Efficient emulator for solving 3N Faddeev equation with contact terms of chiral 3NF at N4LO

R.Skibiński, J.Golak, H.Witała

JAGIELLONIAN UNIVERSITY

LENPIC Collaboration

Jagiellonian University, Kraków
Ruhr-Universität, Bochum
Forschungszentrum, Jülich
Bonn Universität,
Ohio State University
Iowa State University
Technische Universität, Darmstadt
Kyutech, Fukuoka
IPN, Orsay
TRIUMF, Vancouver

www.lenpic.org

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Outline

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. C105 (2022) 054004 *„Significance of chiral 3NF contact terms for understanding of elastic nucleon-deuteron scattering*”

1. Formalism – new set of equations

2. Proof of concept: tests and the first results on fixing short-range 3NF parameters

Our standard approach to Nd scattering

Prepare and solve the Faddeev equation

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

Compute amplitudes

$$U = PG_0^{-1} + V_{123}^{(1)}(1+P)\varphi + PT + V_{123}^{(1)}(1+P)G_0T$$

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

We work in the PWD scheme

3N state: $\left|pq\alpha\right\rangle \equiv \left|pq(ls)j(\lambda\tfrac{1}{2})I(jI)JM_J(t\tfrac{1}{2})TM_T\right\rangle$

what means, that PWD of appearing in this equation operators has to be performed.

$$\left\langle p'q'(l's')j'(\lambda'\tfrac{1}{2})I'(j'I')J'M_{J'}(t'\tfrac{1}{2})T'M_{T'}\right|\hat{O}\left|pq(ls)j(\lambda\tfrac{1}{2})I(jI)JM_J(t\tfrac{1}{2})TM_T\right\rangle$$

After decomposing 3NF:

CPU time required for one run (i.e. one reaction energy, one NN+3NF potential) amounts from approx. 1-8 hrs., depending on number of partial waves, computer parameters, disk space available). Some hardware (GPU, fast memory) or software (parallelization) improvements are still possible but the cake's not worth the candle.

Fixing parmeters of 3NF

- Up to know, i.e. when working at N2LO there are only two free parameters cD and cE.
- Typically ^{3}H and the $^2a_{nd}$ or the differential Nd elastic scattering cross section at one or few energies are used.
  The latter requieres solving the triton many times and the Fadddeev equation 10-20 times.

- However, now 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 opertors, one expect 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 - algorithm

- 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 spilt 3NF

$$\theta = \{c_1, c_2, \ldots$$

$$\theta_0 = \{0, 0, \ldots$$

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

- 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: ΔV(θ).
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 with one equation for $T(\theta_0)$ which is a standard Faddeev equation but with $V(\theta_0)$ and

$$\langle\alpha|\Delta T(\theta)|\phi\rangle = \langle\alpha|tPG_0\Delta T(\theta)|\phi\rangle + \langle\alpha|(1+tG_0)V(\theta_0)(1+P)G_0\Delta T(\theta)|\phi\rangle$$

$$\begin{aligned}\langle\beta|\Delta T(\theta)|\phi\rangle = {} & \langle\beta|(1+tG_0)\Delta V(\theta)(1+P)|\phi\rangle + \langle\beta|(1+tG_0)\Delta V(\theta)(1+P)G_0T(\theta_0)|\phi\rangle \\ & +\langle\beta|(1+tG_0)[V(\theta_0)+\Delta V(\theta)](1+P)G_0\Delta T(\theta)|\phi\rangle \\ & +\langle\beta|tPG_0\Delta T(\theta)|\phi\rangle \ .\end{aligned}$$

- We neglect term $\sim\Delta V\Delta T$, which allows to separate contributions from different ΔV_i and leads to set of equations for a corresponding ΔT_i .
  Next, for single parameter dependent component of V: $V_i=c_iV$ we may solve that equation separately (at $c_i=1$) obtaining corresponding $<\beta|\Delta T_i|\phi>$ and build

$$\langle\beta|\Delta T(\theta)|\phi\rangle = \sum_{i=1}^{N} c_i\langle\beta|\Delta T_i|\phi\rangle$$

and find also $<\alpha|\Delta T_i|\phi>$.

Emulator for Nd scattering - algorithm

- In this way we have matrix elements of T

$$\langle\alpha|T(\theta)|\phi\rangle = \langle\alpha|T(\theta_0)|\phi\rangle + \sum_i c_i\langle\alpha|\Delta T_i|\phi\rangle,$$

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

- Let us now come back to the scattering amplitudes

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

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

- They are linear in T: the dependence on the c_i parameters carries over to them

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

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

- **Summarizing: one needs to solve N+1 Faddeev equations (one for T(θ_0)) and N for <β|ΔT$_i$|ϕ>) and next build transition amplitudes for any set of c_i .**

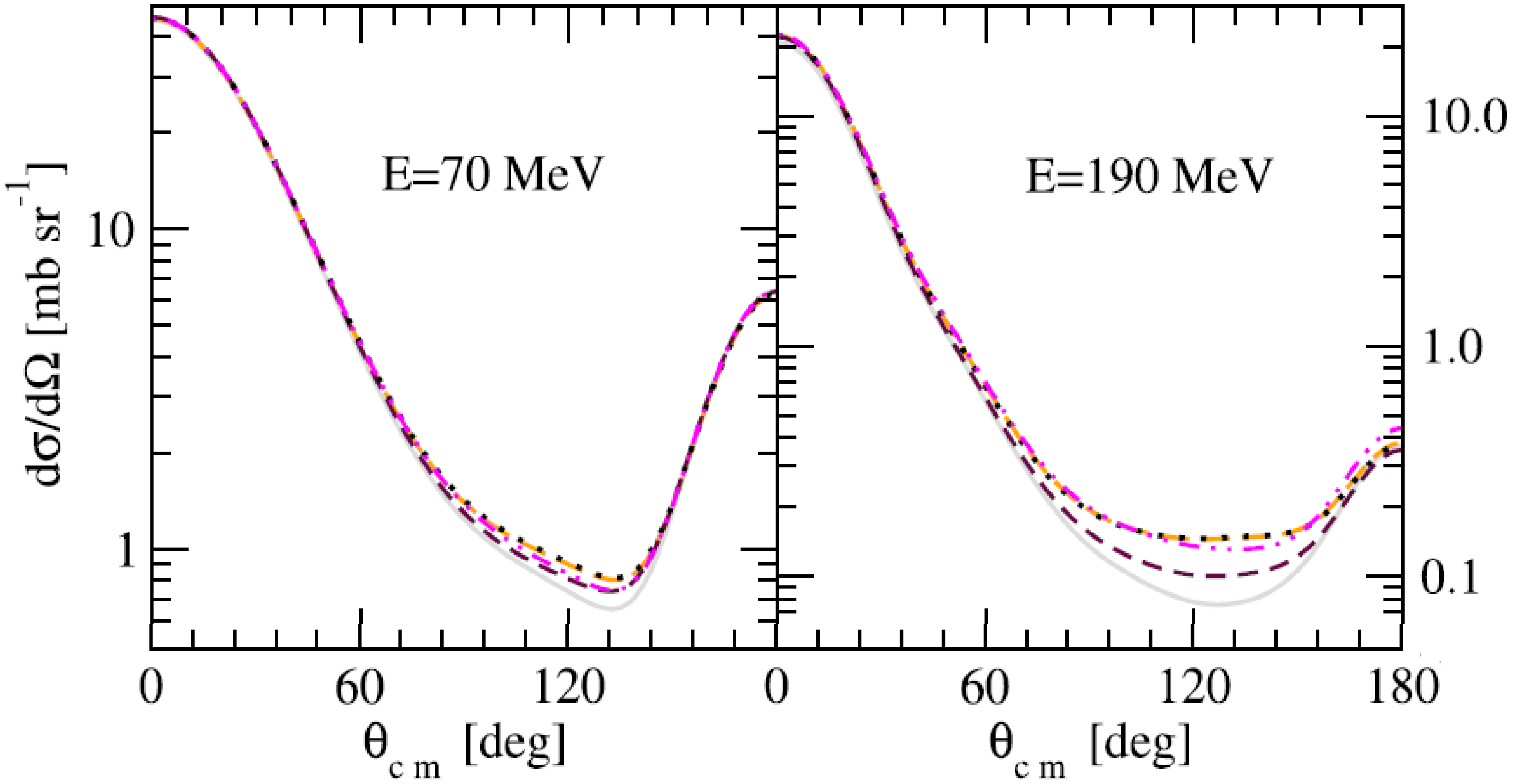
Emulator for Nd scattering – algorithm - application

- We used SMS N4LO+ NN potential at Λ=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 cD and cE, and thirteen from N4LO with the strengths E_i, i = 1, . . . , 13. However, for two pairs of the E_i terms matrix elements are identical, thus finaly there are 13 unknown parameters.

Emulator for Nd scattering – test



Exact:

NN N4LO+

NN N4LO+ + 3NF N2LO (c_D=c_E=cE_7=0.0)

NN N4LO+ + 3NF N2LO+E_7
(c_D = −8.2053, c_E=−1.0019, cE_7=2.0)

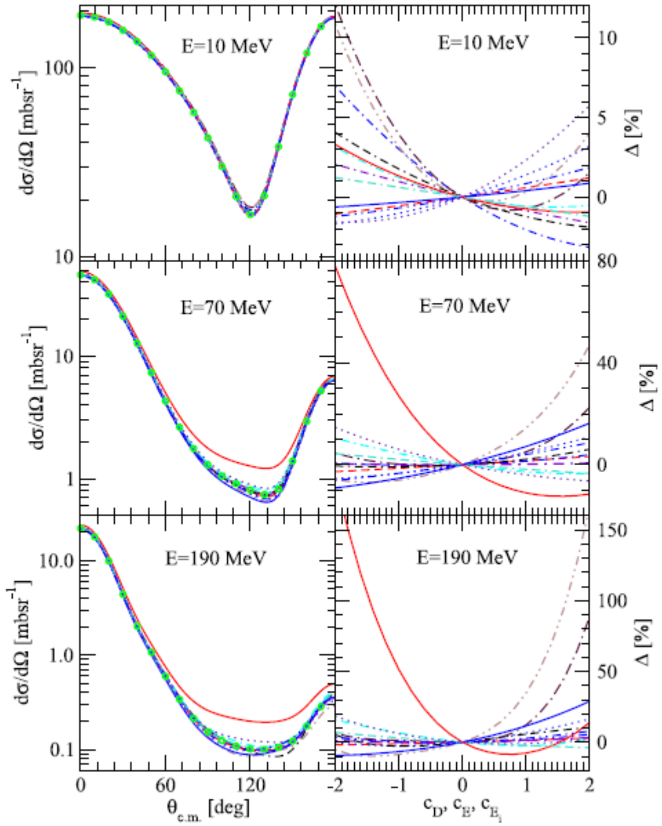
Emulator:

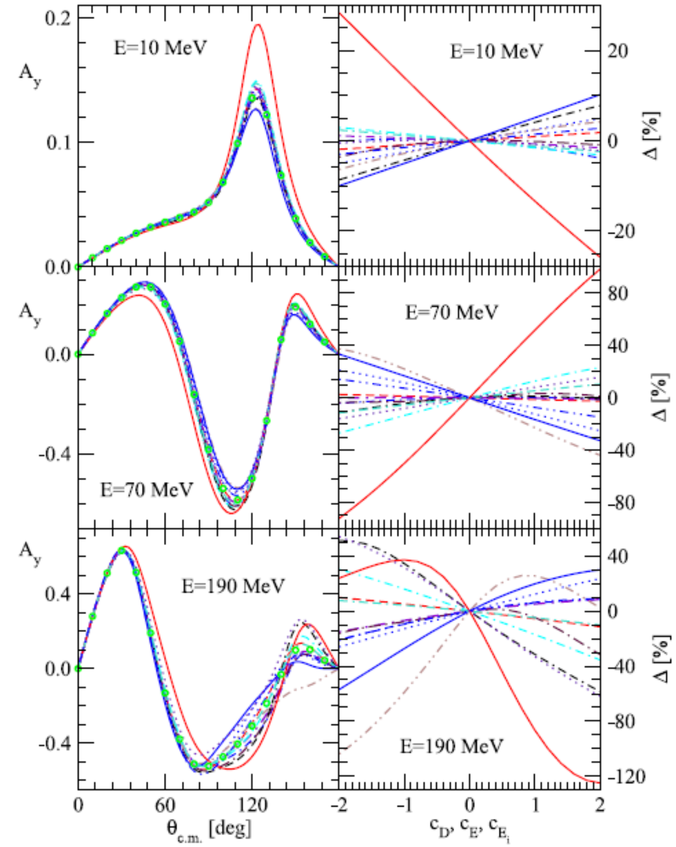
NN N4LO+ + 3NF N2LO+E_7 (β=$^1S_0$, $^3S_1$-$^3D_1$)

NN N4LO+ + 3NF N2LO+E_7 (β= j≤2)

Emulator for Nd scattering – algorithm - 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 dottted E_5

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

- N2LO D and E terms do not dominate
- Some observables are more sensitive to specific terms, e.g. T_{22} to E_{10}

Emulator for Nd scattering – application
V_i expectation values in ^{3}H at c_i=1.0

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

V_i	$\langle \psi_{^3H} \| V_i \| \psi_{^3H} \rangle$ [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

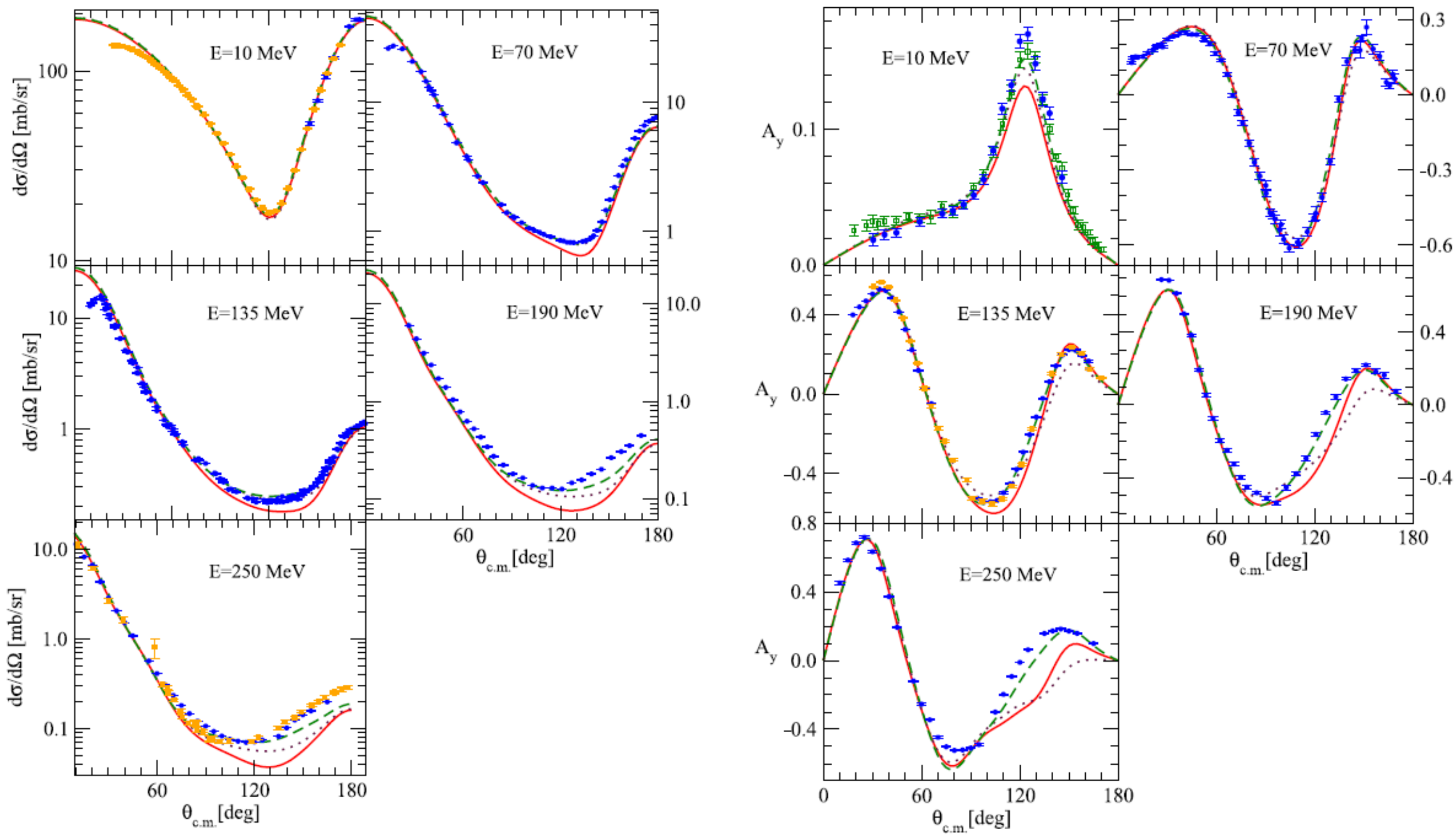
TABLE IV. The covariance matrix for the strengths c_i determined by the least squares fit of data from Table II at the three energies $E = 10$, 70, and 135 MeV [the values shown are $\mathrm{Cov}(c_i, c_j) \times 1000$].

	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 $c_{E1}, c_{E2}, c_{E3}, c_{E7}, c_{E9}$
- 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_{Ei}),(c_E,c_{Ei})
- χ^2/data≈35

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

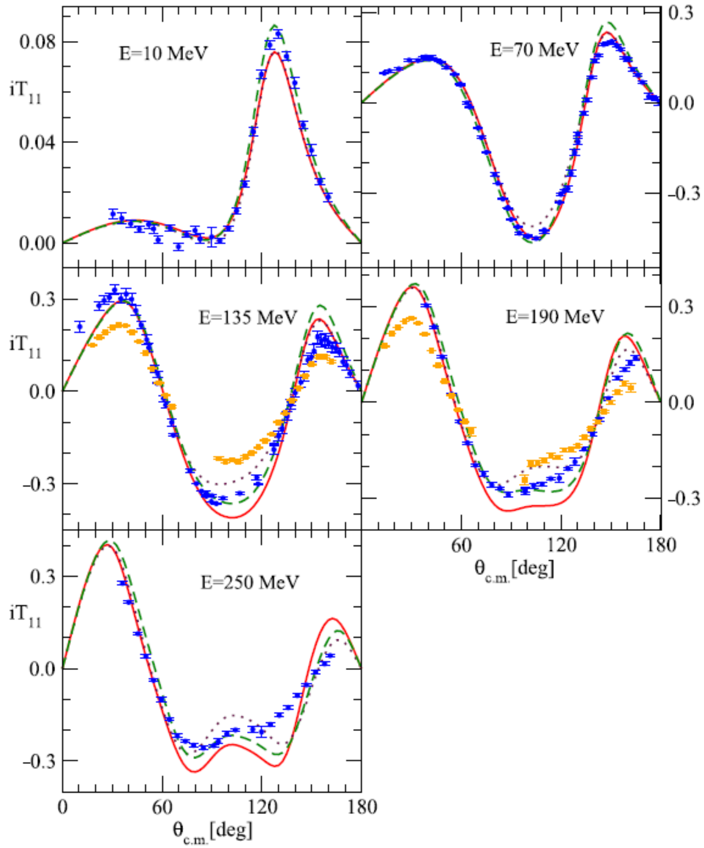
- Data at 10, 70 and 135 MeV
- Results at 190 and 250 MeV are predictions

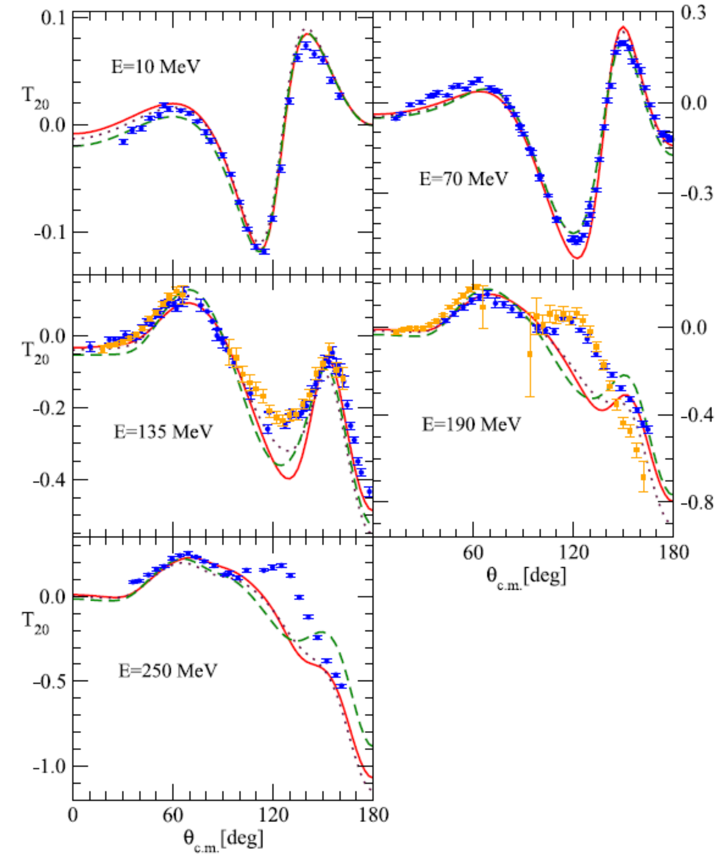


NN N4LO+ NN N4LO+ + 3NF N2LO NN N4LO+ + 3NF N2LO + E_i

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

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Summary

- 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 correction (if needed) and 3NF at N3LO has to be included for final conclusions.