The Validation and Falsification of Chiral Nuclear Forces

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with Rodrigo Navarro Pérez, José Enrique Amaro Soriano
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INTRODUCTION
Error Analysis and Nuclear Structure

What is the predictive power of theoretical nuclear physics?

INPUT from Experiment $\rightarrow$ CALCULATION $\rightarrow$ OUTPUT vs Experiment

Experiment much more precise than theory, but how much?

$$\Delta M^{\text{exp}} < 1\text{KeV} \ll \Delta M^{\text{th}} = ?$$

Theoretical Predictive Power Flow: From light to heavy nuclei

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

Chiral expansion allows to compute $V_{2N}, V_{3N}, V_{4N} \ldots$ systematically so that one has the hierarchy

$$V_{2N} \gg V_{3N} \gg V_{4N} \gg \ldots$$

Forces depend on the renormalization scale allowing to adjust $B_2, B_3, \ldots$
Sources of uncertainties/bias

- Input data from experiment
- Choose the form of the potential
- How to estimate theoretical errors based on INPUT data

\[ INPUT = NN, 3N, \cdots \rightarrow OUTPUT = 4N, \ldots \]

- First Step: INPUT=NN scattering data
- OUTPUT=NN scattering amplitudes
The issue of predictive power in Chiral Approach

- Chiral forces are UNIVERSAL at long distances

\[ V^\chi(r) = V^\pi(r) + V^{2\pi}(r) + V^{3\pi}(r) + \ldots \quad r \gg r_c \]

- Chiral forces are SINGULAR at short distances

\[ V^\chi(r) = \frac{a_1}{f_\pi^2 r^3} + \frac{a_2}{f_\pi^4 r^5} + \frac{a_3}{f_\pi^6 r^7} + \ldots \quad r \ll r_c \]

- They trade model independence for regulator dependence
- What is the best theoretical accuracy we can get within “reasonable” cut-offs?
- What is a reasonable cut-off?

\[ r_c = ? \]
Bottomline

THE PROBLEM

- **GOAL:** Estimate uncertainties from IGNORANCE of NN,3N,4N interaction
  Reduce computational cost
- **Statistical Uncertainties:** NN,3N,4N Data
  Data abundance bias
- **Systematic Uncertainties:** NN,3N,4N potential
  Many forms of potentials possible
- **Confidence level of Imperfect theories vs Perfect experiments**

OUR APPROACH

- Start with NN
- Fit data WITH ERRORS with a simple interaction
- Compare different interactions
- Estimate uncertainties of Effective Interactions and Matrix elements
- Propagate errors to A=3,4, etc.
\( \alpha \)-triton calculations find a linear correlation between

\[
B_\alpha = 4B_t - 3B_d
\]

SRG argument with on-shell nuclear forces

Timoteo, Szpigel, ERA, Few Body 2013
Tjon-Lines: numerical accuracy

(with A. Nogga)

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

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

\[ \Delta t^{\text{num}} > 1\text{KeV} \quad \Delta t^{\text{num}} > 20\text{KeV} \]
The question and its consequences

- We have $N$ DATA with UNCERTAINTIES

$$O_1 \pm \Delta O_1 \quad \ldots \quad O_N \pm \Delta O_N$$

- We have a theory depending on $M$-PARAMETERS

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

- Does theory EXPLAIN data?

  YES (Validate) \quad NO (Falsify)

- Statistical Answer:
  If uncertainties are a gaussian distribution

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

Define the LEAST SQUARES SUM

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

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

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

\[
\sigma(\theta, E) \rightarrow \sigma_{\text{Ruth}}(\theta, E)
\]

θ ≪ 1

Total Normalization (mean free path, no Coulomb)

\[
l = \frac{1}{n\sigma_T}, \quad \sigma_T = \int d\Omega \frac{d\sigma}{d\Omega}
\]
Counting statistics

- Binomial distribution ($p$ scattering probability)

\[
P_{N,k} = p^k (1-p)^{N-k} \left( \begin{array}{c} N \\ k \end{array} \right), \quad \langle k \rangle = Np, \quad (\Delta k)^2 = \langle k^2 \rangle - \langle k \rangle^2 = Np(1-p)
\]

- Binomial $\rightarrow$ Poisson $\rightarrow$ Gauss

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

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

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

\[
\sigma(\theta, E) = \bar{\sigma}(\theta, E) \pm \Delta(\theta, E)
\]
Partial wave expansion (No spin)

- Scattering amplitude

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

- 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

\[ u_l(r) \xrightarrow{r \to 0} r^{l+1} , \quad u_l(r) \xrightarrow{r \to \infty} \sin \left( pr - \frac{l\pi}{2} + \delta_l \right) \]

- GOAL: Determine \( V(r) \pm \Delta V(r) \)
Finite range forces

- Meson exchange picture $\rightarrow$ 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
  
  $$V(r) \sim 0 \quad r \gtrsim r_c$$
  $$\delta_l(p) \sim 0 \quad b \gtrsim r_c$$
  
  $$\rightarrow l_{\text{max}} + \frac{1}{2} \sim pr_c \sim p/m_\pi$$

- Truncation in the partial wave expansion
  
  $$f(\theta, \phi) = \sum_{l=0}^{l_{\text{max}}} (2l + 1) \frac{e^{2i\delta_l} - 1}{2in} P_l(\cos \theta) = \frac{e^{2i\delta_0} - 1}{2in} + 3\frac{e^{2i\delta_1} - 1}{2in} \cos \theta + \ldots$$
FITTING
Single energy fits

- Complete data in a GIVEN energy $E$
  \[
  \sigma(\theta, E) \rightarrow \sigma(\theta_1, E), \ldots, \sigma(\theta_N, E)
  \]

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

- Normalization is COMMON for ONE energy
- Phase-shifts are “experimental” and MODEL INDEPENDENT
  \[
  \delta^\text{exp}_l(E) \pm \Delta\delta^\text{exp}_l(E) , \quad l = 0, \ldots, l_{\text{max}}
  \]
Multienergy analysis

- Incomplete Data in several energies and angles

\[ \sigma(\theta, E) \rightarrow \sigma(\theta_1, E_1), \ldots, \sigma(\theta_N, E_N) \]

- The need for interpolation (Smoothness in \((\theta, E)\))

- Fitting function to Fitting MODEL DEPENDENT parameters \(p = (p_1, \ldots, p_M)\)

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

- The statement

\[ \sigma(\theta_i, E_i)^{\text{exp}} = \nu_0 \sigma^{\text{th}}(\theta_i, E_i, p_0) \pm \Delta \sigma(\theta_i, E_i) \]

- Too large \(\chi^2/\nu\)
  - Bad model \(\rightarrow\) SELECT MODEL
  - Bad data \(\rightarrow\) SELECT DATA
  - Bad model and data
The $\chi^2$-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

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

![Graph showing the distribution of $\chi^2$ values with increasing degrees of freedom (dof)]
The need for selection

- Example: THE SAID DATABASE
  - PP Data No=25188 $\chi^2 = 48225.043$ (TLAB $\leq$ 3 GeV)
  - NP Data No=12962 $\chi^2 = 26079.973$ (TLAB $\leq$ 3 GeV)
  - $\pi N$ 41926 Chi2= 166585.05 (TLAB $\leq$ 3 GeV)
  - $\pi N$ 2599 Chi2= 4586.26 (TLAB $\leq$ 300)
  - $\pi N$ 1355 Chi2= 2600.75 (10 $\leq$ TLAB $\leq$ 70)

- Which experiments are INCOMPATIBLE?

- Contribution the $\chi^2$ will be large (discard BOTH ?)
- If errorbar includes BOTH no contribution to the $\chi^2$
- Incompatibility is DESTRUCTIVE
- Real physical effect?
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 \(\chi^2\) (3σ criterion)
3. Refit parameters
4. Re-apply 3σ criterion to all data
5. Repeat until no more data is excluded or recovered

---

![Graphs showing empirical and theoretical quantiles with 3σ consistent data.](image)
To believe or not to believe

$N_{\text{data}}$

<table>
<thead>
<tr>
<th></th>
<th>HJ62</th>
<th>Reid68</th>
<th>TRS75</th>
<th>Paris80</th>
<th>Urb81</th>
<th>Arg84</th>
<th>BonnR</th>
<th>Bonn89</th>
<th>Nijm93</th>
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<tr>
<td>1787</td>
<td>13.5</td>
<td>2.9</td>
<td>3.4</td>
<td>4.5</td>
<td>6.0</td>
<td>7615</td>
<td>1090</td>
<td>25.5</td>
<td>1.8</td>
</tr>
</tbody>
</table>

\[
\chi^2_{\text{min}} / \nu = 1 \pm \sqrt{2/\nu}
\]

- Charge dependence in OPE
- Magnetic-Moments, Vacuum polarization, ...
STATISTICAL CONSEQUENCES
Nucleons exchange JUST one pion

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

\[ g_p^2/(4\pi) = 13.72(7) \neq g_n^2/(4\pi) = 14.91(39) \neq g_c^2/(4\pi) = 13.81(11) \quad \chi^2/\nu = 1.02 \]
Neutron-Neutron vs Proton-Proton (Polarized)

nn interaction is more intense than pp interaction

\[ V_\pi(r) \text{(MeV)} \]

- \[ r \text{(fm)} \]

-4.0
-3.5
-3.0
0.0
0.1
0.2
0.3
0.4
3.0
3.5
4.0
4.5
5.0
r(fm)

\[ V_\pi(r) \text{(MeV)} \]

-1.6
-1.4
-1.2
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
0.1
0.2
0.3
0.4
3.0
3.5
4.0
4.5
5.0
r(fm)
Chiral Two Pion Exchange from Granada-2013 np+pp database

Compatible to Roy-Steiner

\[ c_1 = 1.11 \pm 0.03 \quad c_2 = 3.13 \pm 0.03 \quad c_3 = 5.61 \pm 0.06 \quad c_4 = 4.26 \pm 0.04 \]
\( f_{\pi N\Delta} \) from Granada-2013 np+pp database

- NN potential in the Born-Oppenheimer approximation

\[
\tilde{V}_{NN,NN}^{1\pi+2\pi+\cdots}(r) = V_{NN,NN}^{1\pi}(r) + 2 \frac{|V_{NN,N\Delta}^{1\pi}(r)|^2}{M_N - M_{\Delta}} + \frac{1}{2} \frac{|V_{NN,\Delta\Delta}^{1\pi}(r)|^2}{M_N - M_{\Delta}} + \mathcal{O}(V^3),
\]

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

\[
f_{\pi N\Delta}/f_{\pi NN} = 2.178(14) \quad \chi^2/\nu = 1.12 \rightarrow h_A = 1.397(9)
\]
Frequentist or Bayes?

- **Frequentist:** What is the probability that given a theory the data are correct?
- **Bayesian:** What is the probability that given the data the theory is correct? (priors, random parameters)

\[ \chi^2_{\text{augmented}} \rightarrow \chi^2_{\text{data}} + \chi^2_{\text{parameters}} \]

- Both approaches agree for \( N_{\text{Data}} \gg N_{\text{Parameters}} \). We have \( N_{\text{Dat}} \sim 7000 \) and \( N_{\text{Par}} = 40 \).
Maximal energy vs shortest distance

- The full potential is separated into two pieces

\[ V(r) = V_{\text{short}}(r)\theta(r_c - r) + V_{\text{long}}^\chi(r)\theta(r - r_c) \]

- Data are fitted up to a maximal \( T_{\text{LAB}} \)

\[ T_{\text{LAB}} \leq \text{max} T_{\text{LAB}} \leftrightarrow p_{\text{CM}} \leq \Lambda \]

<table>
<thead>
<tr>
<th>Max ( T_{\text{LAB}} ) MeV</th>
<th>( r_c ) fm</th>
<th>( c_1 ) GeV(^{-1})</th>
<th>( c_3 ) GeV(^{-1})</th>
<th>( c_4 ) GeV(^{-1})</th>
<th>Highest counterterm</th>
<th>( \chi^2/\nu )</th>
</tr>
</thead>
<tbody>
<tr>
<td>350</td>
<td>1.8</td>
<td>-0.4(11)</td>
<td>-4.7(6)</td>
<td>4.3(2)</td>
<td>( F )</td>
<td>1.08</td>
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<tr>
<td>350</td>
<td>1.2</td>
<td>-9.8(2)</td>
<td>0.3(1)</td>
<td>2.84(5)</td>
<td>( F )</td>
<td>1.26</td>
</tr>
<tr>
<td>125</td>
<td>1.8</td>
<td>-0.3(29)</td>
<td>-5.8(16)</td>
<td>4.2(7)</td>
<td>( D )</td>
<td>1.03</td>
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<tr>
<td>125</td>
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<td>-3.89</td>
<td>4.31</td>
<td>( P )</td>
<td>1.70</td>
</tr>
<tr>
<td>125</td>
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<td>-14.9(6)</td>
<td>2.7(2)</td>
<td>3.51(9)</td>
<td>( P )</td>
<td>1.05</td>
</tr>
</tbody>
</table>

- \( D \)-waves, forbidden by Weinberg counting, are indispensable!

- Data and \( \chi \)-N2LO do not support \( r_c < 1.8 \) fm!
  (Several \( \chi \)-potentials take \( r_c = 0.9 - 1.1 \) fm)
Deconstructing chiral forces

- The full potential is separated into two pieces
  \[ V(r) = V_{\text{short}}(r)\theta(r_c - r) + V_{\text{long}}^x(r)\theta(r - r_c) \]

- Under what conditions are the short distance phases compatible with zero
  \[ |\delta_{\text{short}}| \leq \Delta \delta \quad r_c = 1.8\text{fm} \]

- This is equivalent to set counterterms in given partial waves directly to zero
  \[ \delta_{\text{short}} = 0 \iff C_{\text{short}} = 0 \]
PERIPHERAL TESTS
Statistically equivalent interactions with $\chi^2_{\text{min}}/\nu = 1 \pm \sqrt{2/\nu}$ DO NOT overlap.
When are two protons interacting as point-like particles?

- Electromagnetic Form factor

\[ F_i(q) = \int d^3 r e^{i q \cdot r} \rho_i(r) \]

- Electrostatic interaction

\[ V_{pp}^{el}(r) = e^2 \int d^3 r_1 d^3 r_2 \frac{\rho_p(r_1)\rho_p(r_2)}{|\vec{r}_1 - \vec{r}_2 - \vec{r}|} \rightarrow \frac{e^2}{r} \quad r > r_e \approx 2\text{fm} \]
Angular momentum conservation

\[ L = bp \quad L^2 = \hbar l(l + 1) \approx (l + \frac{1}{2})^2 \quad p = \hbar k \]
Outliers

• Statistical

$$\xi^i_{\text{stat}} = \frac{\Delta^i - \Delta_{\text{Gr}}}{\Delta(\Delta_{\text{Gr}})} = \frac{\delta^i - \delta_{\text{Gr}}}{\Delta\delta_{\text{Gr}}},$$  \hspace{1cm} (1)

• Systematic (6 Gr-potentials, 6 Gr+7 HQ (Nijm, CD-Bonn,..))

$$\xi^i_{\text{sys}} = \frac{\Delta^i - \text{Mean}(\Delta)}{\text{Std}(\Delta)} = \frac{\delta^i - \text{Mean}(\delta)}{\text{Std}(\delta)},$$ \hspace{1cm} (2)

• Prob. of not being an outlier.

$$p(|\xi| > |\xi_0|) = 1 - \int_{-\xi_0}^{\xi_0} dx \frac{e^{-x^2/2}}{\sqrt{2\pi}}.$$  \hspace{1cm} (3)

- $\xi_0 = 1, 2, 3$ for $p = 0.32, 0.05, 0.01$
SAID peripheral waves

\[ L = 4 \]

\[ L = 5 \]

\[ L = 6 \]

\[ \xi_{\text{SAID}}^{G_4} \]

\[ \xi_{\text{SAID}}^{G_3} \]

\[ \xi_{\text{SAID}}^{G_5} \]

\[ \xi_{\text{SAID}}^{H_5} \]

\[ \xi_{\text{SAID}}^{H_6} \]

\[ \xi_{\text{SAID}}^{I_6} \]

\[ \xi_{\text{SAID}}^{I_5} \]
N5LO peripheral waves

\[ L = 4 \]

\[ L = 5 \]

\[ L = 6 \]

\[ \xi_{N5LO} \]

\[ b (fm) \]

\[ \epsilon_{4} \]

\[ \epsilon_{5} \]

\[ \epsilon_{6} \]
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.

$\text{N2LO-Chiral TPE + N3LO-Counterterms} \rightarrow \text{Residuals are normal}$

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 $\sigma$ incompatible