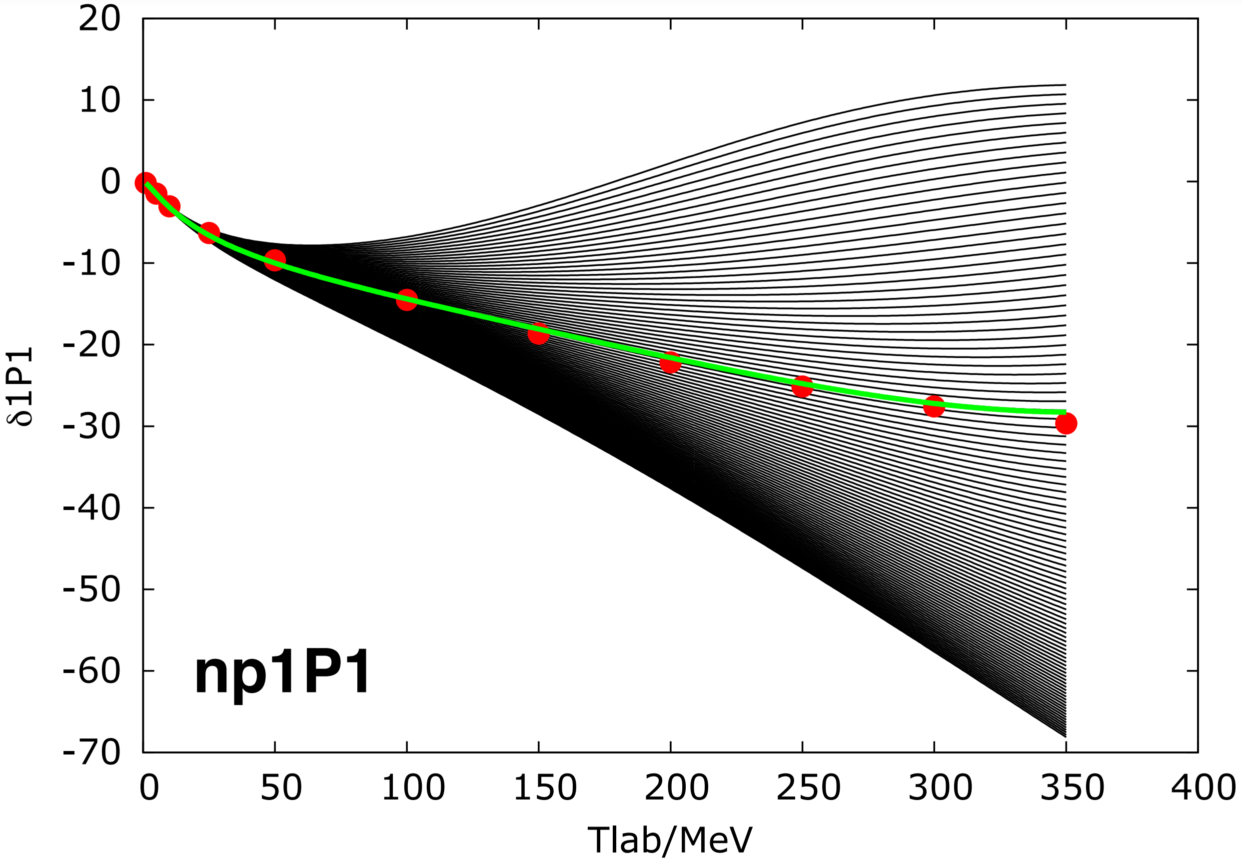
Phase shift sensitivity

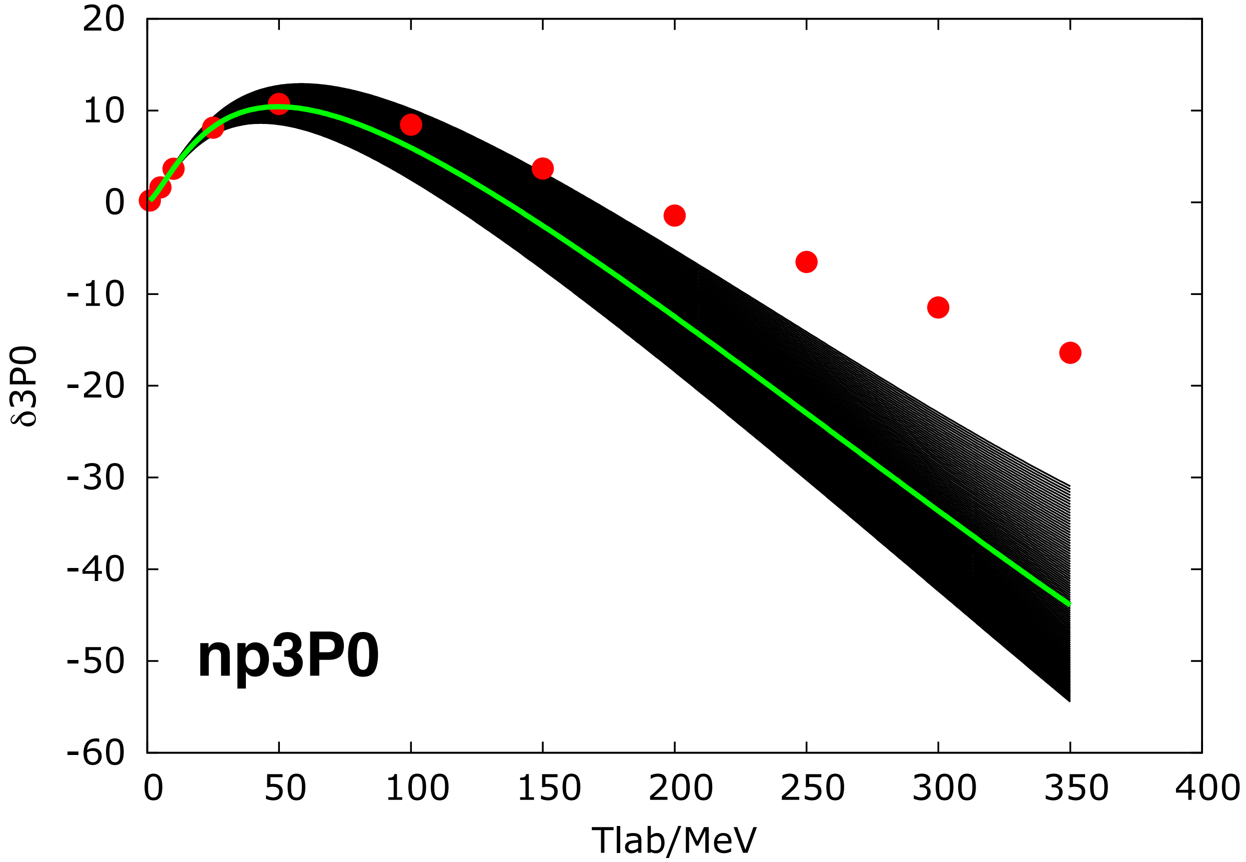




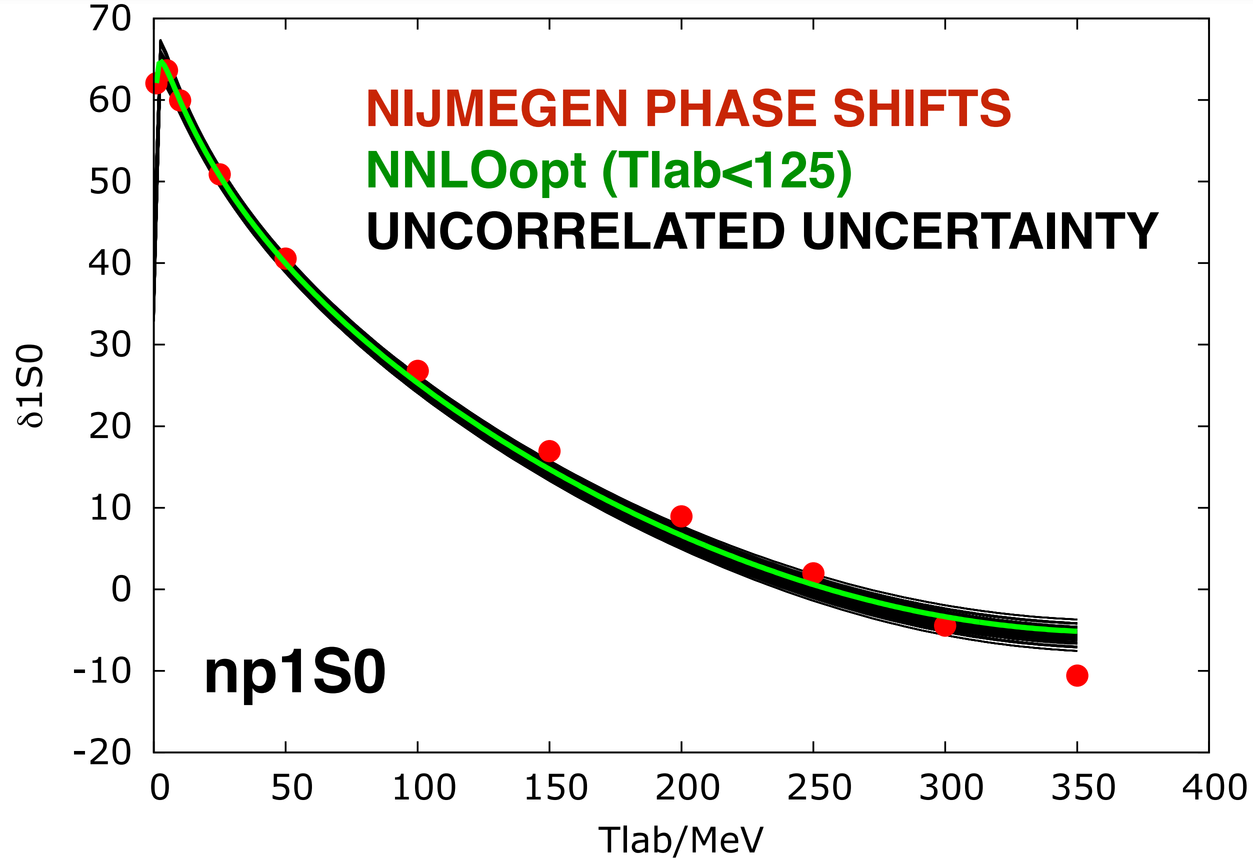
Phase shift sensitivity

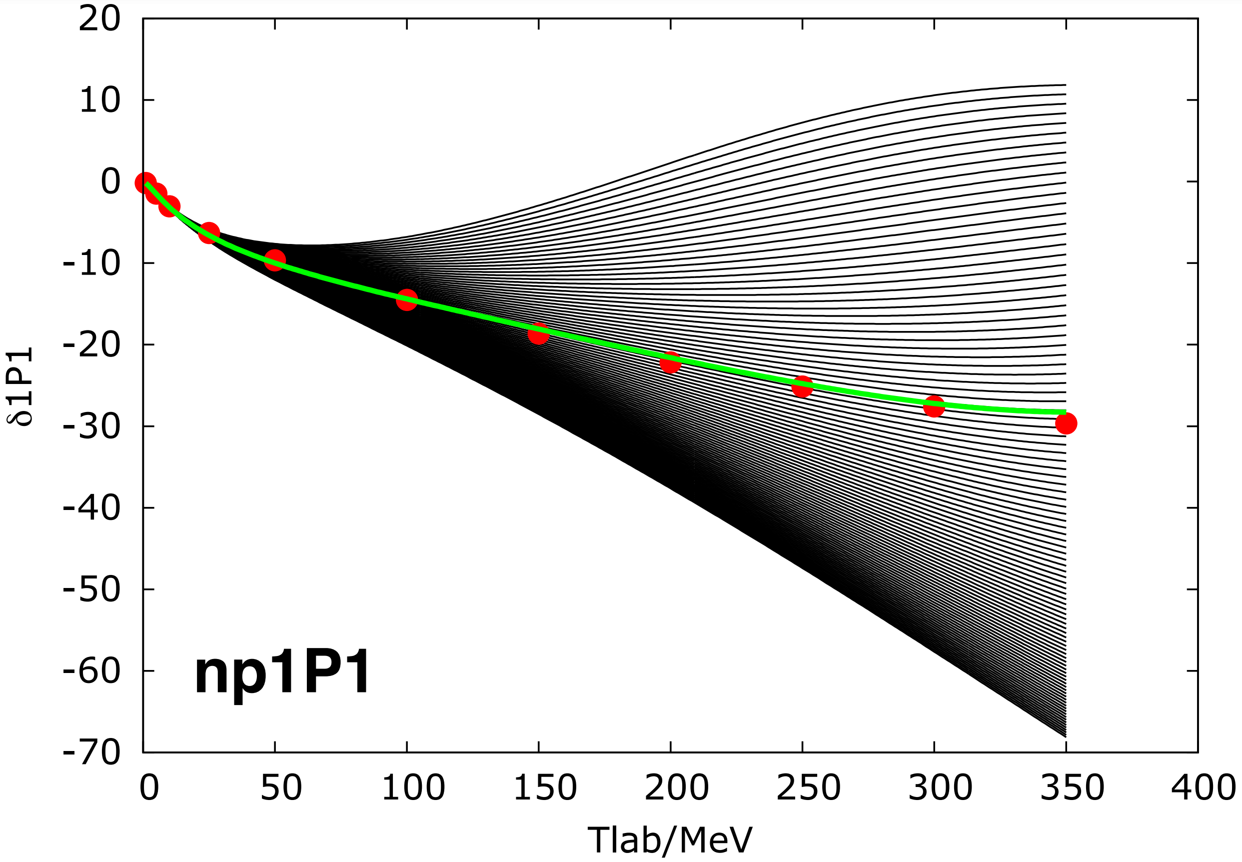


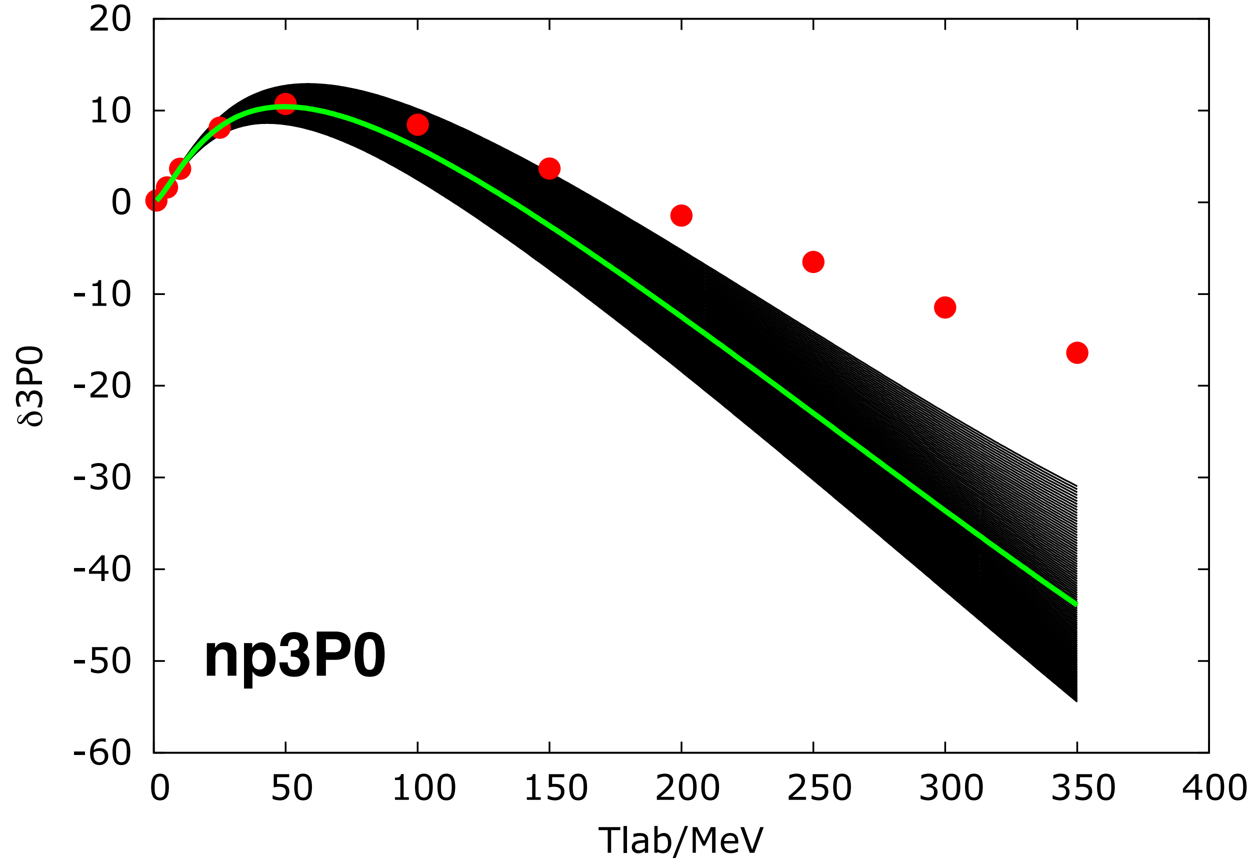




Phase shift sensitivity





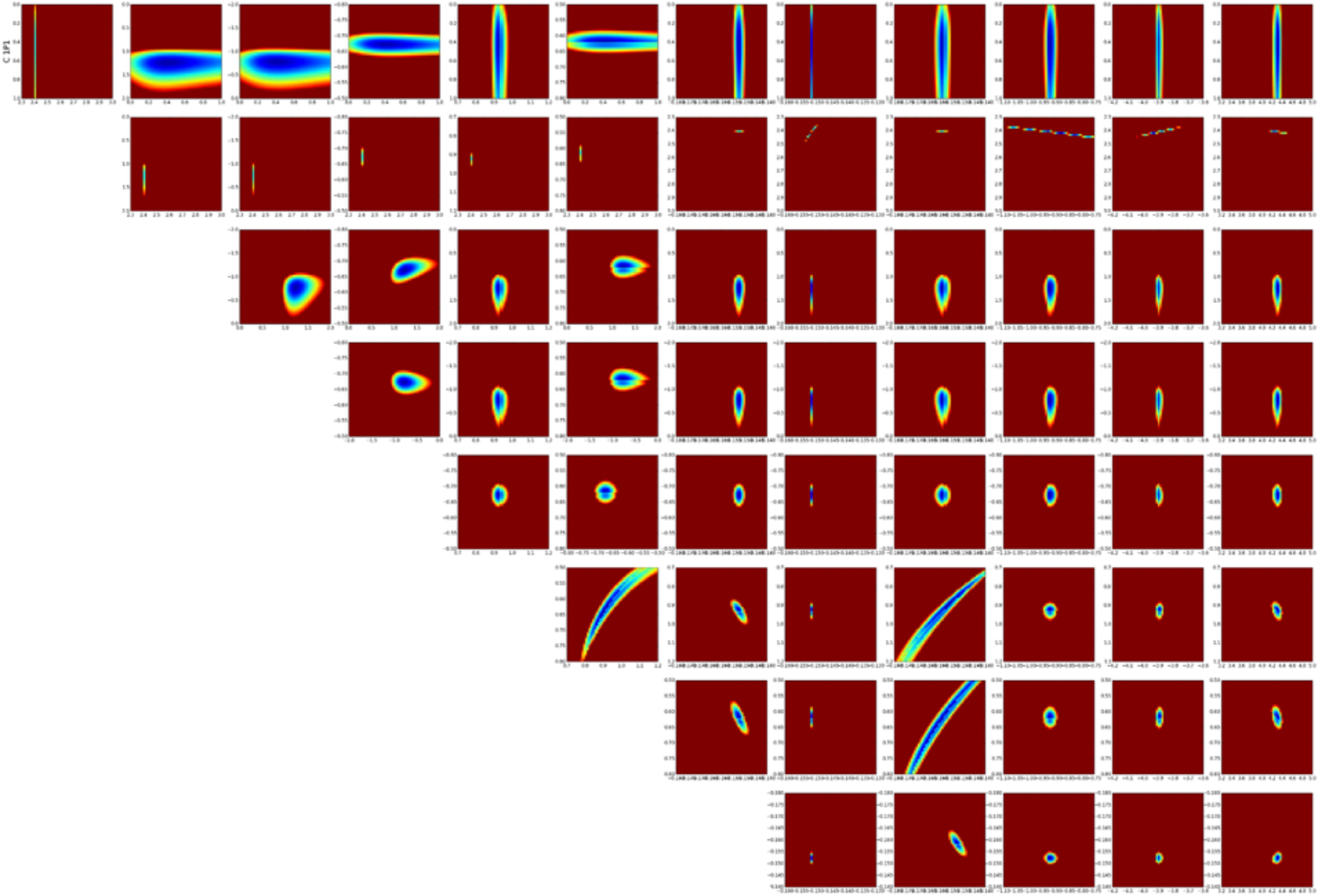


1S0: well reproduced.

3P0: sensitive to data and impossible to reproduce above 125 MeV at NNLO

1P1: data beyond 125 MeV very important for constraining the uncertainty.

Correlations will be important



Summary

The expanded objective function can generate N2LO interactions that simultaneously describe the ground state energy and radii in the oxygen isotopic chain.

POUNDerS shows great promise to deliver state-of-the-art optimized nuclear forces for practical calculations.

The piN LECs require a careful analysis, and might be attributed with large uncertainties.

Outlook: Correlated uncertainty estimates.

Collaboration

UNIVERSITY OF OSLO

University of Idaho

Argonne NATIONAL LABORATORY

THE UNIVERSITY of TENNESSEE

OAK RIDGE National Laboratory

MICHIGAN STATE UNIVERSITY

CHALMERS

NSCL

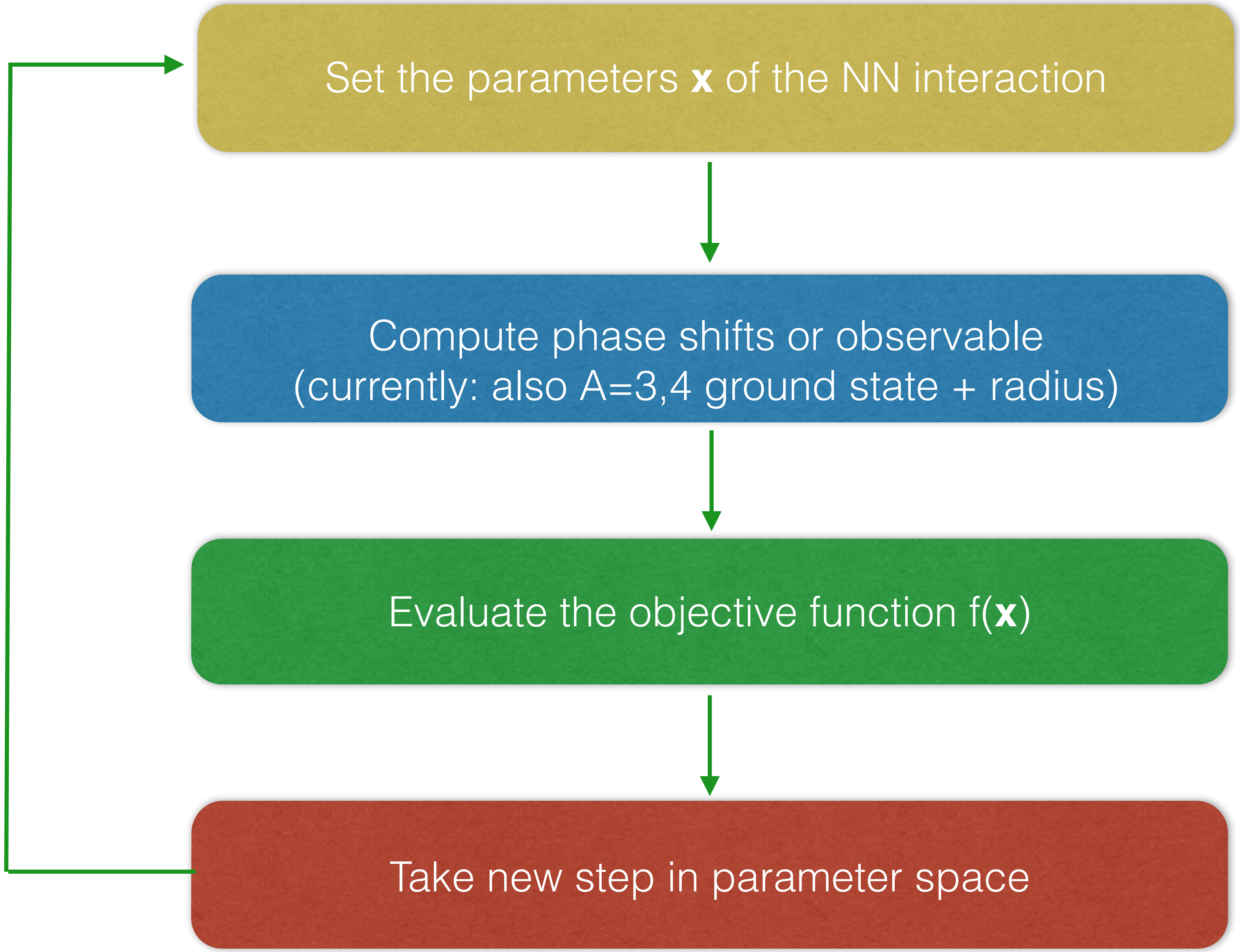
Collaboration

Gustav Baardsen
Boris Carlsson
Christian Forssen
Gaute Hagen
Morten Hjorth-Jensen
Gustav Jansen
Ruprecht Machleidt
Witold Nazarewicz
Thomas Papenbrock
Jason Sarich
Kyle Wendt
Stefan Wild

UNIVERSITY OF OSLO
University of Idaho
Argonne NATIONAL LABORATORY
THE UNIVERSITY of TENNESSEE UT
OAK RIDGE National Laboratory
MICHIGAN STATE UNIVERSITY
CHALMERS
NSCL

thank you for your attention!

Optimization strategy

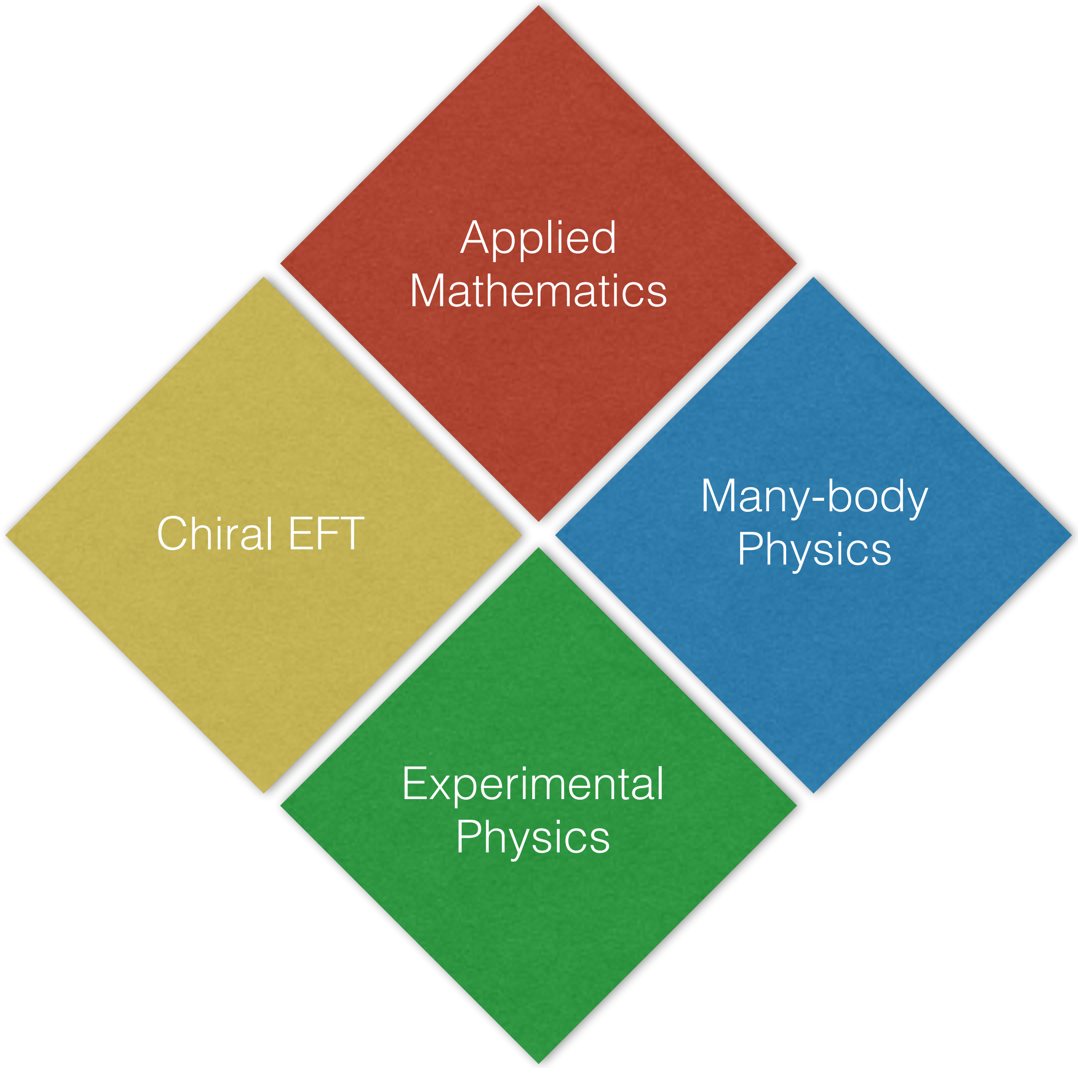


Set the parameters **x** of the NN interaction

Compute phase shifts or observable
(currently: also A=3,4 ground state + radius)

Evaluate the objective function f(**x**)

Take new step in parameter space



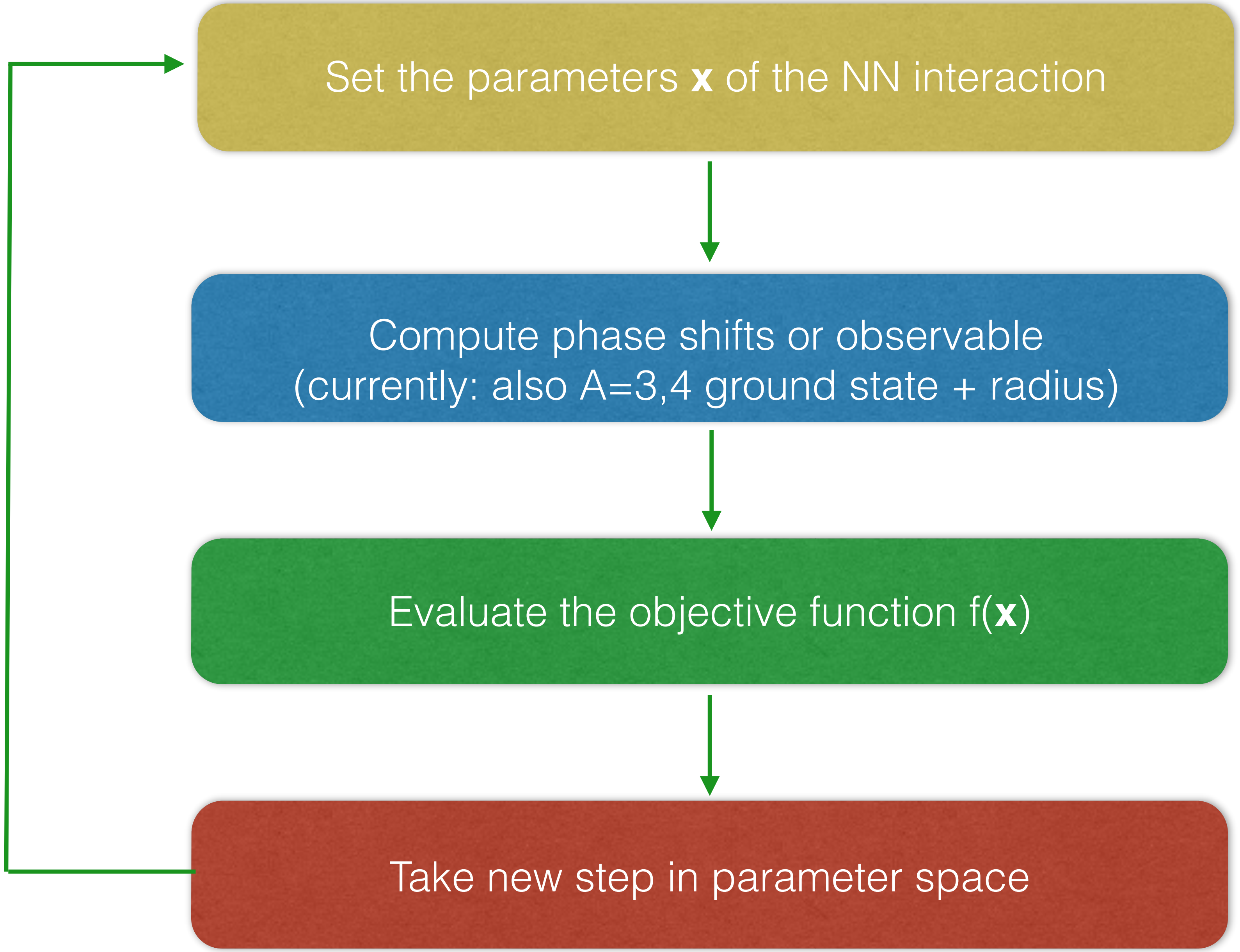
Applied Mathematics

Chiral EFT

Many-body Physics

Experimental Physics

Optimization strategy



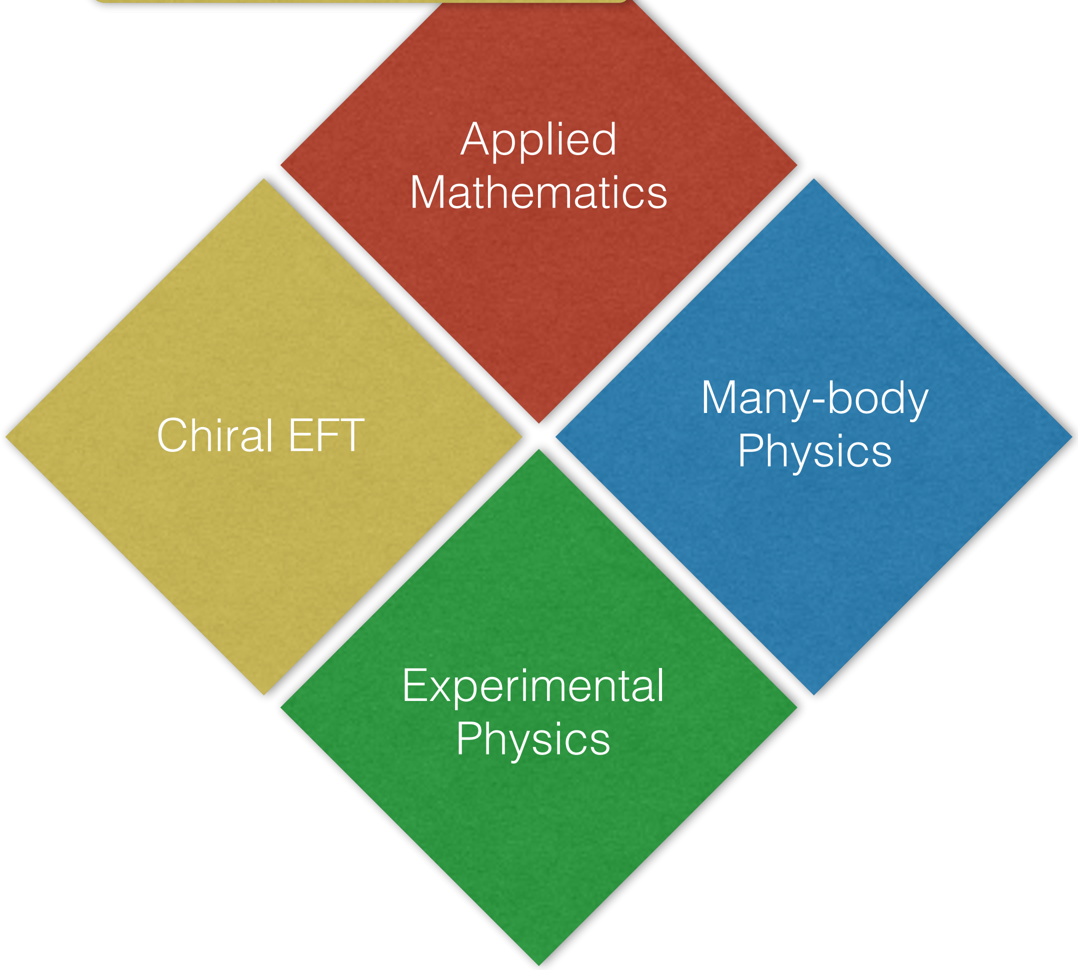
Set the parameters **x** of the NN interaction

Compute phase shifts or observable
(currently: also A=3,4 ground state + radius)

Evaluate the objective function f(**x**)

Take new step in parameter space

LO,..,N3LO
NNN & piN
available



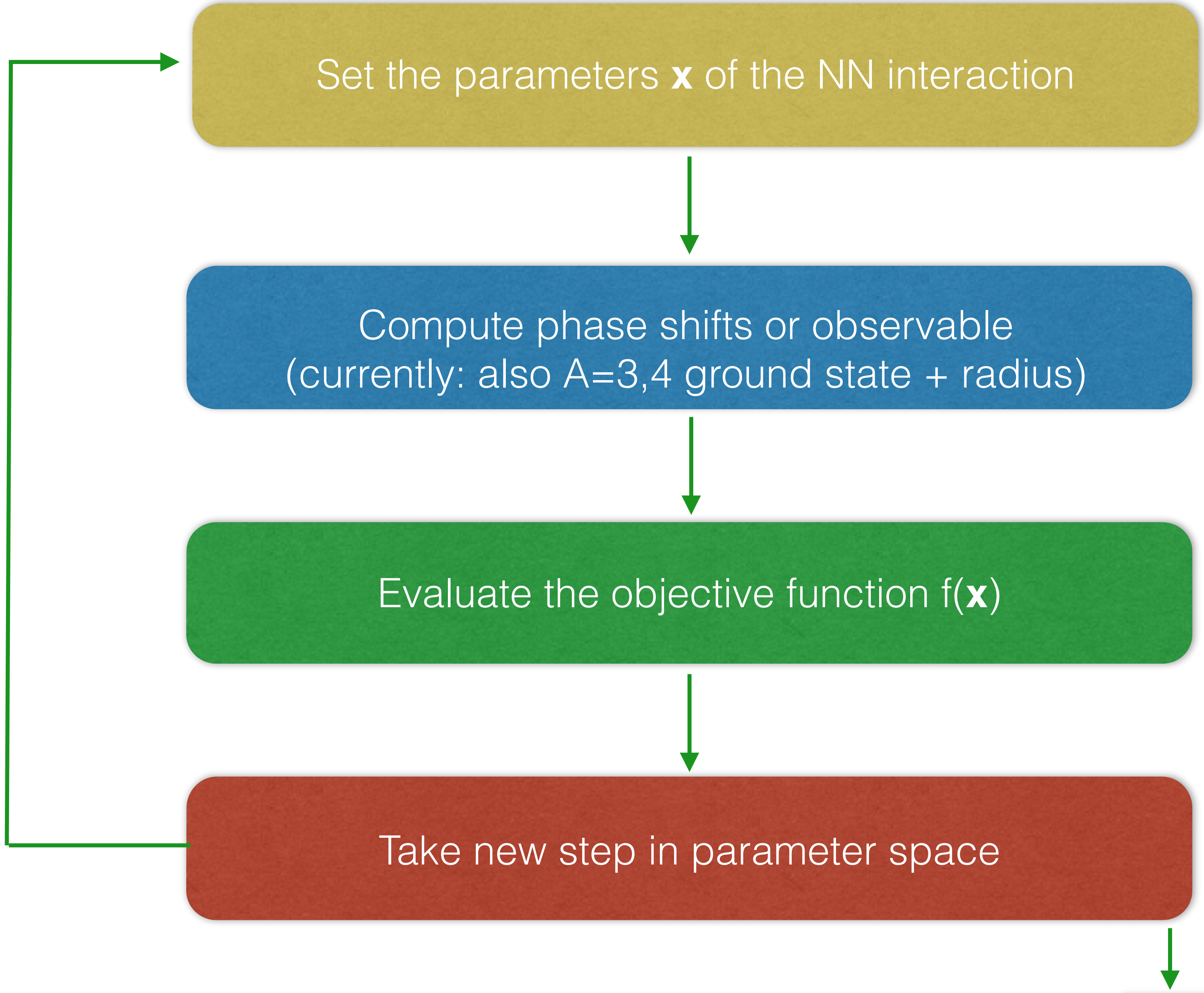
Applied Mathematics

Chiral EFT

Many-body Physics

Experimental Physics

Optimization strategy



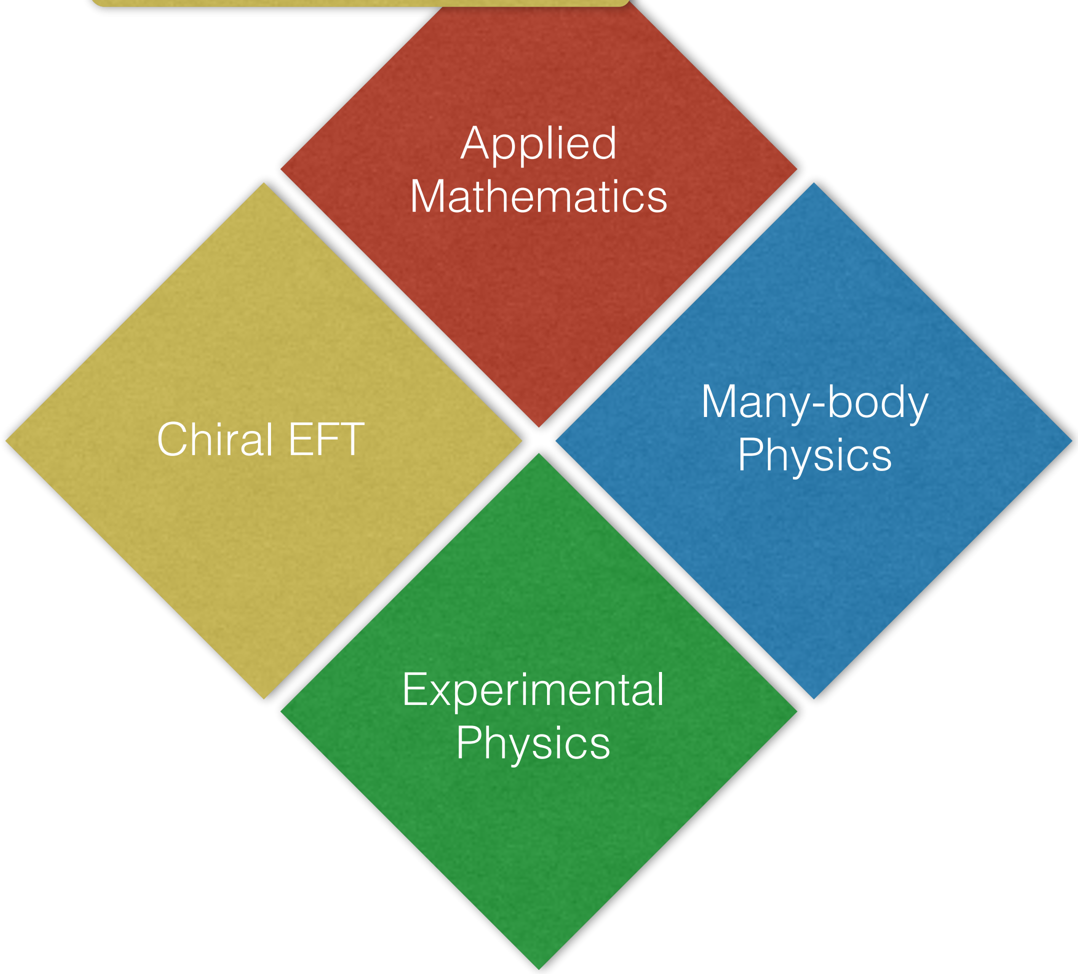
Set the parameters **x** of the NN interaction

Compute phase shifts or observable
(currently: also A=3,4 ground state + radius)

Evaluate the objective function f(**x**)

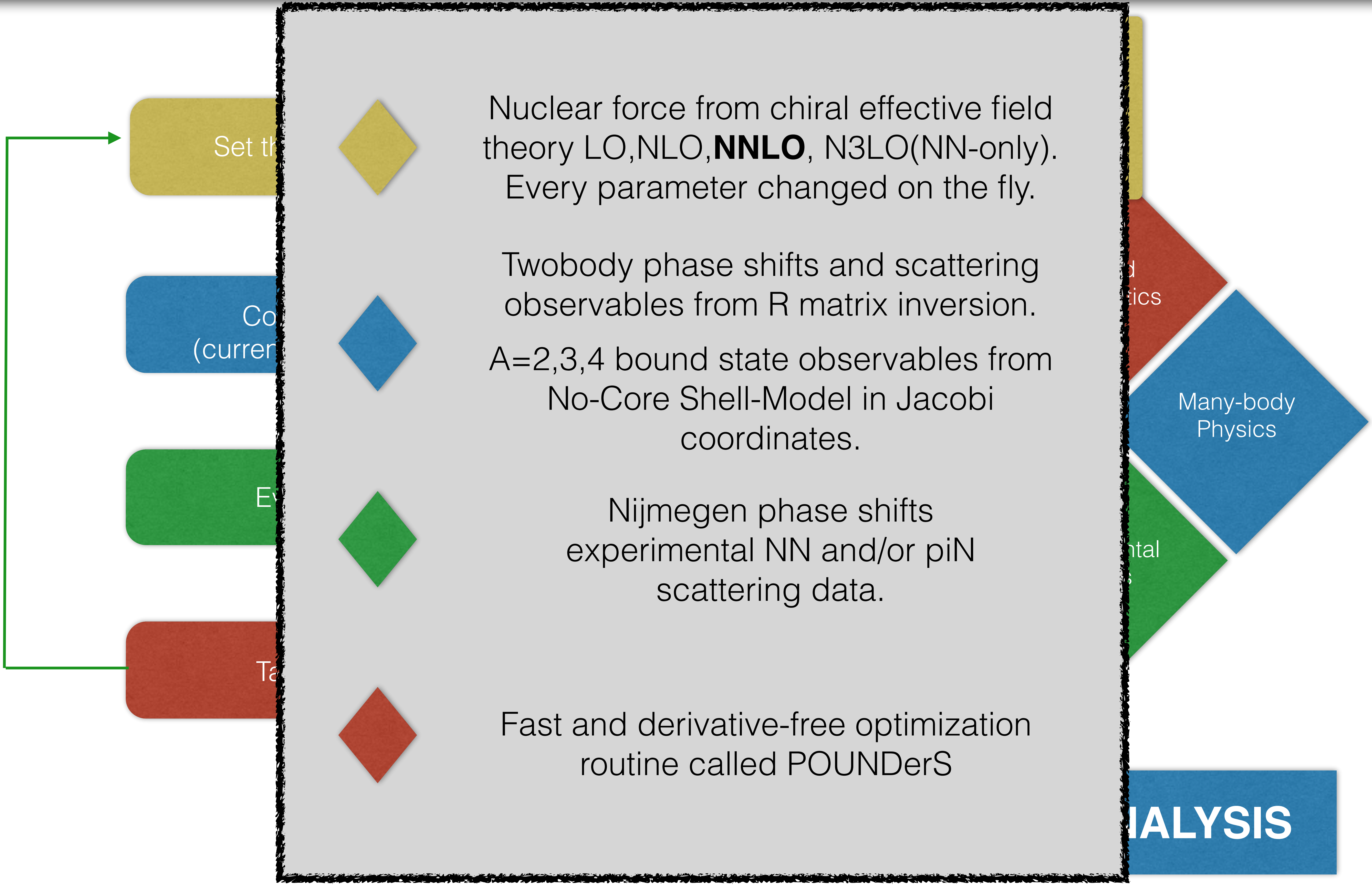
Take new step in parameter space

LO,..,N3LO
NNN & piN
available



SENSITIVITY ANALYSIS

Optimization strategy



- Nuclear force from chiral effective field theory LO,NLO,**NNLO**, N3LO(NN-only). Every parameter changed on the fly.

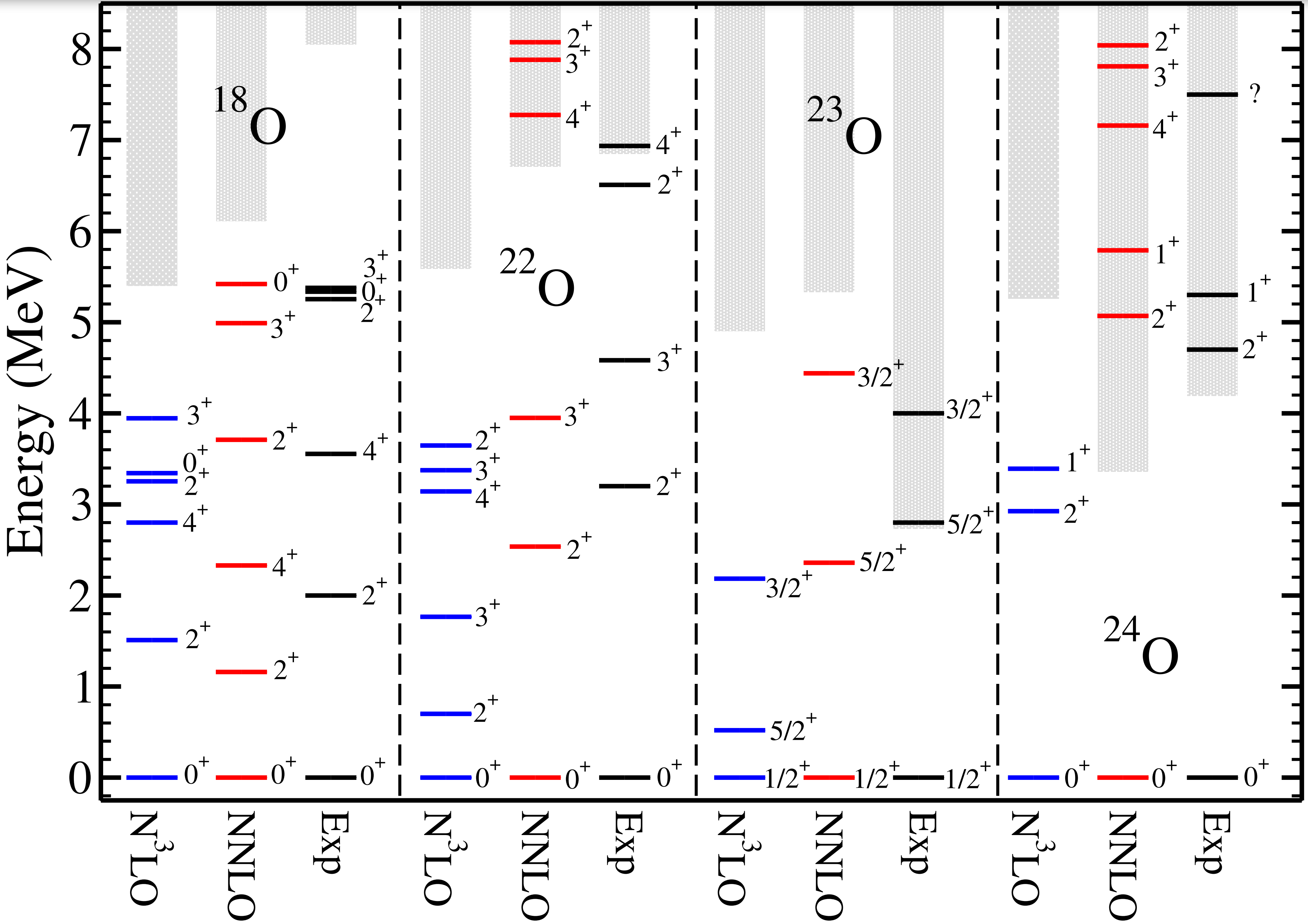
- Twobody phase shifts and scattering observables from R matrix inversion.

  A=2,3,4 bound state observables from No-Core Shell-Model in Jacobi coordinates.

- Nijmegen phase shifts experimental NN and/or piN scattering data.

- Fast and derivative-free optimization routine called POUNDerS

Oxygen excitation energies from NNLOopt



Oxygen24	2+	1+	4+	3+
NNLOopt	5.06	5.79	7.17	7.82
NNLO(EGM 450/500)	9.62	10.54	12.78	13.35
Experiment	4.7	5.3	?	?