

Fitting and selecting scattering data

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The question

- We have N DATA with UNCERTAINTIES

$$O_1 \pm \Delta O_1 \quad \dots \quad O_N \pm \Delta O_N$$

- We have a theory depending on M -PARAMETERS

$$O_1(p_1, \dots, p_M) \quad \dots \quad O_N(p_1, \dots, p_M)$$

$$O_i^{\text{exp}} = O_i^{\text{th}} + \xi_i \Delta O_i$$

Define the LEAST SQUARES SUM

$$\chi^2_{\min} \equiv \min_{p_1, \dots, p_M} \sum_{i=1}^N \left[\frac{O_i(p_1, \dots, p_M) - O_i^{\text{exp}}}{\Delta O_i} \right]^2$$

The probability p that the theory explains the DATA is $> 68\%$ if

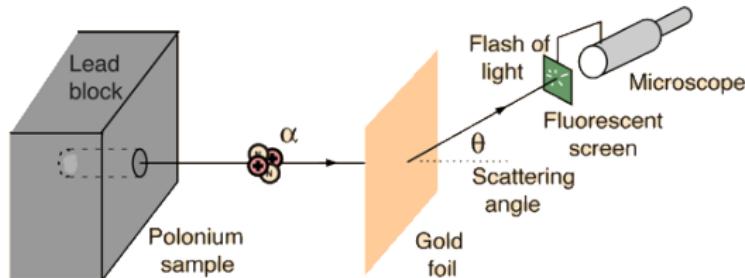
$$\frac{\chi^2_{\min}}{\nu} = 1 \pm \sqrt{\frac{2}{\nu}} \quad \nu = N - M \quad \text{d.o.f (degrees of freedom)}$$

Theory versus experiment

- A good theory can tell us what experiments are wrong
- A good experiment can tell us what theories are wrong
 - ① Assume theory AND experiment to be correct
 - ② If we find no contradiction we validate theory and experiment
 - ③ Experiment , finite number of data, finite precision
 - ④ Theory , approximations
- Important questions
 - ① Does QCD describe hadronic interactions ?
 - ② Does ChPT describe low energy hadronic interactions ?
- Confidence level (statistics)
Example: **AB scattering is described by scheme S with 68 percent confidence**

SCATTERING

Scattering experiment



- Scattering experiments measure FORCES
- Counting rates

$$\frac{R^2 N_{\text{out}}(\theta, \phi)}{N_{\text{in}}} \rightarrow \sigma(\theta, E) \equiv \frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2$$

- Local Normalization

$$\sigma(\theta, E) \underbrace{\rightarrow}_{\theta \ll 1} \sigma_{\text{Ruth}}(\theta, E)$$

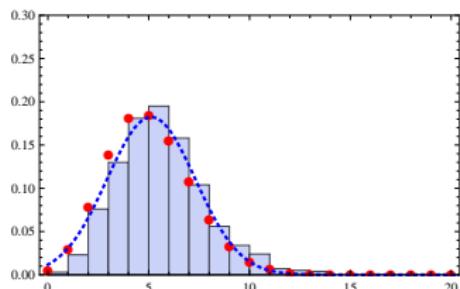
- Total Normalization (mean free path, no Coulomb)

$$l = \frac{1}{n\sigma_T} \quad , \quad \sigma_T = \int d\Omega \frac{d\sigma}{d\Omega}$$

Counting statistics

- Binomial distribution (p scattering probability)

$$P_{N,k} = p^k (1-p)^{N-k} \binom{N}{k}, \quad \langle k \rangle = Np, \quad (\Delta k)^2 = \langle k^2 \rangle - \langle k \rangle^2 = Np(1-p)$$



- Binomial \rightarrow Poisson \rightarrow Gauss

$$\begin{aligned} P_{N,k} &\xrightarrow[p \ll 1]{} \frac{e^{-Np}(Np)^k}{k!} \\ &\xrightarrow[k \gg 1]{} \frac{e^{-(k-Np)^2/2}}{\sqrt{2\pi}\Delta k} \end{aligned}$$

$$p = 0.1 \quad N = 50$$

$$N_{\text{out}} = \bar{N}_{\text{out}} \pm \Delta N_{\text{out}}, \quad \Delta N_{\text{out}} = \sqrt{\bar{N}_{\text{out}}}$$

- $\sigma(\theta, E)$ is Gauss distributed

$$\sigma(\theta, E) = \bar{\sigma}(\theta, E) \pm \Delta(\theta, E)$$

Partial wave expansion (No spin)

- Scattering amplitude

$$f(\theta, \phi) = \sum_{l=0}^{\infty} (2l+1) \frac{e^{2i\delta_l} - 1}{2ip} P_l(\cos \theta) \quad , \quad E = \frac{p^2}{2\mu}$$

- Schrödinger Equation

$$\left[-\frac{\nabla^2}{2\mu} + V(\vec{x}) \right] \Psi(\vec{x}) = E\Psi(\vec{x})$$

- Spherical symmetry $V(r)$

$$\Psi(\vec{x}) = \frac{u_l(r)}{r} Y_{lm}(\hat{x})$$

- Reduced radial equation

$$-u_l''(r) + \left[\frac{l(l+1)}{r^2} + 2\mu V(r) \right] u_l(r) = p^2 u_l(r)$$

- Asymptotic conditions

$$u_l(r) \underset{r \rightarrow 0}{\underbrace{\sim}} r^{l+1} \quad , \quad u_l(r) \underset{r \rightarrow \infty}{\underbrace{\sim}} \sin \left(pr - \frac{l\pi}{2} + \delta_l \right)$$

- GOAL : Determine $V(r) \pm \Delta V(r)$

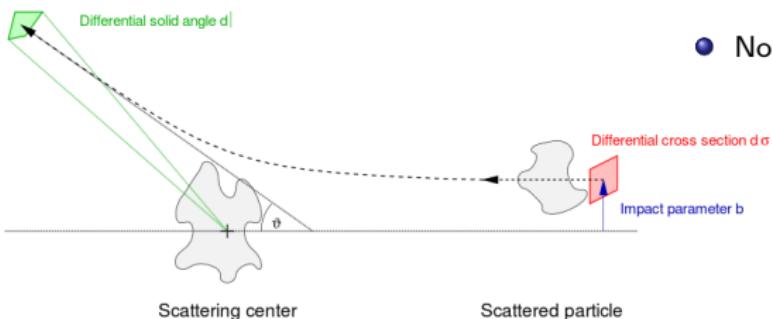
Finite range forces

- Meson exchange picture → Longest range \equiv Lightest particle

$$r_c \sim \frac{\hbar}{m_\pi c} \sim 1.4\text{fm}$$

- Impact parameter

$$|\vec{L}| = |\vec{x} \wedge \vec{p}| \rightarrow bp \quad L^2 = l(l+1)^2 \sim (l+1/2)^2 \rightarrow l + \frac{1}{2} = bp$$



- No scattering condition

$$\begin{aligned} V(r) &\sim 0 & r \gtrsim r_c \\ \delta_l(p) &\sim 0 & b \gtrsim r_c \\ \rightarrow l_{\max} + \frac{1}{2} &\sim pr_c \sim p/m_\pi \end{aligned}$$

- Truncation in the partial wave expansion

$$f(\theta, \phi) = \sum_{l=0}^{l_{\max}} (2l+1) \frac{e^{2i\delta_l} - 1}{2ip} P_l(\cos \theta) = \frac{e^{2i\delta_0} - 1}{2ip} + 3 \frac{e^{2i\delta_1} - 1}{2ip} \cos \theta + \dots$$

FITTING

Single energy fits

- Complete data in a GIVEN energy E

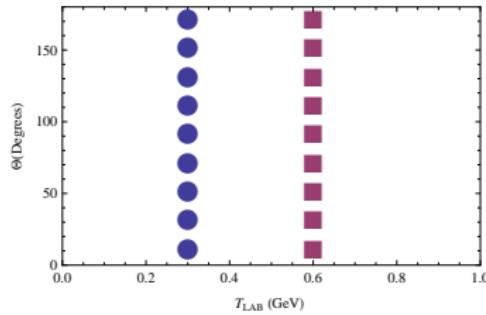
$$\sigma(\theta, E) \rightarrow \sigma(\theta_1, E), \dots, \sigma(\theta_N, E)$$

- Fitting function \rightarrow Fitting parameters $\delta_1(E), \dots, \delta_l(E)$

$$\chi^2(\delta_1(E), \dots, \delta_l(E), \nu) = \sum_{i=1}^N \left[\frac{\sigma^{\text{exp}}(\theta_i, E) - \nu \sigma^{\text{th}}(\theta_i, \delta_1(E), \dots, \delta_l(E))}{\Delta \sigma(\theta_i, E)} \right]^2 + \left(\frac{1 - \nu}{\Delta \nu} \right)^2$$

- Normalization is COMMON for ONE energy
- Phase-shifts are “experimental” and MODEL INDEPENDENT

$$\delta_l^{\text{exp}}(E) \pm \Delta \delta_l^{\text{exp}}(E) \quad , \quad l = 0, \dots, l_{\max}$$



Multienergy analysis

- Incomplete Data in several energies and angles

$$\sigma(\theta, E) \rightarrow \sigma(\theta_1, E_1), \dots, \sigma(\theta_N, E_N)$$

- The need for interpolation (Smoothness in (θ, E))
- Fitting function to Fitting MODEL DEPENDENT parameters $\mathbf{p} = (p_1, \dots, p_M)$

$$\chi^2(\mathbf{p}, \nu) = \sum_{i=1}^N \left[\frac{\sigma(\theta_i, E_i)^{\text{exp}} - \nu \sigma^{\text{th}}(\theta_i, E_i, \mathbf{p})}{\Delta \sigma(\theta_i, E_i)} \right]^2 + \left(\frac{1 - \nu}{\Delta \nu} \right)^2$$

- The statement

$$\sigma(\theta_i, E_i)^{\text{exp}} = \nu_0 \sigma^{\text{th}}(\theta_i, E_i, \mathbf{p}_0) \pm \Delta \sigma(\theta_i, E_i)$$

- Too large χ^2/ν

- Bad model → SELECT MODEL
- Bad data → SELECT DATA
- Bad model and data

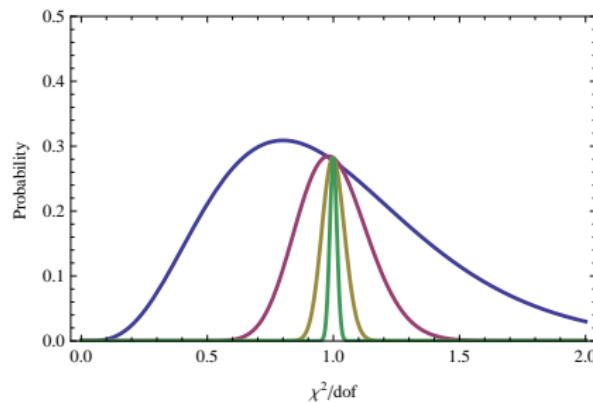
The χ^2 -test

- If $\xi_n \in N(0, 1)$

$$P_\nu(\chi^2) = \prod_{n=1}^N \left(\int_{-\infty}^{\infty} d\xi_i \frac{e^{-\xi_i^2/2}}{\sqrt{2\pi}} \right) \delta(\chi^2 - \sum_{n=1}^N \xi_n^2) = \frac{e^{-\chi^2} \chi^{\nu-2}}{2^{\nu/2} \Gamma(\frac{\nu}{2})}$$

- Mean and Variance

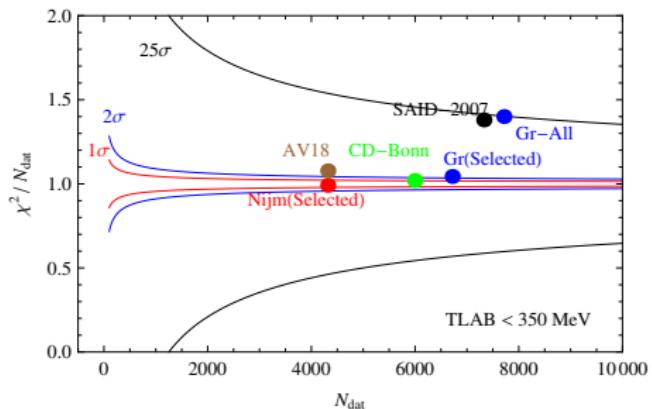
$$\langle \chi^2 \rangle = \nu, \quad \langle (\chi^2 - \langle \chi^2 \rangle)^2 \rangle = 2\nu^2, \quad \rightarrow \chi^2 = \nu \pm \sqrt{2\nu}$$



ν	χ^2/ν (68%)
10	1 ± 0.447
100	1 ± 0.141
1000	1 ± 0.044
10000	$1 \pm 0.014.$

To believe or not to believe

N_{data}	HJ62	Reid68	TRS75	Paris80	Urb81	Arg84	BonnR	Bonn89	Nijm93
1787	13.5	2.9	3.4	4.5	6.0	7615	1090	25.5	1.8

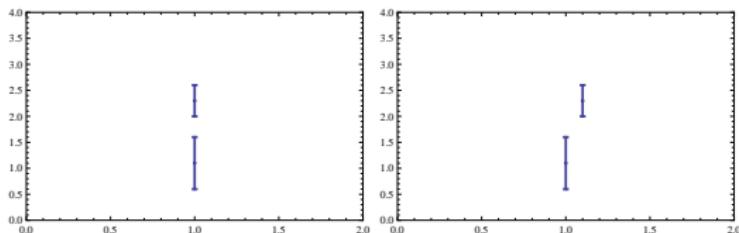


$$\chi^2_{\min}/\nu = 1 \pm \sqrt{2/\nu}$$

- Charge dependence in OPE
- Magnetic-Moments, Vacuum polarization, ...

The need for selection

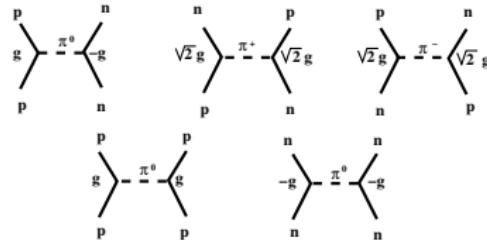
- Example: THE SAID DATABASE
 - PP Data No=25188 Chi2= 48225.043
 - NP Data No=12962 Chi2= 26079.973
 - πN 41926 Chi2= 166585.05
 - πN 2599 Chi2= 4586.26 (TLAB i 300)
- Which experiments are INCOMPATIBLE ?



- Contribution the χ^2 will be large (discard BOTH ?)
- If errorbar includes BOTH no contribution to the χ^2
- Incompatibility is DESTRUCTIVE
- Real physical effect ?

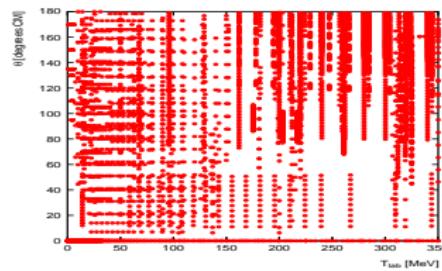
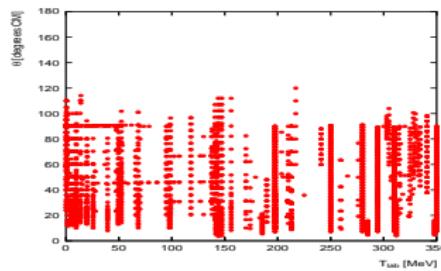
Long distances

- Nucleons exchange JUST one pion



- Low energies (about pion production) 8000 pp + np scattering data (polarizations etc.)
- Granada coarse grained analysis (2016) (isospin breaking !!)

$$g_p^2/(4\pi) = 13.72(7) \neq g_n^2/(4\pi) = 14.91(39) \neq g_c^2/(4\pi) = 13.81(11) \quad \chi^2/\nu = 1.02$$



COARSE GRAINING NN (LOW ENERGY)

Nucleon-Nucleon Scattering

- Scattering amplitude

$$\begin{aligned} M &= a + m(\sigma_1 \cdot \mathbf{n})(\sigma_2 \cdot \mathbf{n}) + (g - h)(\sigma_1 \cdot \mathbf{m})(\sigma_2 \cdot \mathbf{m}) \\ &+ (g + h)(\sigma_1 \cdot \mathbf{l})(\sigma_2 \cdot \mathbf{l}) + c(\sigma_1 + \sigma_2) \cdot \mathbf{n} \\ \mathbf{l} &= \frac{\mathbf{k}_f + \mathbf{k}_i}{|\mathbf{k}_f + \mathbf{k}_i|} \quad \mathbf{m} = \frac{\mathbf{k}_f - \mathbf{k}_i}{|\mathbf{k}_f - \mathbf{k}_i|} \quad \mathbf{n} = \frac{\mathbf{k}_f \wedge \mathbf{k}_i}{|\mathbf{k}_f \wedge \mathbf{k}_i|} \end{aligned}$$

- 5 complex amplitudes \rightarrow 24 measurable cross-sections and polarization asymmetries
- Partial Wave Expansion

$$\begin{aligned} M_{m'_s, m_s}^s(\theta) &= \frac{1}{2ik} \sum_{J, l', l} \sqrt{4\pi(2l+1)} Y_{m'_s - m_s}^{l'}(\theta, 0) \\ &\times C_{m_s - m'_s, m'_s, m_s}^{l', s, J} i^{l-l'} (S_{l, l'}^{J, s} - \delta_{l', l}) C_{0, m_s, m_s}^{l, s, J}, \end{aligned} \quad (1)$$

- S-matrix

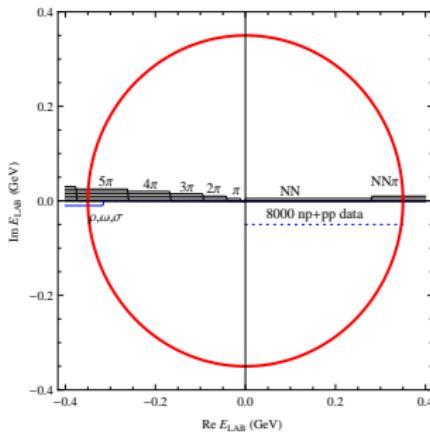
$$S^J = \begin{pmatrix} e^{2i\delta_{J-1}^{J,1}} \cos 2\epsilon_J & ie^{i(\delta_{J-1}^{J,1} + \delta_{J+1}^{J,1})} \sin 2\epsilon_J \\ ie^{i(\delta_{J-1}^{J,1} + \delta_{J+1}^{J,1})} \sin 2\epsilon_J & e^{2i\delta_{J+1}^{J,1}} \cos 2\epsilon_J \end{pmatrix}, \quad (2)$$

Analytical Structure

- $s = 4(M_N^2 + p^2) \rightarrow E_{\text{LAB}} = 2p^2/M_N$
- Partial Wave Scattering Amplitude analytical for $|p| \leq m_\pi/2$

$$T_{ll'}^J(p) \equiv S_{ll'}^J(p) - \delta_{l,l'} = p^{l+l'} \sum_n C_{n,l,l'} p^{2n}$$

- Nucleons behave as elementary (AT WHAT SCALE ?)



- Nucleons are heavy → Local Potentials

$$V_{n\pi}(r) \sim \frac{g^{2n}}{r} e^{-nm_\pi r}$$

- Crucial long range electromagnetic effects are local

The number of parameters (for $E_{\text{LAB}} \leq 350$ MeV)

- At what distance look nucleons point-like ?

$$r > 2\text{fm}$$

- When is OPE the **ONLY** contribution ?

$$r_c > 3\text{fm}$$

- What is the minimal resolution where interaction is elastic ?

$$p_{\max} \sim \sqrt{M_N m_\pi} \rightarrow \Delta r = 1/p_{\max} = 0.6\text{fm}$$

- How many partial waves must be fitted ?

$$l_{\max} = p_{\max} r_c = r_c / \Delta r = 5$$

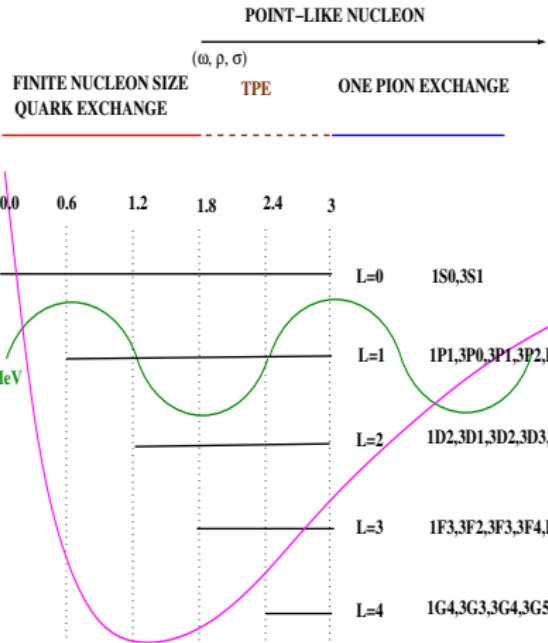
- Minimal distance where centrifugal barrier dominates

$$\frac{l(l+1)}{r_{\min}^2} \leq p^2$$

- How many parameters ?

$(^1S_0, ^3S_1), (^1P_1, ^3P_0, ^3P_1, ^3P_2), (^1D_2, ^3D_1, ^3D_2, ^3D_3), (^1F_3, ^3F_2, ^3F_3, ^3F_4)$

$$2 \times 5 + 4 \times 4 + 4 \times 3 + 4 \times 2 + 4 \times 1 = 50$$



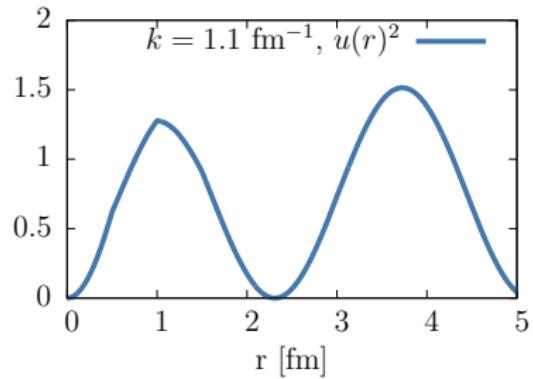
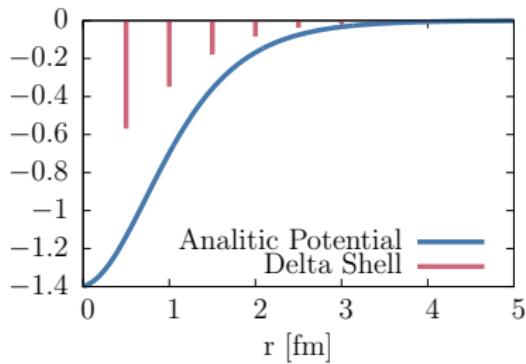
Delta Shell Potential

- A sum of delta functions

$$V(r) = \sum_i \frac{\lambda_i}{2\mu} \delta(r - r_i)$$

[Aviles, Phys.Rev. C6 (1972) 1467]

- Optimal and minimal sampling of the nuclear interaction
- Pion production threshold $\Delta k \sim 2 \text{ fm}^{-1}$
- Optimal sampling, $\Delta r \sim 0.5 \text{ fm}$



Delta Shell Potential

- 3 well defined regions
- Innermost region $r \leq 0.5$ fm
 - Short range interaction
 - No delta shell (No repulsive core)
- Intermediate region $0.5 \leq r \leq 3.0$ fm
 - Unknown interaction
 - λ_i parameters fitted to scattering data
- Outermost region $r \geq 3.0$ fm
 - Long range interaction
 - Described by OPE and EM effects
 - Coulomb interaction V_{C1} and relativistic correction V_{C2} (pp)
 - Vacuum polarization V_{VP} (pp)
 - Magnetic moment V_{MM} (pp and np)

Fitting NN observables

- Delta shell potential in every partial wave

$$V_{l,l'}^{JS}(r) = \frac{1}{2\mu_{\alpha\beta}} \sum_{n=1}^N (\lambda_n)_{l,l'}^{JS} \delta(r - r_n) \quad r \leq r_c = 3.0\text{fm}$$

- Strength coefficients λ_n as fit parameters
- Fixed and equidistant concentration radii $\Delta r = 0.6$ fm
- EM interaction is crucial for pp scattering amplitude

$$V_{C1}(r) = \frac{\alpha'}{r},$$

$$V_{C2}(r) \approx -\frac{\alpha\alpha'}{M_p r^2},$$

$$V_{VP}(r) = \frac{2\alpha\alpha'}{3\pi r} \int_1^\infty dx e^{-2m_e rx} \left[1 + \frac{1}{2x^2} \right] \frac{(x^2 - 1)^{1/2}}{x^2},$$

$$V_{MM}(r) = -\frac{\alpha}{4M_p^2 r^3} [\mu_p^2 S_{ij} + 2(4\mu_p - 1)\mathbf{L} \cdot \mathbf{S}]$$

STATISTICS

Self-consistent fits

- We test the assumption

$$O_i^{\text{exp}} = O_i^{\text{th}} + \xi_i \Delta O_i \quad i = 1, \dots, N_{\text{Data}} \quad \xi_i \in N[0, 1]$$

- Least squares minimization $\mathbf{p} = (p_1, \dots, p_M)$

$$\chi^2(\mathbf{p}) = \sum_{i=1}^N \left(\frac{O_i^{\text{exp}} - F_i(\mathbf{p})}{\Delta O_i^{\text{exp}}} \right)^2 \rightarrow \min_{\mathbf{p}} \chi^2(\mathbf{p}) \equiv \chi^2(\mathbf{p}_0) \quad (3)$$

- Are residuals Gaussian ?

$$R_i = \frac{O_i^{\text{exp}} - O_i^{\text{th}}}{\Delta O_i} \quad O_i^{\text{th}} = F_i(\mathbf{p}_0) \quad i = 1, \dots, N \quad (4)$$

If $R_i \in N[0, 1]$ self-consistent fit.

- Normality test for a finite sample with N elements \rightarrow Probability (Confidence level) p-value

$$\chi^2_{\min} = 1 \pm \sigma \sqrt{\frac{2}{\nu}} \quad \nu = N_{\text{Dat}} - N_{\text{Par}} \quad p = 1 - \int_{\sigma}^{\infty} dt \frac{e^{-t^2}}{\sqrt{2\pi}}$$

Histograms, Moments, Kolmogorov-Smirnov, Tail Sensitive QQ-plots

Normality tests

- Does the sequence

$$x_1^{\text{exp}} \leq x_2^{\text{exp}} \leq \cdots \leq x_N^{\text{exp}} \in N[0, 1]$$

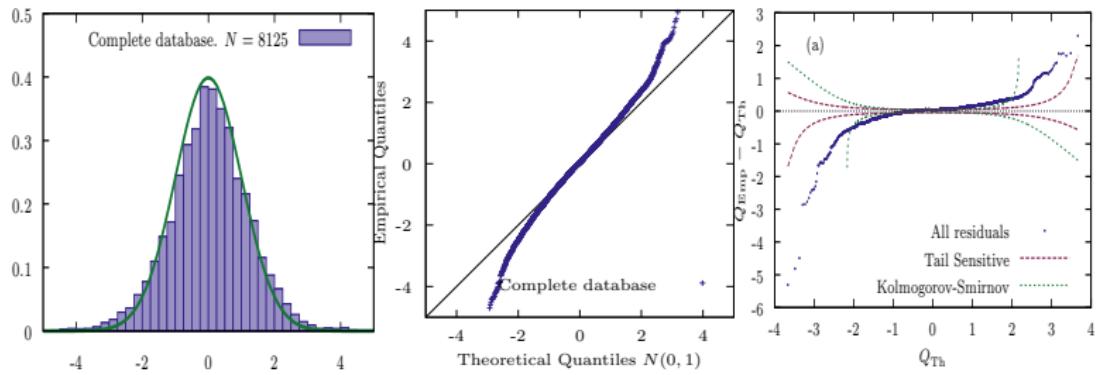
- We compute the theoretical points

$$\frac{n}{N+1} = \int_{-\infty}^{x_n^{\text{th}}} dt \frac{e^{-t^2/2}}{\sqrt{2\pi}}$$

- The Q-Q plot is x_n^{th} vs x_n^{exp}

- For large N

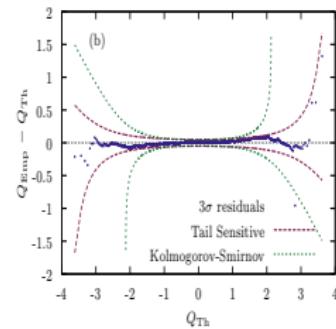
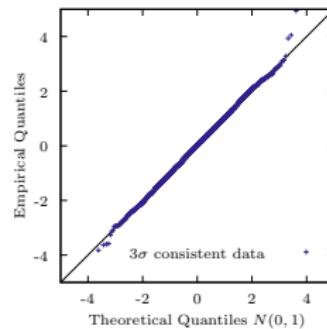
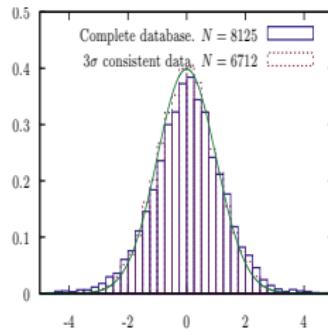
$$x_n^{\text{th}} - x_n^{\text{exp}} = \mathcal{O}(1/\sqrt{N})$$



Granada-2013 np+pp database

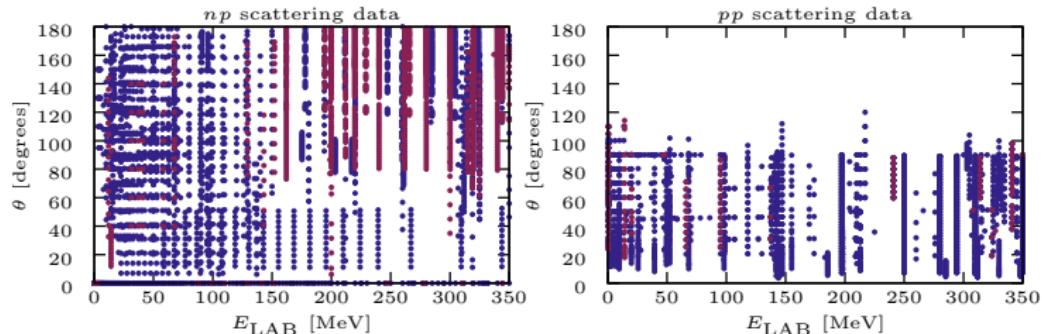
Selection criterium

- 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
 - ① Fit to all data ($\chi^2/\nu > 1$)
 - ② Remove data sets with improbably high or low χ^2 (3σ criterion)
 - ③ Refit parameters
 - ④ Re-apply 3σ criterion to all data
 - ⑤ Repeat until no more data is excluded or recovered

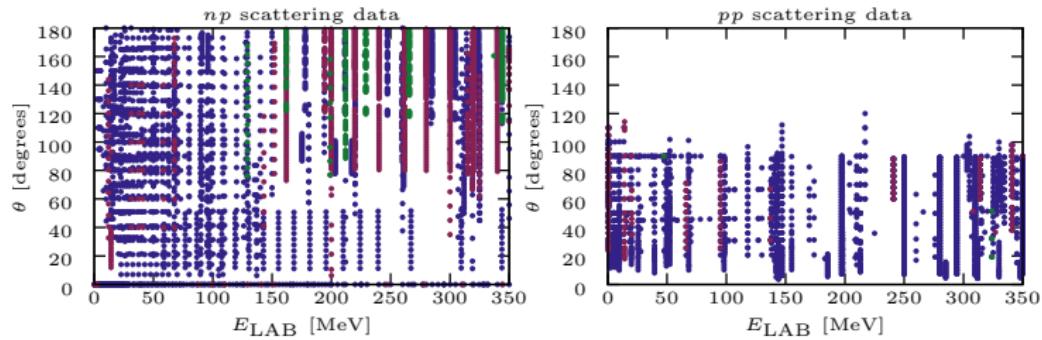


Selection of data

Usual Nijmegen 3σ criterion (1677 rejected data)

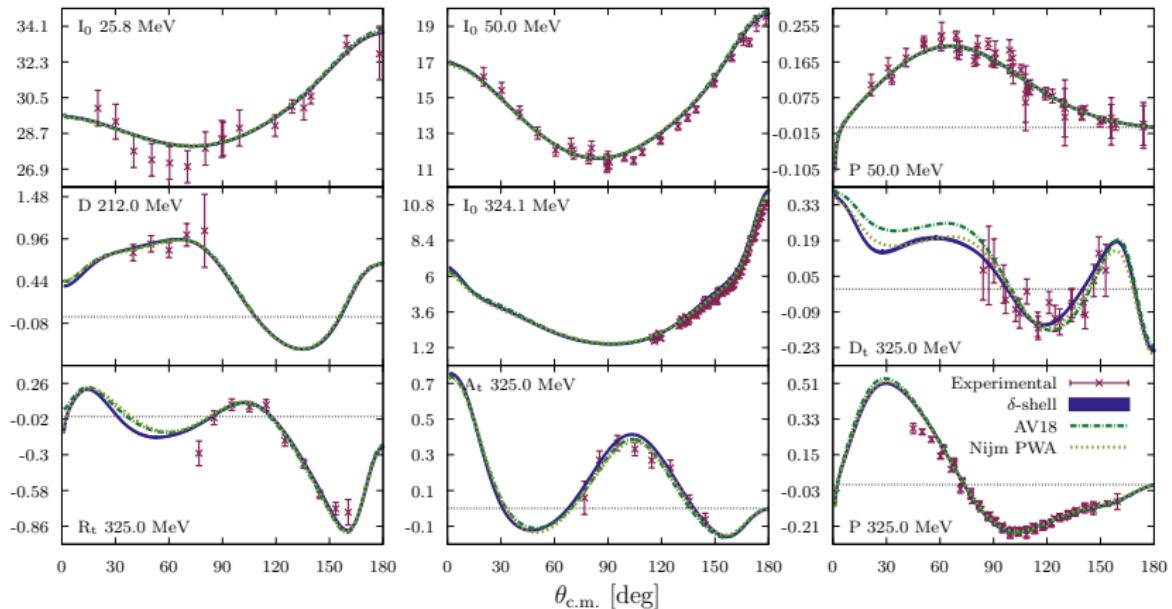


300 recovered data with Granada procedure (consistent database)



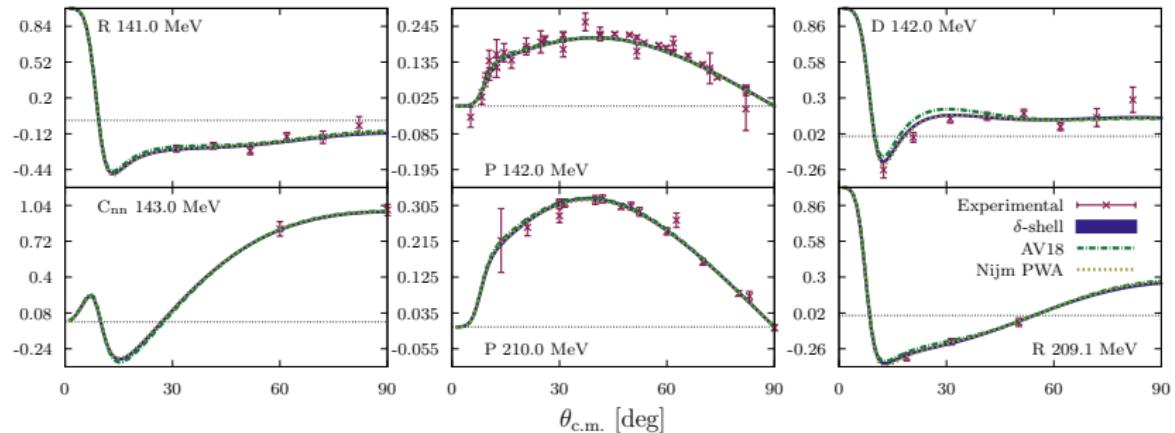
Scattering Observables

- Comparing with Potentials and Experimental data
- np data



Scattering Observables

- Comparing with Potentials and Experimental data
- pp data

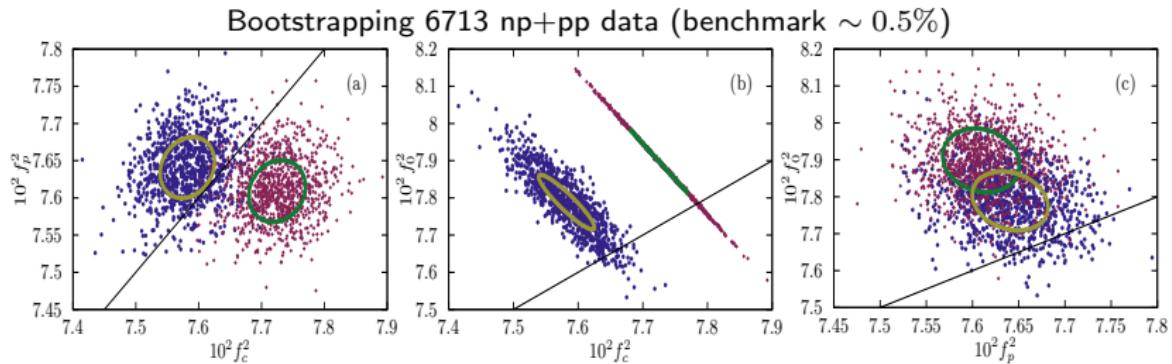


- $\chi^2/\text{d.o.f.} = 1.06$ with $N = 2747|_{\text{pp}} + 3691|_{\text{np}}$

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

STATISTICAL CONSEQUENCES

Coupling constants

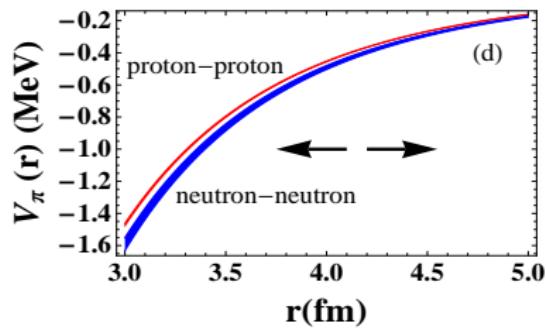
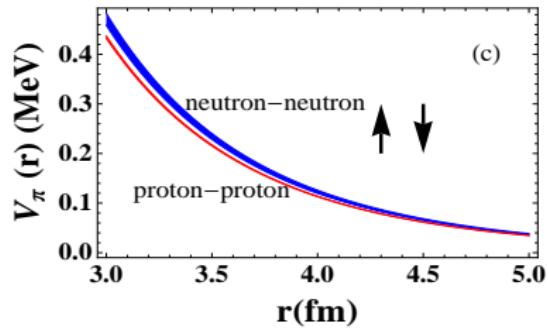
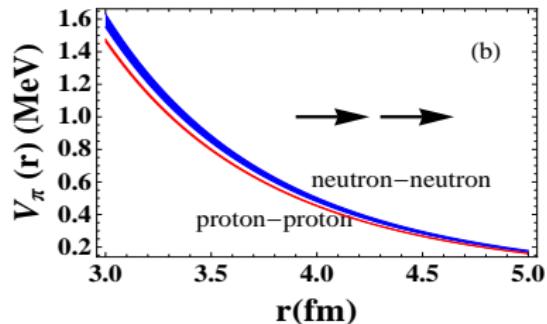
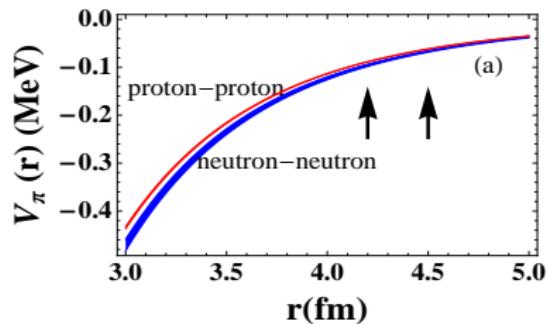


Fits to the Granada-2013 database.

f^2	f_0^2	f_c^2	CD-waves	χ^2_{pp}	χ^2_{np}	N_{Dat}	N_{Par}	χ^2/ν
0.075	idem	idem	1S_0	3051	3951	6713	46	1.051
0.0761(3)	idem	idem	1S_0	3051	3951	6713	46+1	1.051
-	-	-	${}^1S_0, P$	2999	3951.40	6713	46+3	1.043
0.0759(4)	0.079(1)	0.0763(6)	${}^1S_0, P$	3045	3870	6713	46+3+9	1.039

Neutron-Neutron vs Proton-Proton (Polarized)

nn interaction is more intense than pp interaction



Arqueological Flashback

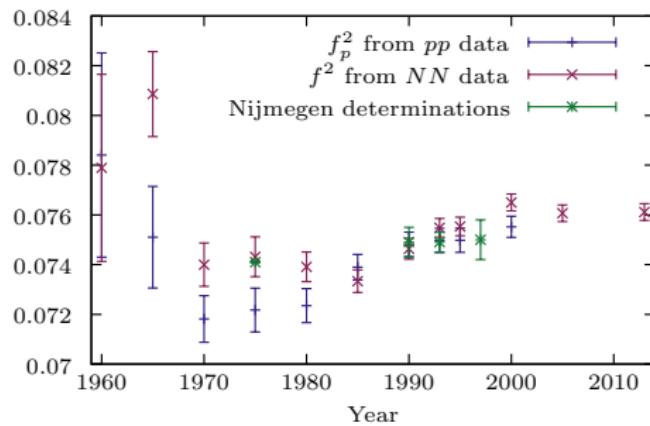
- Can we witness isospin breaking in the couplings ?

$$\frac{dg}{g} \Big|_{\text{QCD}} = \mathcal{O}(\alpha, \frac{m_u - m_d}{\Lambda_{\text{QCD}}}) = \mathcal{O}(\alpha, \frac{M_n - M_p}{\Lambda_{\text{QCD}}}) \sim 0.01 - 0.02$$

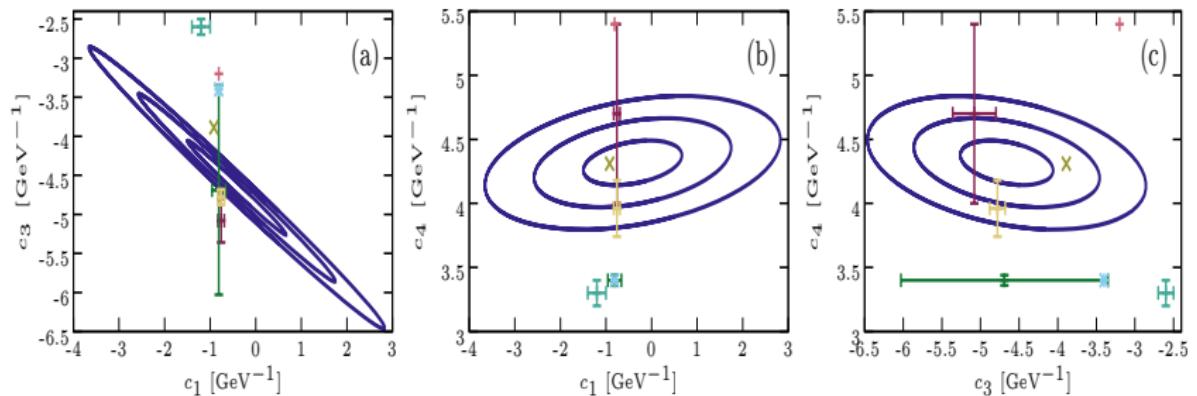
- Statistically yes ! Granada NN $N = 6713$

$$\frac{dg}{g} \Big|_{\text{stat}} = \mathcal{O}\left(\frac{\Delta N_{\text{Dat}}}{N_{\text{Dat}}}\right) = \mathcal{O}\left(\frac{1}{\sqrt{N_{\text{Dat}}}}\right) \rightarrow N \sim 7000 - 10000$$

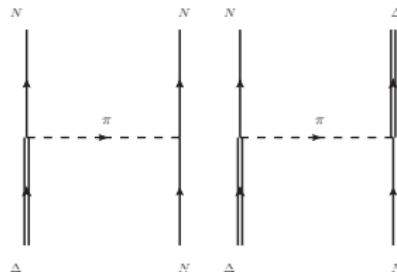
- Chronological recreation of pion-nucleon coupling constants



Chiral Two Pion Exchange from Granada-2013 np+pp database



$f_{\pi N \Delta}$ from Granada-2013 np+pp database



- NN potential in the Born-Oppenheimer approximation

$$\bar{V}_{NN,NN}^{1\pi+2\pi+\dots}(\mathbf{r}) = V_{NN,NN}^{1\pi}(\mathbf{r}) + 2 \frac{|V_{NN,N\Delta}^{1\pi}(\mathbf{r})|^2}{M_N - M_\Delta} + \frac{1}{2} \frac{|V_{NN,\Delta\Delta}^{1\pi}(\mathbf{r})|^2}{M_N - M_\Delta} + \mathcal{O}(V^3),$$

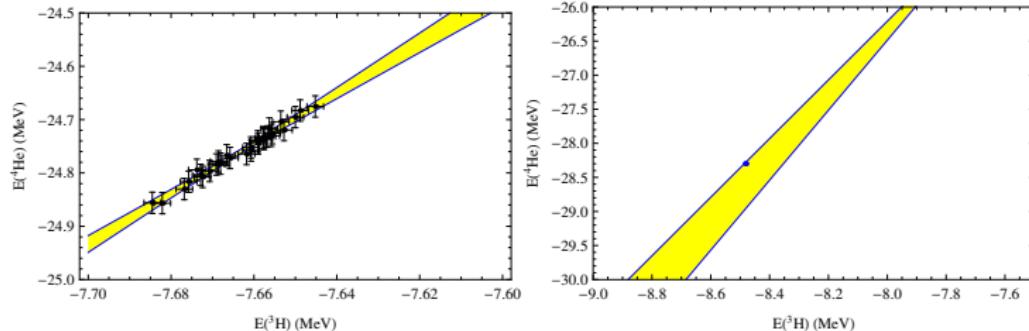
- Bulk of TWO-Pion Exchange Chiral forces reproduced
- Fit with $r_e = 1.8\text{fm}$ to $N = 6713\text{pp} + np$ scattering data

$$f_{\pi N \Delta}/f_{\pi N N} = 2.178(14) \quad \chi^2/\nu = 1.12 \rightarrow h_A = 1.397(9)$$

Tjon-Lines: numerical accuracy of $A = 2, 3, 4$ Nuclei

(with A. Nogga)

$$\Delta E_{\text{triton}}^{\text{stat}} = 15 \text{ KeV} \quad \Delta E_{\alpha}^{\text{stat}} = 50 \text{ KeV}$$



- 4-Body forces are masked by numerical noise in the 3 and 4 body calculation if

$$\Delta_t^{\text{num}} > 1 \text{ KeV} \quad \Delta_t^{\text{num}} > 20 \text{ KeV}$$

To count or not to count: The Falsification of Chiral Forces

- We can fit CHIRAL forces to ANY energy and look if counterterms are compatible with zero within errors
- We find that if $E_{\text{LAB}} \leq 125\text{MeV}$ Weinberg counting is INCOMPATIBLE with data.
- You have to promote D-wave counterterms.
N2LO-Chiral TPE + N3LO-Counterterms → Residuals are normal
[Piarulli, Girlanda, Schiavilla, Navarro Pérez, Amaro, RA, PRC](#)
- We find that if $E_{\text{LAB}} \leq 40\text{MeV}$ TPE is INVISIBLE
- We find that peripheral waves predicted by 6th-order chiral perturbation theory ARE NOT consistent with data within uncertainties

$$|\delta^{\text{Ch,N5LO}} - \delta^{\text{PWA}}| > \Delta\delta^{\text{PWA,stat}}$$

5 σ incompatible

CONCLUSIONS

Conclusions

- Fitting and selecting scattering databases allows to pose and ANSWER important questions
- Coarse graining is a simple method to analyze and select data using a statistical framework
- Self-consistent databases allow to determine coupling constants
- Validate power countings in NN (Weinberg is not)
- It could be a possible way to do Nuclear Physics AND Hadronic physics

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