Connecting Lattice QCD Nucleon-Pion Scattering to Nuclear Ab Initio Calculations

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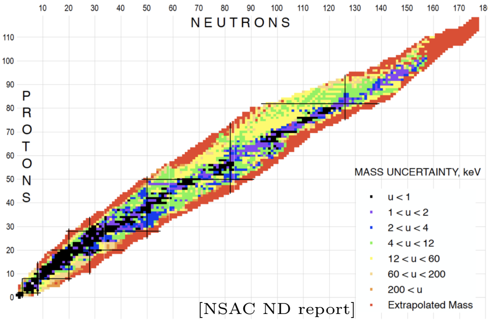
Outline

- Introduction
- Chiral Effective Field Theory and $N\pi$ Scattering
- Combined Fits with Lattice QCD
- Outlook/Conclusions

Nucleon-Pion Scattering

Nuclear Theory



[NSAC ND report]

Nuclear landscape is vast

Many short-lived nuclei with unknown properties

To describe full decay chains,
need predictions of intermediate nuclei

Chiral Effective Field Theory
is powerful tool to characterize nuclei
that are not directly accessible to experiments

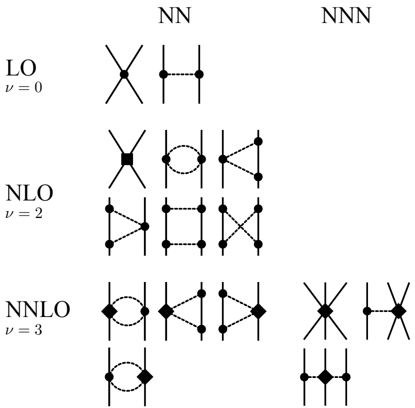
Chiral Effective Field Theory

Nuclear properties from effective interactions
between nucleons (N, solid) & pions (π, dashed)

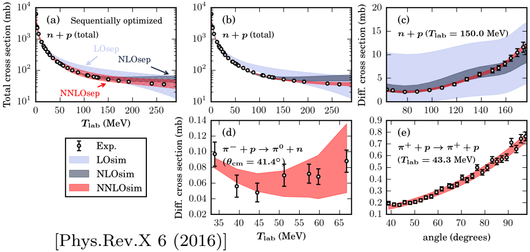
Parameterized by Low Energy Constants (LECs)
calibrated with fits to observables

c_1–$c_4 \in$ LO LECs (fit at N3LO) for $N\pi$ scattering
$\implies$ contribute to N2LO NN effective interaction

Powerful tool for predicting nuclear properties



Uncertainty Quantification



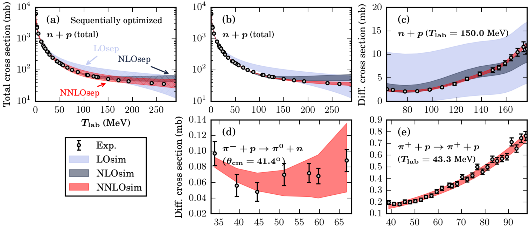
[Phys.Rev.X 6 (2016)]

LECs for χEFT typically fixed by fits to scattering phase shifts

$\Longrightarrow$ scattering phase shifts reported without uncertainties

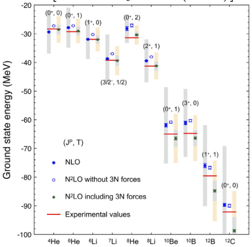
$\Longrightarrow$ scattering phase shifts well described, but nontrivial uncertainty propagation

Uncertainty Quantification



[Phys.Rev.X 6 (2016)]

[Front.Phys. 11 (2023)]



LECs for χEFT typically fixed by fits to scattering phase shifts

$\Longrightarrow$ scattering phase shifts reported without uncertainties

$\Longrightarrow$ scattering phase shifts well described, but nontrivial uncertainty propagation

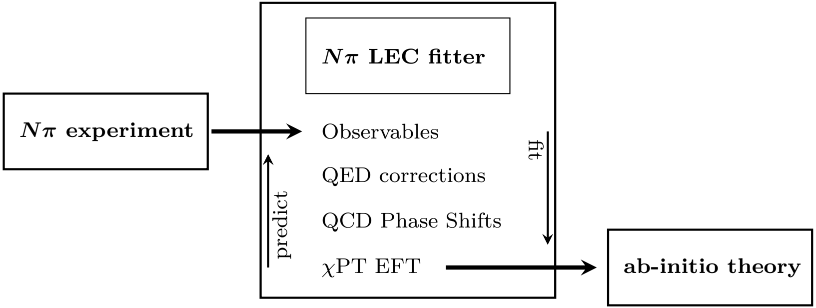
$\Longrightarrow$ some derived quantities not well described (large uncertainties, not accurate)

Improvement limited by available data, no new $N\pi$ scattering experiments forthcoming:

How can we improve predictions?

$\Longrightarrow$ Lattice Quantum Chromodynamics (LQCD)

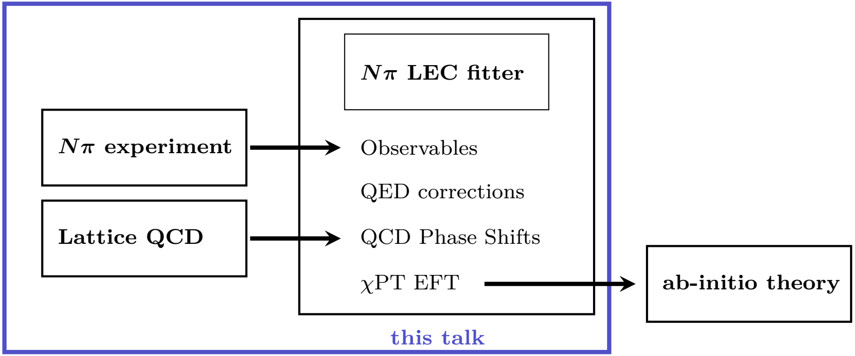
Fit Workflow



Framework to fit $N\pi$ scattering cross section data [arXiv:1410.0646[nucl-th]] [Phys.Rev.X 6 (2016)]

$\implies$ Differential unpolarized, differential singly-polarized cross sections from Washington Institute Group database [Phys.Rev.C 86 (2012)] ($N_{\text{data}} = 1347$)

Fit Workflow



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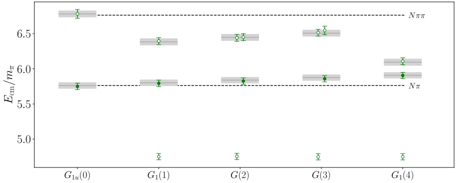
Addition of LQCD spectra to improve $N\pi$ LECs constraints [Nucl.Phys.B 987 (2023)]

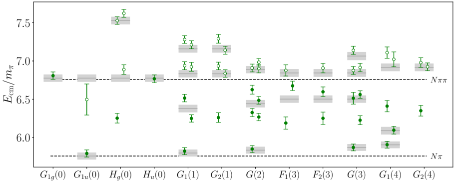
$\implies$ Isospin 3/2 $N\pi$ scattering phase shifts ($N_{\text{LQCD}} = 14$)

LQCD Combined Fit

LQCD Details

Isospin 1/2 [Nucl.Phys.B 987 (2023)] Isospin 3/2

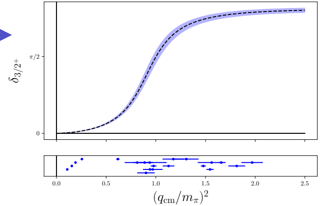




Use $M_\pi \approx 200$ result from [Bulava *et al.*]

explicit $N\pi$ operators with stochastic LapH method

$64^3 \times 128$, $a \approx 0.633$ fm; 2000 measurements



$\boldsymbol{d}$	Λ	dim.	contributing $(2J,\ell)^{n_{occ}}$ for $\ell_{max}=2$
(0,0,0)	G_{1u}	2	(1,0)
	G_{1g}	2	(1,1)
	H_g	4	(3,1), (5,2)
	H_u	4	(3,2), (5,2)
	G_{2g}	2	(5,2)
(0,0,1)	G_1	2	(1,0), (1,1), (3,1), (3,2), (5,2)
	G_2	2	(3,1), (3,2), $(5,2)^2$
(0,1,1)	G	2	(1,0), (1,1), $(3,1)^2$, $(3,2)^2$, $(5,2)^3$
(1,1,1)	G	2	(1,0), (1,1), (3,1), (3,2), $(5,2)^2$
	F_1	1	(3,1), (3,2), (5,2)
	F_2	1	(3,1), (3,2), (5,2)

Fit Procedure

Fits using determinant residual method:

$$r_i = \det\left[\mathbb{1} - B\tilde{K}\right] \qquad B: \text{ box matrix} \qquad \tilde{K}: \text{ rescaled } K \text{ matrix}$$

$$K^{-1}_{L'S'a';LSa} = u_{a'}^{-L'-\frac{1}{2}} \tilde{K}^{-1}_{L'S'a';LSa} u_a^{-L-\frac{1}{2}} \qquad u_a = \frac{L|\boldsymbol{q}_{\mathrm{cm},a}|}{2\pi}$$

Use residuals to construct covariance:

$$\chi^2_{\mathrm{LQCD}} = \sum_{ij} r_i C^{-1}_{ij} r_j$$

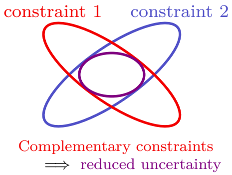
C_{ij} includes complete LQCD covariance, constructed from gradients using Gaussian error propagation

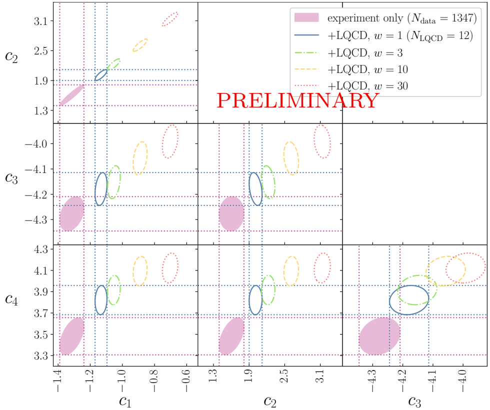
K matrix truncated to $J \leq 3/2, 5/2$; I=3/2 spectrum only

K matrix parameterized by χEFT

- NB: power series in $\boldsymbol{q}_{\mathrm{cm}}$ – no possible way to reproduce Δ channel ($K \to \infty$ for finite $\boldsymbol{q}_{\mathrm{cm}}$)
- Cut high $\boldsymbol{q}_{\mathrm{cm}}$ LQCD data in $J^P = 3/2^+$ channel

Combined Fit Covariance





$$\chi^2_{\text{total}} = \chi^2_{\text{experiment}} + w \cdot \chi^2_{\text{LQCD}}$$

$w = 1$: normal χ^2 definition including LQCD and experiment

$w = 30$: each LQCD point counted 30 times in fit

Some reduction of uncertainties (tension from LQCD?)

Drifting based on strength of LQCD weight $\Longrightarrow$ Included spectra still too high?

Concluding Remarks

Outlook

Big to-do list:

- More LQCD spectra (add isospin 1/2, *subthreshold expansion*)
- Better LQCD spectra ($M_\pi \approx 200$ MeV $\rightarrow$ 140 MeV)
- Add full χPT dependence on M_π, F_π
- Combined χPT with ERE?
- Refit NN LECs using updated $N\pi$ LECs
- Predictions with ab initio nuclear theory

Takeaway messages:

- $N\pi$ LECs are essential for quantifying interactions between nucleons
- Without modern experimental measurements, potential improvement of LEC constraints limited
- LQCD as complement to experimental data: use near threshold spectrum to better constrain LECs?

Thank you for your attention!

Backup

χET at $O(Q^4)$

$$f^{\pm}_{\ell\pm}(s) = \frac{E+m}{16\pi\sqrt{s}} \int_{-1}^{+1} dz \Big[g^{\pm} P_\ell(z) + \vec{q}^{\,2} h^{\pm} \big(P_{\ell\pm1}(z) - z P_\ell(z) \big) \Big]$$

$$\tan\, \delta^{\pm}_{\ell}(s) = |\vec{q}|\ \mathrm{Re}\Big[f^{\pm}_{\ell\pm}(s) \Big]$$

Contributions at order Q:

$$g^+ = 0\,, \qquad g^- = \frac{g_A^2\left(2M_\pi^2 - t - 2\,\omega^2\right) + 2\,\omega^2}{4F_\pi^2\,\omega}\,, \qquad h^+ = -\frac{g_A^2}{2F_\pi^2\,\omega}\,, \qquad h^- = 0\,, \tag{B.1}$$

Contributions at order Q^2:

$$g^+ = -\frac{4c_1 M_\pi^2 - 2c_2\,\omega^2 - c_3\left(2M_\pi^2 - t\right)}{F_\pi^2}\,, \qquad g^- = 0\,, \qquad h^+ = 0\,, \qquad h^- = \frac{c_4}{F_\pi^2}\,, \tag{B.2}$$

Contributions at order Q^3:

$$\begin{aligned}
g^+ &= \frac{i\sqrt{\omega^2 - M_\pi^2}\left(g_A^4\left(M_\pi^2 - \omega^2\right)\left(2M_\pi^2 - t - 2\,\omega^2\right) + 3\,\omega^4\right)}{24\pi F_\pi^4\omega^2} - \frac{g_A^2 \tilde{K}_0(t)\left(2M_\pi^4 - 5M_\pi^2 t + 2t^2\right)}{8F_\pi^4} \\
&+ \frac{g_A^2 M_\pi\left(4g_A^2 M_\pi^2\left(2M_\pi^2 - t - 2\,\omega^2\right) + 3\,\omega^2\left(M_\pi^2 - 2t\right)\right)}{96\pi F_\pi^4\omega^2} - \frac{g_A^2\left(4M_\pi^4 - 4M_\pi^2 t + t\left(t + 4\omega^2\right)\right)}{16F_\pi^2 m\,\omega^2}\,, \\
g^- &= \frac{(\bar{d}_1 + \bar{d}_2)\left(4M_\pi^2\,\omega - 2t\,\omega\right)}{F_\pi^2} + \frac{4\bar{d}_3\,\omega^3}{F_\pi^2} + \frac{8\bar{d}_5 M_\pi^2\,\omega}{F_\pi^2} + \frac{\bar{d}_{18} g_A M_\pi^2\left(-2M_\pi^2 + t + 2\,\omega^2\right)}{F_\pi^2\,\omega} \\
&+ \frac{\tilde{J}_0(\omega)\left(g_A^4\left(M_\pi^2 - \omega^2\right)\left(2M_\pi^2 - t - 2\,\omega^2\right) + 6\,\omega^4\right)}{12F_\pi^4\,\omega^2} + \frac{i\sqrt{\omega^2 - M_\pi^2}\left(g_A^4\left(M_\pi^2 - \omega^2\right)\left(2M_\pi^2 - t - 2\,\omega^2\right) + 6\,\omega^4\right)}{96\pi F_\pi^4\,\omega^2} \\
&+ \frac{g_A^4\left(3M_\pi^2 - 2\,\omega^2\right)\left(2M_\pi^2 - t - 2\,\omega^2\right) - g_A^2\,\omega^2\left(12M_\pi^2 + t\right) + \omega^2\left(t - 6M_\pi^2\right)}{288\pi^2 F_\pi^4\,\omega} \\
&+ \frac{\tilde{I}_{20}(t)\,\omega\left(-4\left(2g_A^2 + 1\right)M_\pi^2 + 5g_A^2 t + t\right)}{12F_\pi^4} - \frac{\left(-4M_\pi^2 + t + 4\,\omega^2\right)\left(g_A^2\left(2M_\pi^2 - t + 2\,\omega^2\right) - 2\,\omega^2\right)}{16F_\pi^2 m\,\omega^2}\,, \\
h^+ &= \frac{2(\bar{d}_{14} - \bar{d}_{15})\,\omega}{F_\pi^2} + \frac{2\bar{d}_{18} g_A M_\pi^2}{F_\pi^2\,\omega} + \frac{g_A^4 \tilde{J}_0(\omega)\left(\omega^2 - M_\pi^2\right)}{6F_\pi^4\,\omega^2} + \frac{i g_A^4\left(\omega^2 - M_\pi^2\right)^{3/2}}{48\pi F_\pi^4\,\omega^2} - \frac{g_A^4\left(3M_\pi^2 + 4\,\omega^2\right)}{144\pi^2 F_\pi^4\,\omega} + \frac{g_A^2\left(t - 4M_\pi^2\right)}{8F_\pi^2 m\,\omega^2}\,, \\
h^- &= \frac{i g_A^4\left(\omega^2 - M_\pi^2\right)^{3/2}}{24\pi F_\pi^4\,\omega^2} + \frac{g_A^2 \tilde{K}_0(t)\left(4M_\pi^2 - t\right)}{8F_\pi^4} - \frac{4g_A^4 M_\pi^3 + 3g_A^2 M_\pi\,\omega^2}{96\pi F_\pi^4\,\omega^2} + \frac{g_A^2\left(2M_\pi^2 - t - 2\,\omega^2\right) + 2\,\omega^2}{8F_\pi^2 m\,\omega^2}\,,
\end{aligned} \tag{B.3}$$

Contributions at order Q^4:

$$\begin{aligned}
g^+ &= \frac{2c_1 \tilde{I}_{20}(t) M_\pi^2\left(M_\pi^2 - 2t\right)}{F_\pi^4} + c_2\left(-\frac{\tilde{I}_{20}(t)\left(4M_\pi^4 - 9M_\pi^2 t + 2t^2\right)}{12F_\pi^4} - \frac{6M_\pi^4 - 13M_\pi^2 t + 2t^2}{288\pi^2 F_\pi^4} + \frac{\omega\left(-4M_\pi^2 + t + 4\,\omega^2\right)}{F_\pi^2 m}\right) \\
&- \frac{c_3 \tilde{I}_{20}(t)\left(2M_\pi^4 - 5M_\pi^2 t + 2t^2\right)}{2F_\pi^4} + \frac{4\bar{e}_{14}\left(t - 2M_\pi^2\right)^2}{F_\pi^2} + \frac{8\bar{e}_{15}\,\omega^2\left(2M_\pi^2 - t\right)}{F_\pi^2} + \frac{16\bar{e}_{16}\,\omega^4}{F_\pi^2} \\
&+ \frac{4M_\pi^2\left(2\bar{e}_{19} - \bar{e}_{22} - \bar{e}_{36} + 2\bar{l}_3 c_1 F_\pi^{-2}\right)\left(2M_\pi^2 - t\right)}{F_\pi^2} + \frac{16\left(\bar{e}_{20} + \bar{e}_{35}\right)M_\pi^2\,\omega^2}{F_\pi^2} + \frac{8\left(\bar{e}_{22} - 4\bar{e}_{38} - \bar{l}_3 c_1 F_\pi^{-2}\right)M_\pi^4}{F_\pi^2}\,, \\
g^- &= -\frac{i c_1 M_\pi^2\,\omega\sqrt{\omega^2 - M_\pi^2}}{\pi F_\pi^4} + \frac{i c_2\,\omega^3\sqrt{\omega^2 - M_\pi^2}}{2\pi F_\pi^4} \\
&+ c_3\left(\frac{g_A^2 M_\pi^3\left(2M_\pi^2 - t - 2\,\omega^2\right)}{12\pi F_\pi^4\,\omega} + \frac{i\sqrt{\omega^2 - M_\pi^2}\left(g_A^2\left(M_\pi^2 - \omega^2\right)\left(2M_\pi^2 - t - 2\,\omega^2\right) + 6\,\omega^4\right)}{12\pi F_\pi^4\,\omega}\right) \\
&+ c_4\left(-\frac{i g_A^2\left(\omega^2 - M_\pi^2\right)^{3/2}\left(-2M_\pi^2 + t + 2\,\omega^2\right)}{12\pi F_\pi^4\,\omega} + \frac{g_A^2 M_\pi^3\left(-2M_\pi^2 + t + 2\,\omega^2\right)}{12\pi F_\pi^4\,\omega} + \frac{t\,\omega}{2F_\pi^2 m}\right)\,, \\
h^+ &= (c_3 - c_4)\left(\frac{i g_A^2\left(\omega^2 - M_\pi^2\right)^{3/2}}{6\pi F_\pi^4\,\omega} - \frac{g_A^2 M_\pi^3}{6\pi F_\pi^4\,\omega}\right)\,, \\
h^- &= c_4\left(\frac{4g_A^2 \tilde{J}_0(\omega)\left(M_\pi^2 - \omega^2\right)}{3F_\pi^4\,\omega} + \frac{-6\left(5g_A^2 + 1\right)M_\pi^2 + 8g_A^2\,\omega^2 + t}{144\pi^2 F_\pi^4} + \frac{i g_A^2\left(M_\pi^2 - \omega^2\right)\sqrt{\omega^2 - M_\pi^2}}{6\pi F_\pi^4\,\omega}\right. \\
&+ \left.\frac{\tilde{I}_{20}(t)\left(t - 4M_\pi^2\right)}{6F_\pi^4} + \frac{\omega}{F_\pi^2 m}\right) + \frac{\bar{e}_{17}\left(8M_\pi^2 - 4t\right)}{F_\pi^2} + \frac{8\bar{e}_{18}\,\omega^2}{F_\pi^2} + \frac{8\left(\bar{e}_{21} - \frac{\bar{e}_{37}}{2}\right)M_\pi^2}{F_\pi^2}\,.
\end{aligned} \tag{B.4}$$

[Phys.Rev.C 85 (2012)]