

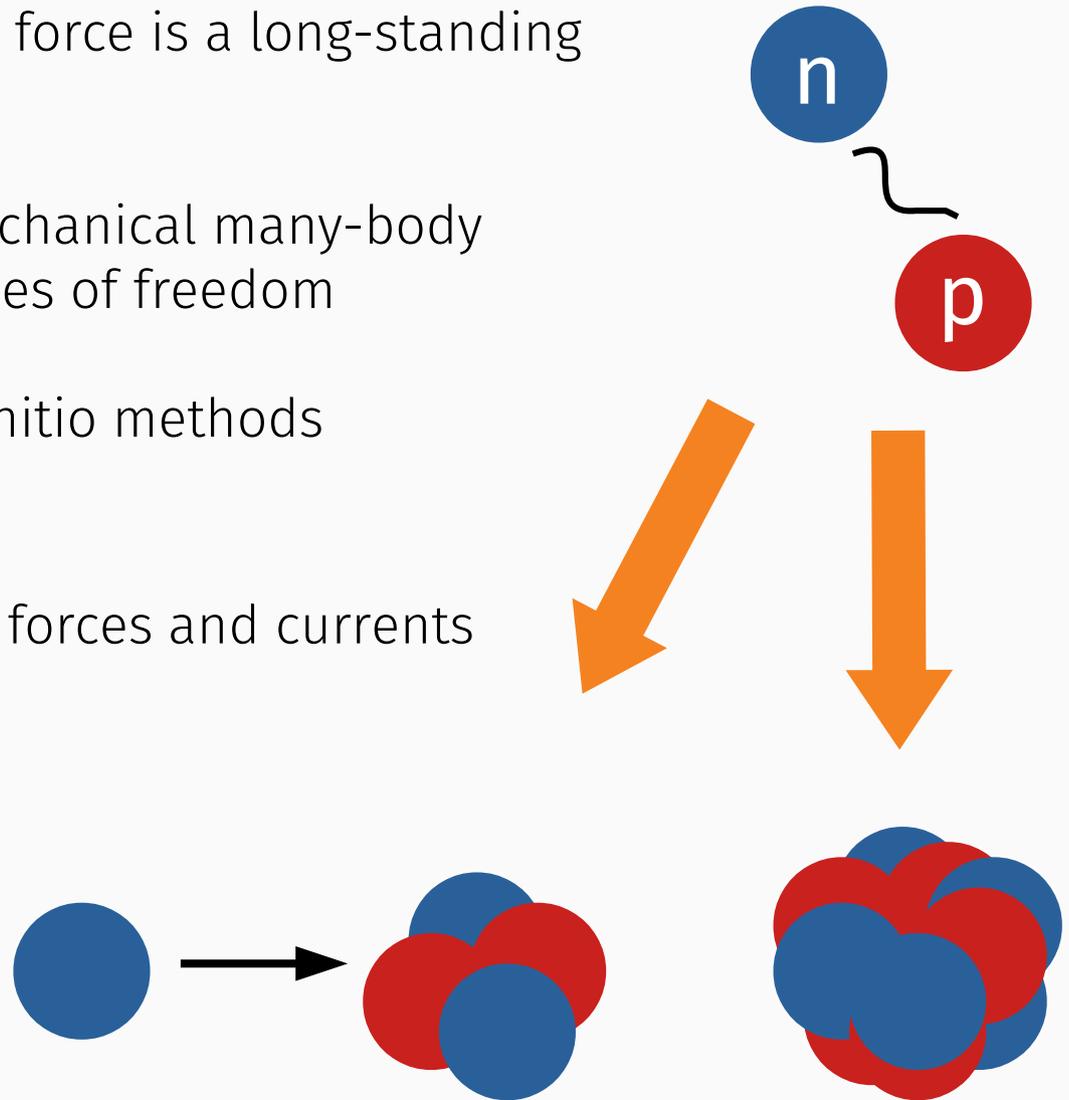
High-quality nuclear forces from chiral EFT

Patrick Reinert
Ruhr-Universität Bochum

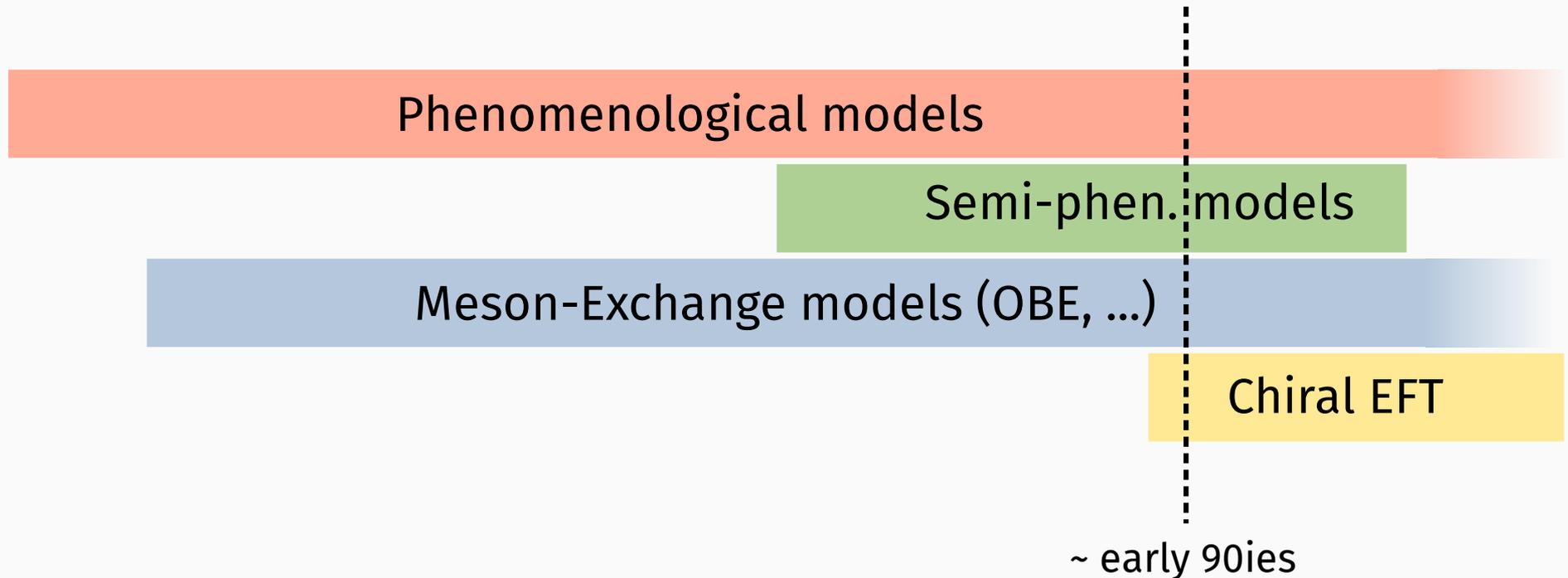
Dr. Klaus Erkelenz Kolloquium
December 17, 2019

Motivation

- Proper description of the strong force is a long-standing problem
- Formulate nuclear quantum-mechanical many-body problem with nucleons as degrees of freedom
- Computational advances in ab initio methods
 - **Precise forces required**
- Need for consistent many-body forces and currents



A short history of NN potentials



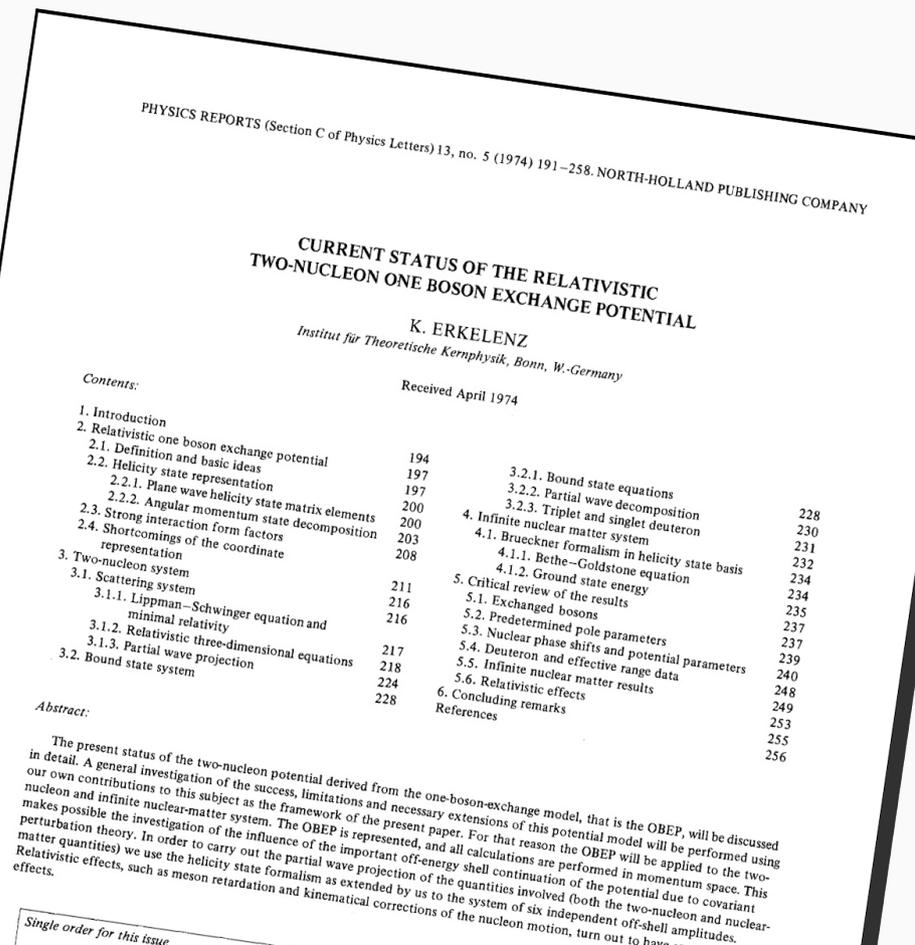
- 1935: One-Pion-Exchange (Yukawa)
- 1960ies: Phenomenological potentials & One-Boson-Exchange (OBE)
- 1970ies: Bonn Potential (Erkelenz)
- 1990ies: Nijmegen PWA & semi-phenomenological potentials achieve $\chi^2/\text{datum} \sim 1$ description, Chiral EFT as QCD-inspired approach

Erkelenz' work in the light of today



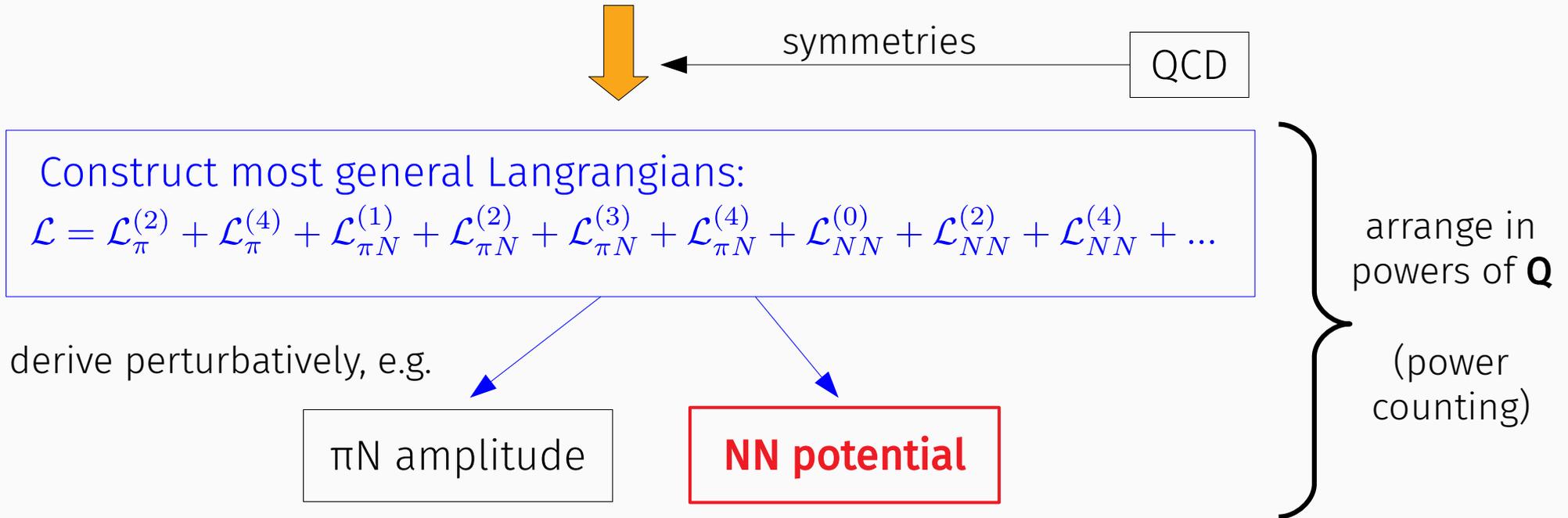
Driven by the same goals as today:

- Rejection of phenomenological models
- too many parameters
- Performance beyond the two-nucleon system
- Derivation of potential from field theory



Chiral nuclear EFT

- Degrees of freedom: Nucleons & Pions



Chiral nuclear EFT

- Degrees of freedom: Nucleons & Pions



Construct most general Lagrangians:

$$\mathcal{L} = \mathcal{L}_\pi^{(2)} + \mathcal{L}_\pi^{(4)} + \mathcal{L}_{\pi N}^{(1)} + \mathcal{L}_{\pi N}^{(2)} + \mathcal{L}_{\pi N}^{(3)} + \mathcal{L}_{\pi N}^{(4)} + \mathcal{L}_{NN}^{(0)} + \mathcal{L}_{NN}^{(2)} + \mathcal{L}_{NN}^{(4)} + \dots$$

arrange in powers of \mathbf{Q}

(power counting)

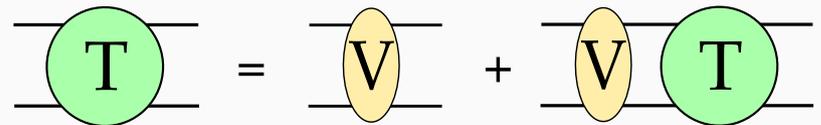
derive perturbatively, e.g.

πN amplitude

NN potential

Nuclear forces require **non-perturbative resummation**

- Iterations UV-divergent → apply regulator



Expansion in \mathbf{Q}



- Systematic improvement
- Uncertainty estimation

Hierarchy of nuclear forces

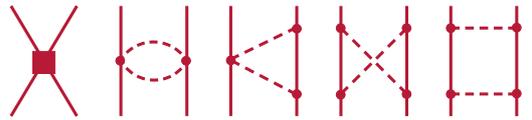
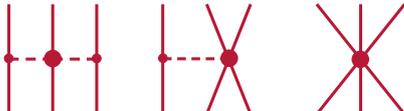
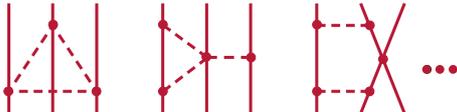
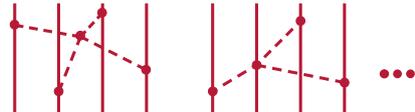
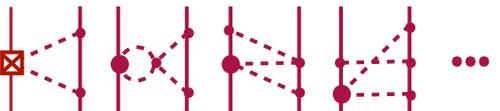
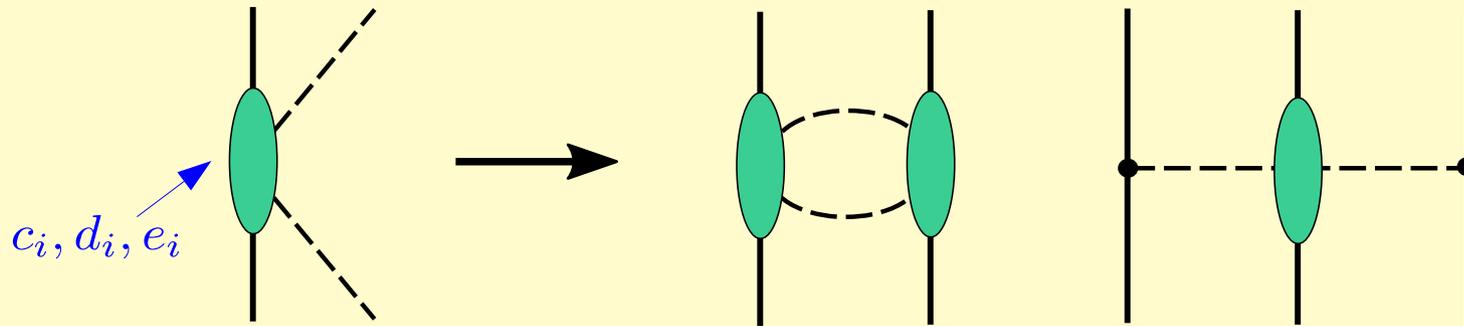
	Two-nucleon force	Three-nucleon force	Four-nucleon force
LO (Q^0)			
NLO (Q^2)			
N ² LO (Q^3)			
N ³ LO (Q^4)			
N ⁴ LO (Q^5)			have not been worked out yet

Figure courtesy of E. Epelbaum

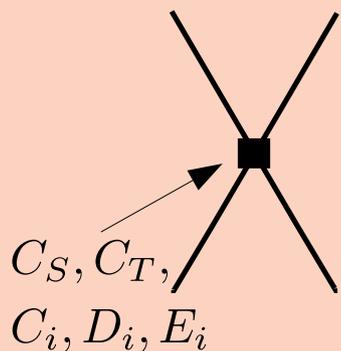
Parameters in chiral nuclear EFT

Consistent derivation of many-body forces & currents from same Lagrangian:

Long-range part of nuclear forces due to pion exchanges:



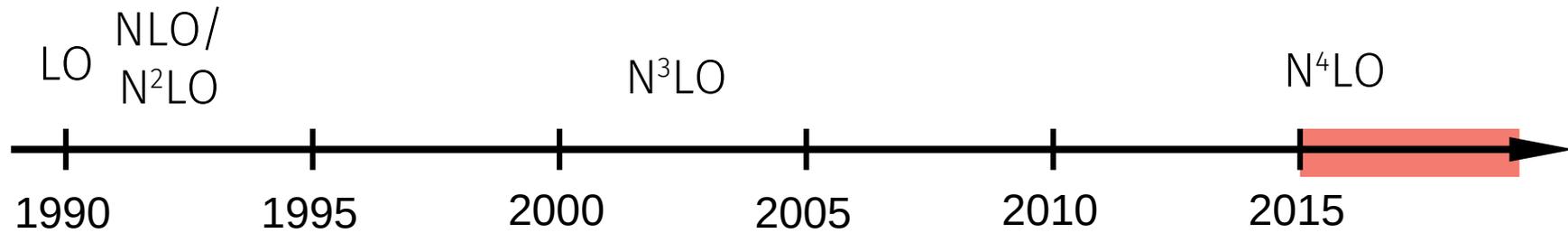
- **π N LECs** from recent Roy-Steiner eq. analysis of π N scattering [[Phys. Rev. Lett. 115, 192301](#)] (Dr. Klaus Erkelenz Preis 2015)
- **Parameter-free** for nuclear forces



Short-range part of 2NF due to contact interactions

- **NN LECs** determined from NN scattering data, $B_d = 2.224575(9)$ MeV and $b_{np} = -3.7405(9)$ fm
- Use self-consistent 2013 Granada database [[Phys. Rev. C 88.064002](#)]

Current generation of chiral NN potentials



New generation of N⁴LO forces

- Semilocal coordinate-space regularized (EKM) [EPJA 51 (2015) 53; PRL 115 (2015) 122301]
- **Semilocal momentum-space regularized (SMS), this work**
- Nonlocal momentum-space regularized (EMN) [PRC 96 (2017) 024004]

Also:

- Interactions fitted to properties of heavier nuclei (e.g. NNLOsat [PRC 91 (2015) 051301]), Delta-full,...

Important differences in regularization & fitting protocol!

Regularization of SMS forces

“Semilocal momentum-space regularized (SMS) NN forces”



Non-local regulator for short-range contacts (same as EKM)

+

New **local** regularization for long-range potential *in momentum space*

$$\langle p' | V_{\text{cont}} | p \rangle_{\text{reg.}} = \langle p' | V_{\text{cont}} | p \rangle \exp \left[-\frac{p'^2 + p^2}{\Lambda^2} \right]$$

Regularization of long-range part

EKM potential used local regularization [in coordinate space](#):

$$V_{\pi,\text{reg}}(\vec{r}) = V_{\pi}(\vec{r}) \left[1 - e^{-\frac{r^2}{R^2}} \right]^n$$

✓ Minimization of long-range cutoff artifacts
✗ inconvenient for currents & N³LO 3NF

New local regularization [in momentum space](#) (inspired by [Annals Phys. 208, 253](#)):

Main idea: regularize static pion-propagators with gaussian form factor

$$\frac{1}{\vec{l}^2 + M_{\pi}^2} \rightarrow \frac{1}{\vec{l}^2 + M_{\pi}^2} e^{-\frac{\vec{l}^2 + M_{\pi}^2}{\Lambda^2}}$$

e.g. $V_{1\pi,\text{reg.}}(q) \propto \frac{1}{q^2 + M_{\pi}^2} e^{-\frac{q^2 + M_{\pi}^2}{\Lambda^2}} = \frac{1}{q^2 + M_{\pi}^2} + \text{short-range terms}$

- Polynomial short-range contribution chosen such that $V(r)|_{r=0} = 0$

and $\left. \frac{d^n V}{dr^n}(r) \right|_{r=0} = 0$

- ✓ similar to previous coordinate-space regulator
- ✓ scheme extendable to many-body forces & currents

χ^2/datum ($\Lambda=450$ MeV)

E_{lab} bin	LO	NLO	N ² LO	N ³ LO	N ⁴ LO	N ⁴ LO ⁺
neutron-proton scattering data						
0–100	73	2.2	1.2	1.07	1.07	1.07
0–200	62	5.4	1.7	1.09	1.08	1.06
0–300	75	14	4.2	2.01	1.16	1.06
proton-proton scattering data						
0–100	2290	10	2.2	0.90	0.88	0.86
0–200	1770	90	37	1.99	1.42	0.95
0–300	1380	90	41	3.43	1.67	1.00

χ^2/datum ($\Lambda=450$ MeV)

E_{lab} bin	LO	NLO	N ² LO	N ³ LO	N ⁴ LO	N ⁴ LO ⁺
neutron-proton scattering data						
0–100	73	2.2	1.2	1.07	1.07	1.07
0–200	62	5.4	1.7	1.09	1.08	1.06
0–300	75	14	4.2	2.01	1.16	1.06
proton-proton scattering data						
0–100	2290	10	2.2	0.90	0.88	0.86
0–200	1770	90	37	1.99	1.42	0.95
0–300	1380	90	41	3.43	1.67	1.00

2 + 1 IB LECs
 +7 LECs
 No new LECs
 +12 LECs
 +1 IB LEC
 +4 LECs

- (Almost) parameter-free improvements show importance of chiral 2 π -exchange

χ^2/datum ($\Lambda=450$ MeV)

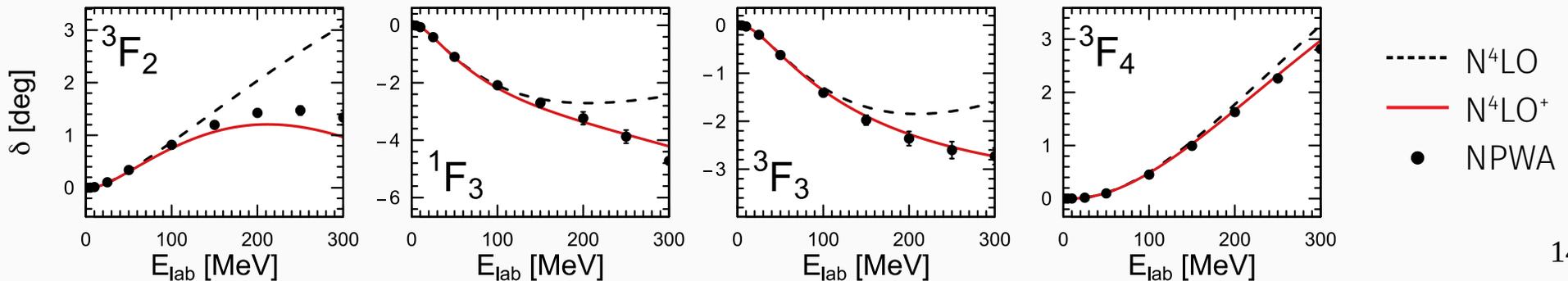
E_{lab} bin	LO	NLO	N ² LO	N ³ LO	N ⁴ LO	N ⁴ LO ⁺
neutron-proton scattering data						
0–100	73	2.2	1.2	1.07	1.07	1.07
0–200	62	5.4	1.7	1.09	1.08	1.06
0–300	75	14	4.2	2.01	1.16	1.06
proton-proton scattering data						
0–100	2290	10	2.2	0.90	0.88	0.86
0–200	1770	90	37	1.99	1.42	0.95
0–300	1380	90	41	3.43	1.67	1.00

2 + 1 IB
LECs +7 LECs

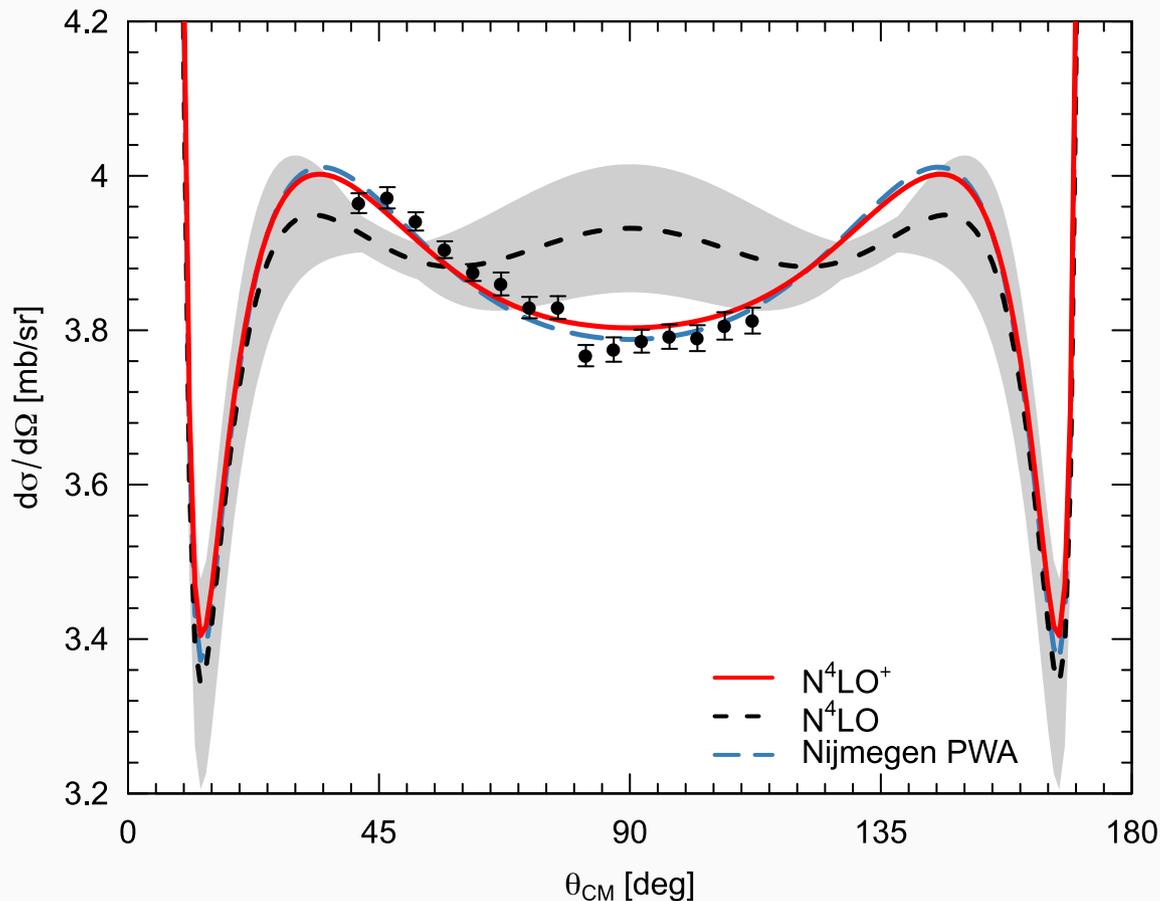
+12 LECs

+4 LECs

N⁴LO⁺ = N⁴LO + leading F-Wave contacts: $\langle {}^S F_j, p' | V_{\text{cont}} | {}^S F_j, p \rangle = E_{i_F} p^3 p'^3$



CO(67)

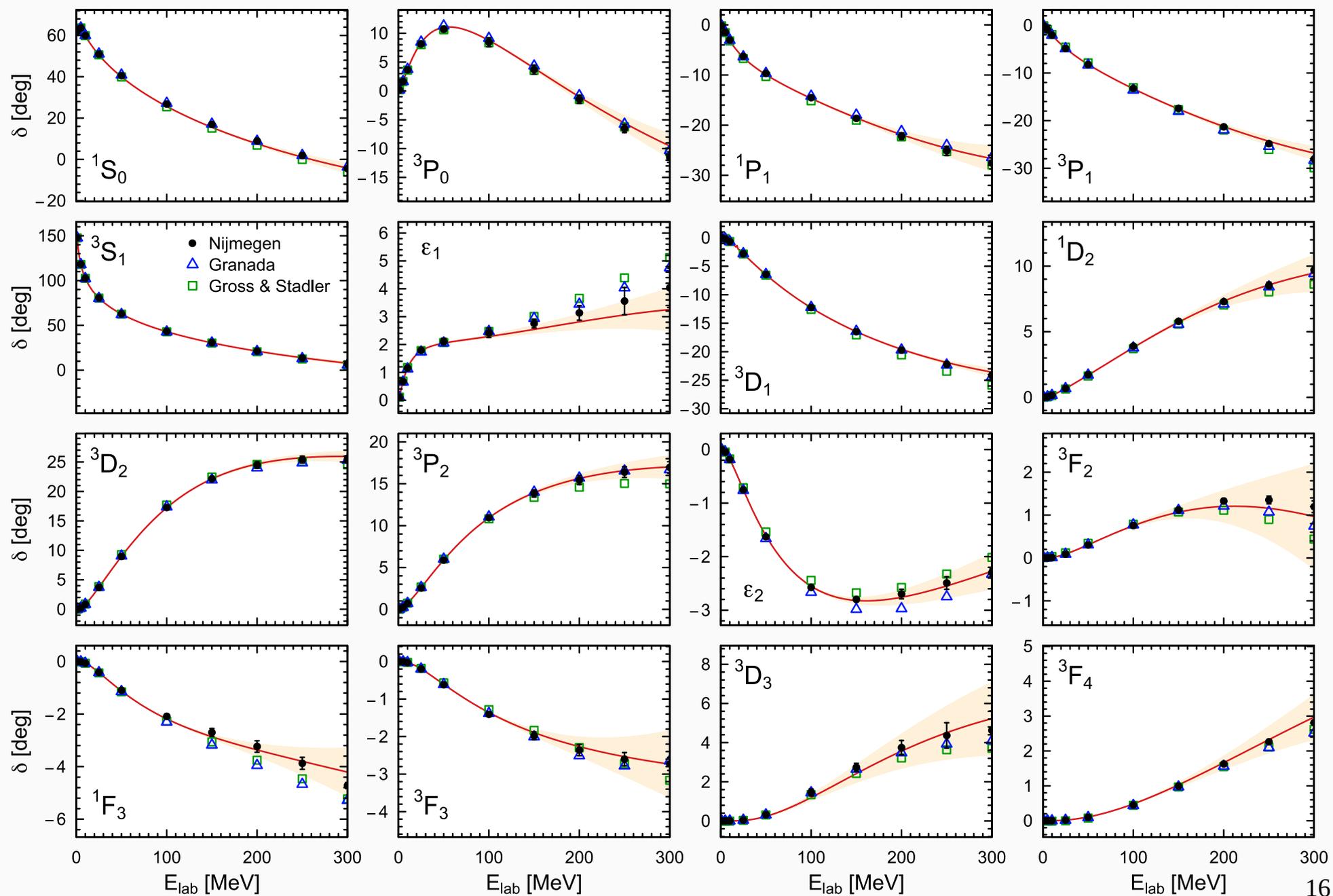


About this dataset:

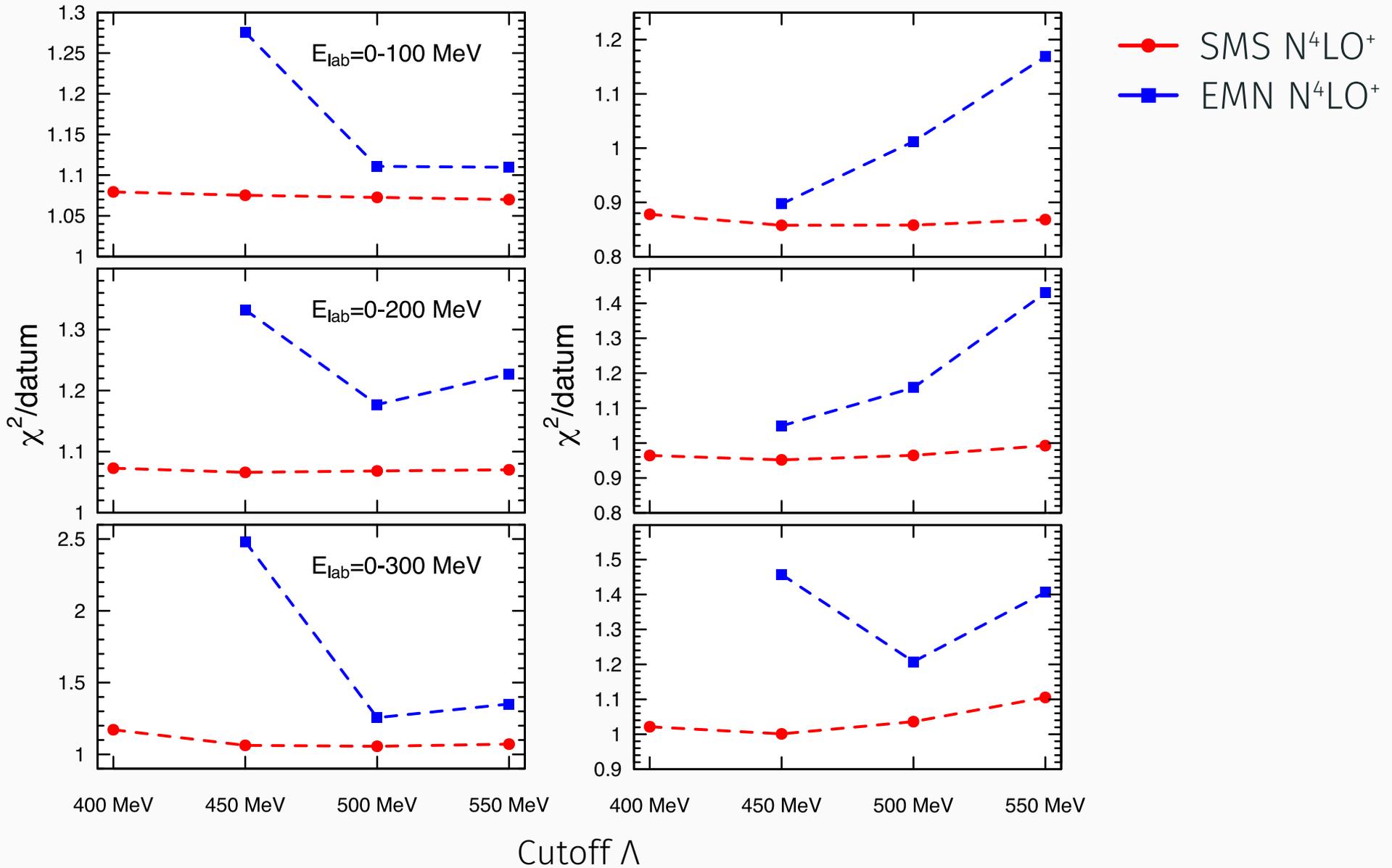
- differential cross section $d\sigma/d\Omega$
- $E_{lab} = 144.1$ MeV
- experimental errors $\sim 0.5\%$

- Need accurate F-Waves (in particular 3F_2) at energies ~ 150 MeV to describe such observables well
- Estimated truncation error and naturalness of F-Wave LECs suggest **no failure of power counting**

Phaseshifts N^4LO^+ ($\Lambda = 450$ MeV)



χ^2/datum Cutoff Dependence



➔ Best precision for $\Lambda = 450$ MeV in 2N system

Quantile-Quantile plot

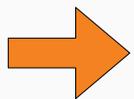
Check assumption: $r_i = \frac{O_i^{\text{exp}} - O_i^{\text{th}}}{\Delta O_i^{\text{exp}}} \sim \mathcal{N}(0, 1)$

- Plot $F_{\text{emp}}^{-1}(x)$ vs $F_{\text{th}}^{-1}(x)$

$$F_{\text{emp}}(x) = \frac{1}{N} \sum_{i=1}^N \theta(x - r_i)$$

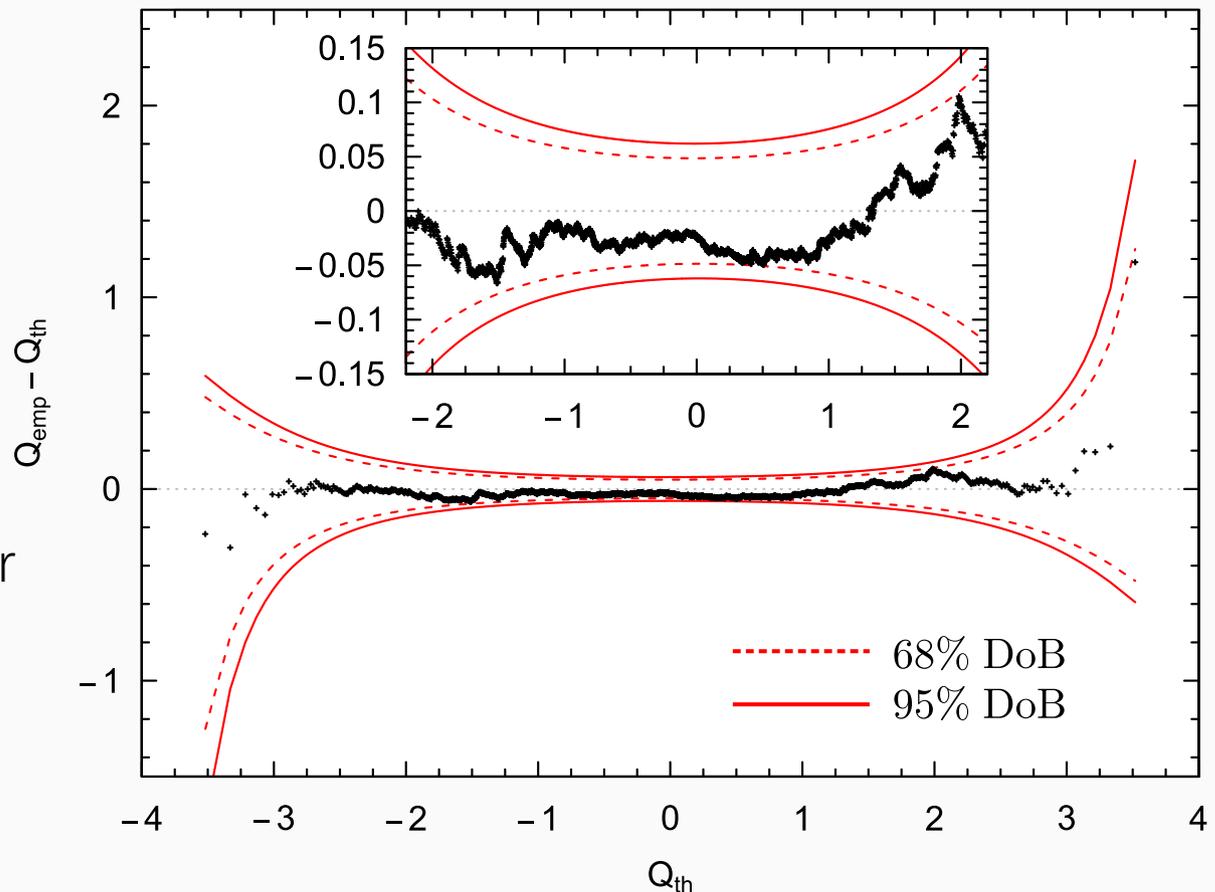
$$F_{\text{th}}(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x dt e^{-t^2/2}$$

- Tail-sensitive error bands for Q-Q plot **Am. Stat. Phys. 67, 249**



High quality of fit confirmed at N⁴LO⁺

$\Lambda = 450 \text{ MeV}$



χ^2 Comparison with other potentials

E_{lab} bin	CD Bonn	Nijm I	Nijm II	Reid93	Idaho N ³ LO*	EMN N ⁴ LO+*	SMS N ⁴ LO+†
neutron-proton scattering data							
0–100	1.07	1.06	1.07	1.08	1.17	1.11	1.07
0–200	1.08	1.07	1.07	1.09	1.17	1.17	1.06
0–300	1.08	1.08	1.08	1.10	1.24	1.25	1.06
proton-proton scattering data							
0–100	0.89	0.87	0.88	0.85	1.01	1.01	0.86
0–200	0.98	0.98	1.00	0.99	1.32	1.16	0.95
0–300	1.01	1.03	1.05	1.04	1.39	1.21	1.00
No. of Parameters	43	41	47	50	28+x	29+x	27+1

* $\Lambda = 500$ MeV , † $\Lambda = 450$ MeV

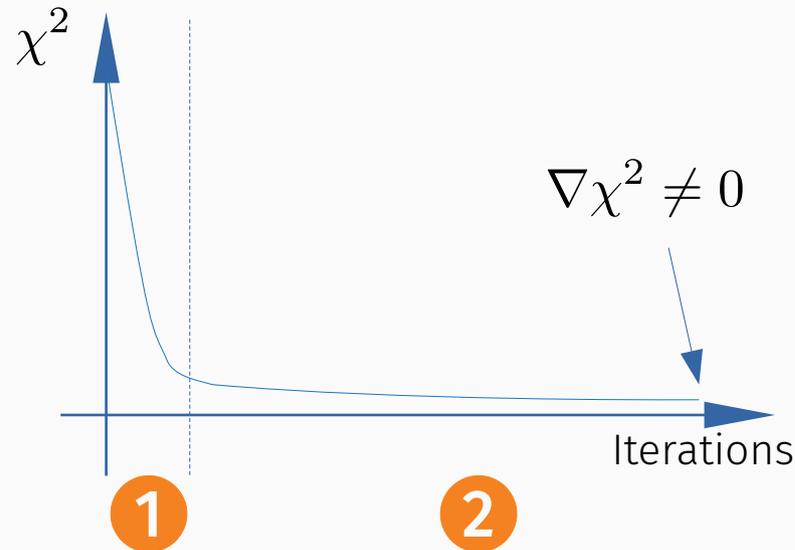


SMS N⁴LO⁺ achieves same precision as high-precision phenomenological potentials with notably less parameters

Redundant Contact Interactions at Q^4

Peculiar convergence behavior of fits:

→ Strong correlations?



Look at S-wave contact potentials:

$$\begin{aligned}
 \langle {}^1S_0, p' | V_{\text{cont}} | {}^1S_0, p \rangle &= \tilde{C}_{1S0} + C_{1S0}(p^2 + p'^2) + D_{1S0}p^2p'^2 + \boxed{D_{1S0}^{\text{off}}(p'^2 - p^2)^2} \\
 \langle {}^3S_1, p' | V_{\text{cont}} | {}^3S_1, p \rangle &= \tilde{C}_{3S1} + C_{3S1}(p^2 + p'^2) + D_{3S1}p^2p'^2 + \boxed{D_{3S1}^{\text{off}}(p'^2 - p^2)^2} \\
 \langle {}^3S_1, p' | V_{\text{cont}} | {}^3D_1, p \rangle &= C_{\epsilon 1}p^2 + D_{\epsilon 1}p^2p'^2 + \boxed{D_{\epsilon 1}^{\text{off}}p^2(p'^2 - p^2)}
 \end{aligned}$$

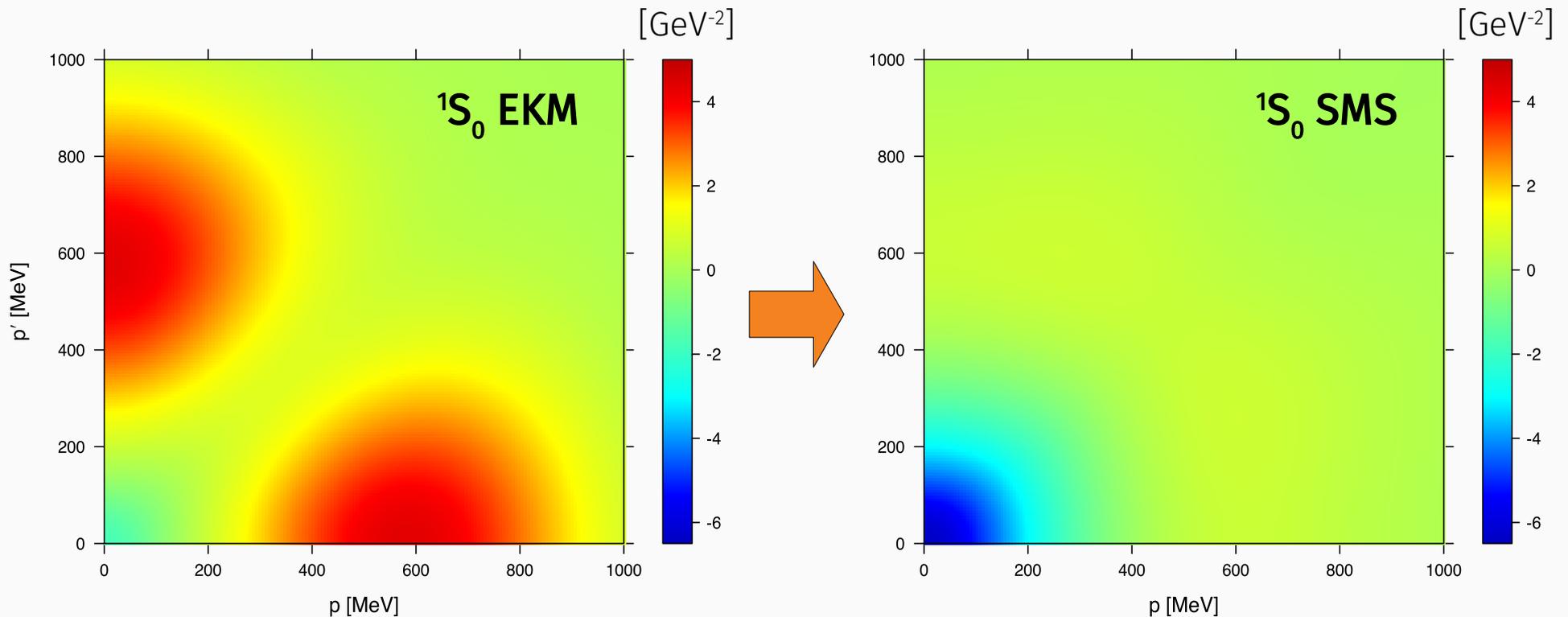
pure off-shell contributions

Can be changed by unitary transformation

→ affects only values of other contact LECs modulo higher order terms

Redundant Contact Interactions at Q^4

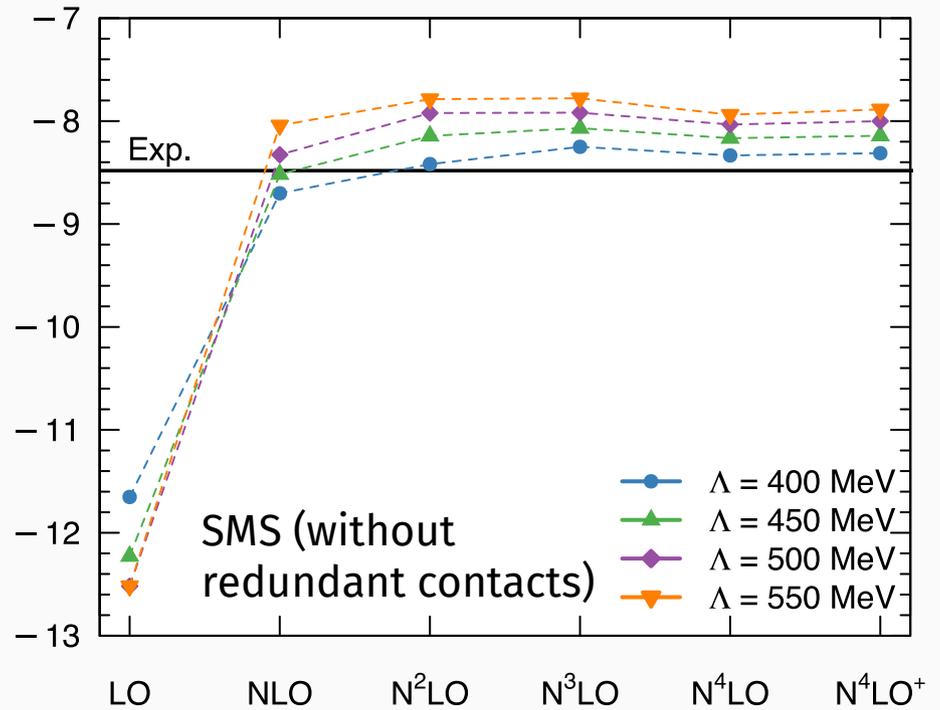
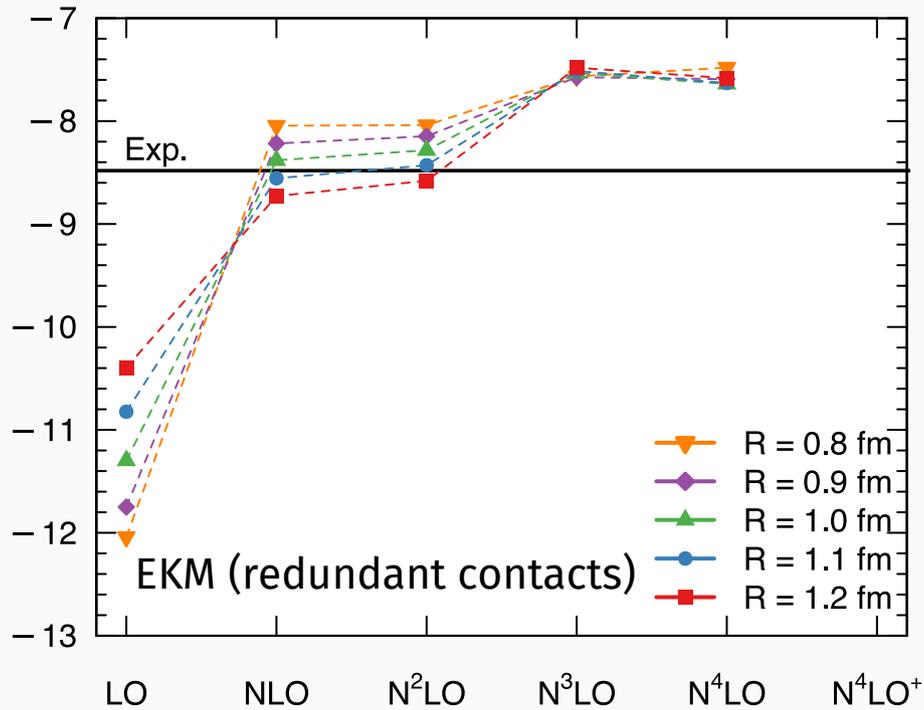
Choice: $D_{1S_0}^{\text{off}} = D_{3S_1}^{\text{off}} = D_{\epsilon_1}^{\text{off}} = 0$



- Impact on 2N observables negligible
- Leads to **softer, more perturbative interactions** (confirmed in Weinberg eigenvalue analysis)
- Fast convergence of fits, stable LECs

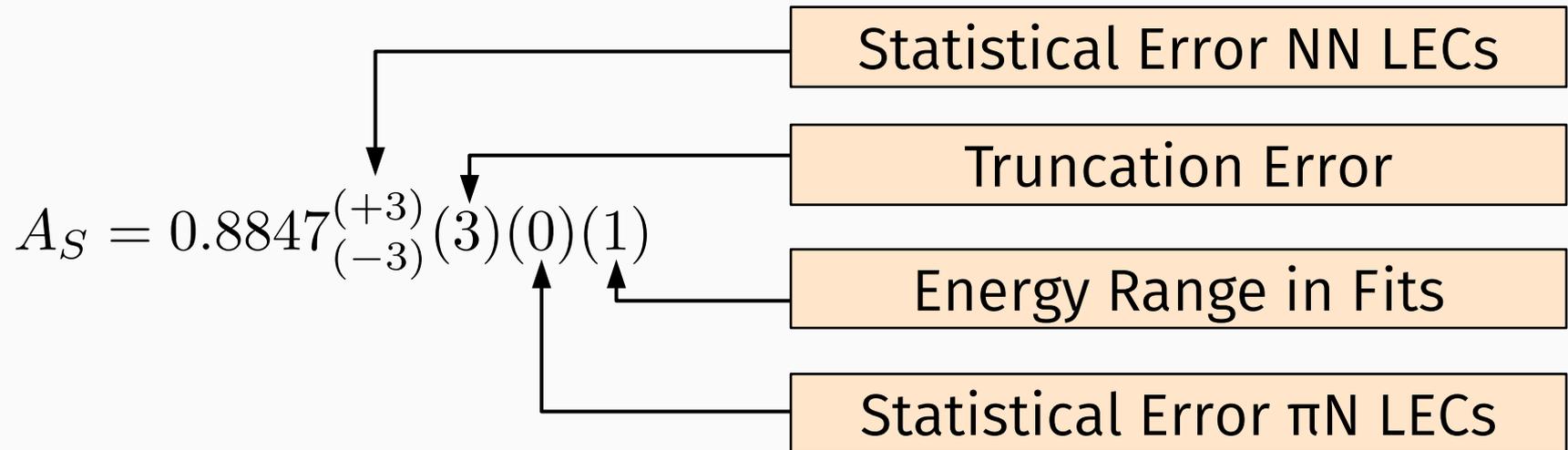
Triton binding energy

Faddeev equation without 3NF:



- Unitary transformation also induces short-range 3NF
- Smaller 3NF strength to compensate Triton underbinding with new choice
- Caution: 3NF contributions are generally not smaller than before

Uncertainty Estimation



- **Statistical errors of NN LECs** based on **covariance matrix** of the fit and second-order Taylor expansion of observables [**Phys. Rev. X 6.011019**]
- Recently switched to **Bayesian model** for estimation of **truncation errors** [**Phys. Rev. C 92.024005, Phys. Rev. C 96.024003**]
- For Energy Range Errors, compare observables from fits up to $E_{\text{lab}} = 220, 260 \text{ \& } 300 \text{ MeV}$
- Finally, propagate statistical uncertainty of Roy-Steiner π N LECs
→ usually smallest error

Uncertainty Estimation

$$A_S = 0.8847^{(+3)}_{(-3)} (3)(0)(1)$$

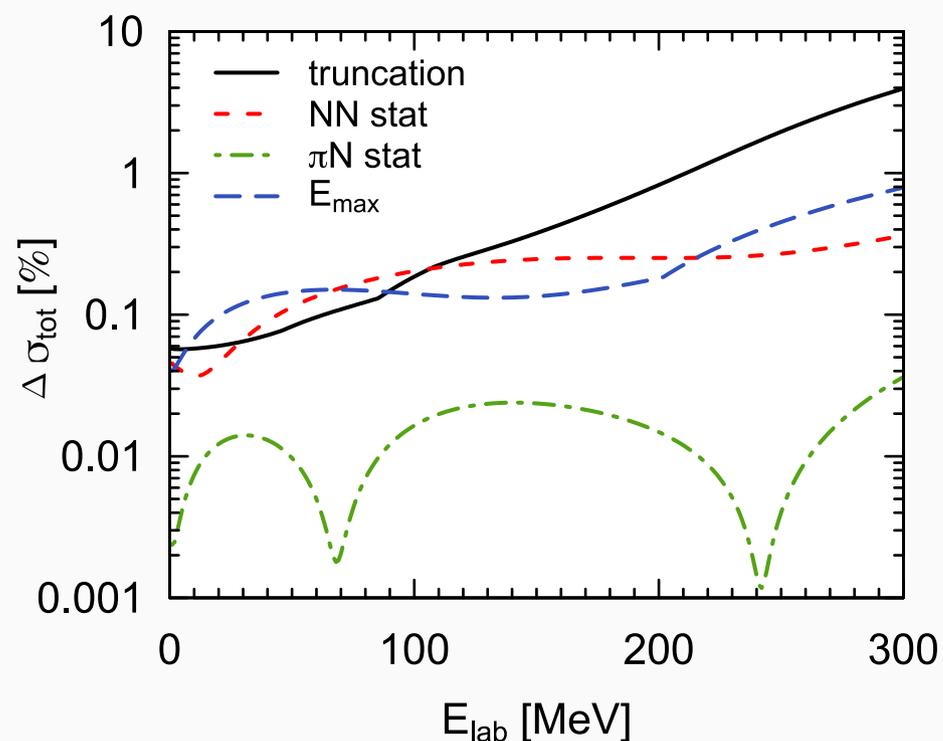
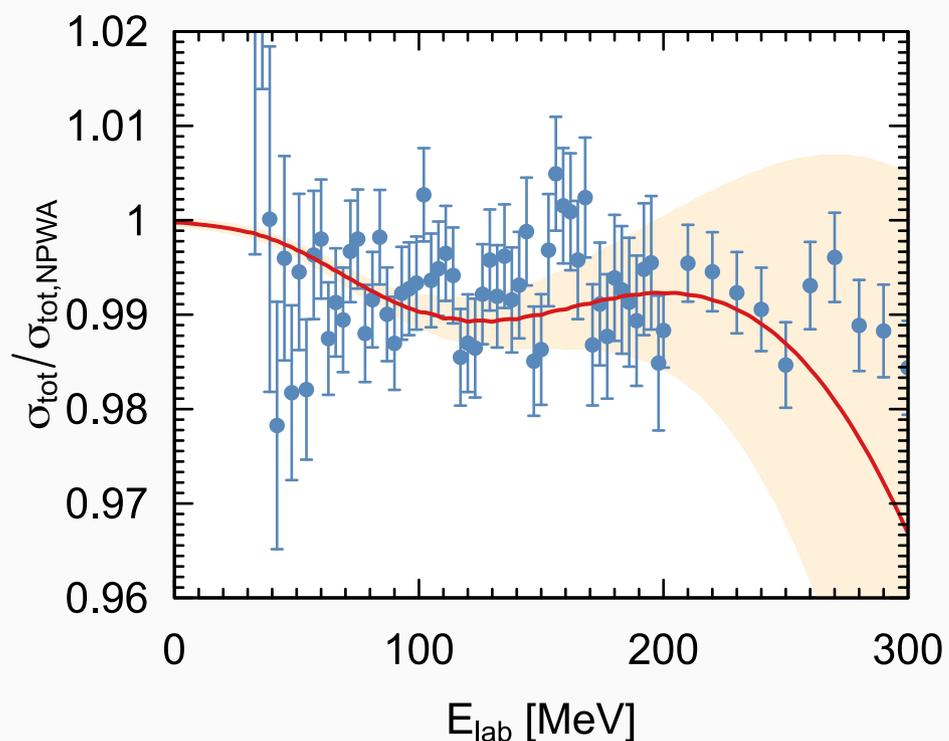
Statistical Error NN LECs

Truncation Error

Energy Range in Fits

Statistical Error π N LECs

np total cross section:



Isospin-breaking (IB) 2N force

- SMS potential achieves $\chi^2/\text{datum} \sim 1$
- But isospin-breaking (IB) limited to pion-mass splitting in One-pion-exchange and charge-dependent short-range interactions in 1S_0
- Chiral EFT allows systematic incorporation of IB effects:

Standard Model:

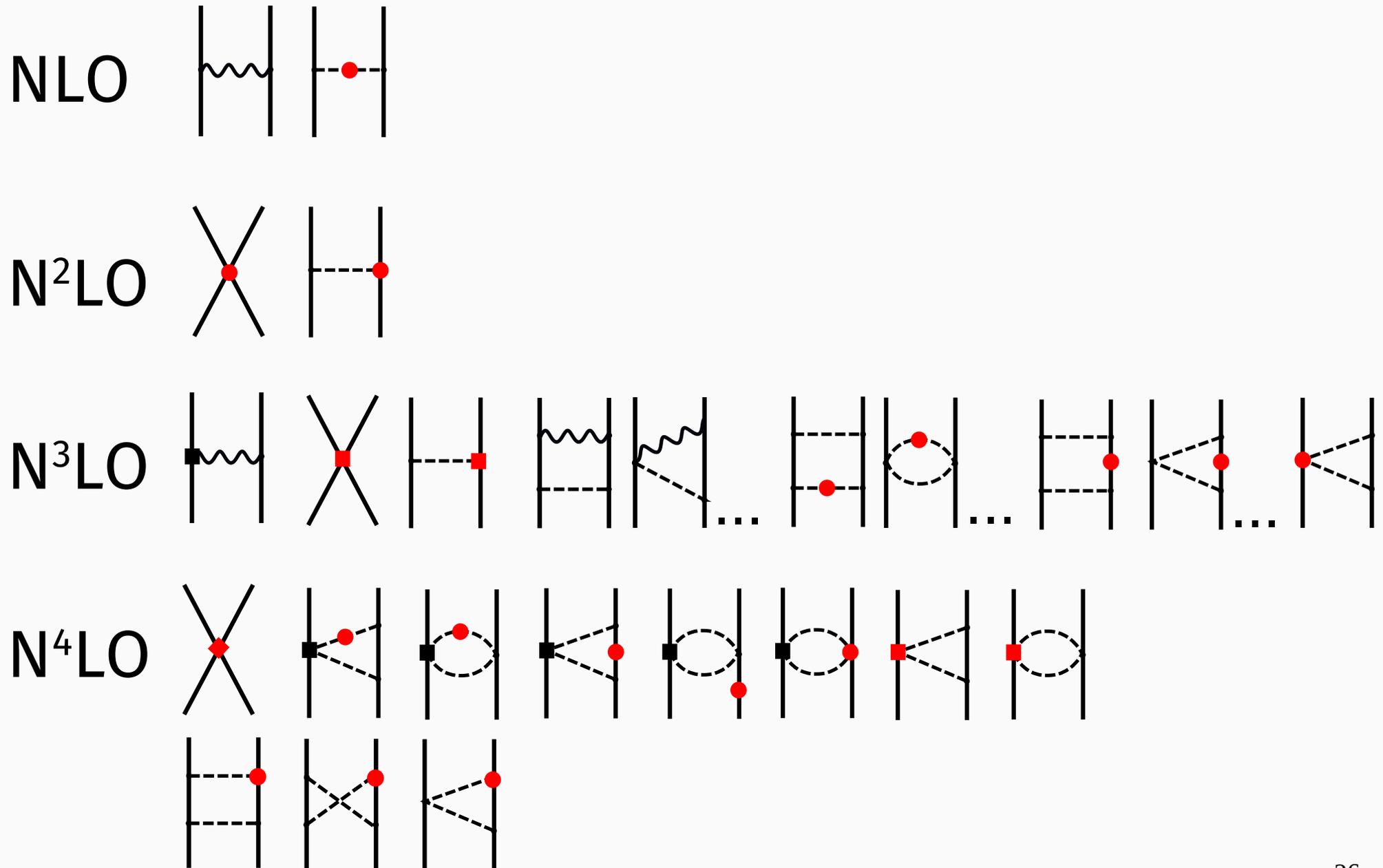
- strong IB due to $m_d \neq m_u$
- electromagnetic IB due to $q_d \neq q_u$



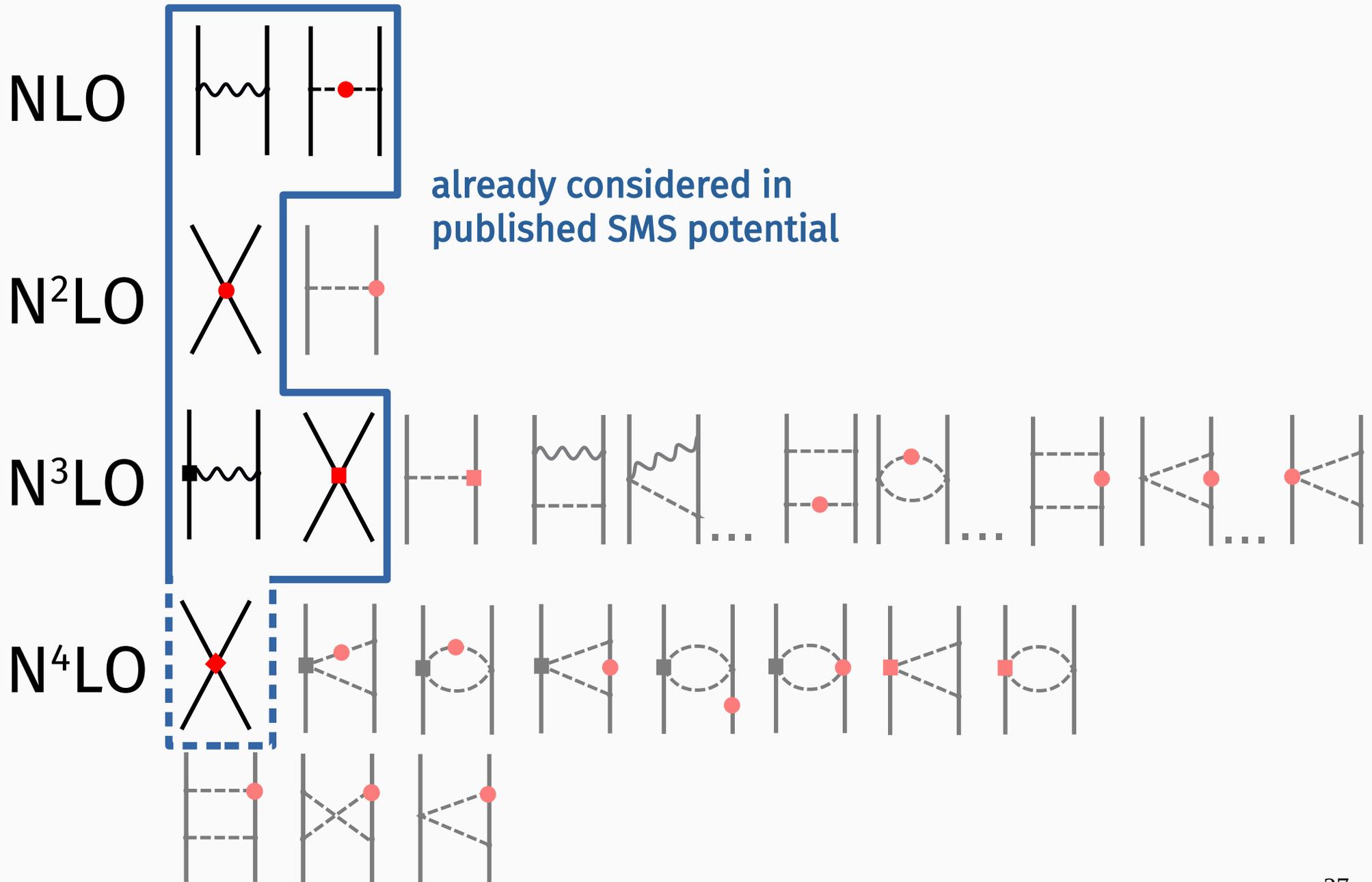
ChEFT: String of IB interaction vertices between nucleons and pions $\propto \epsilon = \frac{m_d - m_u}{m_d + m_u}$ and e

- Count IB contributions in terms of chiral expansion parameter [Epelbaum & Meißner '04]

Overview of isospin-breaking contributions

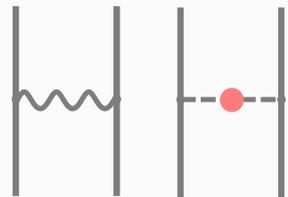


Overview of isospin-breaking contributions

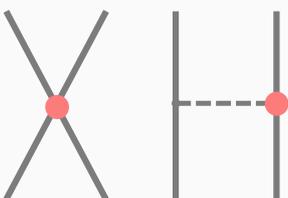


Overview of isospin-breaking contributions

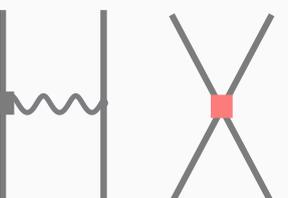
NLO



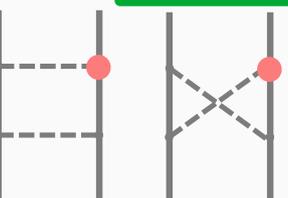
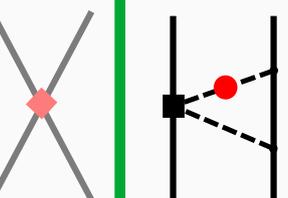
N²LO



N³LO

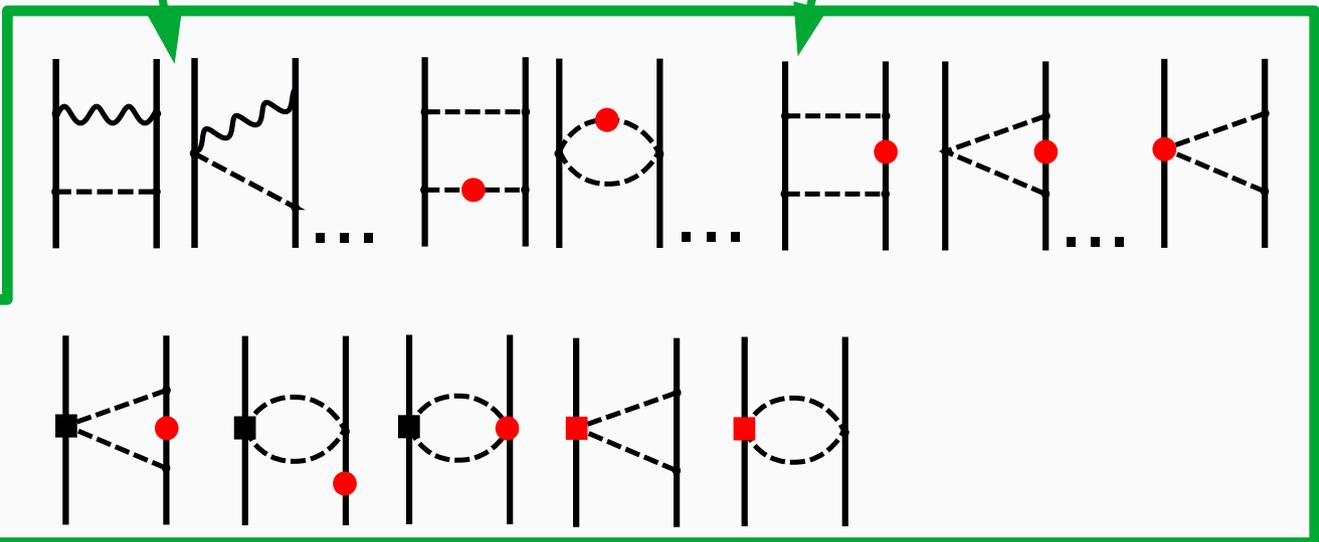


N⁴LO



$\pi\gamma$ -exchange
[van Kolck '98]

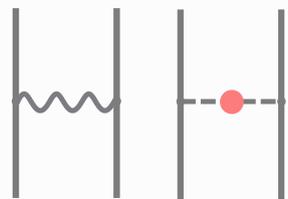
TPEP $\propto \delta M_\pi, \delta m_N$ and
 $\delta m_N^{\text{str.}} = -2.05(30) \text{ MeV}$
[Gasser, Leutwyler '82]



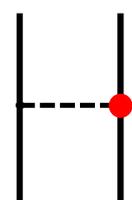
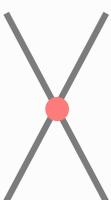
parameter-free

Overview of isospin-breaking contributions

NLO

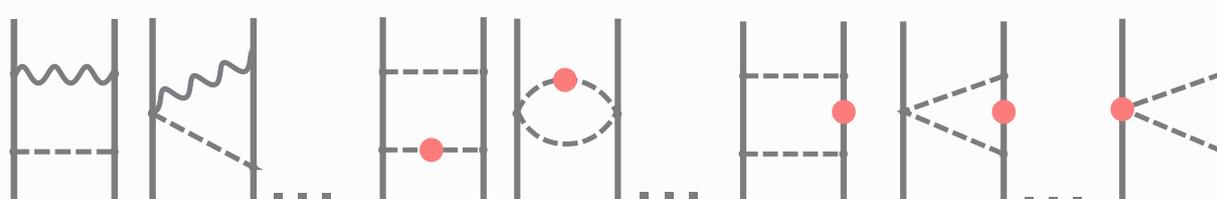
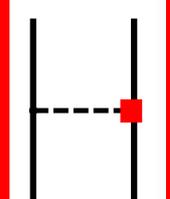
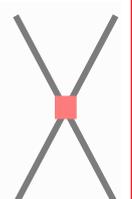


N²LO

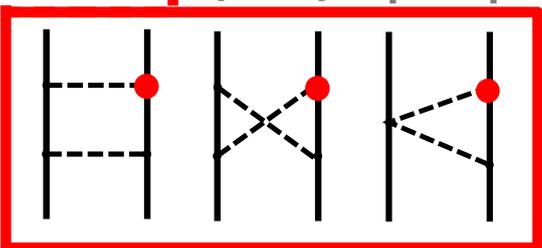
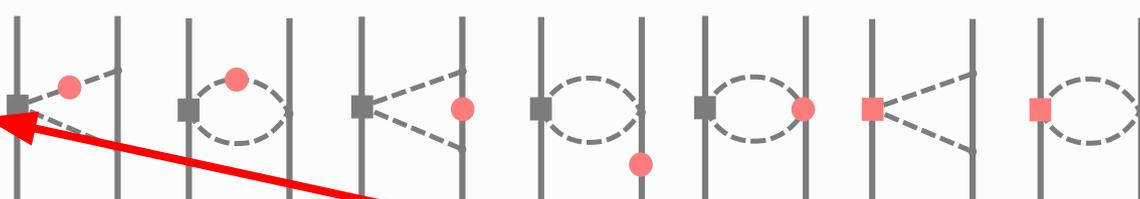
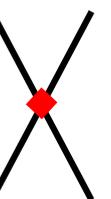


additional unknown parameters

N³LO



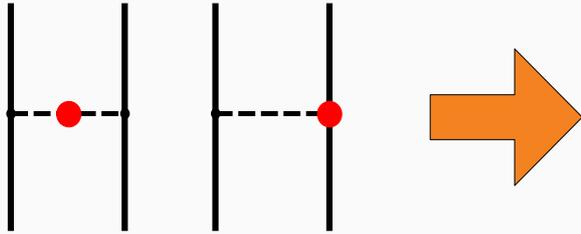
N⁴LO



charge-dependent short-range interactions in P-waves

Charge-dependent π NN couplings

General OPE without isospin limit:



$$V_{1\pi}(pp) = f_p^2 V_\pi(M_{\pi^0})$$

$$V_{1\pi}(np) = -f_0^2 V_\pi(M_{\pi^0}) + (-1)^{t+1} 2f_c^2 V(M_{\pi^\pm})$$

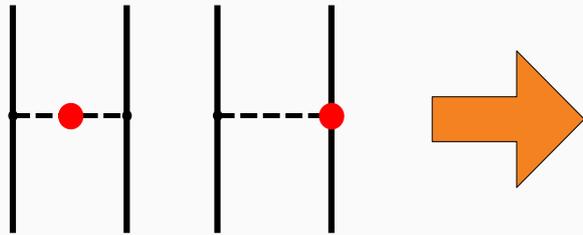
$$V_{1\pi}(nn) = f_n^2 V_\pi(M_{\pi^0})$$

$$\text{with } V_\pi(M_i) = -\frac{4\pi}{M_{\pi^\pm}^2} \frac{\vec{\sigma}_1 \cdot \vec{q} \vec{\sigma}_2 \cdot \vec{q}}{\vec{q}^2 + M_i^2}, \quad f_0^2 = f_p f_n$$

Long-standing question regarding charge-dependence of the π NN coupling constant!

Charge-dependent π NN couplings

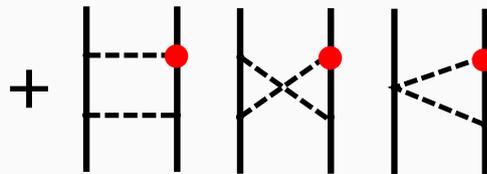
General OPE without isospin limit:



$$V_{1\pi}(pp) = f_p^2 V_\pi(M_{\pi^0})$$

$$V_{1\pi}(np) = -f_0^2 V_\pi(M_{\pi^0}) + (-1)^{t+1} 2f_c^2 V(M_{\pi^\pm})$$

$$V_{1\pi}(nn) = f_n^2 V_\pi(M_{\pi^0})$$



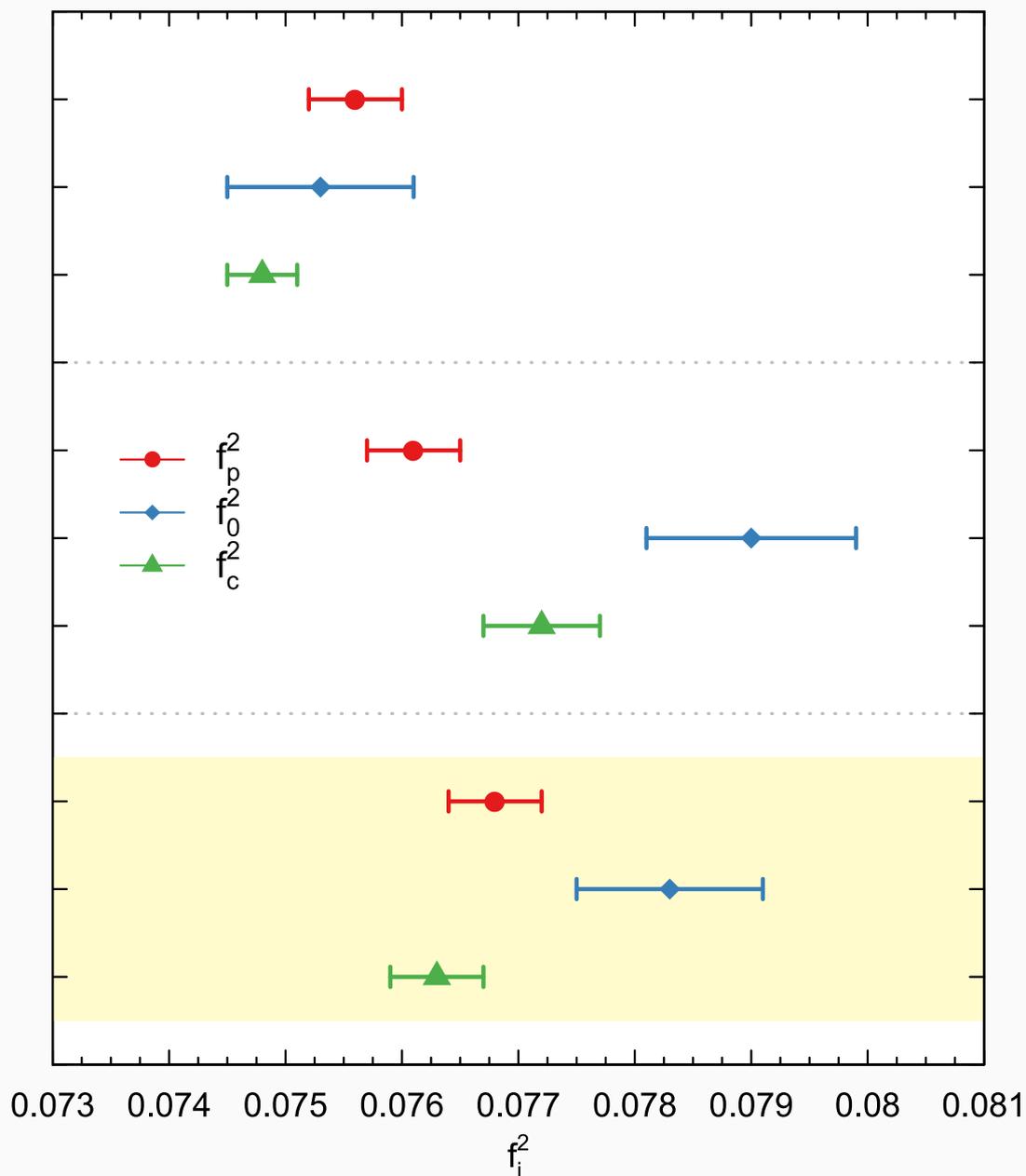
IB two-pion exchange $\propto \mathcal{O}(\Delta f)$

Determine f_i 's from NN data

- Combined fit of np- and pp- scattering data from self-consistent 2013 Granada database for $E_{\text{lab}} = 0 - 280$ MeV
- Integrate („marginalize“) over Λ and short-range LECs:

$$p(\{f_i^2\}|D) = \int d\Lambda dC \frac{p(D|\{f_i^2\}, \{C_i\}, \Lambda) p(\{f_i^2\}, \{C_i\}, \Lambda)}{p(D)}$$

Results for πNN couplings (preliminary)



Nijmegen

[Phys Rev Lett 82, 4992 (1999),

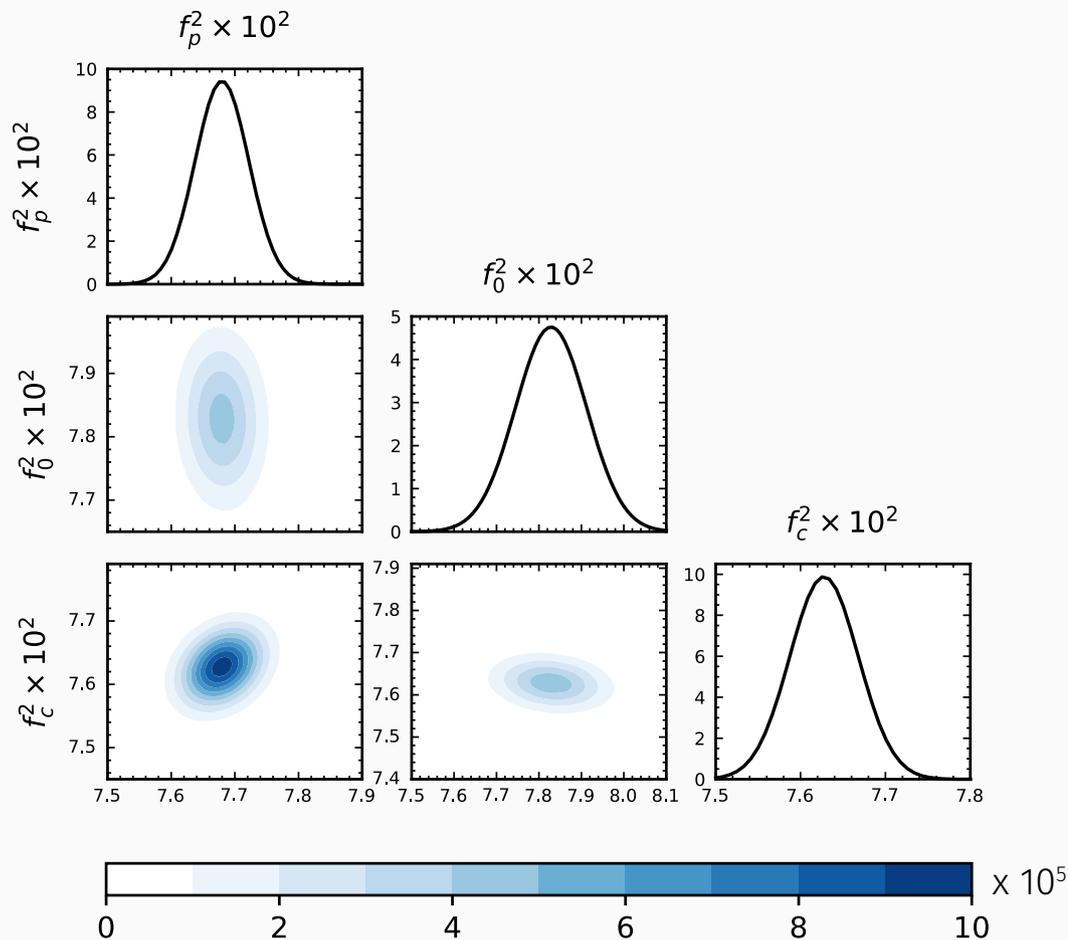
Phys Rev C 44, R1258 (1991),

Phys Rev C 47, 512 (1993)]

Granada '17 [Phys Rev C 95, 064001]

this work

Results for πNN couplings (preliminary)

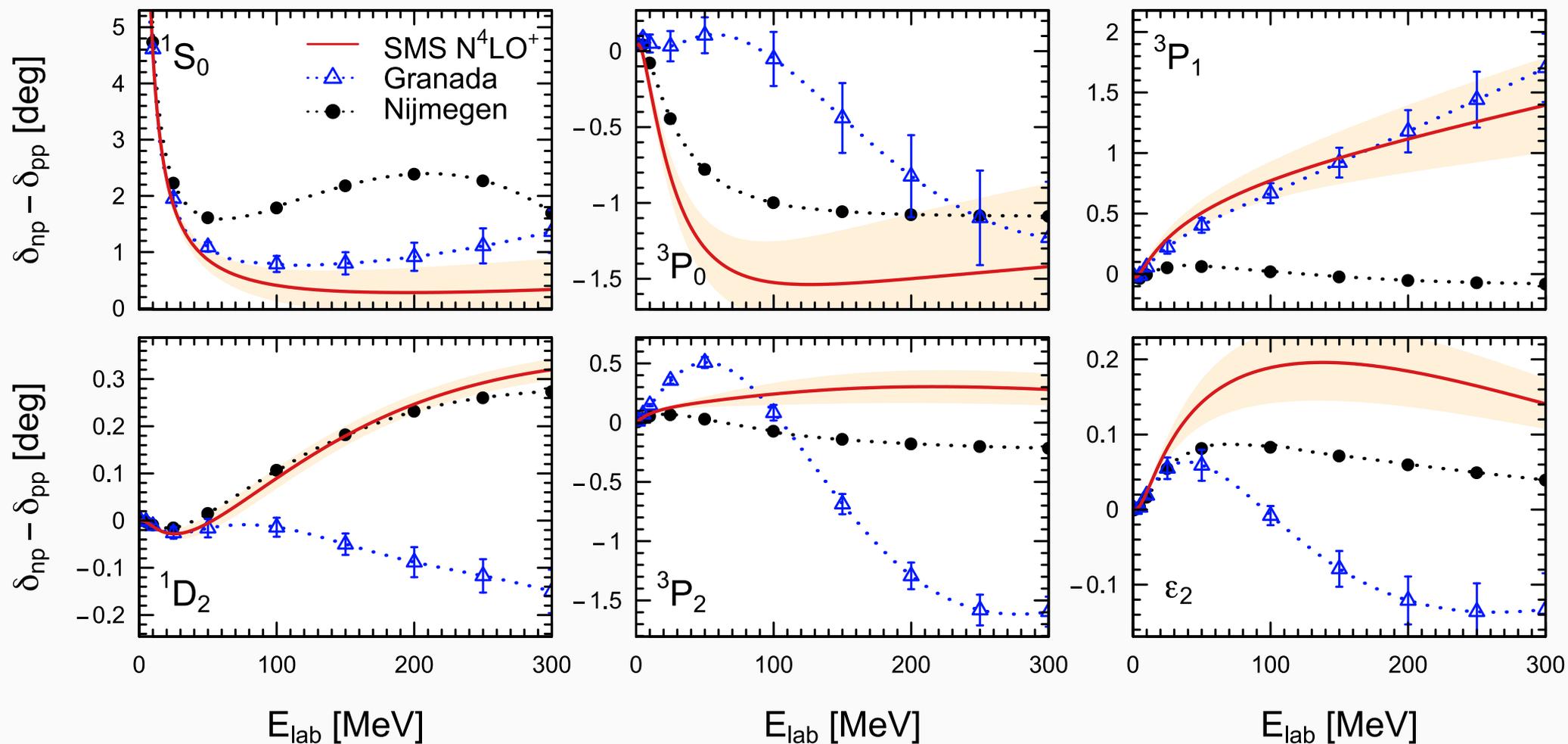


- $p(\{f_i^2\}|D)$ is **gaussian** to a high degree of approximation
- Integrand over cutoff is strongly peaked at $\Lambda = 453 \text{ MeV}$
- Implicit dependence on data selection by Granada group

What is the impact on 2N data (total IB)?

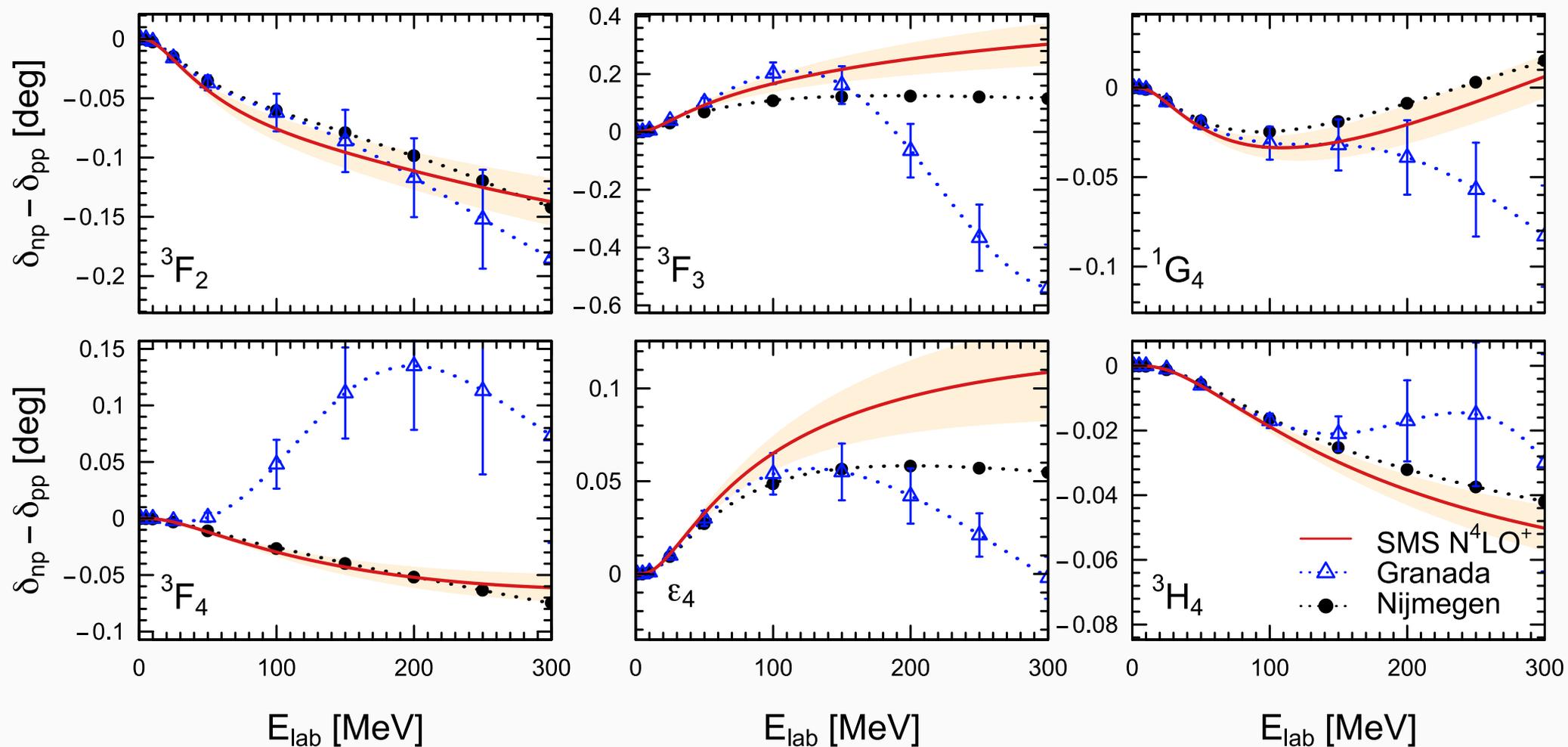
χ^2/datum $E_{\text{lab}} = 0\text{-}280 \text{ MeV}$	Without additional IB effects	➔	With additional IB effects	($\Lambda = 450 \text{ MeV}$)
	1.022		1.015	
			+ 6 parameters	

np-pp phaseshift difference (lower partial waves)



preliminary

np-pp phaseshift difference (higher partial waves)



preliminary

Summary

- 1 The N⁴LO+ SMS potential is currently the most precise interaction from chiral EFT, rivaling high-quality semi-phenomenological potentials
- 2 Local regularization in momentum space preserves long-range behavior of the interactions and paves the way for consistent regularization of higher-order 3NF & currents
- 3 Softer forces due to removal of redundant off-shell contributions to the Q⁴ contact potential
- 4 Complete treatment of isospin-breaking effects up to N⁴LO
- 5 Extraction of charge-dependent π NN couplings using Bayesian methods

Database

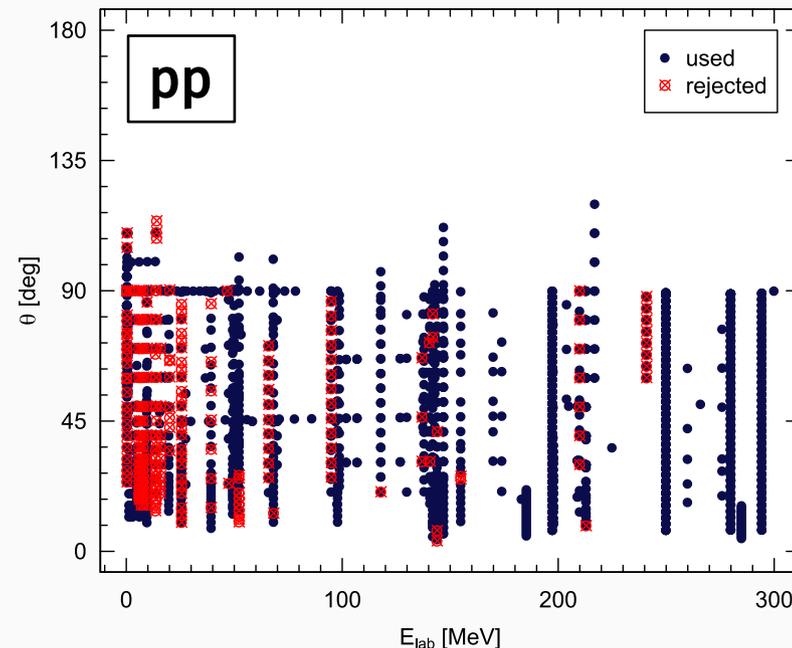
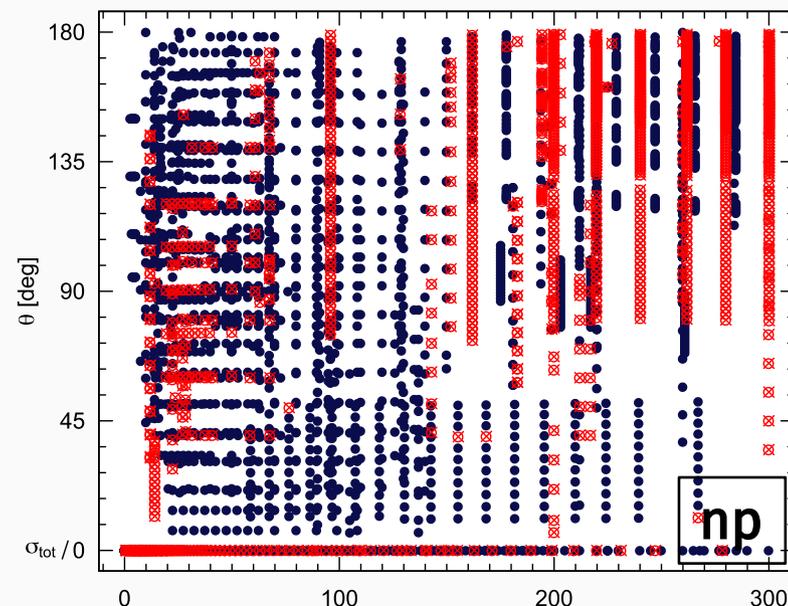
Use self-consistent 2013 Granada database
[Phys. Rev. C 88.064002]

- Includes scattering data from 50ies up to 2013
- uses "3 σ -criterion" to reject non-normal-distributed data
- rejection rate 0-300 MeV: np: 31%, pp: 11%

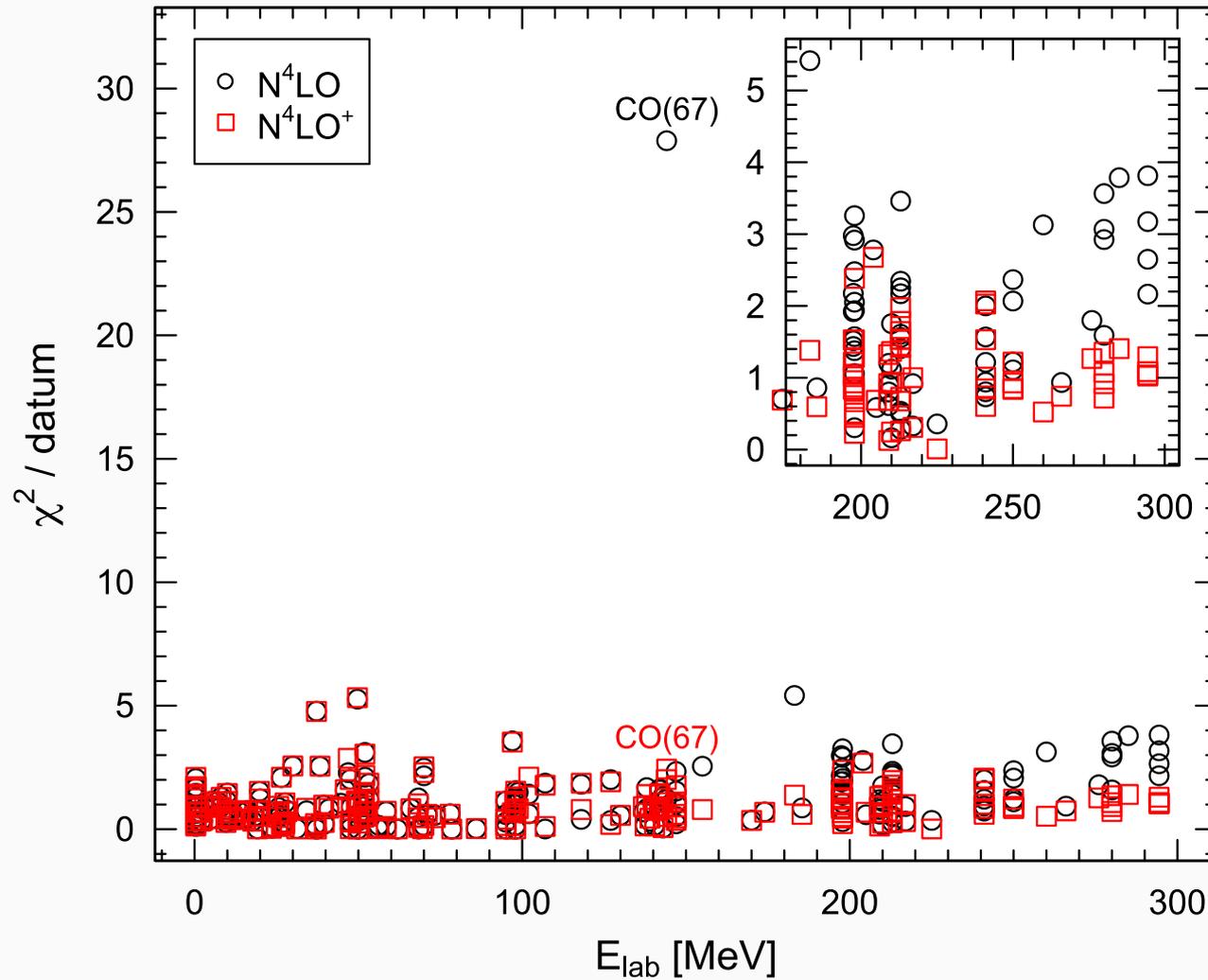
Comparison between theory and experiment via standard χ^2 approach:

$$\chi_j^2 = \sum_{i=1}^{n_j} \left(\frac{O_i^{\text{exp}} - ZO_i^{\text{theo}}}{\delta O_i} \right)^2 + \left(\frac{Z - 1}{\delta_{\text{sys}}} \right)^2$$

- Z (inverse relative norm) is chosen to minimize χ_j^2



F-Wave sensitivity of pp data



- Higher accuracy also improves extraction of other LECs

Repulsive WE

$$\lim_{\epsilon \rightarrow 0} G_0(E + i\epsilon)V|\psi_i(E)\rangle = \eta_i(E)|\psi_i(E)\rangle$$

