Ab initio nuclear physics with chiral EFT

Andreas Ekström (UT/ORNL)
- Simultaneous optimization
- UQ applied to proton-proton fusion
- Chiral EFT tailored to the HO-basis
- Optimizing the 3NF at N3LO
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Overview

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1. Diversify and extend the statistical analysis and perform a sensitivity analysis of input data.
Overview

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2. Explore alternative strategies of informing the model about low-energy many-body observables.

Robust parameter estimation
Three-nucleon scattering data.
The information content of heavy nuclei.

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   Robust parameter estimation
   Three-nucleon scattering data.
   The information content of heavy nuclei.

2. Explore alternative strategies of informing the model about low-energy many-body observables.

3. Continue efforts towards higher orders of the chiral expansion, and possibly revisit the power counting.

   Delta resonances
   Other regulators
   Lattice QCD data
   Modified PC

Simultaneous optimization
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Optimizing the 3NF at N3LO

Simultaneous optimization

*chiral EFT is our tool to analyze the nuclear interaction*

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We optimize the LECs such that the chiral interactions reproduces some calibration data, then we predict!

E. Epelbaum et al. Rev. Mod. Phys. 81, 1773 (2009)
Simultaneous optimization

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the same LECs appear in the expressions for various low-energy processes e.g. the $c_i$ (green dot) and $c_D$ (blue square)

- two-nucleon interaction
- pion-nucleon scattering
- three-nucleon interaction
- three-nucleon interaction
- external probe current
Simultaneous optimization

**chiral EFT is our tool to analyze the nuclear interaction**

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$
\chi^2(p) \equiv \sum_{i \in M} R_i^2(p) = \sum_{k \in \pi N} R_{k}^{2}(p) + \sum_{j \in NN} R_{j}^{2}(p) + \sum_{l \in NNN} R_{l}^{2}(p)
$
Simultaneous optimization is critical in order to
  • find the optimal set of LECs.
  • capture all relevant correlations between them.
  • reduce the statistical uncertainty.
  • attain order-by-order convergence.

Within such an approach we find that statistical errors are, in general, small, and that the total error budget is dominated by systematic errors.
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All 42 different sim/sep potentials, as well as the respective covariance matrices are available as supplemental material.

LO-NLO-NNLO
7 different cutoffs: 450, 475, ..., 600 MeV
6 different NN-scattering datasets

\[
\text{Cov}(A, B) \equiv \mathbb{E}[(O_A(p) - \mathbb{E}[O_A(p)])(O_B(p) - \mathbb{E}[O_B(p)])]
\approx \mathbb{E}[(\tilde{J}_{A,i} x_i + \frac{1}{2} \tilde{H}_{A,ij} x_i x_j - \frac{1}{2} \tilde{H}_{A,ii} \sigma_i^2) \times (\tilde{J}_{B,k} x_k + \frac{1}{2} \tilde{H}_{B,kl} x_k x_l - \frac{1}{2} \tilde{H}_{B,kk} \sigma_k^2)]
= \tilde{J}_A^T \Sigma \tilde{J}_B + \frac{1}{2} (\sigma^2)^T (\tilde{H}_A \circ \tilde{H}_B) \sigma^2,
\]

compute the derivatives of your own observables wrt LECs, then explore:

- cutoff variations
- order-by-order evolution
- LEC UQ/correlations
In the core of the Sun, energy is released through sequences of nuclear reactions that convert hydrogen into helium. The primary reaction is thought to be the fusion of two protons with the emission of a low-energy neutrino and a positron.

\[
p + p \rightarrow d + e^+ + \nu_e
\]

\[
S(E) = \sigma(E) E e^{2\pi\eta}
\]

\[
\sigma(E) = \int \frac{d^3 p_e}{(2\pi)^3} \frac{d^3 p_\nu}{(2\pi)^3} \frac{1}{2E_e} \frac{1}{2E_\nu} \times 2\pi\delta \left(E + 2m_p - m_d - \frac{q^2}{2m_d} - E_e - E_\nu\right)
\]

\[
\frac{1}{\nu_{\text{rel}}} F(Z, E_e) \frac{1}{4} \sum |\langle f | \hat{H}_W | i \rangle|^2
\]

In collaboration with B. Acharya, L. Platter, B. D. Carlsson, and C. Forssen

L. E. Marcucci et al. PRL 110, 192503 (2013)
R. Schiavilla et al. PRC 58, 1263 (1998)
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\[
S(0) \left( 10^{-23} \text{ MeV fm}^3 \right)
\]

\[
c_4 \left( \text{GeV}^{-1} \right)
\]

In collaboration with B. Acharya, L. Platter, B. D. Carlsson, and C. Forssen
UQ applied to proton-proton fusion

\[ S(0) \left(10^{-23} \text{ MeV fm}^2\right) \]

\[ \Lambda_{EFT} \text{ (MeV)} \]

Preliminary

Statistical uncertainty

cutoff variation

[Graph showing the relationship between \( S(0) \) and \( \Lambda_{EFT} \), with \( T_{Lab} \) variations indicated]
UQ applied to proton-proton fusion

\[ S(0) \text{ (10}^{-23} \text{ MeV fm}^2) \]

\[ \Lambda_{\text{EFT}} \text{ (MeV)} \]

\[ T_{\text{Lab}} \]

\[ \text{correlation analysis:} \]
\[ S(0) - E(2H): \text{phase space} \]
\[ \Lambda^2 - r(2H): \text{radial overlap} \]
\[ \Lambda^2 - rQ(2H): \text{radial overlap} \]
\[ \delta_{2B} - E1A: 2B-current operator \]
UQ applied to proton-proton fusion

**Correlation analysis:**

- $S(0) - E(2\text{H})$: phase space
- $\Lambda^2 - r(2\text{H})$: radial overlap
- $\Lambda^2 - Q(2\text{H})$: radial overlap
- $\delta_{2B} - E_1(3\text{He})$: $2B$-current operator
- $r_{pt-p}(3\text{He})$
- $r_{pt-p}(4\text{He})$
- $E(3\text{He})$
- $E(3\text{He})$
- $E(4\text{He})$
- $D(2\text{H})$
- $Q(2\text{H})$
- $r_{pt-p}(2\text{H})$
- $E(2\text{H})$
- $S(0)$
- $\Lambda^2$
- $\delta_{2B}$

---

- Insofar most consistent xEFT-study of this reaction
- Correlation study indicates sound statistical analysis
- Cutoff variation not large source of error
- Statistical error in $S(0)$ is 3 times larger than what was previously thought
- Central value is most likely also larger due to previously neglected systematic uncertainties.

**Preliminary**

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- $S(0)$ (10$^{-23}$ MeV fm$^2$)
- $\Lambda_{\text{EFT}}$ (MeV)
- $T_{\text{Lab}}$
- cutoff variation
- statistical uncertainty
- $\Sigma_0$ - $\Lambda^2$ - $\delta_{2B}$ - $E(2\text{H})$ - $r_{pt-p}(2\text{H})$ - $Q(2\text{H})$ - $D(2\text{H})$ - $E(3\text{He})$ - $r_{pt-p}(3\text{He})$ - $E_1(3\text{He})$ - $E(4\text{He})$ - $r_{pt-p}(4\text{He})$
converging heavy nuclei with \textit{ab initio} methods
Nuclei in the Harmonic Oscillator basis

\[ (N_{max}, \omega) \rightarrow (\Lambda_{UV}, L) \]

\[ \Lambda_{UV} \approx \sqrt{2N_{max} \frac{m\omega}{\hbar}} \]

\[ L \approx \sqrt{2N_{max} \frac{\hbar}{m\omega}} \]

Nucleus needs to fit into the modelspace

\[ L > R_{nucleus} \]

Interaction must be captured

\[ \Lambda_{UV} > \Lambda_{\chi} \]
Nuclei in the Harmonic Oscillator basis

- Converging calculations beyond ~calcium becomes truly expensive, or even impossible.
- *Ab initio* calculations usually carried out at several different oscillator energies $\hbar \omega$ to gauge the model dependence of the results
- To facilitate calculations in heavy nuclei we propose to **tailor the EFT interaction to a finite HO basis**

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Similar ideas in nuclear physics already exist:

\textbf{Arizona group} developed pionless-EFT in HO basis and studied UV/IR cutoff dependencies. Coupling constants depend on the size of the basis.

\textbf{Haxton et al.} proposed HOBET (HO-based effective theory). “Shell-Model” (Bloch-Horowitz) plus resummed kinetic energy and physics beyond a cutoff absorbed by contact-gradient expansion (like EFT contact potential).

\textbf{We propose} to choose (and fix) an oscillator space and evaluate the \textit{existing} chiral EFT interaction operators in this space. This \textit{projection} requires us to refit the LECs of chiral EFT.
EFT interaction in a truncated HO basis

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\[ N = \left\lfloor \frac{N_{\text{max}} - \ell}{2} \right\rfloor \]

EFT interaction in a truncated HO basis

\[ n' \quad n \]

\[ (N_{\text{max}}, \omega) \rightarrow (A_{\text{UV}}, L) \]

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\((N_{\text{max}}, \omega) \to (\Lambda_{UV}, L)\)
EFT interaction in a truncated HO basis

**simple picture:** choose e.g. $N_{\text{max}} = 10$, $\hbar \omega = 40 \text{ MeV}$

set $\langle n|V|n' \rangle$ to zero outside $N_{\text{max}}$

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"thinking inside the box"
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Optimize the LECs to reproduce selected fit-data
we can compute phase shifts using the J-matrix formalism, and finite nuclei using e.g. NCSM, CC, IM-SRG, ….

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However, in the longer perspective, we seek to develop an EFT. So it is important to understand the squared momentum operator

$$\langle n\ell | \hat{p}^2 | n' \ell' \rangle$$

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We start by solving the eigenvalue problem of the squared momentum operator in a finite oscillator space truncated at an energy $(N_{\text{max}} + 3/2)\hbar \omega$. It turns out that momenta $k = k_\mu$ such that $\psi_{N+1}(k) = 0$ solve this eigenvalue problem.

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$$\psi_{n\ell}(k) = \sqrt{\frac{2n!b^3}{\Gamma(n + \ell + \frac{3}{2})}} (kb)^\ell e^{-\frac{1}{2}k^2b^2} L_{n+\frac{1}{2}}^{\ell+\frac{1}{2}}(k^2b^2)$$

This has pleasant consequences for most analytical and numerical evaluations!
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This has pleasant consequences for most analytical and numerical evaluations!

In harmonic oscillator EFT we compute matrix elements of the chiral interaction $V$ as:

$$\langle n \ell | V | n' \ell' \rangle = \sum_{\mu \nu = 0}^{N} c_{\mu \ell}^2 \psi_{n, \ell}(k_\mu, \ell) \langle k_\mu, \ell | V | k_\nu, \ell', \ell' \rangle c_{\nu', \ell'}^2 \psi_{n', \ell'}(k_\nu, \ell') + O(k^{2N+2})$$

Idaho-N3LO in the Harmonic Oscillator basis

S. Binder, A. Ekstrom, G. Hagen, T. Papenbrock, and K. A. Wendt
arXiv:1512.03802 [nucl-th]
selected proton-neutron phase shifts of Idaho-N3LO(500) projected onto an $N_{\text{max}}=10$, $h\nu=40$ MeV oscillator space

\[ \Lambda_{\nu \nu} = 700 \ \text{MeV} > \Lambda_{\chi} = 500 \ \text{MeV} \]
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OBSERVATIONS:

- There are oscillations in the phase shifts
- The period of this oscillation is approximately proportional to the IR cutoff
- Gauss-Laguerre (“HO-EFT”) phases exhibit slightly smaller oscillations than the “exact” phases
- At the energies corresponding to the eigenenergies of the truncated Hamiltonian (solid dots), computed phases are closest to the true N3LO value

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Increasing N and/or hw gives "smaller" oscillations.
Refitting the NLO interaction to CD-Bonn phases

With goal of computing heavy nuclei, we design a HO-NLO interaction with:

- small number of oscillator shells \( N_{\text{max}} = 10 \)
- Lower frequencies, rapid IR convergence
- Lower frequencies, lower UV cutoffs

We choose \( \hbar w = 24 \text{ MeV} \), which gives:
\[ \Lambda_{\text{UV}} = 550 \text{ MeV}, \quad L = 9.6 \text{ fm}. \]
Considering the tail of the chiral regulator function, we set \( \Lambda_{\chi} = 450 \text{ MeV} \).
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<th>$r_d$ [fm]</th>
<th>$Q_d$ [fm$^2$]</th>
<th>$P_d$</th>
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See G. Hagen’s talk for HO-EFT in Coupled Cluster

Some open questions that we are currently addressing
Open questions, and next steps

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Next step: HO-NNLO$_{\text{sat}}$
NNN-N3LO: simple cD/cE scan with Idaho-N3LO

2π  2π-1π  rings  2π-contact

+ rel. corr.

NNN-N3LO: simple cD/cE scan with Idaho-N3LO

Idaho-N3LO + 3NF(N3LO) $\hbar\omega = 36$ MeV $N_{\text{max}} = 40/20$

$^3$H  $^4$He

NNN-N3LO: simple cD/cE scan with Idaho-N3LO

Expectation values (in MeV and fm)

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<td>N3LO</td>
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Initialize by computing phase shifts for $10^5$ random contact LEC values for each partial wave and select the ~1000 best values and optimize. This leads to 192 different optima (for cutoff 450 MeV) with respect to phase shifts. (pi-N LECs from sep-optimization)

The $A=3$ observables weed out several of the S-wave minima, but many P-wave minima remain. Things improve when $A=4$ is included. But still, several local minima remain.

This is where we stand right now.
N3LO optimizations are challenging

Work led by B. D. Carlsson (Chalmers)

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Phase shifts from Granada analysis: Navarro Pérez et al PRC 88, 064002 (2013)
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Summary and conclusions

- **Covariance matrices** for optimized LO-NLO-NNLO potentials available for download

- **Small variations** in the nuclear interaction renders large fluctuations in predictions for heavier nuclei

- **Harmonic Oscillator EFT** could be a promising approach for ab initio studies of heavy atomic nuclei

- **Non-local 3NF at N3LO** is not constrained by \( A=2,3 \) data

- **N3LO optimizations** benefit from gradients
Thank you for your attention

and thanks to all collaborators!

Bijaya Acharya
Sven Binder
Boris D. Carlsson
Christian Forssen
Gaute Hagen
Gustav Jansen
Oskar Lilja
Mattias Lindby
Björn Mattsson
Thomas Papenbrock
Lucas Platter
Dag Fahlin Strömberg
Kyle Wendt