Error quantification and falsification of chiral-EFT interactions

The tower of effective (field) theories and the emergence of nuclear phenomena

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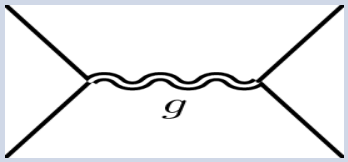
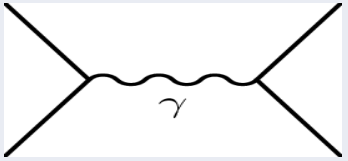
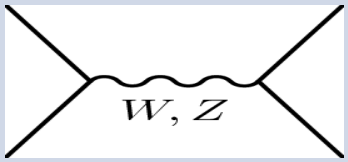
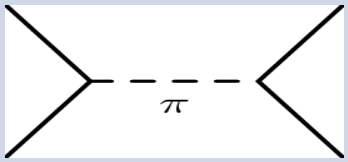
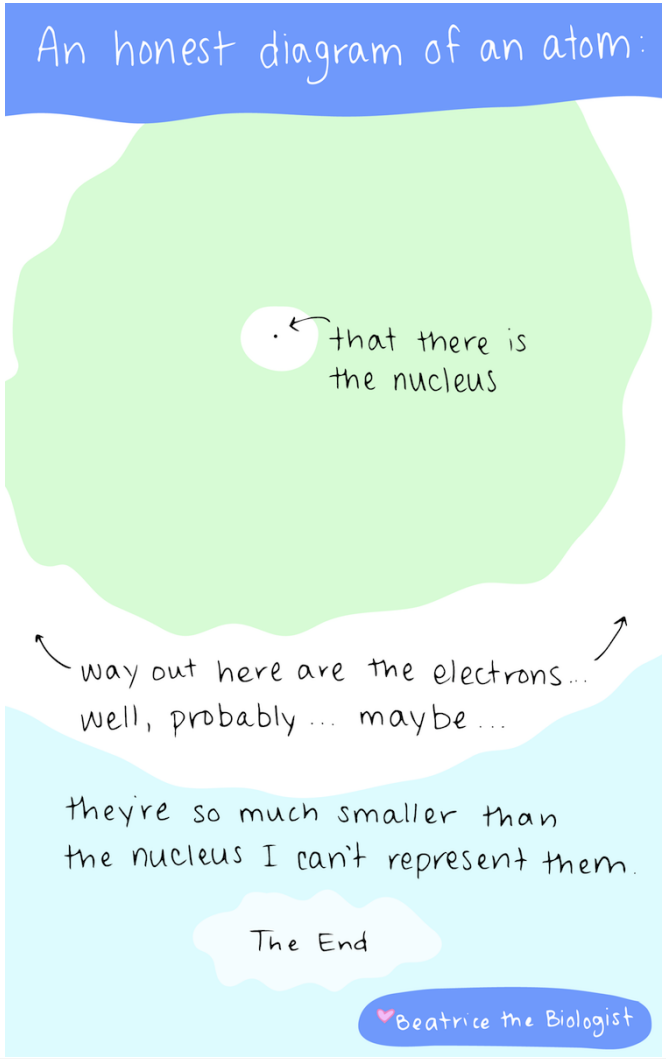
Four fundamental interactions

		Intensity	Range	Exchange
Gravitational		6×10^{-39}	Infinite	Gravitons?
Electromagnetic		1/137	Infinite	photons
Weak		10^{-6}	10^{-8} m	W^+, W^-, Z
Strong		1	10^{-15} m	gluons, π

Strong interaction has the largest intensity
but a very short range.

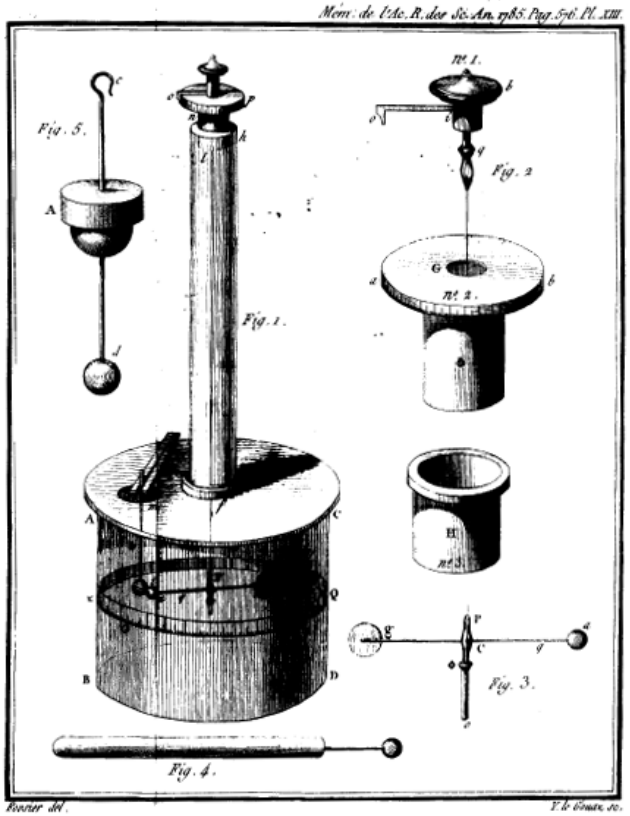
Scales

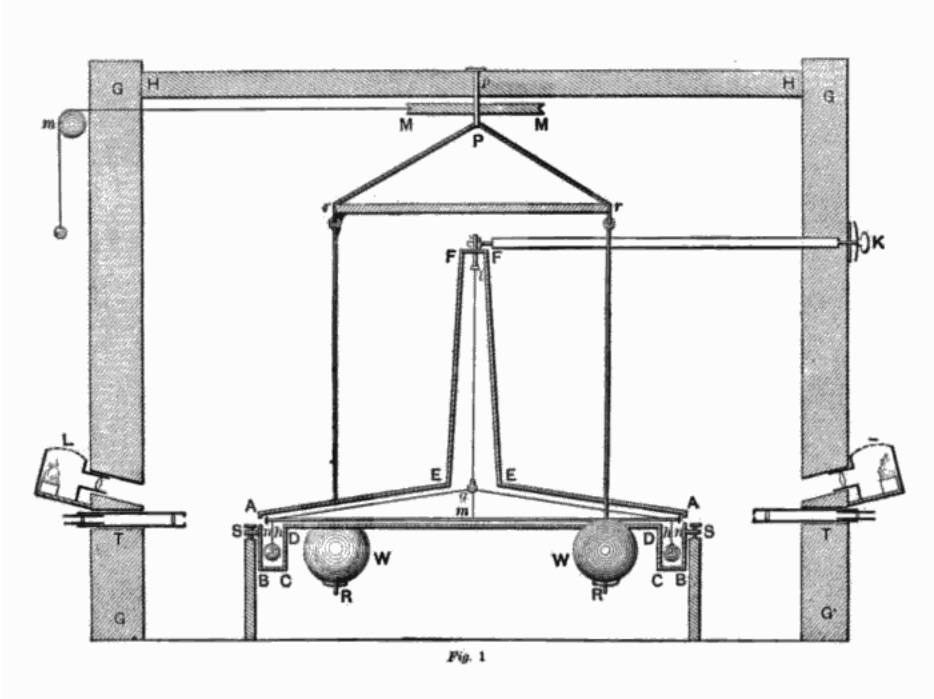


- Atomic scale
  - 1 Angstrom = 10^{-10} m
  - Bohr radius = 0.529 Å
  - Phosphorus atom ~ 1 Å
- Nuclear scale
  - 1 Fermi = 10^{-15} m
  - Proton radius ~ 0.85 fm
  - Inter-nucleon distance ~ 2 fm
  - Gold nucleus ~ 8.45 fm

How to determine the interactions?

"Easy" for infinite range. Direct Measurements



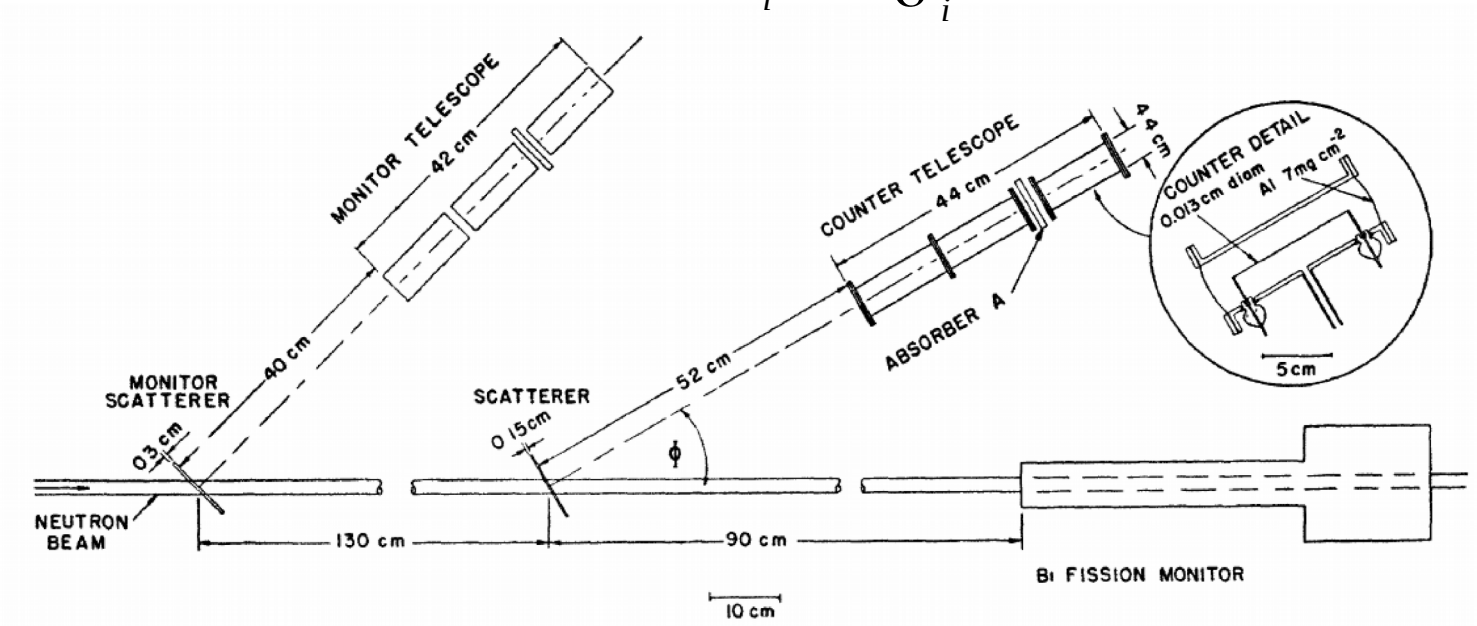


- Coulomb (1785)
  - "Premier mémoire sur l'electrcité et le magnetisme"
- Cavendish (1798)
  - "Experiment to determine the density of the earth"

How to determine the interactions?

"Not so easy" for the short range. Indirect Measurements

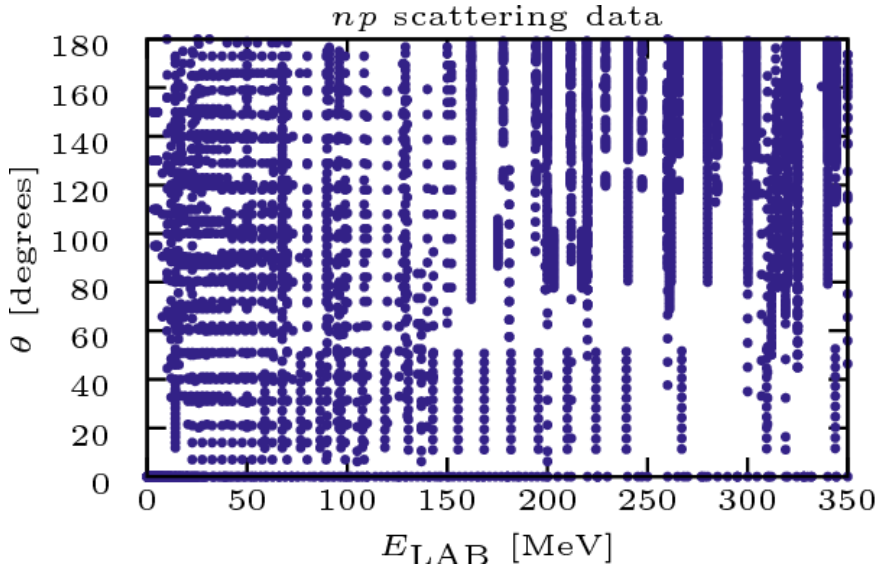
- Scattering experiments
  - Over 20 different observables for energy and angle
- Phenomenological potentials
  - Least squares fit $\chi^2 = \sum_i \frac{(E_i - T_i)^2}{\sigma_i^2}$

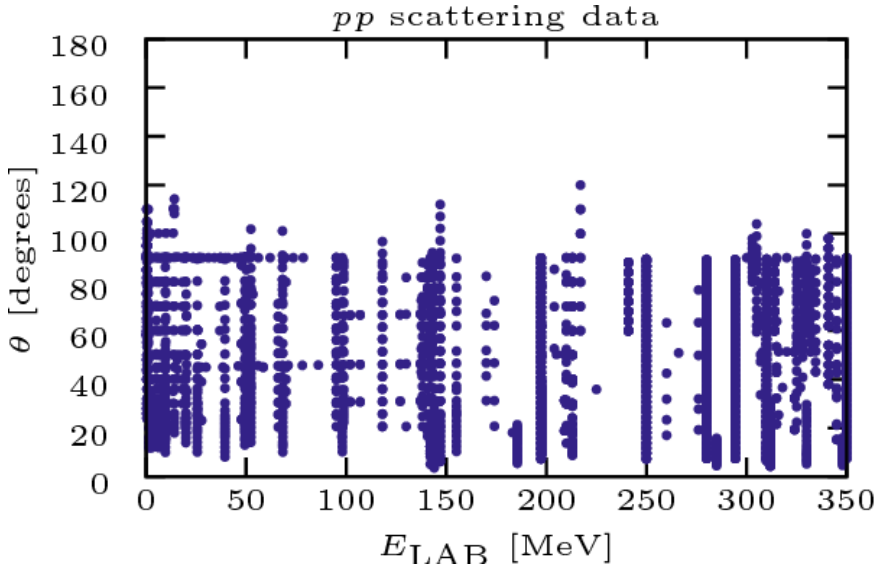


- Quantum chromodynamics (QCD)

Scattering experiments

- Study of the interaction between nucleons for over 60 years
- More than 7800 scattering data since the 1950's
- Several phenomenological models



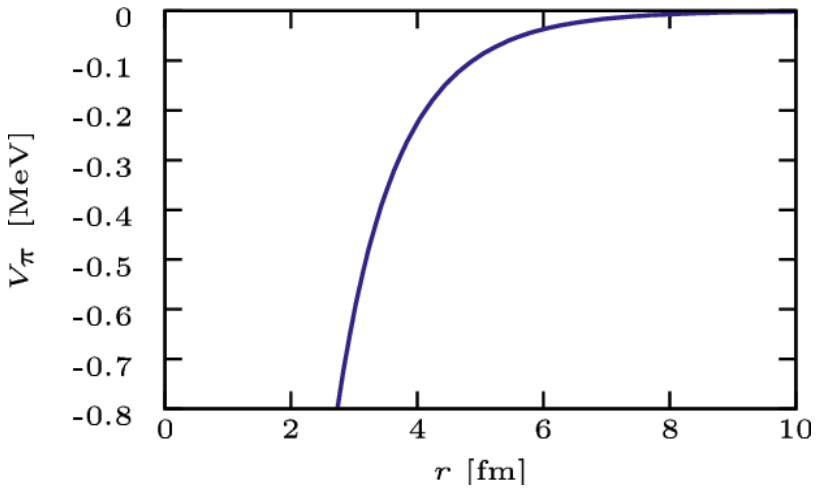


The distribution of the data is relevant

Yukawa potential (1935)

- Exchange of a scalar field with mass
- pion-nucleon coupling constant
- Good description for large distance

$$V_\pi(r) = -f_\pi^2 \frac{e^{-m_\pi r}}{r}$$



Predictive Power in Nuclear Physics

- What is the predictive power of theoretical nuclear physics
  - INPUT from Experiment → CALCULATION → OUTPUT vs. Experiment

- Theoretical Predictive Power Flow: From light to heavy nuclei

$$H(A) = T + V_{2N} + V_{3N} + V_{4N} + \ldots \rightarrow E_2, E_3, E_4, \ldots$$

- Chiral expansion allows to compute V_{2N} ,V_{3N} ,V_{4N} , … systematically

$$V_{2N} >> V_{3N} >> V_{4N}$$

Predictive Power in Nuclear Physics

- Chiral forces are UNIVERSAL at long distances

$V\chi(r) = V^{\pi}(r) + V^{2\pi}(r) + V^{3\pi}(r) + \ldots \qquad r >> r_c$

- Chiral forces at SINGULAR at short distances

$$V^{\chi}(r) = \frac{a_1}{f_\pi^2 r^3} + \frac{a_2}{f_\pi^4 r^5} + \frac{a_3}{f_\pi^6 r^7} + \ldots \qquad r << r_c$$

- Trade between model independence for regulator dependence
- What is the best theoretical accuracy we can get within reasonable cut-offs?
- What is a reasonable cut-offs? r_c = ?

Phenomenological potentials

- One big family of models
- Hamada-Johnston, Yale, Paris, Bonn, Nijmegen, Reid, Argonne, Granada, …
- $\chi^2/N \sim 1$ in 1993
- One pion exchange for long range part
- ~ 40 parameters for short and intermediate range
- Different results in nuclear structure calculations

Statistical and Systematic error estimates are recent

Sources of uncertainty

- Numerical (Implementation)
  - Inexact solution method
  - Inherent to any numerical calculation
- Systematic (Model dependence)
  - Any model makes assumptions
  - Different representations for the NN interaction
- Statistical (Fitting bias)
  - Statistical fluctuations in any measurement
  - Uncertainty in data ➡ Uncertainty in parameters

Assuming independence among them

$$(\Delta F)^2 = (\Delta F^{\text{num}})^2 + (\Delta F^{\text{sys}})^2 + (\Delta F^{\text{stat}})^2$$

Anatomy of phenomenological models
fitted to the Granada database

Short and Intermediate range

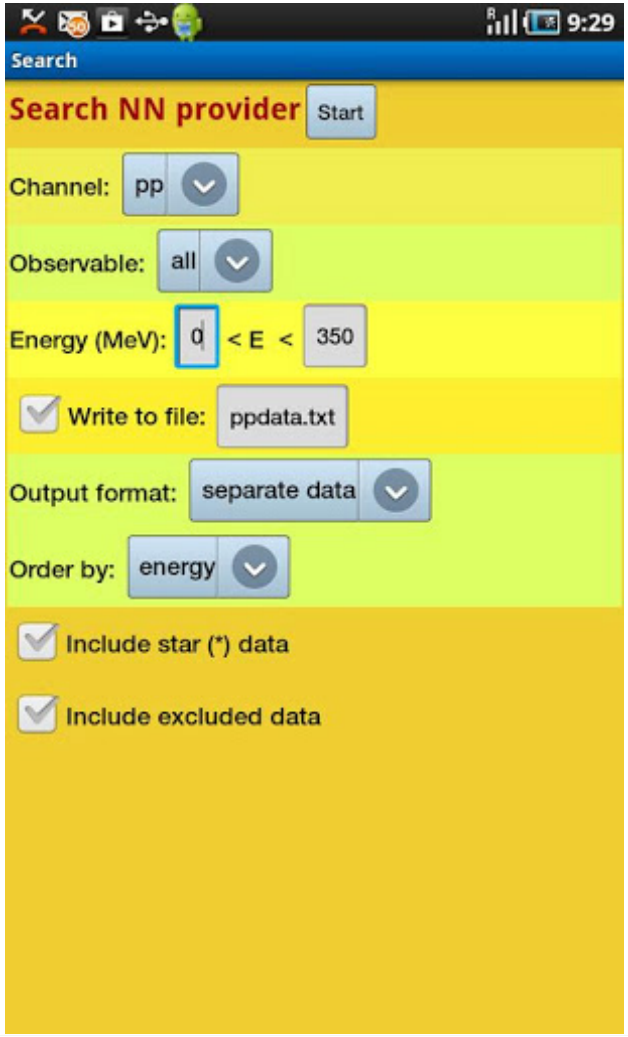
- Delta Shells
  - Coarse grained
  - Simplified calculations
  - High momentum components
- Sum of Gaussian functions
  - Smooth and soft
  - Nuclear structure calculations
  - Not as fast

Long range

- Electromagnetic contributions
  - Small but crucial
- One pion exchange
  - Proper analytic behavior
- Optional
  - Two pion exchange
  - Δ degree of freedom
    - Born approximation

Six different phenomenological models

Granada database

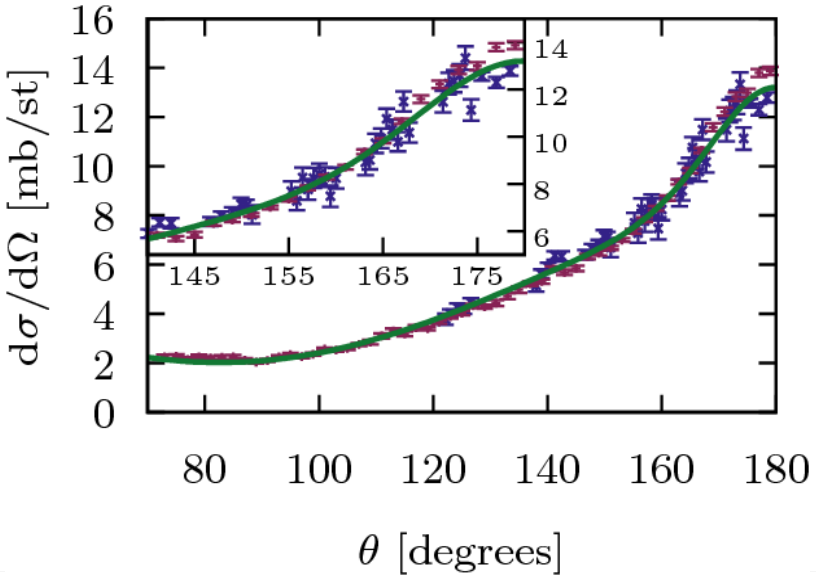


- NN scattering data from 1950 to 2013
  - http://nn-online.org/
  - http://gwdac.phys.gwu.edu/
  - NN Provider for Android
    - Google play store

    [Amaro, RNP, Ruiz-Arriola]
  - http://www.ugr.es/~amaro/nndatabase/
- 2868 pp and 4991 np data

Fitting NN scattering observables
Selection of data

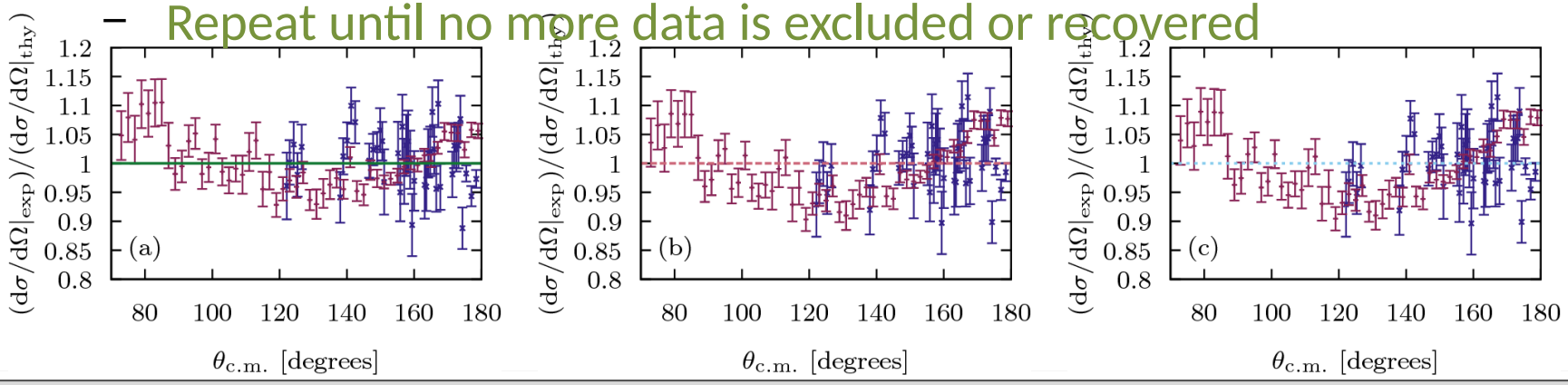
- Direct fits to all data NEVER give χ^2/d.o.f. ≈ 1
  - Restrictive model ? ➡ Improve model
  - Mutually incompatible data ➡ Reject incompatible data
- np $d\sigma/d\Omega$ at 162 MeV
- Statistical and systematic errors may be over or underestimated
- 3σ criterion
  - Fit all data (χ^2/d.o.f. > 1)
  - Remove sets with improbably high or low χ^2
  - Refit parameters



Fitting NN scattering observables

Recovering data

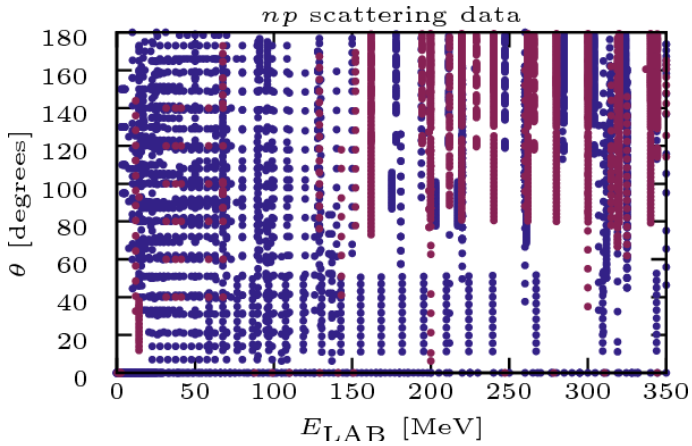
- Mutually incompatible data
  - Which experiment is correct?
  - Is any of the two correct?
  - Maximization of experimental consensus
- Exclude data sets inconsistent with the rest of the database
  - Fit to all data (χ^2/d.o.f. > 1)
  - Remove data sets with improbably high or low χ^2 (3σ criterion)
  - Refit parameters
  - Re-apply 3σ criterion to all data
  - Repeat until no more data is excluded or recovered

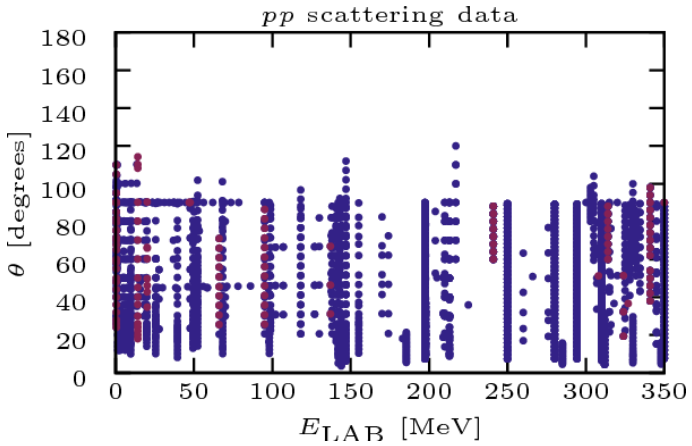


Fitting NN scattering observables

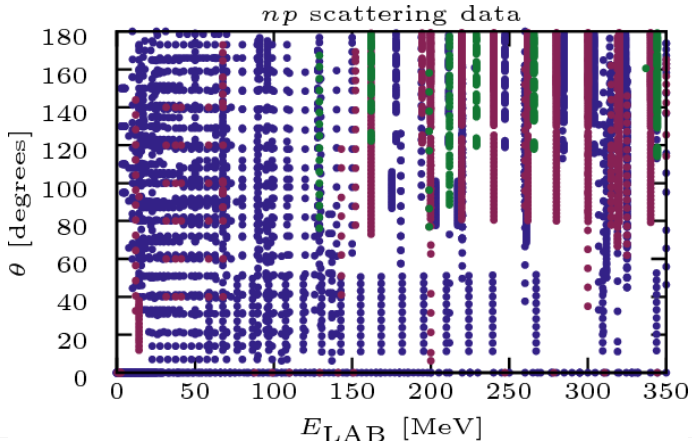
Recovering data

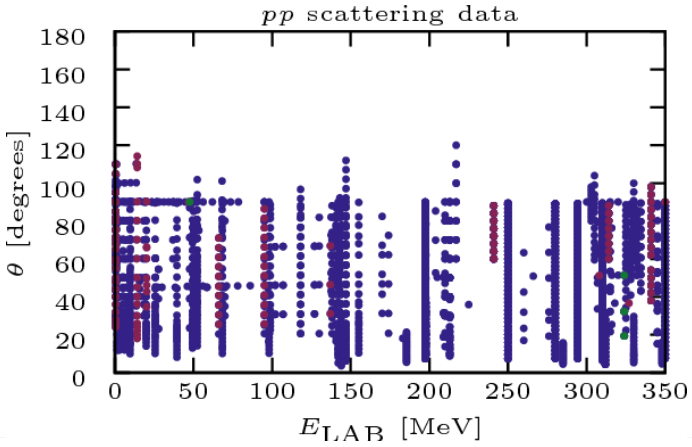
Usual Nijmegen 3σ criterion (1677 rejected data)





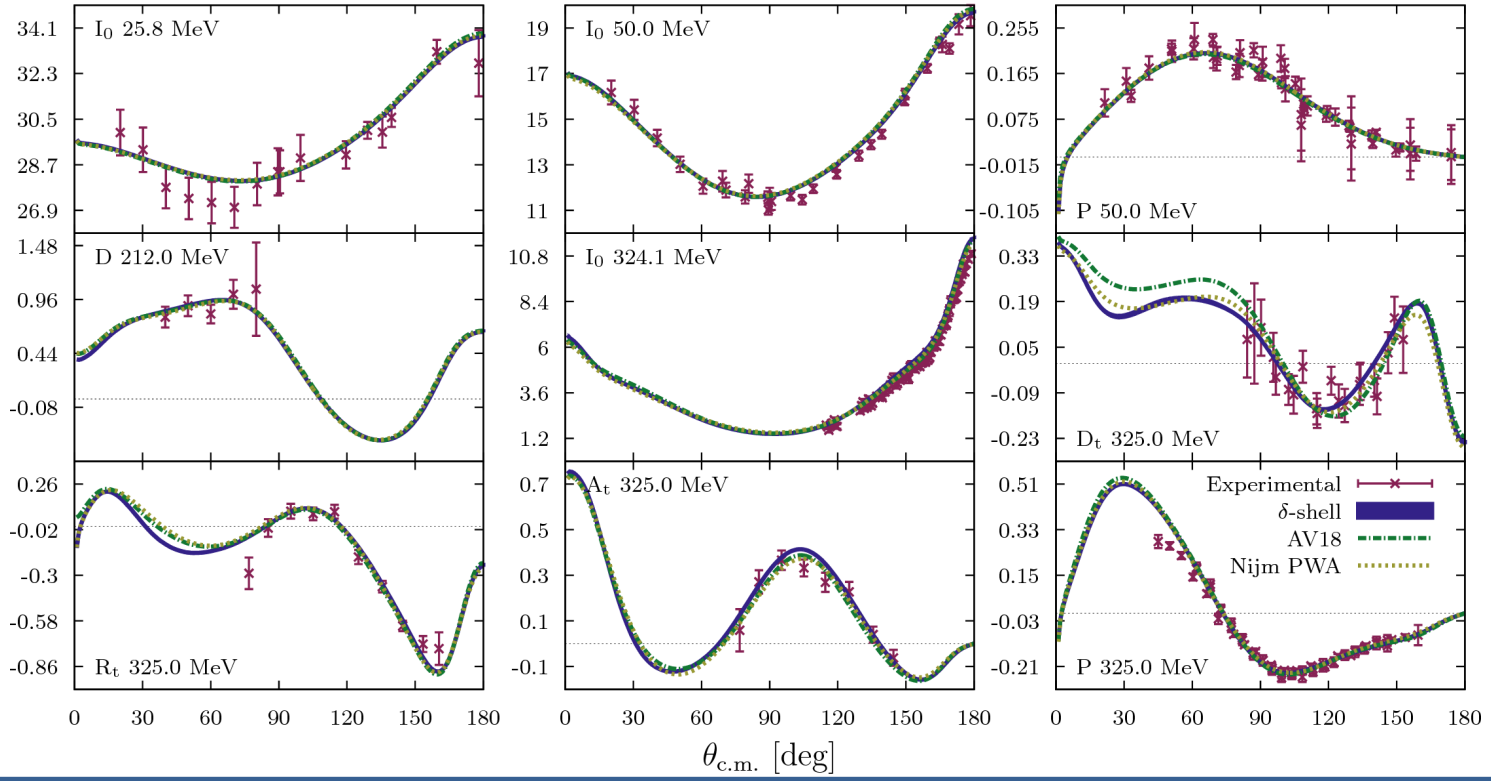
300 recovered data with Granada procedure (consistent database)





Fitting NN scattering observables

- Comparing with other models and experimental data



χ^2/d.o.f. = 1.06 with $N = 2747|_{pp} + 3691|_{np}$

[RNP, Amaro & Ruiz-Arriola. Phys.Rev.C88 (2013) 024002]

Fitting NN scattering observables

- Different models fitted to the *same* database

Potential	T_{LAB}	N_{Data}	$N_{parameters}$	χ^2/d.o.f.
DS - OPE	350	6713	46	1.05
DS - χTPE	350	6712	33	1.08
DS - ΔBorn	350	6719	31	1.06
Gauss - OPE	350	6712	42	1.07
Gauss - χTPE	350	6712	31	1.09
Gauss - ΔBorn	350	6712	30	1.14

[RNP, Amaro & Ruiz Arriola. ArXiv:1410.8097v3]

Predictions are different
Source of *systematic* uncertainties

Fitting NN scattering observables

Testing the normality of residuals

- Experiments by counting events → Poissonian statistics
- Large number of events → Normal statistics
- Crucial assumption

$$R_i = \frac{O_i^{\exp} - O_i^{theor}\left(p_1, p_2, \ldots p_P\right)}{\Delta O_i^{\exp}}$$

  follows the standard normal distribution

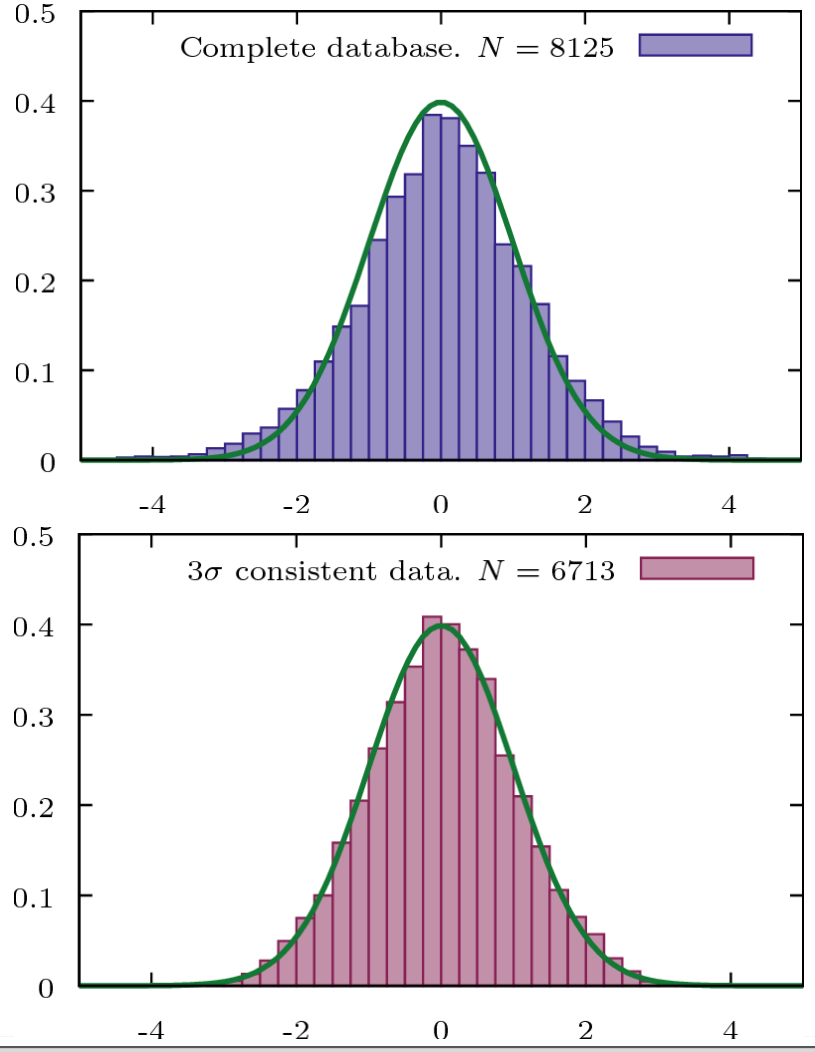
- $\chi^2/\text{d.o.f.} = 1 \pm (2/\text{d.o.f.})^{1/2}$
- Can be different from $N(0,1)$, but it has to be known

Can only be checked *a posteriori*

Fitting NN scattering observables

Testing the normality of residuals

- Empirical distribution P_{emp}
- Normal distribution N(0,1)
- Finite size fluctuations
- Discrepancies between P_{emp} and $N(0,1)$
- How large is too large?
- Normality tests
  - Quantifying discrepancies
  - Test statistic T
  - Critical values



Fitting NN scattering observables

Tail Sensitive test

- Quantitative test with a graphical representation

  Aldor-Noiman et al. The American Statistician, 67(4):249–260, 2013.

- Quantile-Quantile plot
  - Theoretical quantiles

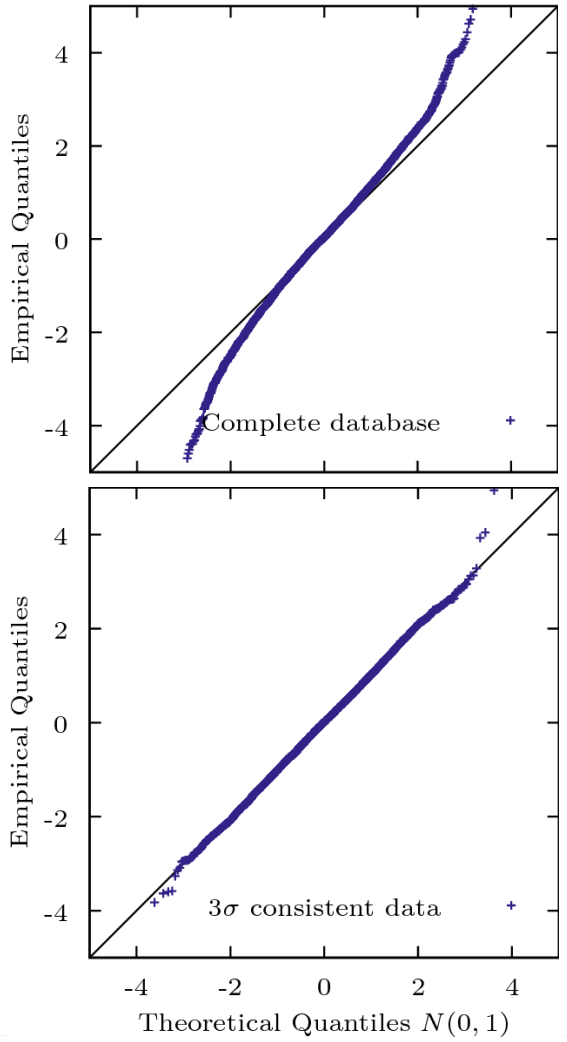
$$\frac{i}{N+1} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x_i^{th}} e^{-\frac{t^2}{2}} dt$$

  - Empirical Quantiles

$$x_1^{emp} < x_2^{emp} < \ldots < x_N^{emp}$$

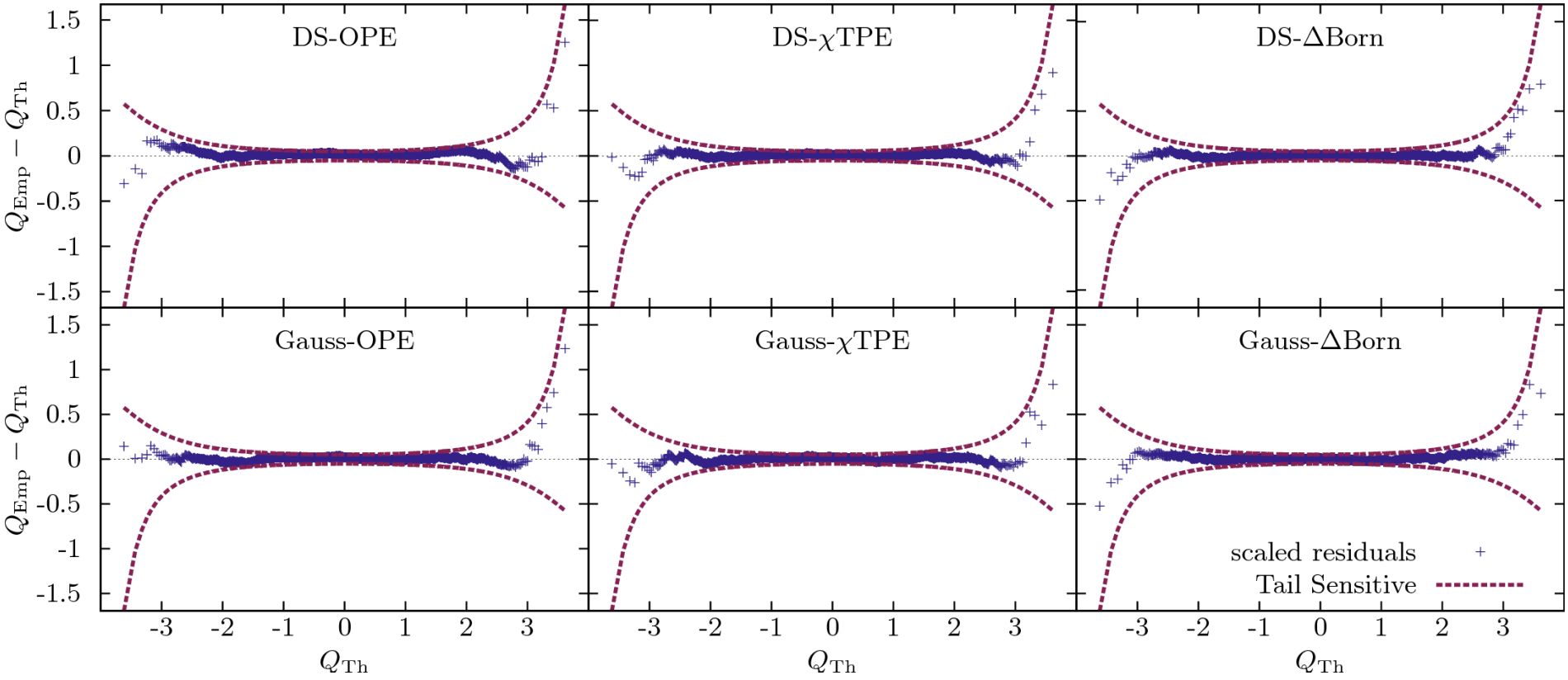
  - Mapping (x_i^{th}, x_i^{emp})
  - $\lim_{N\to\infty} (x_i^{emp} - x_i^{th}) = 0$
  - Confidence bands
    - Recipe and tables available at

      J. Phys. G: Nucl. Part. Phys. 42 (2015) 034013



Fitting NN scattering observables

Testing the normality of residuals



Six statistically equivalent representations of the NN interaction
Their discrepancies won't come from the data

Chiral Two Pion Exchange

- Can χTPE interaction describe the same data
  - OPE, TPE(NLO) and TPE(NNLO)
  - Different cut radious rc = 3.0, 2.4, 1.8 fm
- Fitting the consistent database
  - No further data is excluded or added

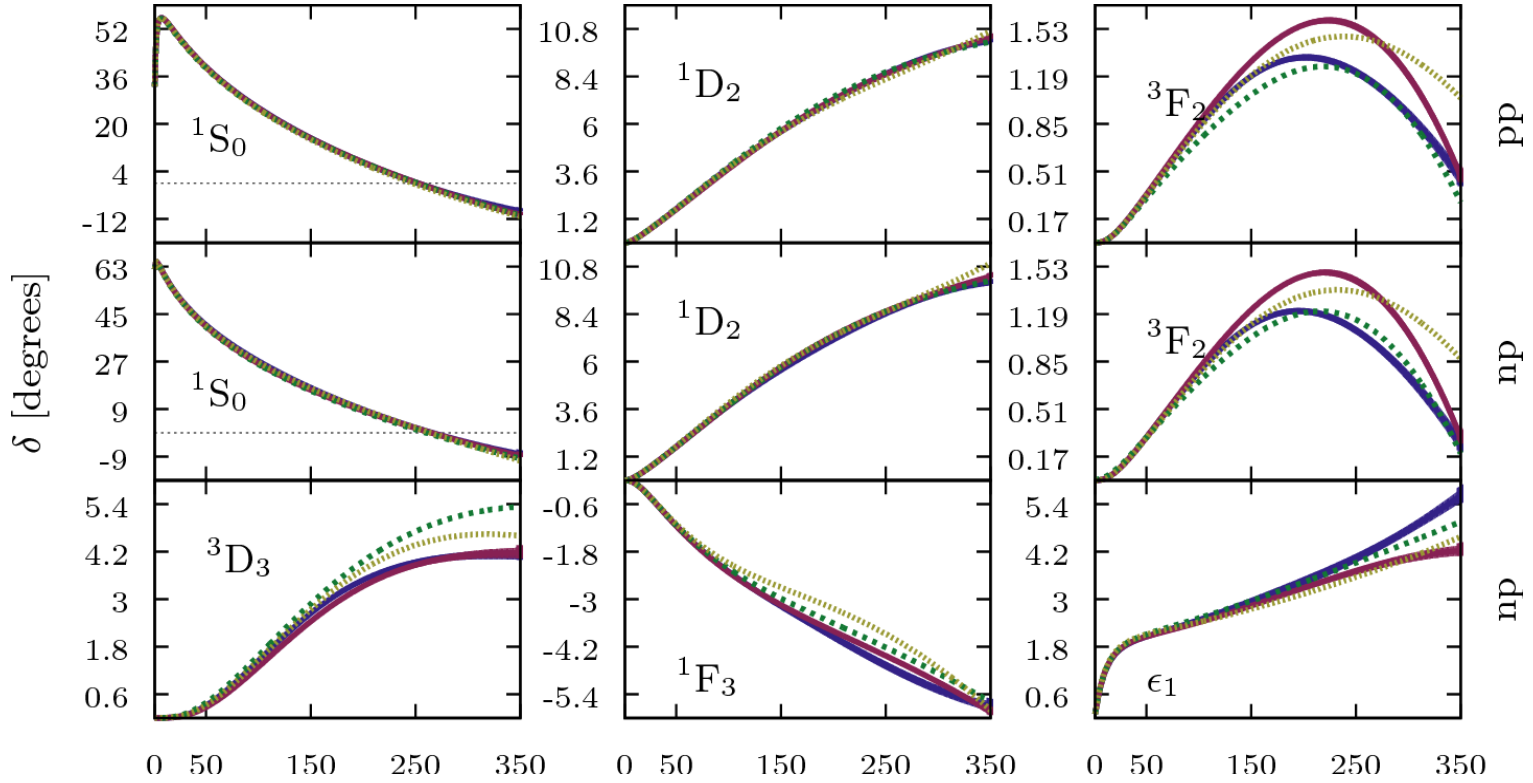
r_c [fm]	*1.8* *Np - χ^2/d.o.f.*	*2.4* *Np - χ^2/d.o.f.*	*3.0* *Np - χ^2/d.o.f.*
OPE	31 – 1.37	39 – 1.09	46 – 1.06
TPE (NLO)	31 – 1.26	38 – 1.08	46 – 1.06
TPE (NNLO)	30+3 – 1.08	38+3 – 1.08	46+3 – 1.06

[RNP, Amaro & Ruiz Arriola. Phys.Rev.C89 (2014) 024004]

Chiral Two Pion Exchange

Phase-shifts

- Comparison of OPE and χTPE

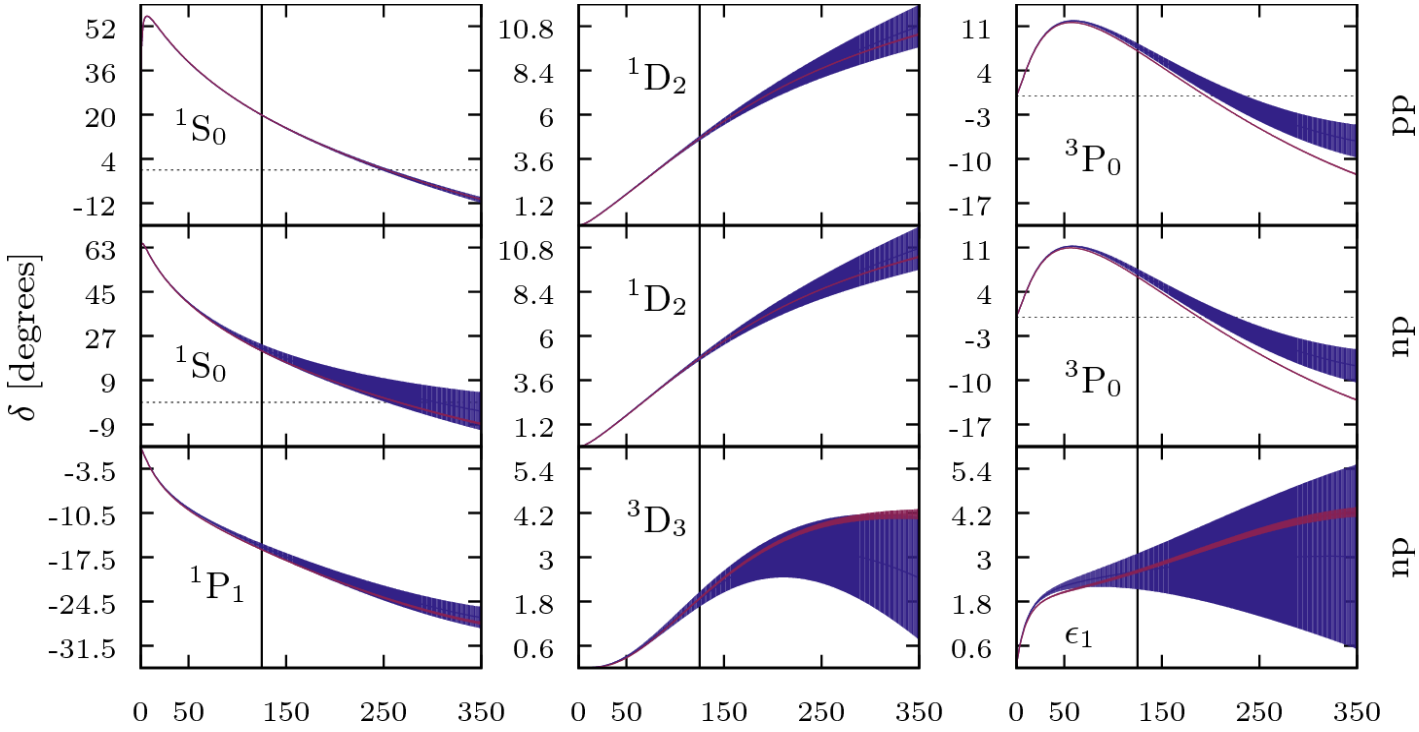


Discrepancies in phase-shifts account for systematic uncertainties

Chiral Two Pion Exchange

Phase-shifts

- Lowering the Energy fitting range from 350 to 125 MeV
  - 20+3 parameters with χ^2/d.o.f. = 1.02

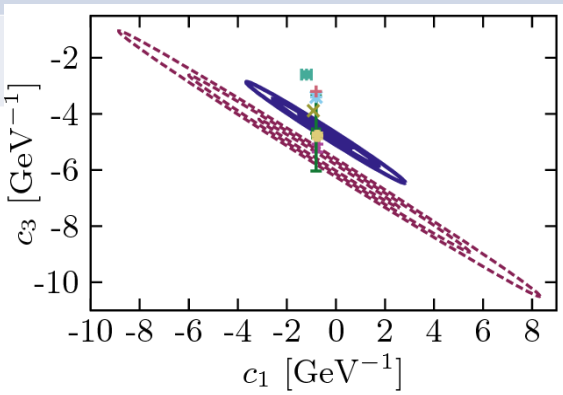


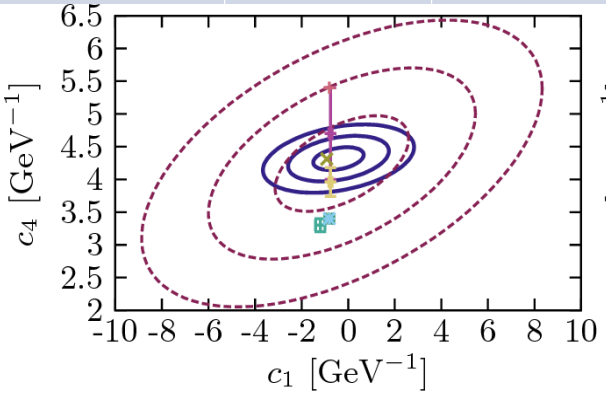
Significant increase of statistical uncertainties

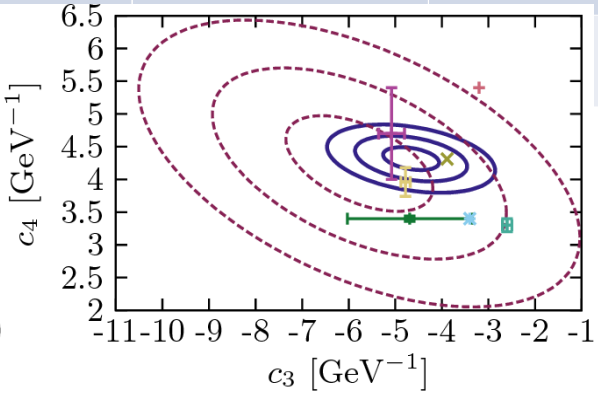
[RNP, Amaro & Ruiz-Arriola Phys.Rev.C91 (2015) 054002]

Determination of Chiral LEC's

	Source	c_1 GeV^{-1}	c_3 GeV^{-1}	c_4 GeV^{-1}
RNP, Amaro and Ruiz-Arriola 350	NN	-0.42±1.08	-4.66±0.60	4.32±0.17
RNP, Amaro and Ruiz-Arriola 125	NN	-0.27±2.87	-5.77±1.58	4.24±0.73
Nijmegen	pp	-0.76±0.07	-5.08±0.28	4.70±0.70
Entem & Machleidt	NN	-0.81	-3.40	3.40
Ekström et. al.	NN	-0.92	-3.89	4.31
Buetikker & Meissner	πN	-0.81±0.15	-4.69±1.34	3.40±0.04

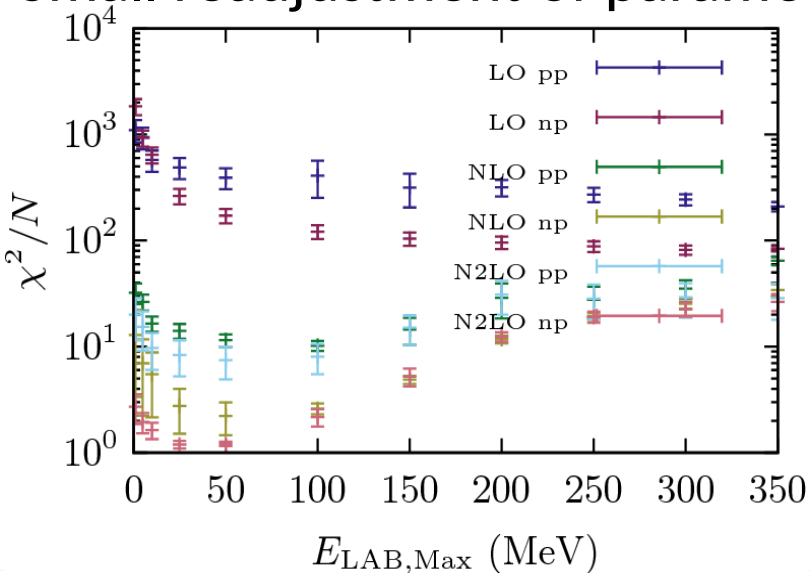






Fit Phases or Fit Data

- Phases are NOT experimental observables
  - Complete set of 10 observables at a given energy and angle
    - Cross sections and polarization asymmetries
- Large χ^2 even at N2LO and low energies
- Small readjustment of parameters may reduce χ^2

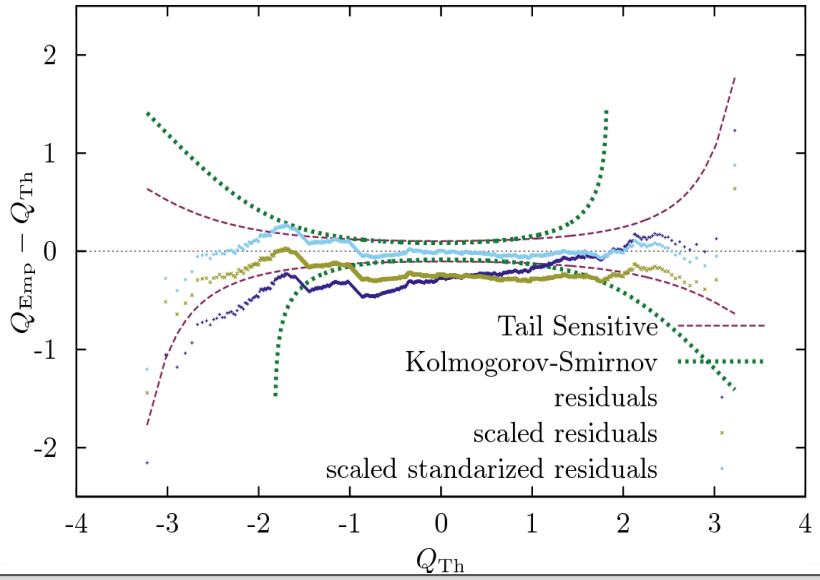


"Local chiral effective field theory interactions and quantum Monte Carlo applications "

Phys.Rev. C90 (2014) no.5, 054323

Are residuals irrelevant?

- Even a good fit (χ^2~1) can be inconsistent
- Non normal residuals
  - Errors can't be propagated via frequentist tools
- Systematic errors seem to be present
  - Regulator dependence?
  - Go to a higher order?



"Optimized Chiral Nucleon-Nucleon Interaction at Next-to-Next-to-Leading Order"

Phys.Rev.Lett. 110 (2013) no.19, 192502

Natural or unnatural?

Cut-off dependence

- Different rc in coordinates → Different Λ in momentum

r_c [fm]	C1 [GeV^{-1}]	C3 [GeV^{-1}]	C4 [GeV^{-1}]	X^2/d.o.f.
3.6	978.3(390)	-961.1(353)	-4.0(148)	1.03
3.0	-35.2(79)	31.3(60)	-6.4(27)	1.04
2.4	-11.9(20)	6.0(12)	-2.3(8)	1.07
1.8	-0.4(11)	-4.7(6)	4.3(2)	1.08
1.2	-9.8(2)	0.3(1)	2.84(5)	1.27
3.6	-0.76	-29.2(27)	-24.4(150)	1.04
3.0	-0.76	3.4(4)	-8.1(26)	1.05
2.4	-0.76	-1.5(1)	-1.9(8)	1.07
1.8	-0.76	-4.25(5)	4.3(2)	1.07
1.2	-0.76	-3.592(4)	3.25(5)	1.27

Natural or unnatural?

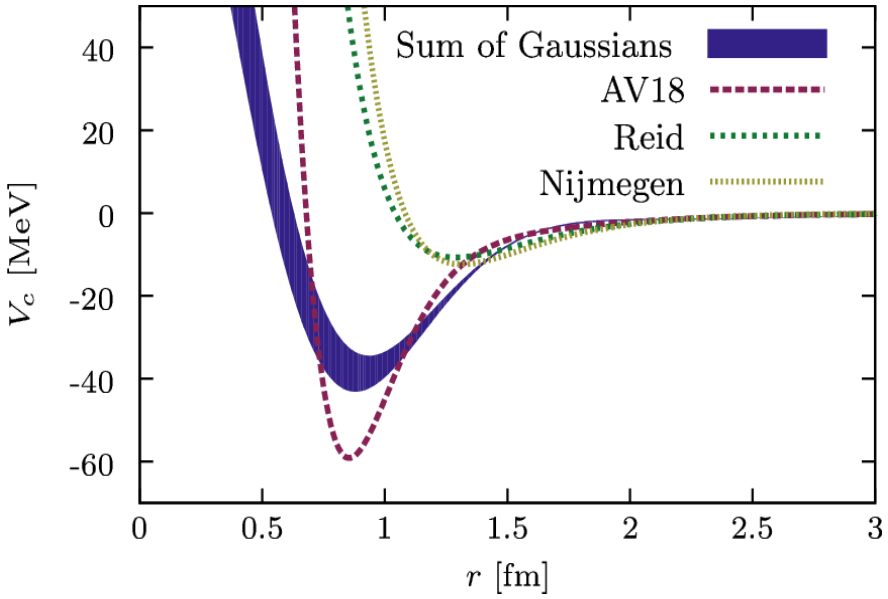
- Which counterterms are needed?

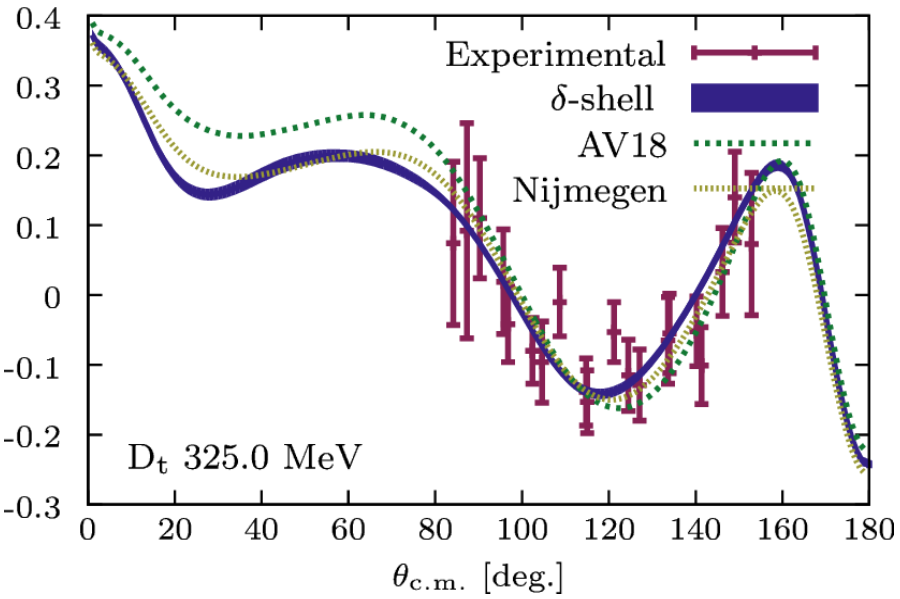
Max Tlab [MeV]	r_c [fm]	*C1* [GeV^{-1}]	C3 [GeV^{-1}]	C4 [GeV^{-1}]	Highest counterterm	X^2/d.o.f.
350	1.8	-0.4(11)	-4.7(6)	4.3(2)	F	1.08
350	1.2	-9.8(2)	0.3(1)	2.84(5)	F	1.27
125	1.8	-0.3(29)	-5.8(16)	-4.2(7)	D	1.03
125	1.2	-0.92	-3.89	4.31	P	1.70
125	1.2	-14.9(6)	2.7(2)	3.51(9)	P	1.05

- D waves needed at N2LO and low energies
  - Contradicting Weinberg

Systematic vs. statistical uncertainties

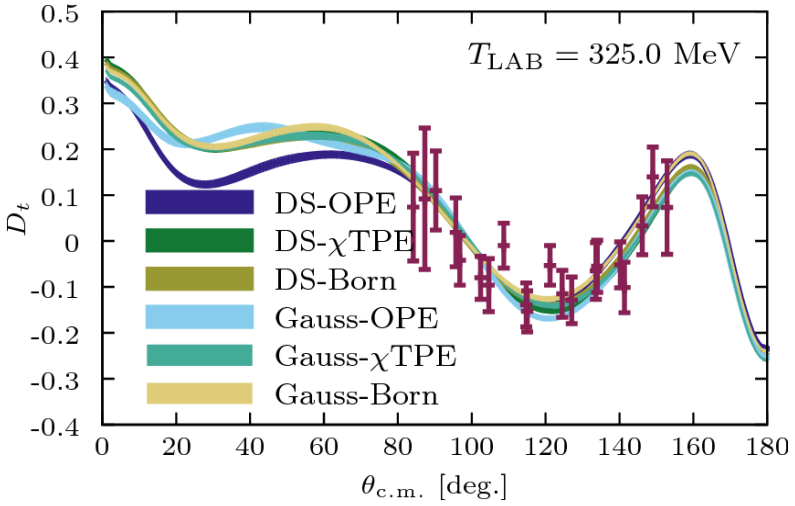
- Same data
- Different representations
- Different predictions
- Who dominates the uncertainty?

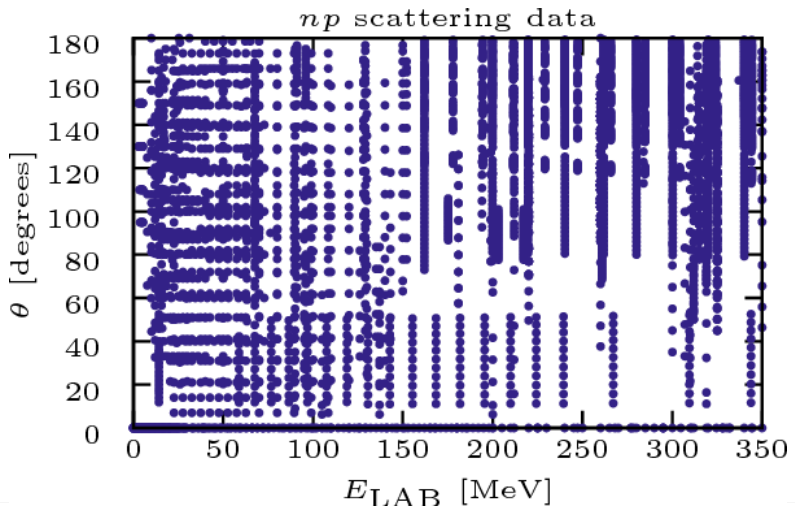




NN Systematic Uncertainty

- Data is unevenly distributed on the (T_{LAB},$\theta_{c.m.}$)
- Same description in probed regions
- Incompatible predictions in unexplored areas
- A uniform experimental exploration is necessary but unlikely





Summary

- Conditions for realistic interaction
  - Reproduce Data $\chi^2/N \sim 1$
  - Reproduce Errors $R_i \sim N(0,1)$
- Nucleon Nucleon interaction
  - Over 8000 scattering data
  - Selection of data is relevant
- Systematic uncertainties
  - Dominate statistical ones
- Lowering the fitting energy range increases statistical uncertainties

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