Chiral effective field theory for nuclear forces and the dense matter equation of state

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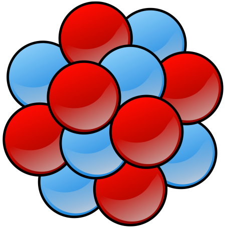
Outline

1. Chiral EFT (χEFT) and nuclear forces
2. Bayesian uncertainty quantification (UQ) in ab initio nuclear theory
3. Many-body perturbation theory (MBPT) calculations of nuclear matter
4. Posterior predictive distributions for nuclear matter (preliminary!)
5. New χEFT bands for dense matter equation of state (EOS)

Making predictions in nuclear theory

The time-independent Schrödinger equation:

$$(\hat{H}_0 + \hat{V})\,|\Psi\rangle = E\,|\Psi\rangle$$



We need:

1. a model for the interaction potential $\hat{V}$:
   chiral effective field theory
2. a many-body method for solving the S.E.

2-body scattering: Solving Lippmann-Schwinger equation

Many-body methods: NCSM, QMC, ... (light systems, $A \lesssim 16$), CC, IMSRG, MBPT, ... (not-so-light systems)

χEFT and nuclear forces

χEFT:

- Systematic expansion in low momenta: $(Q/\Lambda_b)^k$
- Power counting: assigns each contribution to an order k^a
- Orders designated leading order (LO), next-to-leading order (NLO), N^2LO, N^3LO, ...
- Many-body forces enter consistently at sub-leading orders

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^{a}No contributions for $k = 1$.

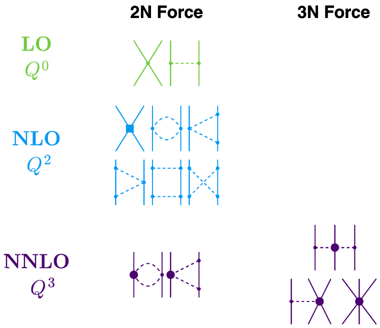


Figure adapted from Entem et al., Phys. Rev. C 96 (2017).

(Weinberg, van Kolck, Kaplan, Savage, Wise, Bernard, Epelbaum, Kaiser, Meißner, ...)

χEFT and nuclear forces

- Two main variants: Δ-less (previous slide) and Δ-full
- Degrees of freedom in Δ-less: nucleons and pions
- Additionally in Δ-full: $\Delta(1232)$-isobar

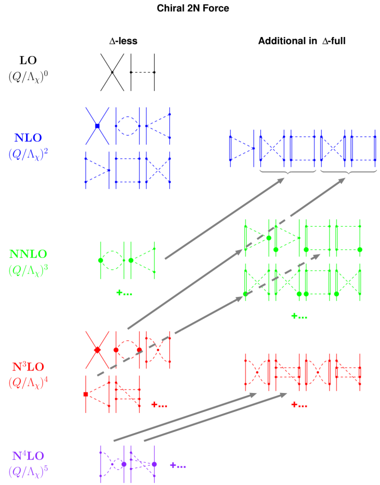


Figure from Machleidt & Entem, Phys. Rept. 503 (2011).

χEFT and nuclear forces - UQ

χEFT (in principle) enables **uncertainty quantification**:

- Each order suppressed by $\sim (Q/\Lambda_b) < 1$ (gives a handle on **truncation errors**)
- Short-range physics accounted for by unknown **low-energy constants** (LECs)
- Number of LECs grows with order: ~ 15 at N^2LO, ~ 30 at N^3LO
- LECs ($\vec{\alpha}$) fitted to scattering and other nuclear observables

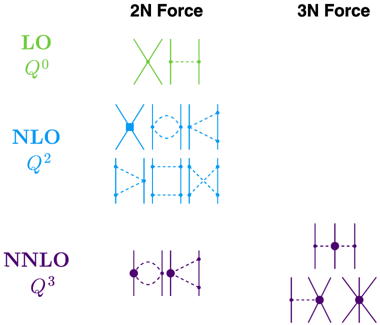


Figure adapted from Entem et al., Phys. Rev. C 96 (2017).

Bayesian UQ for χEFT pioneered by the BUQEYE collaboration: Furnstahl, Melendez, Phillips, Wesolowski ...

Bayesian UQ in ab initio nuclear theory

Based on my PhD work in collaboration with Andreas Ekström and Christian Forssén (and BUQEYE): Svensson et al., Phys. Rev. C 105 (2022), Phys. Rev. C 107 (2023), arXiv:2304:02004; Wesolowski et al., Phys. Rev. C 104 (2021)

Bayesian UQ in ab initio nuclear theory

Most common approach to fitting LECs: optimization to (mainly 2-body) nuclear observables/phaseshifts

Has yielded many accurate interactions. To mention a few: Entem & Machleidt Phys. Rev. C 68 (2003), Hebeler et al. Phys. Rev. C 83 (2011), Carlsson et al. Phys. Rev. X 6 (2016), Jiang et al. Phys. Rev. C 102 (2020)

But rigorous UQ is lacking

Bayesian inference and predictions

We make predictions of y using a **posterior predictive distribution (PPD)**:

$$\mathrm{pr}(y|D,I) = \int \mathrm{pr}(y|\vec{\alpha},I)\mathrm{pr}(\vec{\alpha}|D,I)d\vec{\alpha}$$

For this we need the joint **posterior** for the LECs $\mathrm{pr}(\vec{\alpha}|D,I)$. **Bayes' theorem**:

$$\underbrace{\mathrm{pr}(\vec{\alpha}|D,I)}_{\text{Posterior}} \propto \underbrace{\mathrm{pr}(D|\vec{\alpha},I)}_{\text{Likelihood}} \times \underbrace{\mathrm{pr}(\vec{\alpha}|I)}_{\text{Prior}}$$

We include experimental errors and truncation errors[1] in our analyses. Our priors are grounded in EFT.

[1] Both uncorrelated and (in the latest paper) correlated.

(Breaking) the curse of dimensionality

Problem: $\mathrm{pr}(\vec{\alpha}\vert D, I)$ is multidimensional ($\sim$ 15-30 parameters). Must use Markov chain Monte Carlo (MCMC).

Even with MCMC, sampling $\mathrm{pr}(\vec{\alpha}|D, I)$ is very challenging due to (i) the dimensionality and (ii) computational cost of calculating observables.

Our approach: use **Hamiltonian Monte Carlo**[2] (HMC), which is uniquely suited to high-dimensional problems

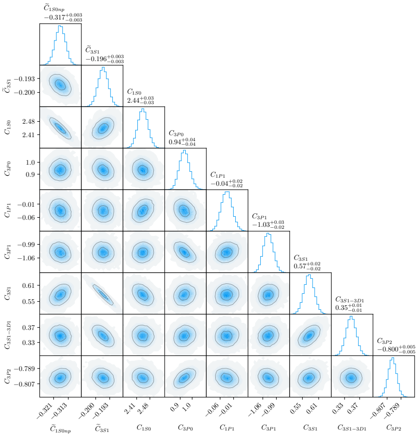
HMC uses **gradients** of the posterior to increase sampling efficiency.

We have found that HMC is $\sim$ **5 times more efficient** than the popular Emcee[3] in our application.

[2] Duane et al., Phys. Lett. B **195**(2) (1987)

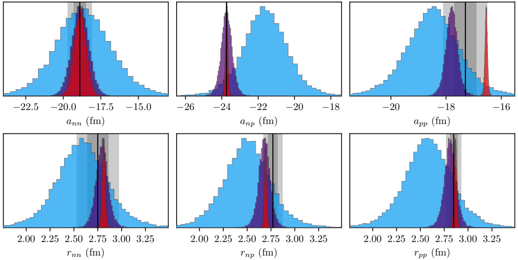
[3] Foreman-Mackey et al., PASP **125** (2013)

LEC posteriors $\longrightarrow$ observable PPDs



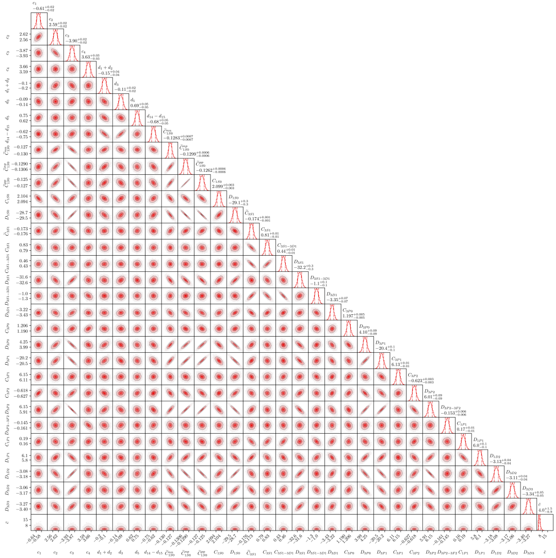
Example 9-dimensional NLO posterior (arXiv:2304:02004).

Blue: NLO
Purple: N^{2}LO
Red: N^{3}LO



PPDs for effective range parameters [Phys. Rev. C 107 (2023)]

Demonstrating the sampling capabilities of HMC



31-dimensional N^3LO LEC posterior [Phys. Rev. C 107 (2023)].

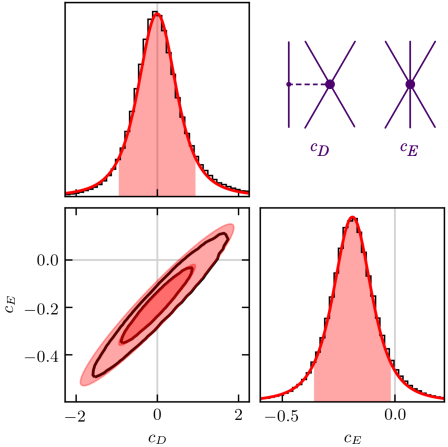
I can zoom in if you want to see details!

Inferring three-nucleon forces

Three-nucleon forces play an essential role in the description of many-body systems.

In collaboration with BUQEYE we have inferred the two leading $3N$ LECs (c_D, c_E).

Practically usable data are rather lacking as many observables provide degenerate constraints.



Posterior for three-nucleon force LECs c_D, c_E [Wesolowski, IS, et al., Phys. Rev. C 104 (2021)]

Some take-aways

Fully Bayesian UQ is now possible in nuclear theory.

but

Much work remains on accurate error modeling[4]. The fixed-LEC interactions mentioned earlier provide more reliable results.

[4] See, e.g., BUQEYE: Millican et al., 2402.13165.

Goal: combine EOS calculations with Bayesian UQ

MBPT calculations of nuclear matter EOS by Keller et al.:

PHYSICAL REVIEW LETTERS **130,** 072701 (2023)

Nuclear Equation of State for Arbitrary Proton Fraction and Temperature Based on Chiral Effective Field Theory and a Gaussian Process Emulator

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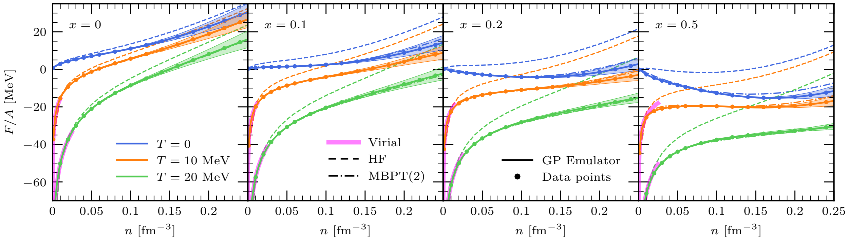
See also previous work by Christian Drischler

MBPT calculations of nuclear matter EOS at N^{3}LO

Pure neutron matter Symmetric nuclear matter



Energy per particle as a function of number density for temperature $T = 0$, 10, 20 MeV and proton fraction $x = 0.0$, 0.1, 0.2, 0.5.

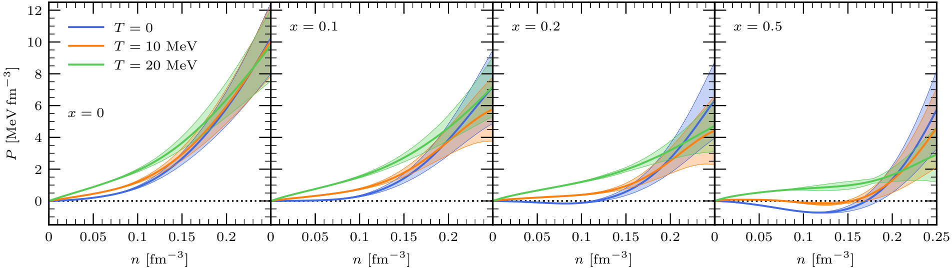
Uncertainty bands using the **EKM prescription**[5] (i.e., not a Bayesian approach):

$$\Delta y^{(k)} = \frac{Q}{\Lambda_b} \max\left(|y^{(k)} - y^{(k-1)}|, \Delta y^{(k-1)}\right)$$

[5] Epelbaum et al., Eur. Phys. J. A 51 (2015)

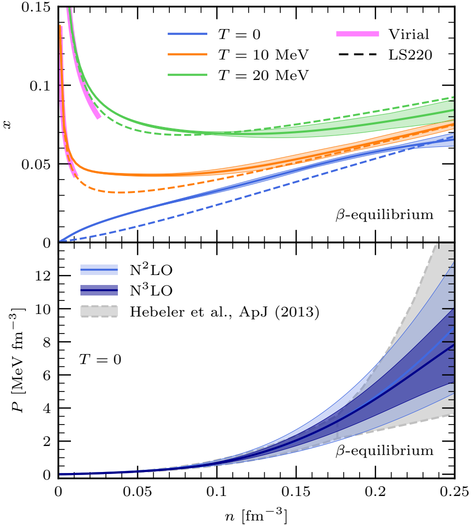
MBPT calculations of nuclear matter EOS at N^{3}LO

Pure neutron matter Symmetric nuclear matter



Pressure as a function of number density for temperature $T = 0$, 10, 20 MeV and proton fraction $x = 0.0$, 0.1, 0.2, 0.5.

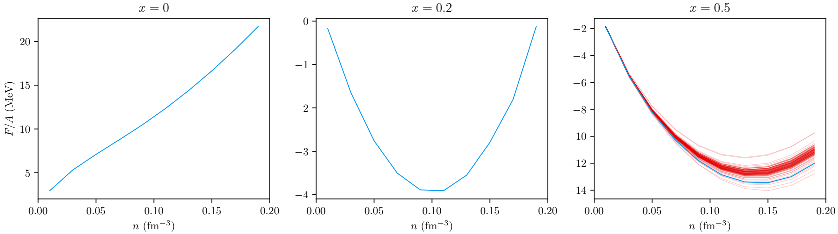
MBPT calculations of nuclear matter EOS at N^3LO



Top: Proton fraction in β-equilibrium as a function of density

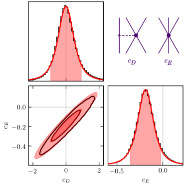
Bottom: Pressure in β-equilibrium as a function of density
N^2LO and N^3LO bands up to $1.5n_0$
Hebeler et al. up to $1.1n_0$, then a piecewise polytrope high-density parametrization

Preliminary: PPD for nuclear matter EOS



Red: PPD for the energy per particle for symmetric nuclear matter at zero temperature.
Blue: results from Keller et al. 2023.

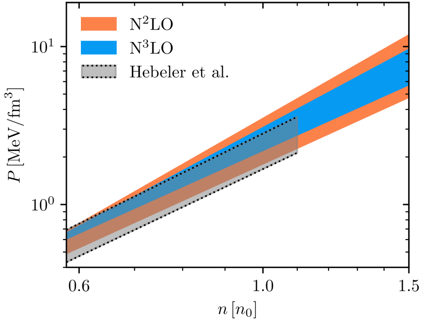
Ongoing work with Achim Schwenk, Kai Hebeler, Hannah Göttling, Alex Tichai: PPDs for nuclear matter EOS including LEC variations, correlated truncation errors, MBPT method error. Arbitrary proton fraction and temperature.



Constraining the dense matter equation of state with new NICER mass-radius measurements and new chiral effective field theory inputs

Nathan Rutherford,[1] Melissa Mendes,[2,3,4] Isak Svensson,[2,3,4] Achim Schwenk,[2,3,4] Anna L. Watts,[5]
Kai Hebeler,[2,3,4] Jonas Keller,[2,3] Chanda Prescod-Weinstein,[1] Devarshi Choudhury,[5]
Geert Raaijmakers,[6] Tuomo Salmi,[5] Patrick Timmerman,[5] Serena Vinciguerra,[5]
Sebastien Guillot,[7,8] and James M. Lattimer[9]

Submitted to ApJL a few weeks ago; see Melissa's talk tomorrow



Pressure as a function of density for matter in β-equilibrium.

- New bands include muons in addition to electrons and neutrons/protons
- We trust χEFT to higher density ($1.5 n_0$)
- New bands calculated directly in β-equilibrium; Hebeler bands use an empirical parametrization
- Plan: map bands to LECs

Outlook

- Simultaneous Bayesian inference for 2- and 3-body forces
- Improved modeling of errors—lots of work remains
- Improved UQ for nuclear matter calculations with correlated truncation errors using Gaussian processes (talk to Hannah Göttling!)
- Improved inferences of neutron star properties as new data become available (see Melissa's talk)

Thank you! Collaborators:

Yannick Dietz
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Jonas Keller
Jordan Melendez
Melissa Mendes
Daniel Phillips
Nathan Rutherford
Achim Schwenk
Alex Tichai
Anna L. Watts
Sarah Wesolowski
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