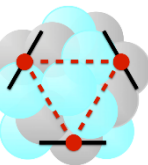


Towards accurate nuclear interaction - recent works in three-nucleon sector

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Nuclear Theory in
Supercomputer Era
5.06.2023,
Lanzhou

Outline

Part I: currently available forces:

the SMS: 2NF up to N4LO+ and 3NF at N2LO

Based on:

R. Skibiński et al., Front. Phys. 11:1084040 (2023) „The nucleon-induced deuteron breakup process as a laboratory for chiral dynamics.”

J. Golak et al., Acta Phys. Polon. B 16, 4-A23 (2023) „Few-nucleon systems for nuclear physics”

1. Formalism
2. Quality of the SMS force tested in $n+d \rightarrow n+n+p$ reaction

Part II: Towards 3NF at higher orders - emulator for the Nd scattering:

Based on:

H. Witała et al., Few-Body Syst. 62 (2021) 23 „Perturbative Treatment of Three Nucleon Force Contact Terms in Three-Nucleon Faddeev Equations.”

H. Witała et al., Eur. Phys. J. A 57 (2021) 241 „Efficient emulator for solving 3N continuum Faddeev equations with chiral 3NF comprising any number of contact terms.”

H. Witała et al., Phys. Rev. C 105 (2022) 054004 „Significance of chiral 3NF contact terms for understanding of elastic nucleon-deuteron scattering”

1. Formalism – new set of equations
2. Tests and the first results on fixing short-range 3NF parameters

Nd scattering

Our standard method to calculate transition amplitude for 3N scattering is to solve:

- the Schrodinger equation -> deuteron

$$(H_0 + V)\Psi_d = E_d \Psi_d$$

- the Lippmann-Schwinger equation -> t-matrix

$$t(E) = V + VG_0(E)V + VG_0VG_0(E)V + \dots = V + VG_0t(E)$$

- the Faddeev equation -> auxiliary operator T

$$T\phi = tP\phi + (1 + tG_0)V_{123}^{(1)}(1 + P)\phi + tPG_0T\phi + (1 + tG_0)V_{123}^{(1)}(1 + P)G_0T\phi$$

where ϕ is the deuteron wf times free nucleon state

- Compute amplitudes for :

$$\text{elastic scattering: } U = PG_0^{-1} + V_{123}^{(1)}(1 + P)\phi + PT + V_{123}^{(1)}(1 + P)G_0T$$

$$\text{deuteron breakup: } U_0 = (1 + P)T$$

Nd breakup

- Within the LENPIC collaboration we work with the chiral SMS potential; Here:
 - 2NF up to N4LO+ (P. Reinert, H. Krebs, E. Epelbaum, Eur. Phys. A54 (2018) 86)
 - 3NF up to N2LO (P. Maris, E. Epelbaum et al., Phys. Rev. C 103 (2021) 054001)
- We studied, using various combinations of NN and 3N forces, the deuteron breakup reaction $n+d \rightarrow n+n+p$, performing global search over the available phase space
- Five independent variables: $\theta_1, \phi_1=0, \theta_2, \phi_2$, and S
- We use for $\theta_1, \theta_2, \phi_2$ grids in range 2.5° - 177.5° step 5° and for S step 0.5 MeV, which results in approx. $5 \cdot 10^6$ kinematical configurations
- For each (θ_1, θ_2) we look for **maximum** of given effect over $\phi_{12}=\phi_2-\phi_1$ and $S(=E_1, E_2)$
- We are interested in:
 1. Dependence of predictions on the regulator parameter Λ
 2. Dependence of predictions on the order of chiral force – here on 2NF
 3. Role of the 3N interaction

Nd breakup

The SMS potential is given for a few values of regulator $\Lambda=400, 450, 500,$ and 550 MeV.

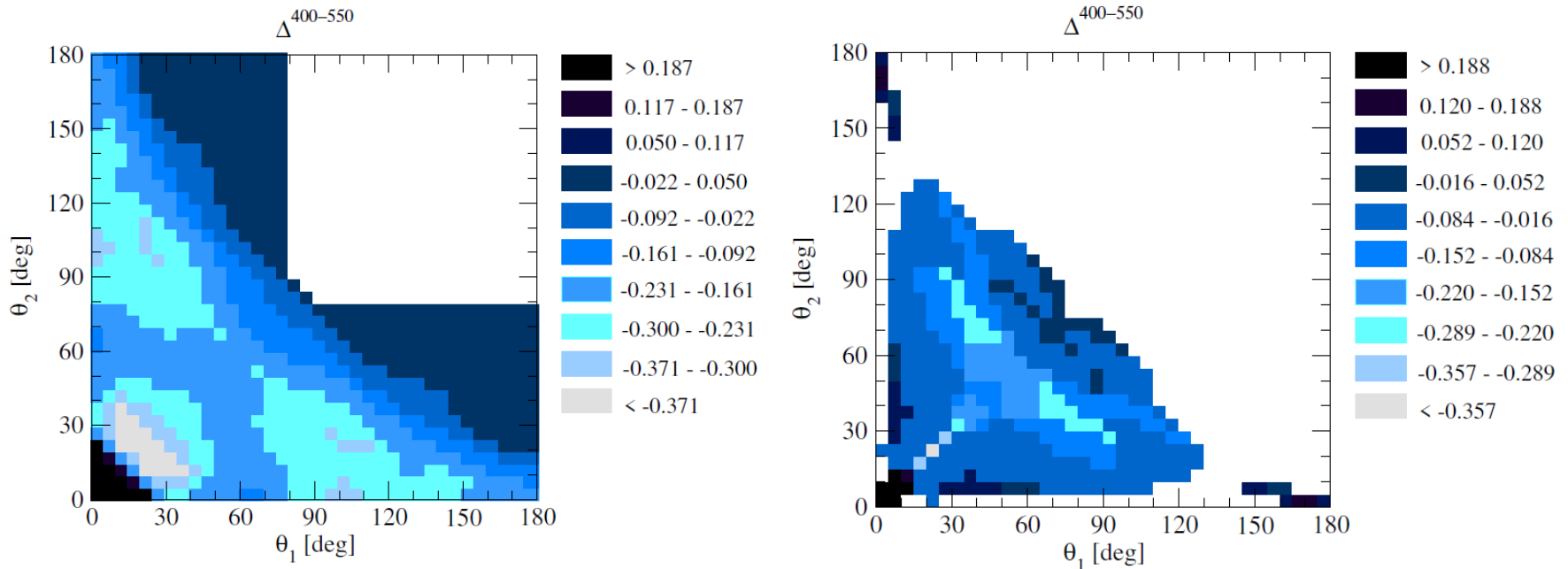
1. Dependence of predictions on the regulator parameter Λ

$$\delta^{400-550}(\theta_1, \theta_2, \phi_2, S) \equiv \frac{\left(\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dS}\right)^{400} - \left(\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dS}\right)^{550}}{\frac{1}{2} \left(\left(\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dS}\right)^{400} + \left(\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dS}\right)^{550} \right)}$$

For each (θ_1, θ_2) we look for maximum of $\delta^{400-550}$ over Φ_{12} and $S(=E_1, E_2)$

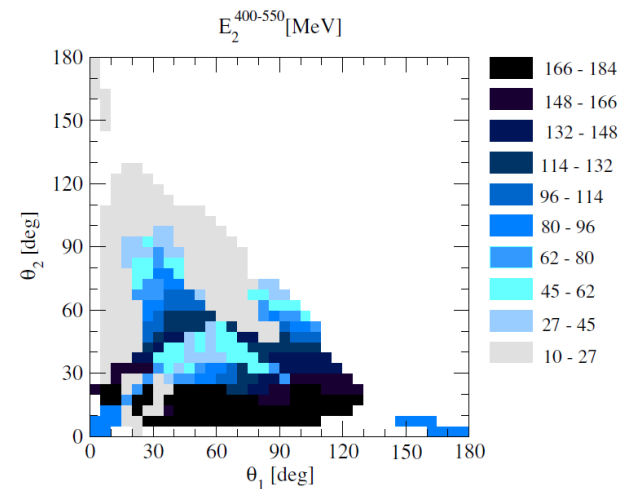
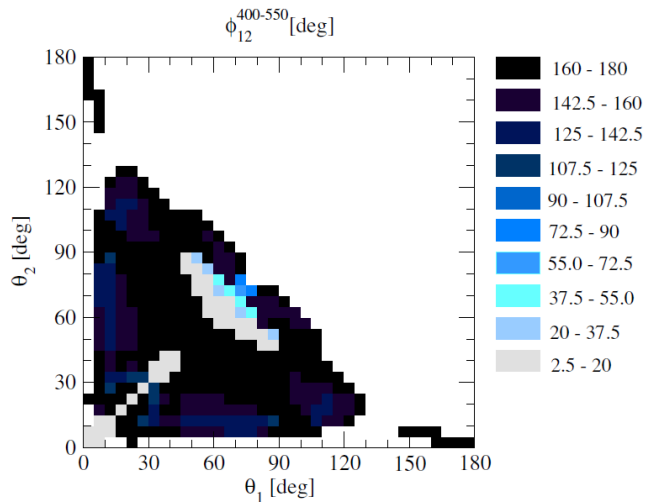
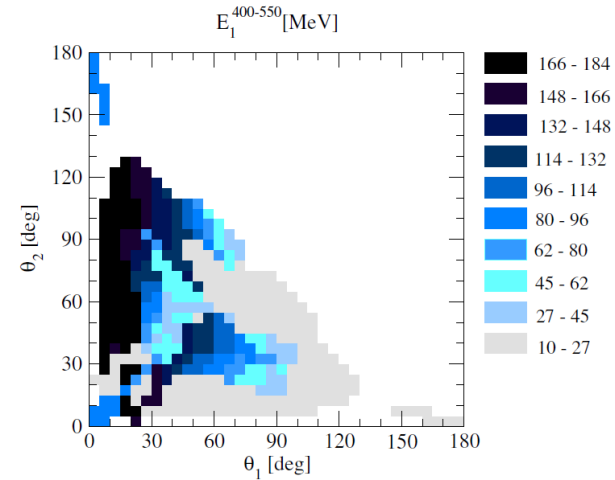
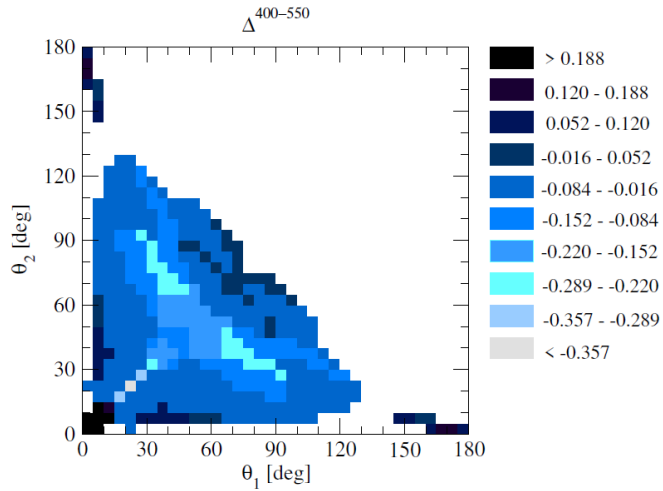
$$\Delta^{400-550} \equiv \Delta^{400-550}(\theta_1, \theta_2) \equiv \max_{\{\phi_2, S\}} \delta^{400-550}(\theta_1, \theta_2, \phi_2, S).$$

Results: $E=200$ MeV regulator dependence: N4LO+ +N2LO at $\Lambda=400$ MeV vs $\Lambda=550$ MeV

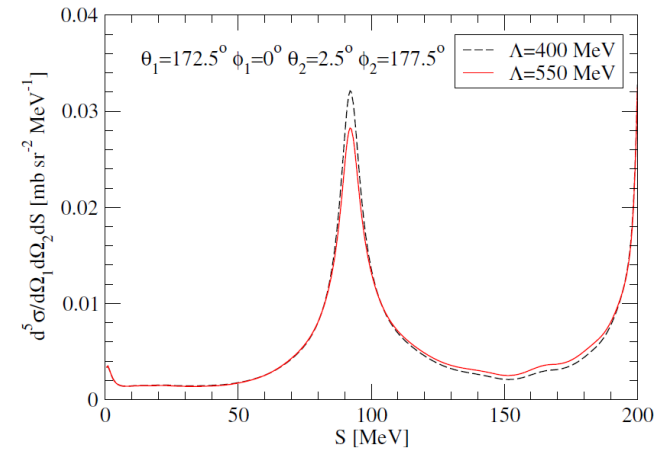
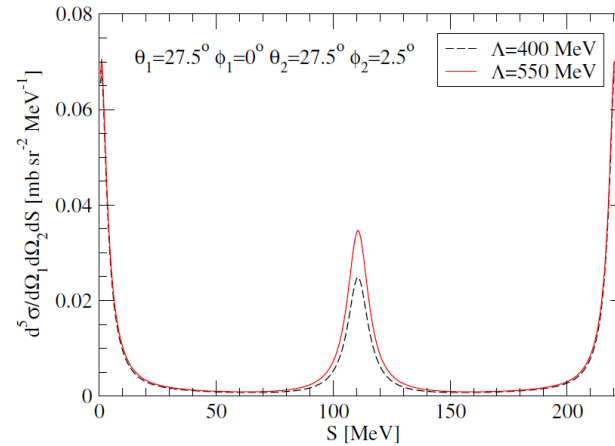
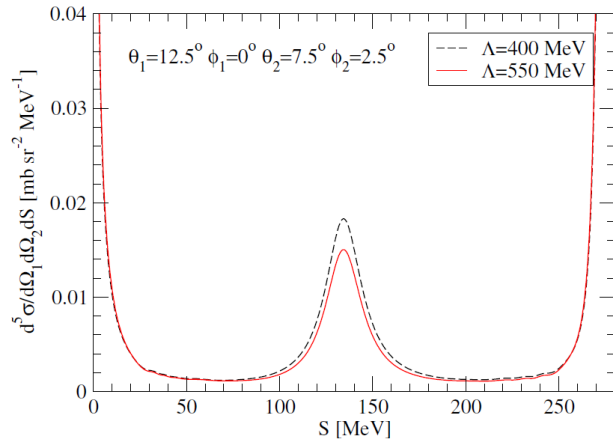


- Right: with additional thresholds:
 $d^5\sigma/d\Omega_1 d\Omega_2 dS \geq 0.01 \text{ mb}$, $E_1 \geq 10 \text{ MeV}$, $E_2 \geq 10 \text{ MeV}$

Results: $E=200$ MeV regulator dependence: N4LO+ + N2LO at $\Lambda=400$ MeV vs $\Lambda=550$ MeV



Results: $E=200$ MeV regulator dependence: N4LO+ + N2LO at $\Lambda=400$ MeV vs $\Lambda=550$ MeV



→ the biggest effects are seen for the FSI configurations

Nd breakup

2. Dependence of predictions on the chiral order (in NN force, 3NF at N2LO)

$$\delta^{N2LO-N4LO+}(\theta_1, \theta_2, \phi_2, S) \equiv \frac{\left(\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dS}\right)^{N2LO} - \left(\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dS}\right)^{N4LO+}}{\frac{1}{2}\left(\left(\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dS}\right)^{N2LO} + \left(\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dS}\right)^{N4LO+}\right)}$$

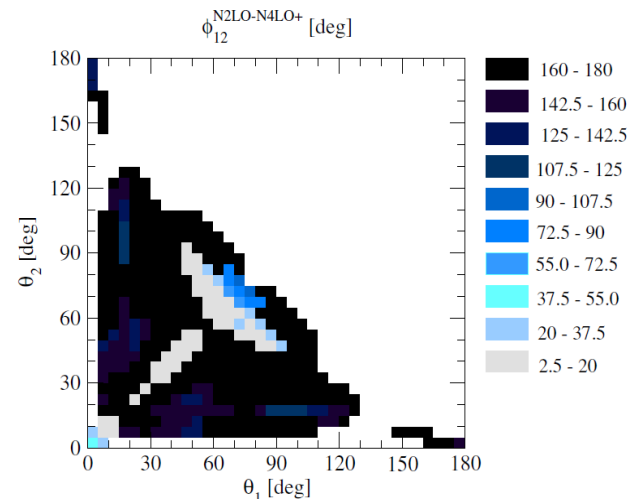
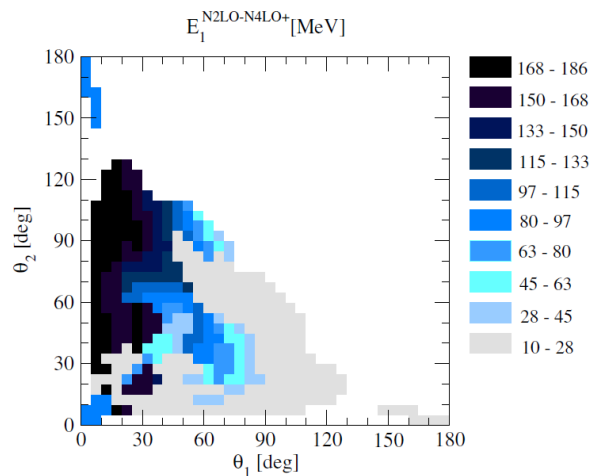
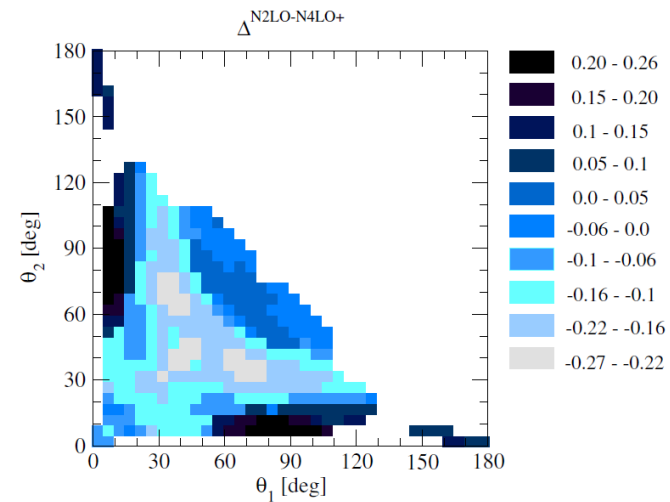
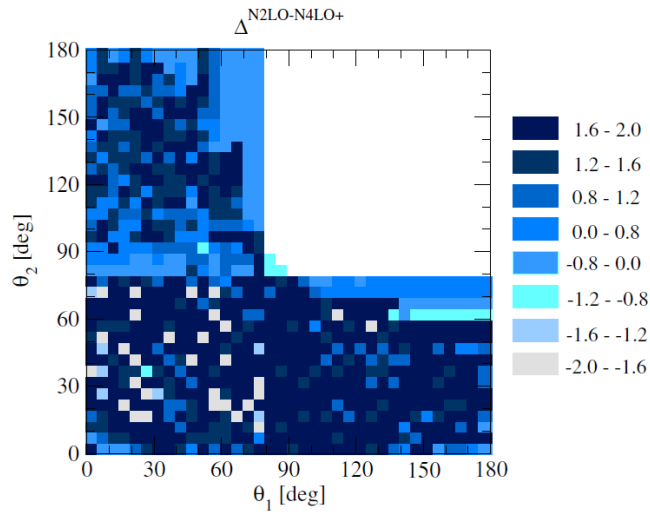
$$\Delta^{N2LO-N4LO+} \equiv \Delta^{N2LO-N4LO+}(\theta_1, \theta_2) \equiv \max_{\{\phi_2, S\}} \delta^{N2LO-N4LO+}(\theta_1, \theta_2, \phi_2, S)$$

3. 3NF effects

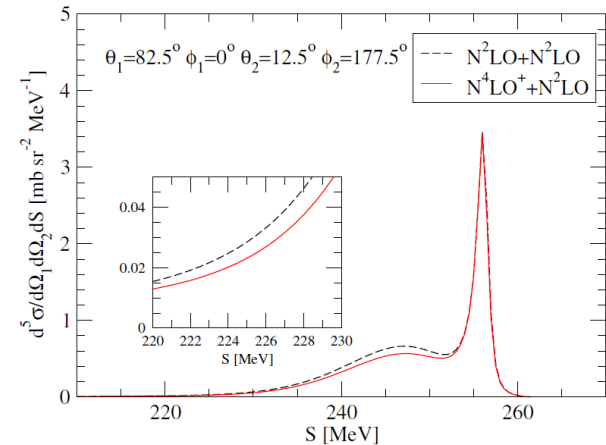
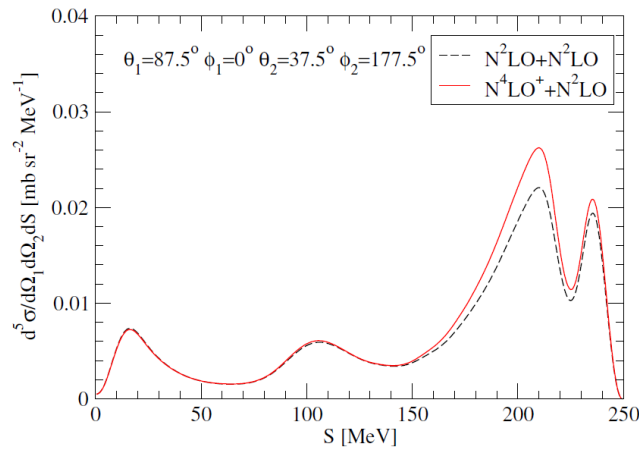
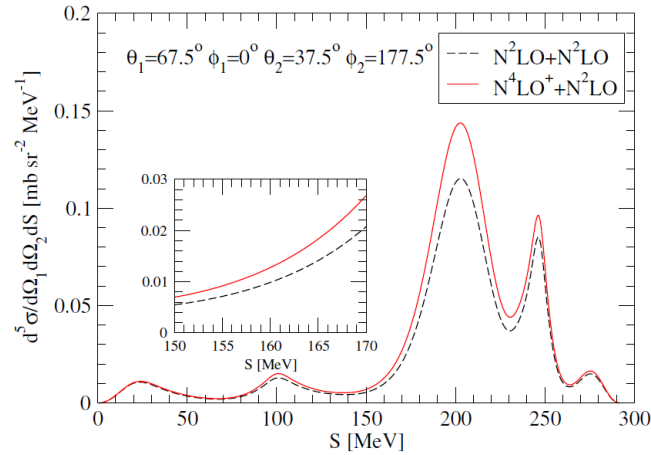
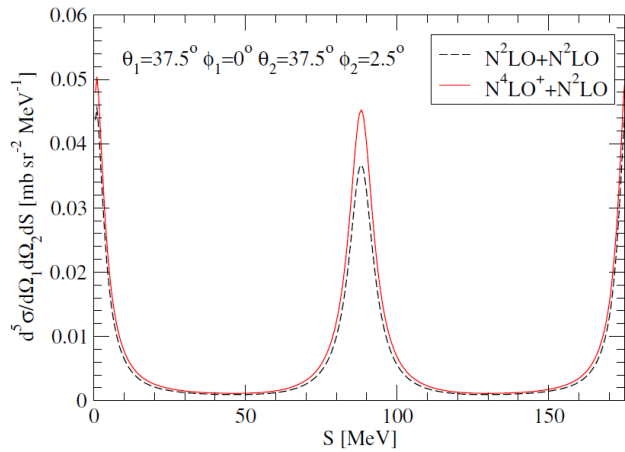
$$\delta^{3NF}(\theta_1, \theta_2, \phi_2, S) \equiv \frac{\left(\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dS}\right)^{NN} - \left(\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dS}\right)^{NN+3NF}}{\frac{1}{2}\left(\left(\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dS}\right)^{NN} + \left(\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dS}\right)^{NN+3NF}\right)}$$

$$\Delta^{3NF} \equiv \Delta^{3NF}(\theta_1, \theta_2) \equiv \max_{\{\phi_2, S\}} \delta^{3NF}(\theta_1, \theta_2, \phi_2, S).$$

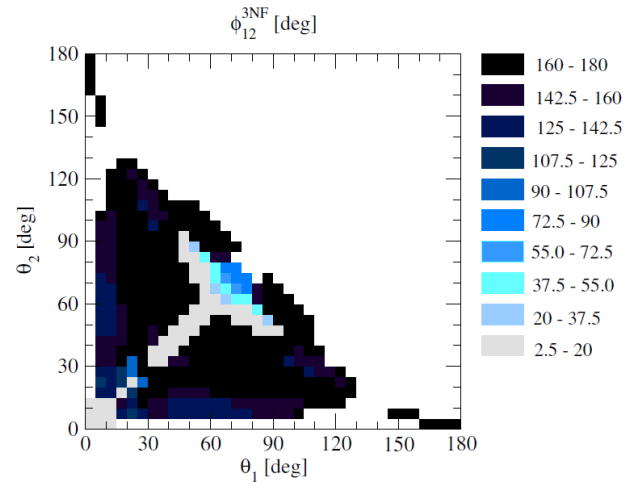
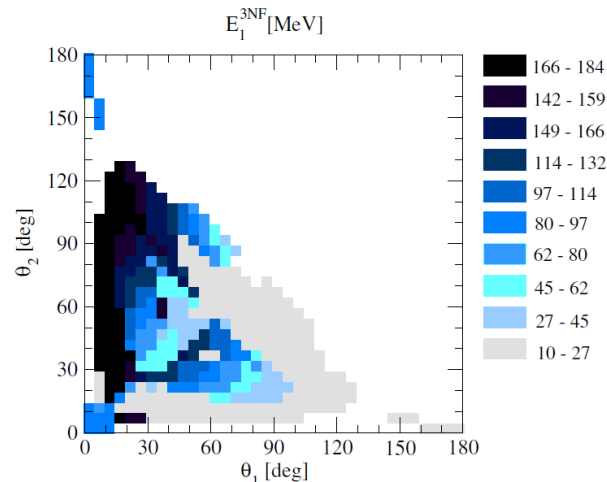
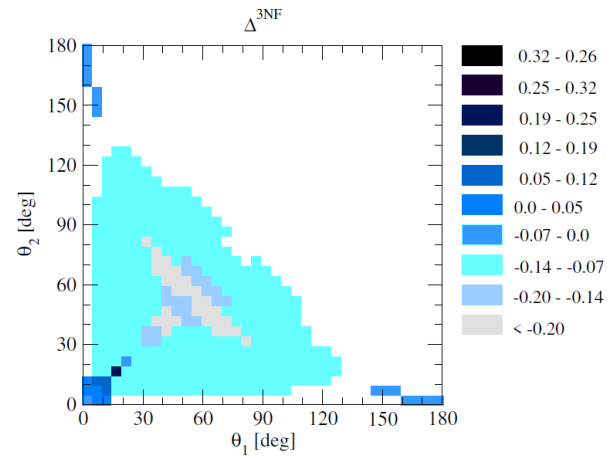
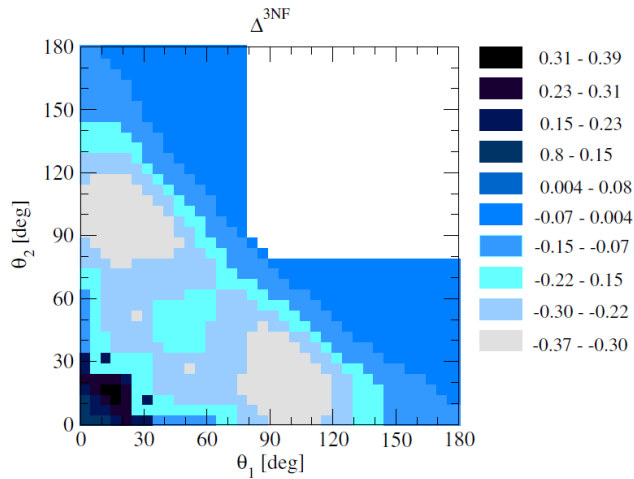
Results: $E=200$ MeV, $\Lambda=450$ MeV, chiral order dependence: N2LO NN+3NF vs N4LO+ NN+N2LO 3NF



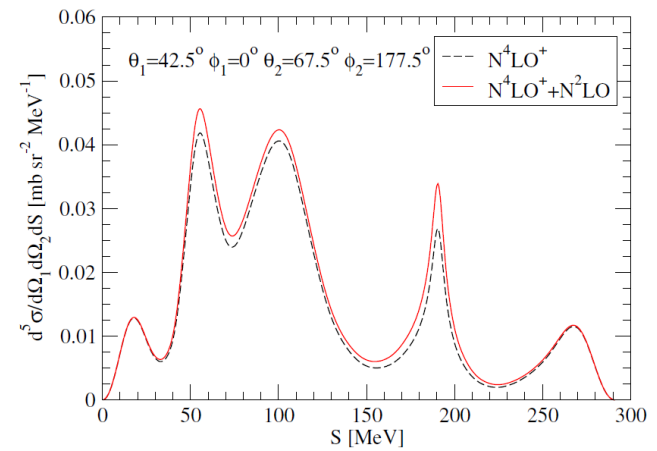
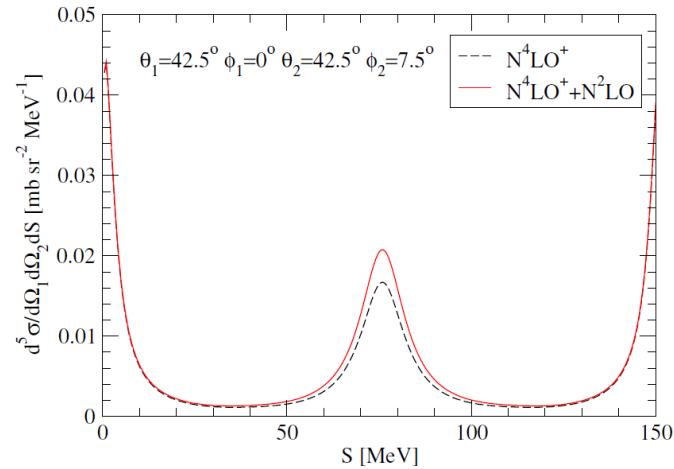
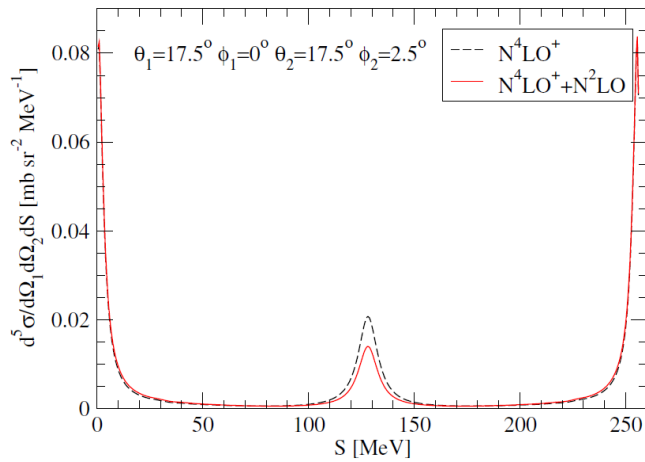
Results: $E=200$ MeV, $\Lambda=450$ MeV, chiral order dependence: N^2LO NN+3NF vs N^4LO + NN+N 2LO 3NF



Results: $E=200$ MeV, $\Lambda=450$ MeV, 3NF effects: N4LO+ NN vs N4LO+ NN+N2LO 3NF



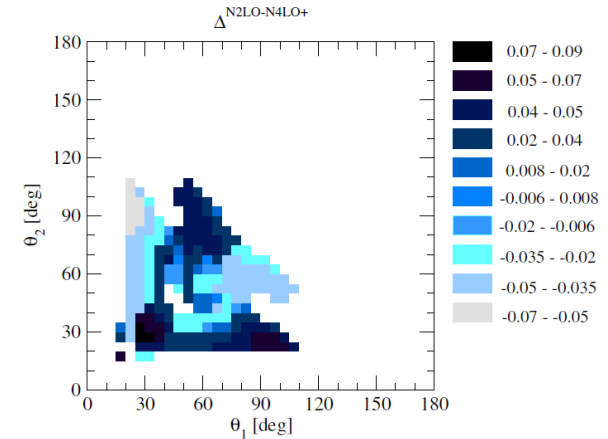
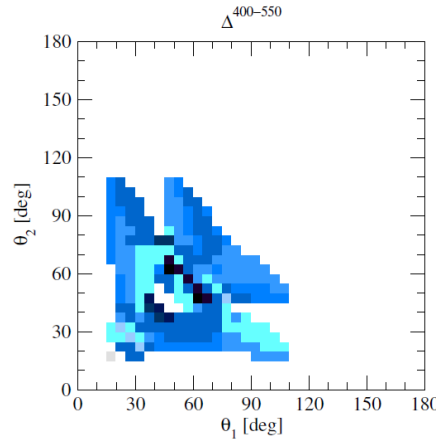
Results: $E=200$ MeV, $\Lambda=450$ MeV, 3NF effects: $N^4LO+ NN$ vs $N^4LO+ NN+N^2LO$ 3NF



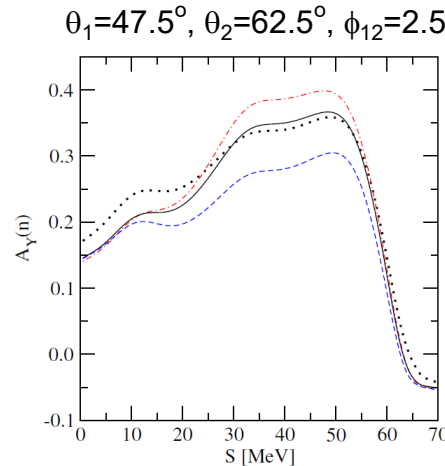
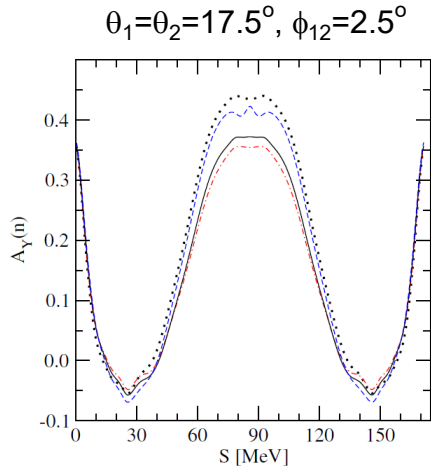
Results for $A_Y(n)$: $E=135$ MeV, $\Lambda=450$ MeV, chiral order and cut-off dependences

$$\delta^{400-550}(\theta_1, \theta_2, \phi_2, S) \equiv (A_Y(n))^{400}(\theta_1, \theta_2, \phi_2, S) - (A_Y(n))^{550}(\theta_1, \theta_2, \phi_2, S)$$

$$\delta^{N^2\text{LO}-N^4\text{LO}+}(\theta_1, \theta_2, \phi_2, S) \equiv (A_Y(n))^{N^2\text{LO}}(\theta_1, \theta_2, \phi_2, S) - (A_Y(n))^{N^4\text{LO}+}(\theta_1, \theta_2, \phi_2, S),$$



Note: $\phi_1=0^\circ$
(not the whole phase space)



- N2LO NN+ N2LO 3NF $\Lambda=450$ MeV
- N4LO+ NN + N2LO 3NF $\Lambda=400$ MeV
- N4LO+ NN + N2LO 3NF $\Lambda=450$ MeV
- N4LO+ NN + N2LO 3NF $\Lambda=550$ MeV

→ $A_Y(n)$ is less sensitive than the cross section,
in addition, in interesting configurations
the magnitude of $A_Y(n)$ is moderate.

Summary I

- We have identified configurations which are sensitive to details of interaction. Mostly they are the FSI or QFS configurations.

For the cross section maximal effects (without, with thresholds) are:

- Cut-off dependence:
E=135 MeV -24%-17%, -19%-12%
E=200 MeV -37%-19%, -36%-19%
- Chiral order dependence (in 2N force):
E=135 MeV -160%-200%, -16%-15%
E=200 MeV -200%-200%, -27%-26%
- 3NF:
E=135 MeV -23%-25%, -20%-24%
E=200 MeV -39%-37%, -20%-26%
- On average the SMS force gives very stable predictions (with $\delta^{***} \leq \text{few } \%$)
→ The SMS NN at N4LO+ interaction meets the expectations → further work should be directed to the three-body force

Fixing parameters of 3NF

- Up to now, i.e. when working at N2LO there are only two free parameters c_D and c_E .
- Typically ^3H and the $^2a_{\text{nd}}$ or the differential Nd elastic scattering cross section at one or few energies are used.
The latter requires solving the triton many times and the Faddeev equation 10-20 times.
- However, beyond N2LO we expect:
- No new 3NF free parameters at N3LO, but three new offshell LECs in the chiral NN force.
- 13 contact terms at N4LO (more precisely, due to some identities between operators, one expects in total 13 free parameters of 3NF at N4LO).
- Thus finding an efficient emulator for solving the 3N Faddeev equation seems to be essential and of high priority.

Emulator for Nd scattering – new results

- In [1] H.Wiła et al., Few-Body Syst. 62 (2021) 23
we proposed such an emulator which enabled us to reduce significantly the required time of computations. We tested its efficiency as well as ability to accurately reproduce exact solution of the 3N Faddeev equations.
- In [2] H.Wiła et al., Eur. Phys. J. A 57 (2021) 241
we introduced a computational scheme based on the perturbative approach of Ref. [1], which even by far more reduced the computer time necessary to obtain the observables in the elastic nucleon-deuteron scattering and deuteron breakup reactions, and which is well suited for calculations with varying strengths of the contact terms in a chiral 3NF
- In [3] H.Wiła et al., Phys. Rev. C105 (2022) 054004
we used the SMS N4LO+ NN potential in combination with the N2LO chiral 3NF supplemented by all the N4LO contact terms. Our aim was to verify if it would be possible to fix strengths of all the contact terms by performing a least squares fit of theory to Nd elastic-scattering data.

Emulator for Nd scattering – algorithm; main steps

- The contact terms are restricted to small 3N total angular momenta and to only few partial-wave states for a given total 3N angular momentum J and parity π

- Let us split 3NF

$$V_{123}^{(1)} = V(\theta_0) + \Delta V(\theta) \equiv V(\theta_0) + \sum_{i=1}^n c_i \Delta V_i$$

$$\theta = \{c_1, c_2, \dots\}$$

$$\theta_0 = \{0, 0, \dots\}$$

- We divide the 3N partial-wave states into two sets:
 1. The β set is defined by non-vanishing matrix elements of parameters dependent short-range 3NF: $\Delta V(\theta)$.
 2. The α set comprises remaining states.

- Similarly to 3NF

$$T = T(\theta_0) + \Delta T(\theta)$$

Emulator for Nd scattering - algorithm

- Inserting this to the Faddeev equation leads to sets of equations: one Eq. is the standard Faddeev equation with $V(\theta_0)$, the second one is for the $\langle \beta | \Delta T(\theta) | \phi \rangle$
- We neglect term $\sim \Delta V \Delta T$
- We split that Eq. to separate equations, each for single parameter dependent component of V : $V_i = c_i V$. We may solve that equation separately at $c_i = 1$ obtaining corresponding ΔT_i .
- Finally:
$$\langle \beta | \Delta T(\theta) | \phi \rangle = \sum_{i=1}^N c_i \langle \beta | \Delta T_i | \phi \rangle.$$
- Summarizing: one needs to solve $N+1$ Faddeev equations (one for $T(\theta_0)$ and N for $\langle \beta | \Delta T_i | \phi \rangle$), next N times find $\langle \alpha | \Delta T_i | \phi \rangle$ by integration.

Emulator for Nd scattering - algorithm

- In this way we have matrix

$$\text{elements of } T \quad \langle \alpha | T(\theta) | \phi \rangle = \langle \alpha | T(\theta_0) | \phi \rangle + \sum_i c_i \langle \alpha | \Delta T_i | \phi \rangle,$$

$$\langle \beta | T(\theta) | \phi \rangle = \langle \beta | T(\theta_0) | \phi \rangle + \sum_i c_i \langle \beta | \Delta T_i | \phi \rangle. \quad (10)$$

- Let us now come back to the scattering amplitudes

$$U = P G_0^{-1} + V_{123}^{(1)} (1 + P) \phi + P T + V_{123}^{(1)} (1 + P) G_0 T$$

$$U_0 = (1 + P) T$$

- They are linear in T: the dependence on the c_i constants carries over to them, except as a complication for elastic scattering, but they can be written as

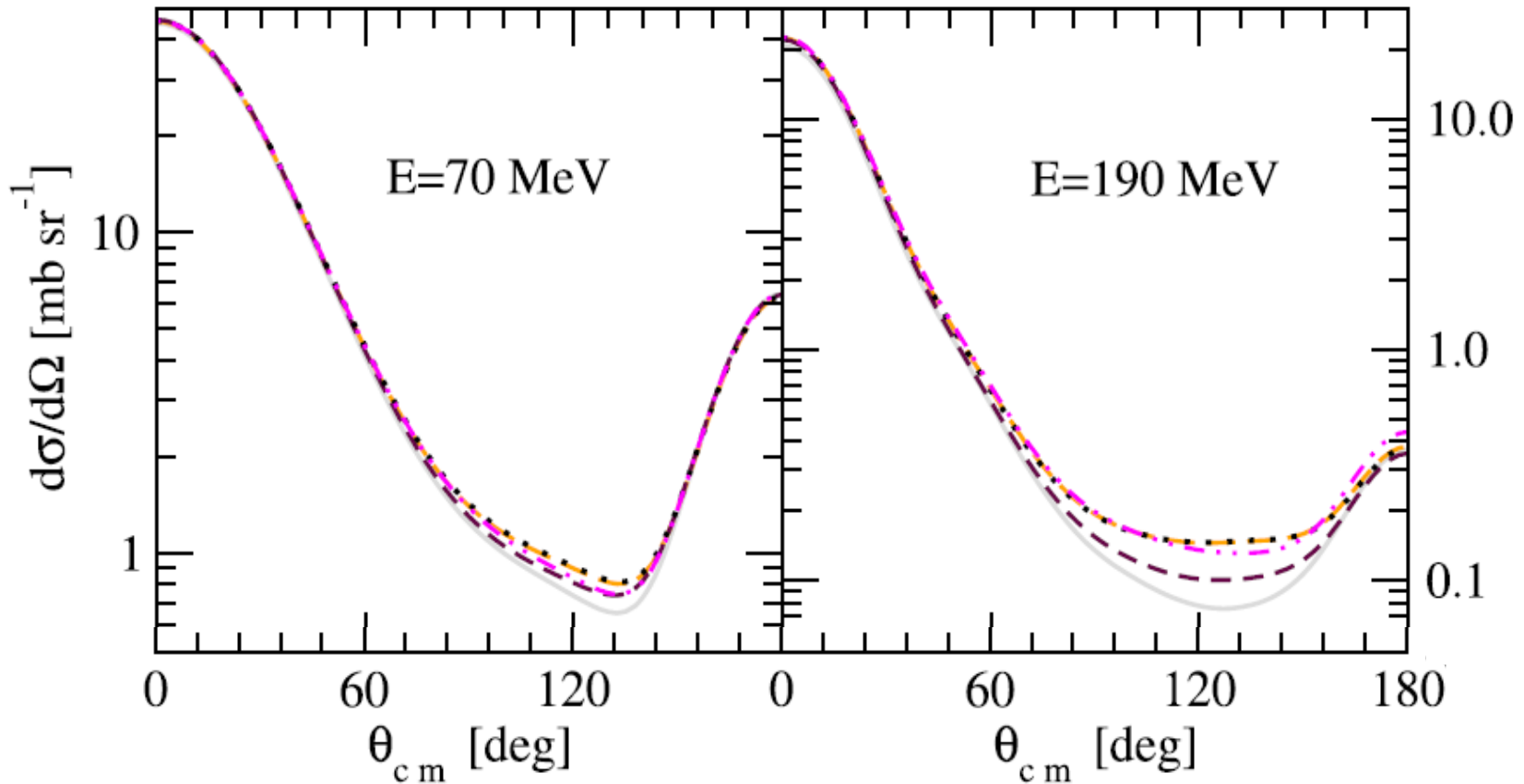
$$U = U(\theta_0) + \sum_i c_i U_i + \sum_{i,k} c_i c_k U_{ik}$$

$$U_0 = U_0(\theta_0) + \sum_i c_i U_{0i}$$

Emulator for Nd scattering – algorithm - application

- We used SMS N4LO+ NN potential at $\Lambda=450$ MeV, combined with the N2LO chiral 3NF and supplemented by all subleading N4LO 3NF contact terms from:
 1. L. Girlanda, A. Kievsky, and M. Viviani, Phys. Rev. C 84, 014001 (2011).,
 2. L. Girlanda, A. Kievsky, and M. Viviani, Phys. Rev. C 102, 019903(E) (2020).
- All terms are regulated with the non-local regulator.
- Such a Hamiltonian comprises altogether 15 short-range contributions to 3NF, two from N2LO with the strengths c_D and c_E , and thirteen from N4LO with the strengths E_i , $i = 1, \dots, 13$. However, for two pairs of the E_i terms matrix elements are identical, thus finally there are 13 unknown parameters.

Emulator for Nd scattering – test



Exact:

NN N4LO+

NN N4LO+ + 3NF N2LO+E7

($c_D = -8.2053$, $c_E = -1.0019$, $c_{E7} = 2.0$)

NN N4LO+ + 3NF N2LO ($c_D = c_E = c_{E7} = 0.0$)

Emulator:

NN N4LO+ + 3NF N2LO+E7 ($\beta = {}^1S_0, {}^3S_1 - {}^3D_1$)

NN N4LO+ + 3NF N2LO+E7 ($\beta = j \leq 2$)

Emulator for Nd scattering – application

Sensitivity of 3N scattering observables to E_i terms

Green circles $V(\theta_0)$

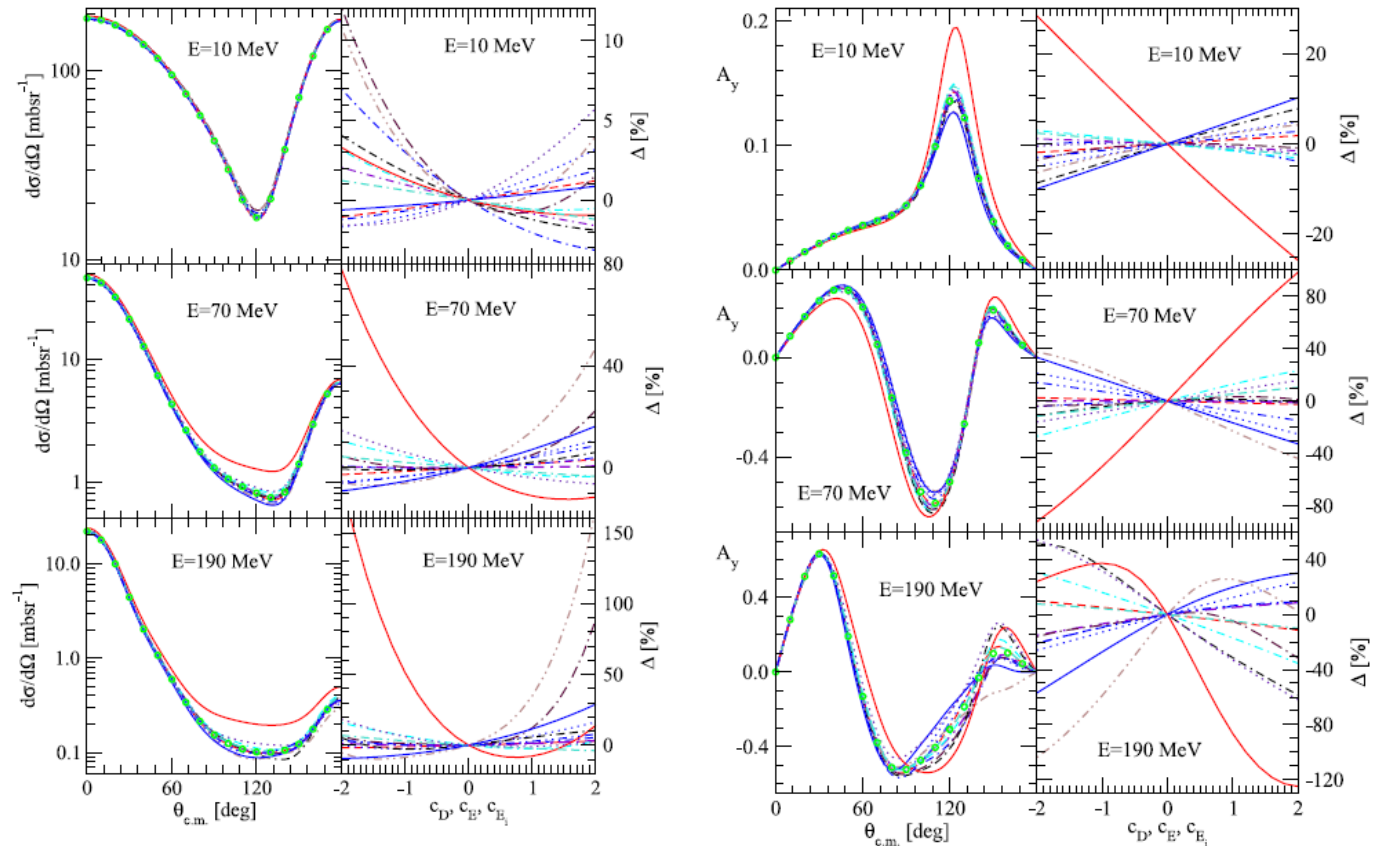
$C_i = -1$ (left)

red solid E_8 ,

blue solid E_7 ,

brown dashed-

double dotted E_5



- N2LO D and E terms do not dominate

- Some observables are more sensitive to specific terms, e.g. T_{22} to E_{10}

$$\Delta \equiv \Delta(c_i) = \frac{1}{N_\theta} \sum_{\theta_k} \frac{Obs(c_i, \theta_k) - Obs(\theta_0, \theta_k)}{Obs(\theta_0, \theta_k)}$$

Emulator for Nd scattering – application

V_i expectation values in ${}^3\text{H}$ at $c_i=1.0$

TABLE I. Contributions of the N^2LO and N^4LO contact terms to the potential energy of the three nucleons in the triton. These expectation values were obtained for the ${}^3\text{H}$ wave function calculated with the SMS chiral N^4LO^+ NN potential ($\Lambda = 450$ MeV) and assuming strengths of contact terms $c_i = 1.0$.

V_i	$\langle \psi_{{}^3\text{H}} V_i \psi_{{}^3\text{H}} \rangle$ [MeV]
V_D	0.1661
V_E	-1.4294
V_{E1}	0.3463
V_{E2}	-0.4173
V_{E3}	-0.2754
V_{E4}	-1.0390
V_{E5}	-0.9559
V_{E6}	-1.0699
V_{E7}	0.1798×10^{-4}
V_{E8}	0.8817×10^{-2}
V_{E9}	-0.2407
V_{E10}	1.0571
V_{E11}	-0.2407
V_{E12}	1.0571
V_{E13}	0.3060

Relative strengths

Nearly all terms are important (for $c_i=1$) with exception of E_7 and E_8 terms

Emulator for Nd scattering – fit to the true data at 10,70, and 135 MeV (786 data points)

TABLE III. The values of strengths c_i found in the least squares fit to the data from Table II at the three energies $E = 10, 70$, and 135 MeV.

c_D	-1.49 ± 0.06
c_E	-1.27 ± 0.06
c_{E_1}	6.40 ± 0.33
c_{E_2}	7.80 ± 0.36
c_{E_3}	6.97 ± 0.34
c_{E_4}	-2.06 ± 0.13
c_{E_5}	-0.36 ± 0.05
c_{E_6}	0.52 ± 0.03
c_{E_7}	-7.40 ± 0.14
c_{E_8}	-2.61 ± 0.05
c_{E_9}	-4.59 ± 0.22
$c_{E_{10}}$	-0.98 ± 0.05
$c_{E_{13}}$	-1.14 ± 0.05

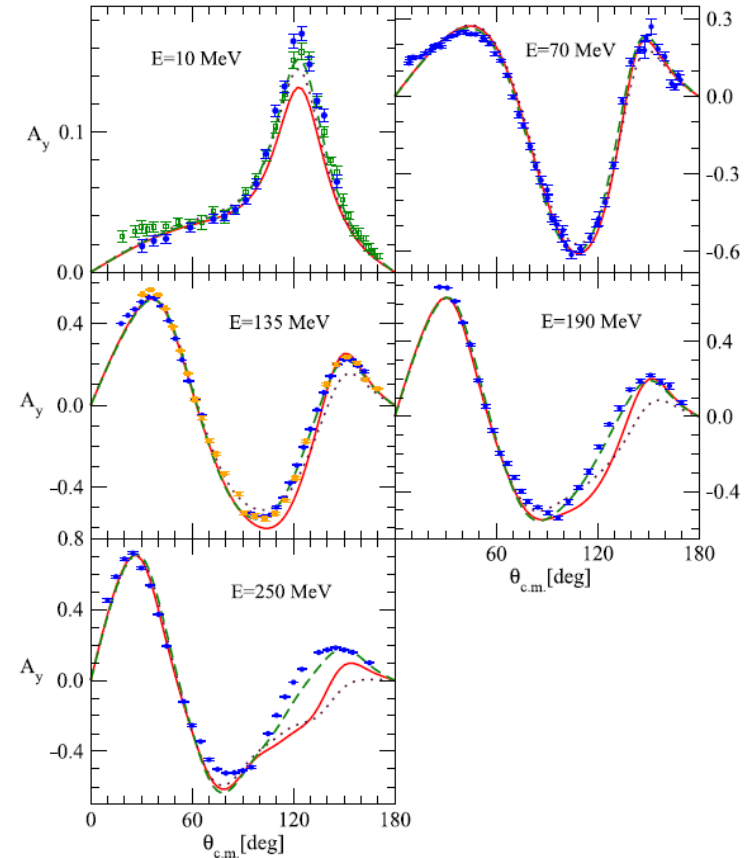
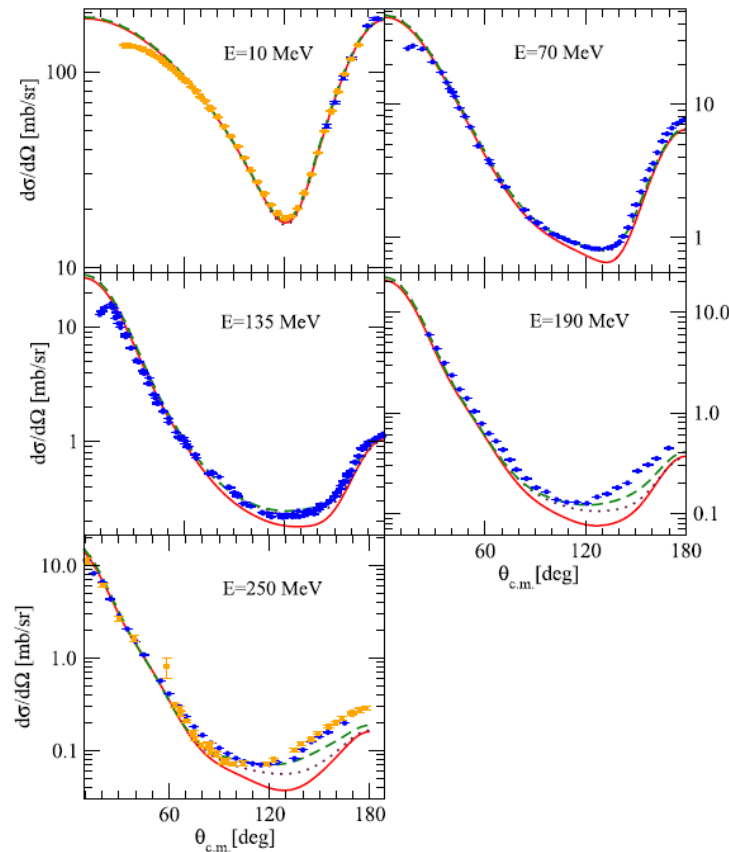
TABLE IV. The covariance matrix for the strengths c_i determined by the least squares fit of data from Table II at the three energies $E = 10, 70$, and 135 MeV [the values shown are $\text{Cov}(c_i, c_j) \times 1000$].

	c_D	c_E	c_{E_1}	c_{E_2}	c_{E_3}	c_{E_4}	c_{E_5}	c_{E_6}	c_{E_7}	c_{E_8}	c_{E_9}	$c_{E_{10}}$	$c_{E_{13}}$
c_D	3.914	-0.456	1.412	4.573	0.843	0.844	-0.729	-0.892	1.109	0.267	-0.726	0.123	-0.207
c_E		3.560	0.947	-3.571	1.345	-0.633	-0.172	-0.217	-2.416	-0.809	-1.702	0.393	0.571
c_{E_1}			108.9	112.8	108.9	-35.13	1.409	-2.418	25.92	7.513	12.99	3.861	0.443
c_{E_2}				130.7	113.4	-35.15	-1.995	-3.241	32.43	9.561	-0.534	0.763	-3.332
c_{E_3}					112.9	-38.92	1.617	-1.814	27.52	8.068	8.366	1.598	-0.193
c_{E_4}						15.97	-1.966	-0.362	-10.50	-3.198	-4.866	0.345	-0.222
c_{E_5}							2.415	0.669	0.791	0.281	9.892	1.311	1.766
c_{E_6}								0.635	-0.874	-0.226	1.426	-0.226	0.210
c_{E_7}									20.33	6.455	3.464	-0.324	-1.463
c_{E_8}										2.071	1.041	-0.158	-0.462
c_{E_9}											50.23	9.133	8.813
$c_{E_{10}}$												2.625	1.910
$c_{E_{13}}$													2.499

- Big values of $c_{E_1}, c_{E_2}, c_{E_3}, c_{E_7}, c_{E_9}$
- Correlation coefficients close to ± 1 : $\rho(E_1, E_2), \rho(E_2, E_3), \rho(E_1, E_3), \rho(E_3, E_4), \rho(E_7, E_8)$
- Correlation coefficients close to 0: $(c_D, c_E), (c_D, c_{E_i}), (c_E, c_{E_i})$
- $\chi^2/\text{data} \approx 35$

Emulator for Nd scattering – fit to the data: cross section and $A_Y(N)$

- Data at 10, 70 and 135 MeV
- Results at 190 and 250 MeV are predictions



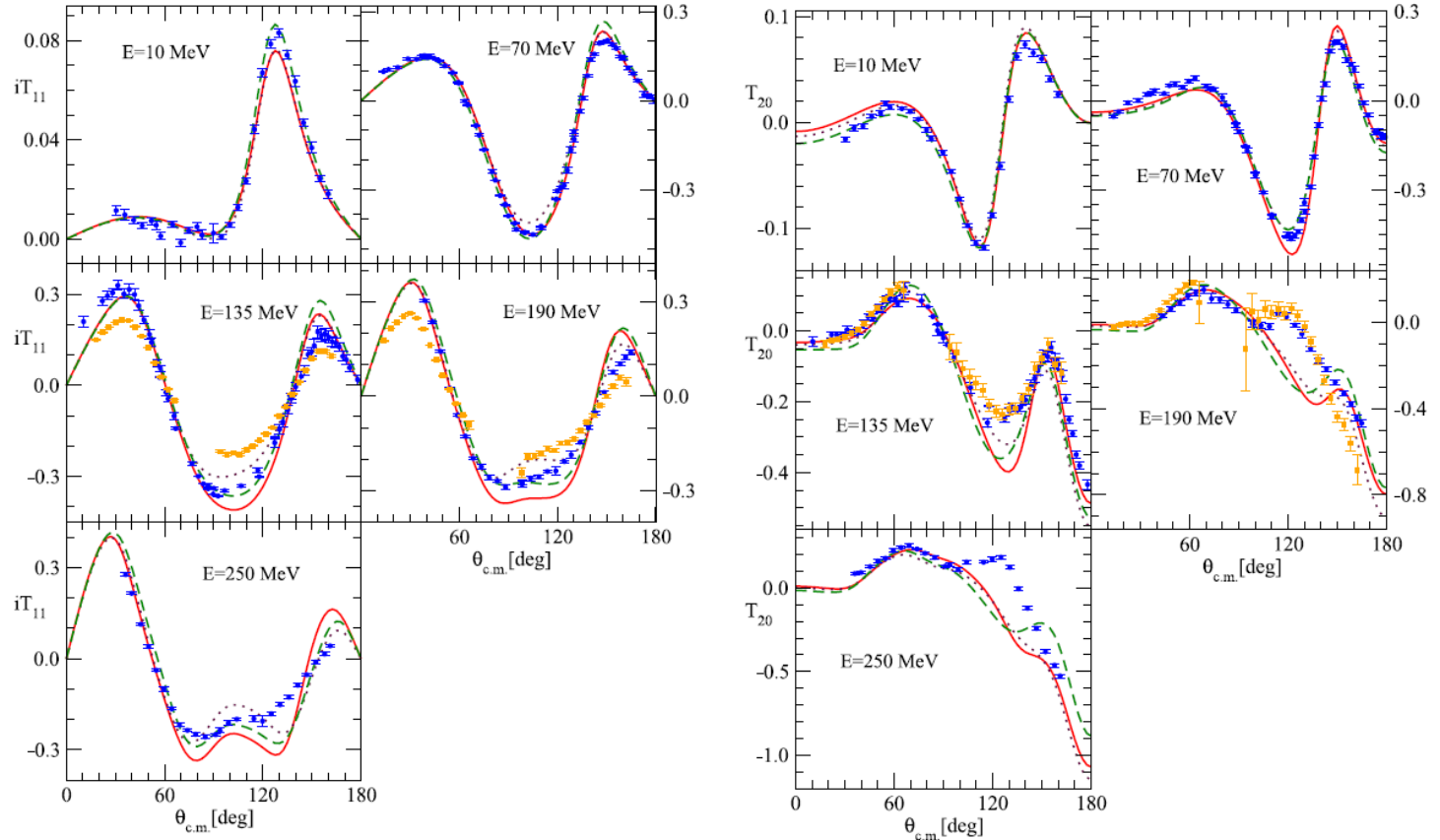
NN N4LO+

NN N4LO+ + 3NF N2LO

NN N4LO+ + 3NF N2LO + E_i

Emulator for Nd scattering – fit to the data: iT_{11} and T_{20}

- Data at 10, 70 and 135 MeV
- Results at 190 and 250 MeV are predictions



NN N4LO+

NN N4LO+ + 3NF N2LO

NN N4LO+ + 3NF N2LO + E_i

Summary II

- We constructed and tested an efficient and accurate emulator for solving 3N Faddeev equation.
- We applied it to the Nd scattering up to $E=250$ MeV, using the chiral SMS NN potential at N4LO+ supplemented by 3NF at N2LO and 13 N4LO contact terms.
- Our emulator allows us to fix free parameters of all short-range terms in the 3NF. We found that even at low energies some observables are sensitive to N4LO 3NF contact terms.
- In general, sensitivity of predictions to N4LO 3NF contact terms depends on observable, energy and scattering angle.
- Usually we observe improvements in data description, but very likely above ≈ 200 MeV 3NF is not sufficient to explain discrepancies with the data.
- The deuteron breakup data can be used in fitting as well.
- Coulomb corrections (if needed) and 3NF at N3LO have to be included for final conclusions.

James,

On behalf of the Kraków group:

- Many interesting scientific challenges and many interesting results;
- Good health to you and your family;
- All the best !