

Bayesian uncertainty analysis of the elastic nucleon-deuteron scattering observables



Yuriy Volkotrub¹, Daniel Phillips², Filomena Nunes³, Frederi Viens³, Özge Sürer⁴, Matthew Plumlee⁴, Pablo Giuliani³, Roman Skibiński⁵, Stefan Wild⁶

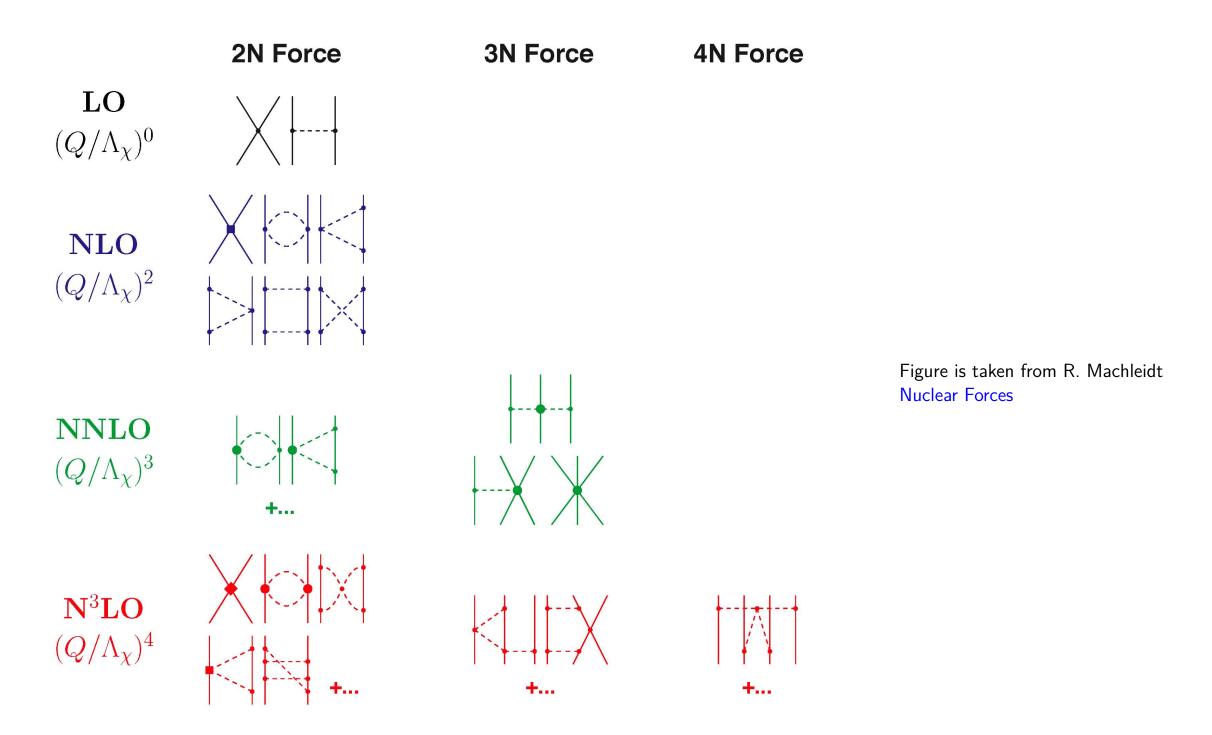
¹AGH University of Science and Technology ²Ohio University ³Michigan State University ⁴Northwestern University ⁵M. Smoluchowski Institute of Physics, Jagiellonian University ⁶Argonne National Laboratory

Introduction

- ▶ We want to study the nuclear force by examining its ability to predict neutron-deuteron scattering.
- ightharpoonup Various observables have been measured for both the elastic reaction and the breakup reaction $\mathrm{nd} \to \mathrm{nnp}$.
- ▶ The Faddeev approach [1, 2] can solve this quantum three-body problems.
- ▶ But it is computationally expensive in both time & memory: running one set of parameters takes on average 4-5 hrs to evaluate neutron-deuteron elastic & inelastic scattering observables.
- ▶ Here we develop a Gaussian Process (GP) "emulator" [5, 6, 7] that is trained at a small number of points in parameter space but can predict elsewhere.
- ► Such emulators make Uncertainty Quantification for this reaction feasible.

Nuclear forces from χEFT

- ► Starting point is Lagrangian for nucleonic and pionic fields with broken chiral symmetry like in QCD.
- ► Effective Hamiltonian for nucleons and pions.
- Power counting perturbative ordering $((Q/\Lambda)^{\nu})$ of various contributions to two- and many-body forces. Finite number of diagrams at given order.
- ➤ Short range interactions are included to the contact terms.



► Three-nucleon forces (3NFs) play a small but critical role in nuclear structure and reactions.

Problems and goals

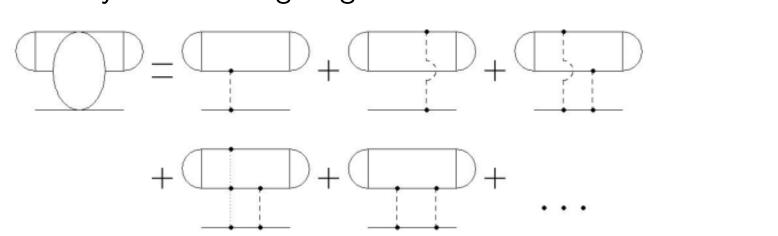
Using surmise's tools to do uncertainty quantification:

- We use 37 training points of NN and 3N LECs (for a total of 12 dimensions). For the 3NF LEC's, we simply use a Latin hypercube design in the range [-2, 2] (20 points) and [-5, 5] (17 points). For the 10 NN LEC's, we start with a Latin hypercube design in the range [-1, 1].
- ▶ Use Principal Components to select more suitable values of parameters & observables.
- ▶ Bayesian calibration of the c_D and c_E parameters based on experimental data and the 3N scattering observables through their posterior distribution function (PDF) allows us to estimate the uncertainty range of 3N observables.

Methods: Formalism for 2N and 3N scattering

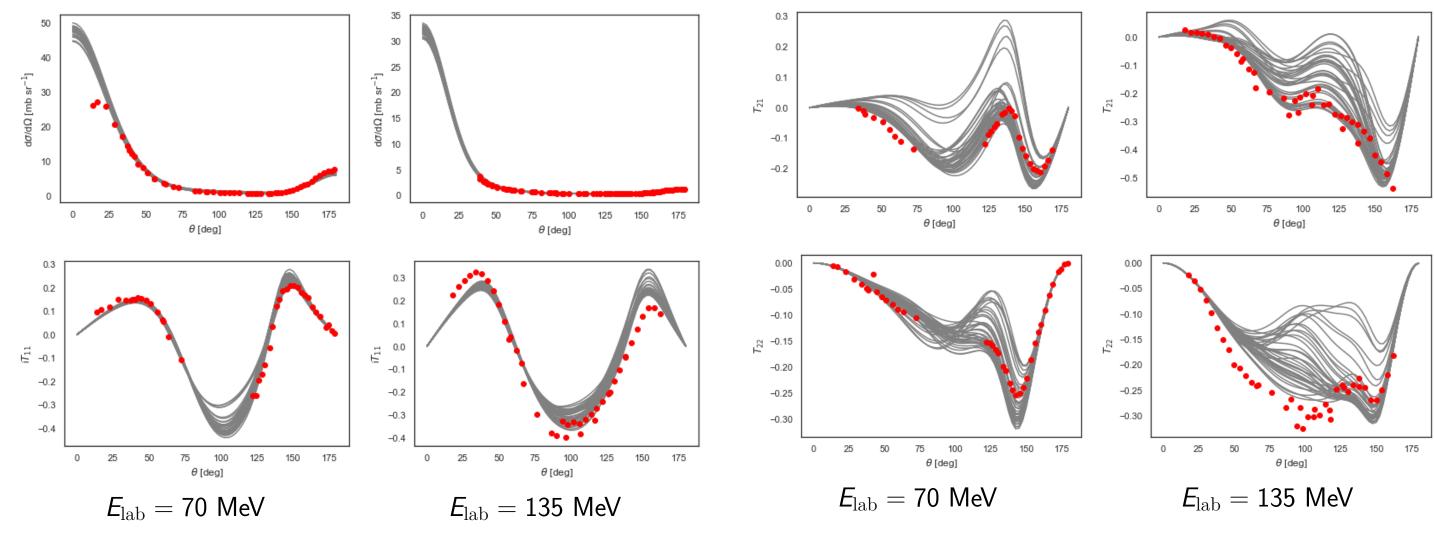
- ► 2N bound state: Schrödinger equation.
- ▶ 2N scattering state: Lippmann-Schwinger equation for the *t*-matrix (interaction + free propagation): $t(E) = V + VG_0(E)V + VG_0(E)VG_0(E)V + \dots$ $G_0(E) \equiv \lim_{\varepsilon \to 0^+} \frac{1}{E H_0 + i\varepsilon}$
- ▶ 3N: Faddeev equation [1, 2]: $T = tP\phi + (1+tG_0)V_{123}^{(1)}(1+P)\phi + tPG_0T + (1+tG_0)V_{123}^{(1)}(1+P)G_0T$
- ► Transition amplitudes

 $U = PG_0^{-1} + V_{123}^{(1)}(1+P)\phi + PT + PT + V_{123}^{(1)}(1+P)G_0T$ (for elastic scattering) and $U_0 = (1+P)T$ (for breakup) can be represented by the following diagram



Constraining three-nucleon forces

- ▶ Dominant piece of 3NF depends on two parameters: c_D and c_E .
- ► Want to constrain them from nd scattering data.
- Curves below shows predictions for various 37 sets of (c_D, c_E) values, together with experimental data [10]:



Tools: surmise BAND application

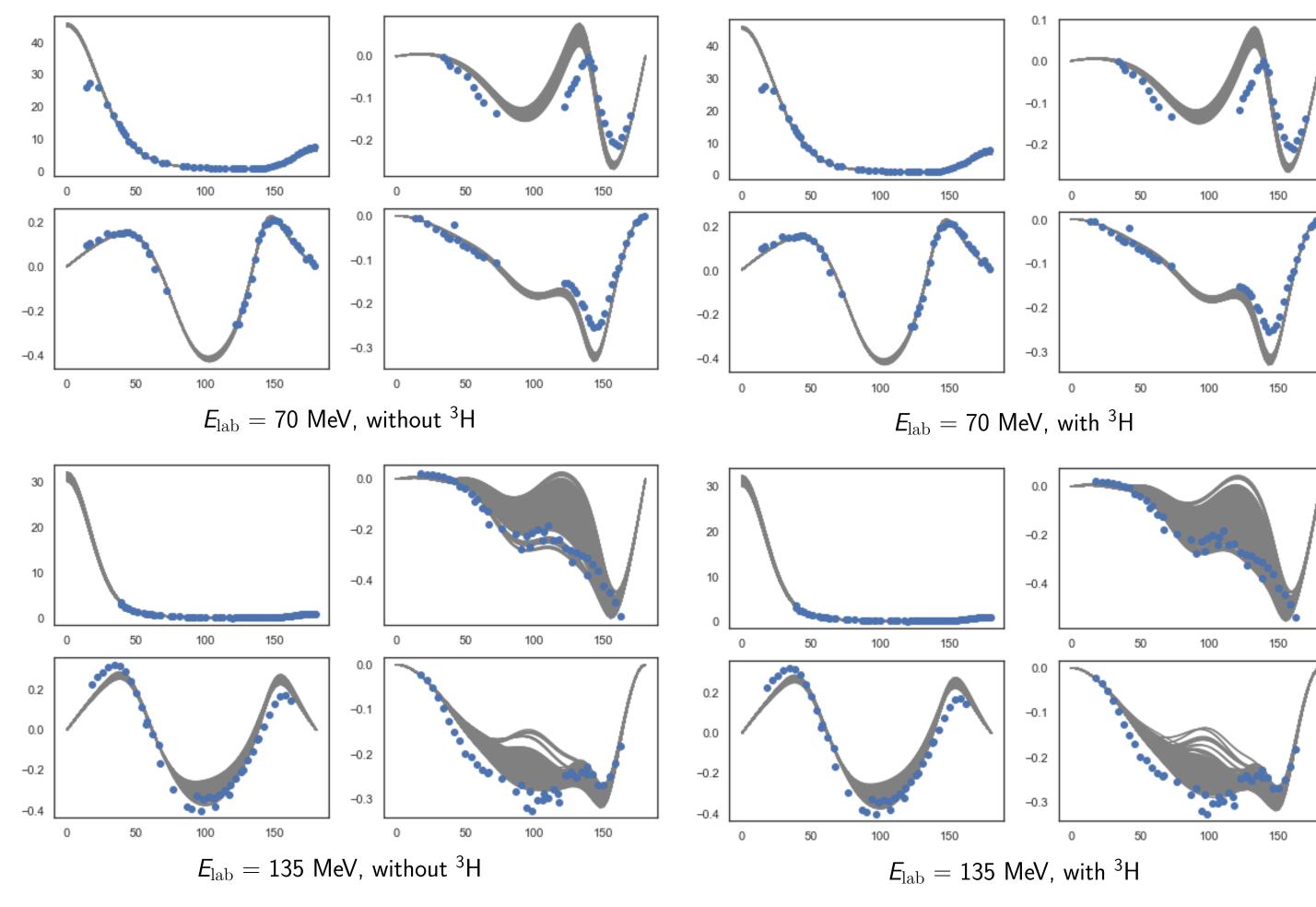
surmise's work is categorized into three routines:

- emulation: carries out Bayesian emulation of the 3N scattering Fadeev calculations using the chiral NN+3NF forces and generates inputs for calibration.
- 1. Emulation via PC's

$$O(\theta; c_D, c_E) = \sum_{i=1}^q \mathbf{k}_i w_i(\theta : c_D, c_E) + \epsilon$$
.

- 2. 10 PC's are enough.
- 3. Employ surmise to link emulation and calibration and run emcee sampler: preliminary calibration of c_D and c_E to nd data at 70 and 135 MeV.
- calibration: generates estimates of the calibration parameters based on field observations of the real process and an output from emulation
- "utilities": performs different utility tasks such as a sampler (e.g., Metropolis-Hastings) to generate posterior draws of calibration parameter

Preliminary results: Posterior predictions after calibration



Summary

- ➤ We applied the SMS chiral NN potentials of Ref. [8], along with the consistently regularized 3NF, both up to N²LO in chiral EFT, to study selected observables in nd elastic scattering.
- ▶ Following the approach of Ref. [6], we have explored the use of a basic GP toolset for reducing the scattering observables predictive uncertainty by calibrating parameters, i.e. c_D and c_E potential parameters directly to the data and 3H binding energy.
- \blacktriangleright We have found the impact of including NN LEC uncertainties on the c_D and c_E posterior is small.
- ► We have shown that thesurmise library as part of the BAND framework allows to use Bayesian parameter estimation and propagation of uncertainties, for example, to draw error bands for the elastic neuron-deuteron predictions using chiral SMS NN+3NF at N²LO order.

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