

# Recent progress in *ab-initio* studies of light nuclei and few-nucleon reactions



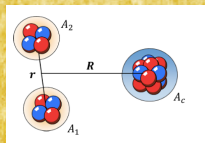
Laura E. Marcucci  
University of Pisa  
INFN-Pisa



Exploring low-energy nuclear properties:  
latest advances on reaction mechanisms with light nuclei

Workshop in honor of Pierre Descouvemont

Bruxelles, June 1, 2023



- **Introduction**

- Microscopic *ab-initio* approach
- Chiral effective field theory ( $\chi$ EFT) framework
- The Hyperspherical Harmonics (HH) *ab-initio* method

- **Selected results**

- $A = 2$  reactions:  $pp$  weak capture, muon capture on deuteron
- $A = 4$  reactions of interest for Big Bang Nucleosynthesis (BBN)

- **Outlook**

## Nuclear observable X

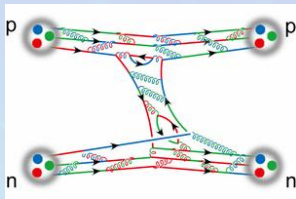
- Microscopic →
  - Nucleus = system of  $A$  nucleons
    - interacting among themselves → structure
    - interacting with external electroweak probes → reactions
- Microscopic → *ab-initio*
  - realistic description of nuclear interactions
  - realistic description of electroweak currents
  - exact<sup>1</sup> (*ab-initio*) method to solve the quantum-mechanical problem

⇒ True predictions for observable X

Ideal case: robust procedure to estimate the theoretical error

<sup>1</sup> exact  $\equiv$  no uncontrolled approximations

# The nuclear Hamiltonian: $H = T + V$



Nuclear interaction:  $V = V_{NN} + V_{NNN}$

Until  $\simeq 20$ – $30$  years ago: **phenomenological potentials**

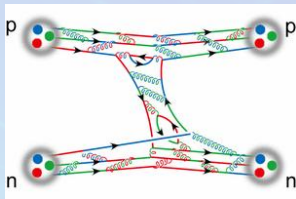
- $V_{NN} + V_{NNN}$  semi-phenomenological
- $V_{NN}$  with  $\simeq 40$  **parameters** fitted to  $A = 2$  data  
 $\rightarrow \chi^2/\text{datum} \simeq 1$
- $V_{NNN}$  with 2-3 parameters fitted to  $B(A = 3, 4)$

Very common models: **AV18+UIX**, **AV18+Illinois**

Very successful, but

- **many parameters**
- no connection with QCD
- no estimate of theoretical uncertainty

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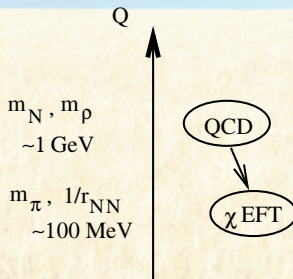
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$\Rightarrow$  **Chiral Effective Field Theory ( $\chi$ EFT)**



# Chiral Effective Field Theory ( $\chi$ EFT): a very short summary

- QCD  $\rightarrow$  quarks and gluons (“high-energy” d.o.f.)
- Nuclear physics  $\rightarrow$  nucleons and pions (“low-energy” d.o.f.)
- EFT  $\rightarrow$  processes with  $E \simeq p \simeq m_\pi \ll \Lambda_{\text{QCD}} \sim 1 \text{ GeV}$ 
  - ★ keep the “l-e” d.o.f.:  $\pi$  and  $N$  (and sometimes  $\Delta$ 's -  $m_\Delta - m_N \sim 300 \text{ MeV}$ )
  - ★ Lagrangians describing the interactions of  $\pi - N(\pi - \Delta)$  are expanded in powers of  $O(p/\Lambda_{\text{QCD}})^\nu \rightarrow$  perturbative expansion
  - ★ “h-e” d.o.f. integrated out  $\rightarrow$  contact interactions with “l-e” d.o.f. and low-energy constants (LECs) obtained from experiment
- $\chi$ EFT  $\rightarrow$  EFT with spontaneous breaking of QCD's  $\chi$ -symmetry
- Regularization of short-range terms with cutoff function  $\rightarrow \Lambda \simeq 400 - 600 \text{ MeV}$

Disadvantage: limited to processes with  $E \leq [2 \div 3] m_\pi$

## Advantages

- nuclear force “hierarchy”  $\rightarrow$  accurate  $V_{NN} + V_{NNN}$
- consistent framework for interactions + currents (just add electroweak field as d.o.f.)
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# $\chi$ EFT potentials

- **Idaho potentials:** N3LO-Idaho ( $\Lambda = 500$  MeV)  $\rightarrow$  EMN  
[D. Entem *et al.*, *Front. Phys.* **8**, 57 (2020)]
- **Norfolk potentials (NV)**  
[M. Piarulli and I. Tews, *Front. Phys.* **7**, 245 (2019)]
- **N2LOsim potentials**  
[B.D. Carlsson *et al.*, *Phys. Rev. X* **6**, 011019 (2016)]
- **SMS-RS:** semi-local regularization scheme (local for TPE and non-local for contact part)  
[P. Reinert, H. Krebs, E. Epelbaum, *Eur. Phys. J. A* **54**, 86 (2018)]

For instance:

Name	DOF	$O_\chi$	$(R_S, R_L)$ or $\Lambda$	$E$ range	Space
NVIa	$\pi, N, \Delta$	N3LO	(0.8, 1.2) fm	0–125 MeV	$r$
NVIb	$\pi, N, \Delta$	N3LO	(0.7, 1.0) fm	0–125 MeV	$r$
NVIIa	$\pi, N, \Delta$	N3LO	(0.8, 1.2) fm	0–200 MeV	$r$
NVIIb	$\pi, N, \Delta$	N3LO	(0.7, 1.0) fm	0–200 MeV	$r$
EMN450	$\pi, N$	up to N4LO	450 MeV	0–300 MeV	$p$
EMN500	$\pi, N$	up to N4LO	500 MeV	0–300 MeV	$p$
EMN550	$\pi, N$	up to N4LO	550 MeV	0–300 MeV	$p$

A. Gnech, L.E. Marcucci, M. Viviani, arXiv:2305.07568



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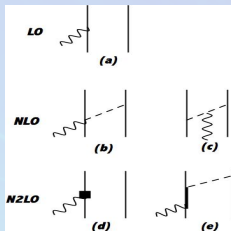
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$V_{NNN} \rightarrow$  see later

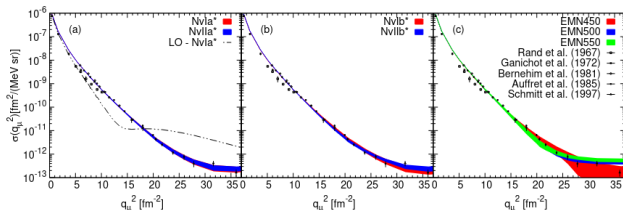
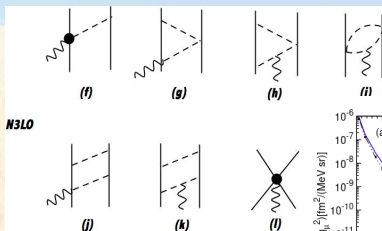
# Electromagnetic current in $\chi$ EFT



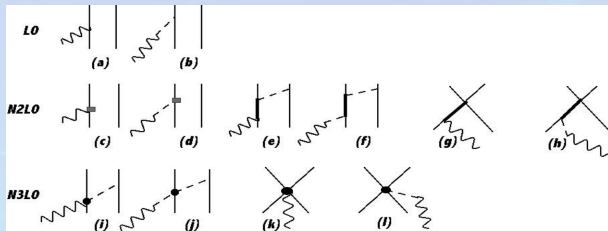
- $\mathbf{j}_{\Delta}^{N2LO}(\mathbf{q})$  in panel (e) absent in  $\Delta$ -EFT
- not included the  $\Delta$  intermediate states at N3LO
- $\mathbf{j}_{\text{OPE}}^{N3LO}(\mathbf{q}) \rightarrow d_2^S, d_2^V; d_3^V$
- $\mathbf{j}_{\text{MIN}}^{N3LO}(\mathbf{q}) \rightarrow$  from  $\pi N$  scattering
- $\mathbf{j}_{\text{NM}}^{N3LO}(\mathbf{q}) \rightarrow d_1^S; d_1^V$

**FIT:** all 5 LECs fitted to  $A = 2, 3$  magnetic moments,  $d$  magnetic form factor and  $d(e, e')pn$  at threshold

A. Gnech and R. Schiavilla, Phys. Rev. C **106**, 044001 (2022)



# Axial current in $\chi$ EFT



A. Baroni et al., Phys. Rev. C 98, 044003 (2018)

- Ignore pion-pole terms [(b), (d), (f), (h), (j), (l)]
- diagrams (g) and (h) vanish; diagram (e)  $\rightarrow c_3^\Delta$ ;  $c_4^\Delta$  (similar to  $c_3$ ;  $c_4$  of diagram (i))
- CTs in (i) and (k)

$$j_{5,a}^{N3LO}(\mathbf{q}; CT) = z_0 e^{i\mathbf{q}\cdot R_{ij}} \frac{e^{-(r_{ij}/R_S)^2}}{\pi^{3/2}} (\boldsymbol{\tau}_i \times \boldsymbol{\tau}_j)_a (\boldsymbol{\sigma}_i \times \boldsymbol{\sigma}_j)$$

$$z_0 = \frac{g_A}{2} \frac{m_\pi^2}{f_\pi^2} \frac{1}{(m_\pi R_S)^3} \left[ -\frac{1}{4} \frac{m_\pi}{g_A \Lambda_\chi} c_D + \frac{m_\pi}{3} (c_3 + 2c_4 + c_3^\Delta + 2c_4^\Delta) + \frac{m_\pi}{6m} \right]$$

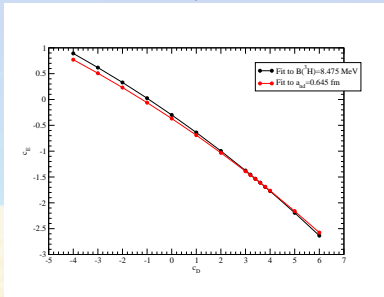
$z_0/d_R \leftrightarrow c_D$  (LEC in  $V_{NNN}$ )  $\rightarrow GT^{exp}$  in  ${}^3\text{H}$   $\beta$ -decay

Factor  $-1/4$  missing in many calculation (error spread in 2012-2018)

# Interplay potential-current in $\chi$ EFT

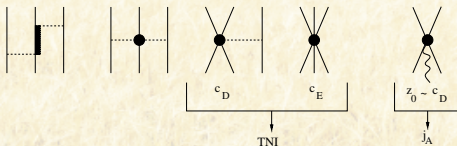
- $NV2+3/nY$ : fit  $c_D$  &  $c_E$  to  $B(^3H)$  and  $a_{nd}^{Exp} = (0.645 \pm 0.010)$  fm

M. Piarulli *et al.*, Phys. Rev. Lett. **120**, 052503 (2018)



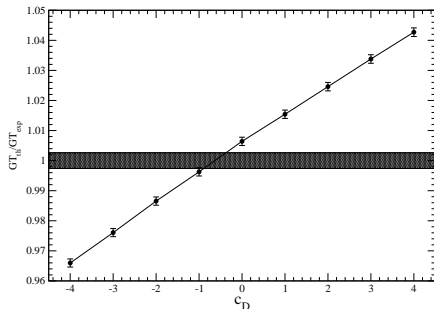
→ correlation  $B(^3H)/a_{nd}$

- Use  $B(^3H)$  and  $GT^{exp}$  of  $^3H$   $\beta$ -decay →  $NV2+3/nY^*$



	NV2+3/1a	NV2+3/1b
$c_D$	3.666	-2.061
$c_E$	-1.638	-0.982
<b>GT</b>	<b>0.9885</b>	<b>0.9730</b>
	NV2+3/1a*	NV2+3/1b*
$c_D$	-0.635	-4.71
$c_E$	-0.09	0.55

$$GT^{exp} = 0.9511 \pm 0.0013$$



### A = 3, 4 HH binding energies and scattering lengths

Model	B( $^3\text{H}$ )	B( $^3\text{He}$ )	B( $^4\text{He}$ )	$a_{nd}^{(2)}$	$a_{nd}^{(4)}$
NV2/1a	8.718	7.090	25.15	1.119	6.326
NV2/1b	7.599	6.885	23.96	1.307	6.327
<b>NV2+3/1a</b>	<b>8.475</b>	<b>7.735</b>	<b>28.33</b>	<b>0.645</b>	6.327
<b>NV2+3/1b</b>	<b>8.475</b>	<b>7.737</b>	<b>28.30</b>	<b>0.645</b>	6.327
<b>NV2+3/1a*</b>	<b>8.477</b>	<b>7.727</b>	<b>28.30</b>	<b>0.638</b>	6.326
<b>NV2+3/1b*</b>	<b>8.469</b>	<b>7.724</b>	<b>28.21</b>	<b>0.650</b>	6.327
Exp.	8.475	7.725	28.30	0.645(10)	6.35(2)

# The Hyperspherical Harmonics (HH) method

## Bound states

$$\Psi^{JJ_z} = \sum_{\mu} c_{\mu} \Psi_{\mu}$$

- $\Psi_{\mu} \rightarrow$  known functions (spin-isospin HH functions)
- **Rayleigh-Ritz var. principle:**  
 $\delta_c \langle \Psi^{JJ_z} | H - E | \Psi^{JJ_z} \rangle = 0$   
 $\Rightarrow$  Solve for  $E$  and  $c_{\mu}$

## Scattering states

$$\Psi_{LSJ} = \Psi_{core}^{LSJ} + \Psi_{asym}^{LSJ}$$

- $\Psi_{core}^{LSJ} = \sum_{\mu} c_{\mu} \Psi_{\mu}$
- $\Psi_{asym}^{LSJ} \propto \Omega_{LS}^R + \sum_{L'S'} R_{LL',SS'} \Omega_{L'S'}^I$
- **Kohn var. principle:**  
 $[R_{LL',SS'}] = R_{LL',SS'} - \langle \Psi_{L'S'J} | H - E | \Psi_{LSJ} \rangle$   
 $\Rightarrow$  Solve for  $c_{\mu}$  and  $R_{LL',SS'}$   $\rightarrow$  **phase-shifts and mixing angles**

## Strength

and

## weakness

- |                                    |                                 |
|------------------------------------|---------------------------------|
| • very accurate                    | • at present limited to $A = 6$ |
| • both $r$ - and $p$ -space        | • in prospective $A = 8$        |
| • both bound and scattering states | • not much more ...             |

# SELECTED RESULTS

- $A = 2$  reactions:  $pp$  and  $\mu - d$  weak captures

# The $pp$ fusion in $\chi$ EFT: an update

B. Acharya, L.E. Marcucci, L. Platter, arXiv:2304.03327

- updated constants (especially  $g_A = 1.2754$ )
- **correct the  $-1/4$  factor**
- better techniques (Bayesian methods) to estimate the theoretical error
- **benchmark of two approaches** (Var. Method and Lippmann-Schwinger)
- various  $\chi$ EFT potentials

Model	Method	$1/m_N^2$ term	$c_D$	Goal
SMS-RS	LS	excluded	from $nd$ scatt.	$\Delta(\chi)$
N2LOsim	LS	excluded	from $GT^{exp}$	update
LO ... N2LO <sup>†</sup>	LS	excluded	from $GT^{exp}$	$\Delta(c_D)$
N3LO-Idaho	VM/LS	included/excluded	from $GT^{exp}$	update + benchmark

<sup>†</sup> Bayesian analysis of S. Wesolowski *et al.*, Phys. Rev. C **104**, 064001 (2021)



## Order-by-order convergence (SMS-RS)

Order	$S(0)$ $\times 10^{-23}$ MeV fm <sup>2</sup>	$S'(0)/S(0)$ MeV <sup>-1</sup>	$S''(0)/S(0)$ MeV <sup>-2</sup>	$S'''(0)/S(0)$ MeV <sup>-3</sup>
LO	4.143	10.75	306.75	-5150
NLO	4.094	10.81	312.78	-5370
NNLO [N3LO]	4.100	10.83	313.72	-5382

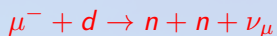
## Benchmark VM vs. LS (N3LO-Idaho)

$ft_{3H}$ -value $s^{-1}$	Method	$S(0)$ $\times 10^{-23}$ MeV fm <sup>2</sup>	$S'(0)/S(0)$ MeV <sup>-1</sup>	$S''(0)/S(0)$ MeV <sup>-2</sup>	$S'''(0)/S(0)$ MeV <sup>-3</sup>
1134.6(3.1)	VM	4.115(4)	10.60	347.1	-6908
	LS	4.101(4)	10.83	313.8	-5382
1129.6(3.0)	VM	4.118(4)	10.60	347.1	-6907
	LS	4.104(4)	10.83	313.8	-5381
1132.1(4.3)	VM	4.117(4)	10.60	347.1	-6908
	LS	4.104(4)	10.83	313.8	-5382

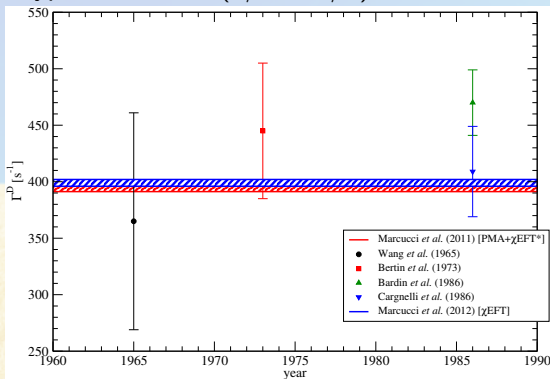
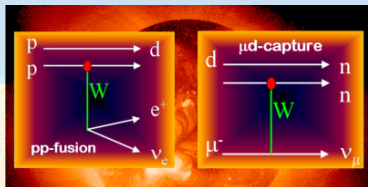
$$S(0) = [4.100 \pm 0.024(\text{syst}) \pm 0.013(\text{stat}) \pm 0.008(g_A)] \times 10^{-23} \text{ MeV fm}^2$$

# The muon capture on deuteron in $\chi$ EFT (I)

A. Gnech, L.E. Marcucci, M. Viviani, arXiv:2305.07568



Two hyperfine states (1/2 & 3/2)  $\Rightarrow \Gamma^D$  &  $\Gamma^Q$



MuSun Collab. at PSI  $\rightarrow$  1.5% exp. error

# The muon capture on deuteron in $\chi$ EFT (II)

$$\Gamma(E'_1) = \frac{G_V'^2}{\pi} |\psi_{1s}(0)|^2 E_1 p_1 \int d \cos \theta_1 \frac{E_2 k_\nu^2}{E_2 + k_\nu + p_1 \cos \theta_1} \sum_{s_1 s_2 h_\nu} \sum_{f_z} |M_{fi}(f_z, s_1, s_2, h_\nu; p_1, \cos \theta_1)|^2$$
$$\Gamma = \int_0^{E'_1 \max} dE'_1 \Gamma(E'_1)$$

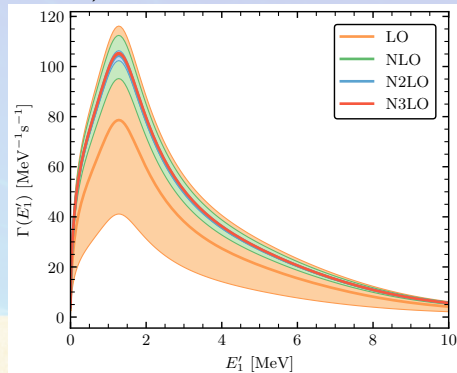
with  $\cos \theta_1 = \mathbf{q} \cdot \mathbf{p}_1$

- update previous work with most recent potentials and currents
- provide  $\Gamma(E'_1)$  to experimentalists (rather than  $\Gamma(p)$ )
- robust estimate of theoretical uncertainties

Theoretical uncertainties from:

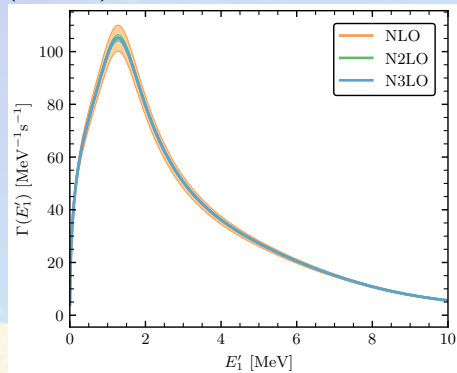
- $g_A(q^2) = g_A \left(1 - \frac{1}{6} r_A^2 q^2\right)$  with  $r_A^2 = 0.46(16) \text{ fm}^2$   
R.J. Hill et al., Rep. Prog. Phys. **81**, 096301 (2018)
- **chiral truncation** of interaction and current (Bayesian analysis)
- **model dependence**

## Chiral truncation error for the current (EMN550 at N3LO)



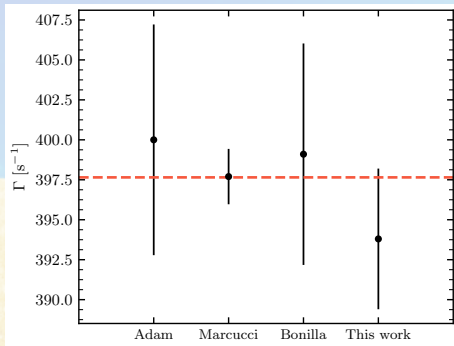
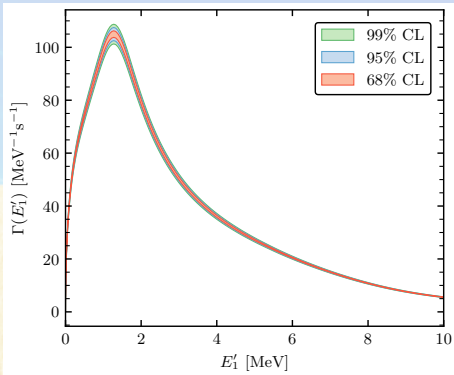
Bands= $2\sigma$  truncation error

## Chiral truncation error for the interaction (EMN550)

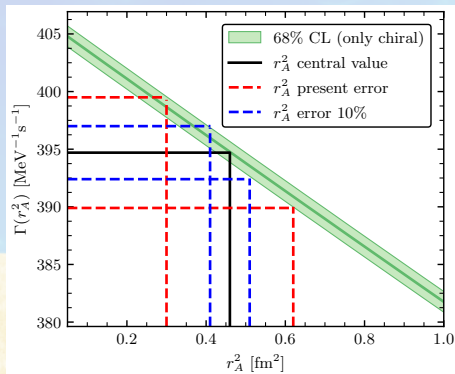
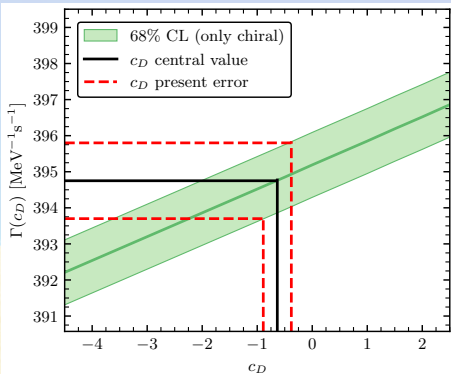


Inter.	$\Gamma(\text{comp})$	$M_{k=3}^C$	$M_{k=4}^I$	$\Gamma(\infty)$	$\sigma_{k=3}^C$ (68% CL)	$\sigma_{k=4}^I$ (68% CL)	$\sigma_{\text{LECs}}$ (68% CL)
NVIa	394.6	0.1	n.a.	394.7	0.8(0.7)	n.a.	3.9
NVib	395.0	0.1	n.a.	395.1	1.4(0.8)	n.a.	3.9
NVIIa	393.6	0.1	n.a.	393.7	0.8(0.7)	n.a.	3.9
NVIIb	394.0	0.1	n.a.	394.1	1.5(0.8)	n.a.	3.9
EMN450	<b>389.8</b>	0.1	-0.2	<b>389.7</b>	0.8(0.7)	0.4(0.4)	3.8
EMN500	393.4	0.1	0.2	393.7	0.8(0.7)	0.3(0.2)	3.9
EMN550	395.2	0.1	0.2	395.5	0.8(0.7)	0.4(0.2)	3.9

$$\Gamma = (393.8 \pm 4.4) \text{ s}^{-1} \quad (68\% \text{ CL})$$



# Impact on the MuSun Experiment



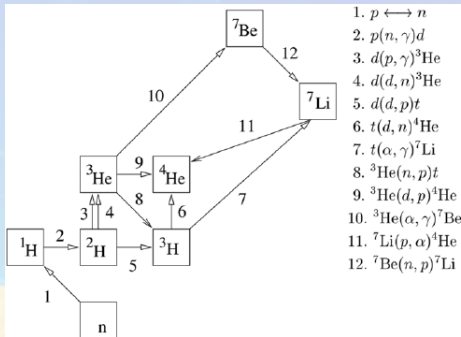
- $c_D$ -uncertainty  $\rightarrow$  minimal impact on  $\Gamma$
- present  $r_A$ -uncertainty  $\rightarrow \sim 1\%$  error on  $\Gamma$

$\Rightarrow r_A$ -uncertainty  $\sim 10\% \rightarrow$  error on  $\Gamma$  of  $0.6\% \ll$  MuSun quoted error (1.5%)

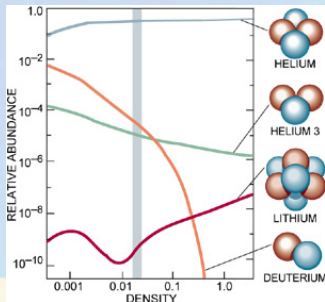
# SELECTED RESULTS

- $A = 4$  reactions of interest for BBN

# The primordial deuterium abundance



1.  $p \leftrightarrow n$
2.  $p(n, \gamma)d$
3.  $d(p, \gamma)^3\text{He}$
4.  $d(d, n)^3\text{He}$
5.  $d(d, p)t$
6.  $t(d, n)^4\text{He}$
7.  $t(\alpha, \gamma)^7\text{Li}$
8.  $^3\text{He}(n, p)t$
9.  $^3\text{He}(d, p)^4\text{He}$
10.  $^3\text{He}(\alpha, \gamma)^7\text{Be}$
11.  $^7\text{Li}(p, \alpha)^4\text{He}$
12.  $^7\text{Be}(n, p)^7\text{Li}$



$$10^5(\text{D}/\text{H})_{\text{exp}} = 2.527 \pm 0.030$$

R.J. Cooke *et al.*, *Astrophys. J.* **885**, 102 (2018)

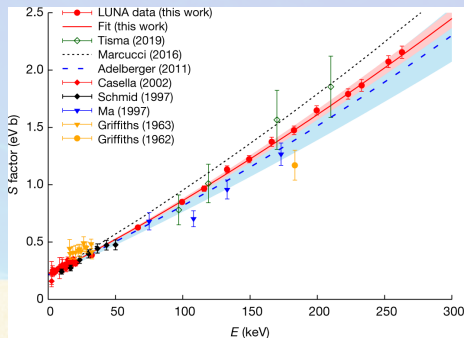
Crucial inputs for BBN

- $p(d, \gamma)^3\text{He}$
- $d(d, p)^3\text{H}$  &  $d(d, n)^3\text{He}$

LUNA experiment for  $p(d, \gamma)^3\text{He}$



# The ${}^2\text{H}(p, \gamma){}^3\text{He}$ reaction - The LUNA experiment



$$10^5 (D/H)_{\text{BBN}} = 2.52 \pm 0.03 \pm 0.06$$

vs.

$$10^5 (D/H)_{\text{exp}} = 2.527 \pm 0.030$$

----- Phenomenological approach (AV18/UIX)

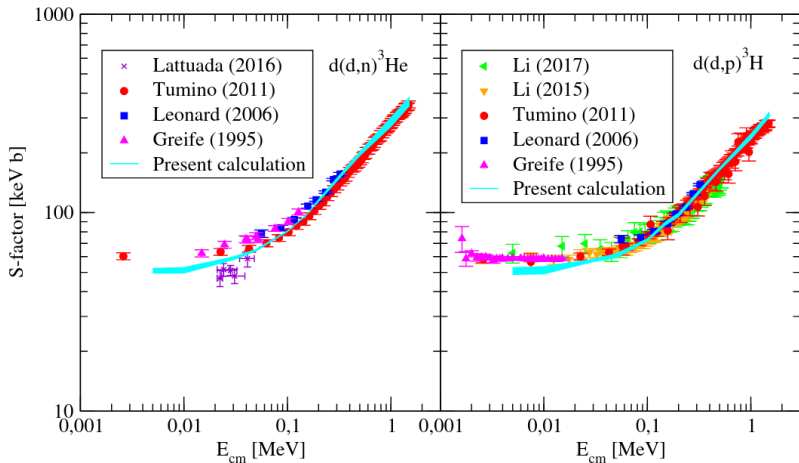
→ what is the theoretical uncertainty?  $\Rightarrow \chi\text{EFT}$  (work in progress)

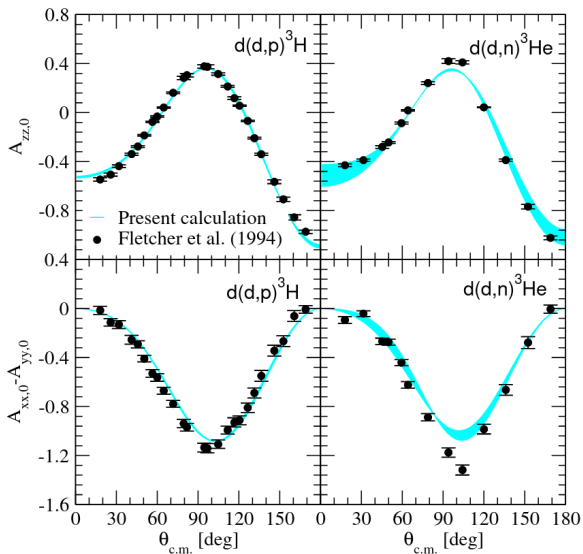
**BBN error now dominated by  $d(d, p){}^3\text{H}$  &  $d(d, n){}^3\text{He}$**

V. Mossa *et al.*, Nature **587**, 210 (2020)

# The $d(d, p)^3\text{H}$ and $d(d, n)^3\text{He}$ processes

M. Viviani *et al.*, Phys. Rev. Lett. **130**, 122501 (2023)

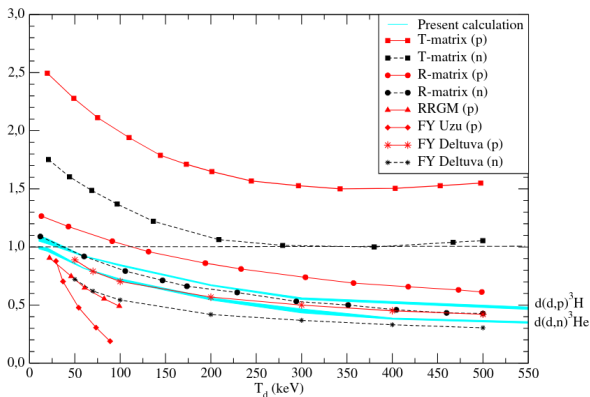
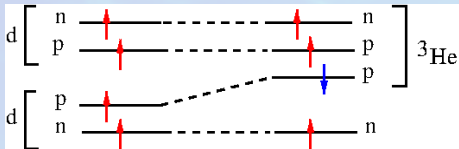




Nice agreement theory vs. experiment

# The “quintic” suppression factor

$\vec{d}(\vec{d}, n)^3\text{He}$  &  $\vec{d}(\vec{d}, p)^3\text{H}$  suppressed in  $S$ -wave



⇒ “neutron lean” reactors

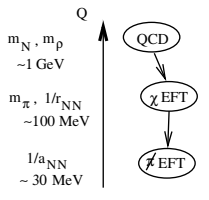
# Outlook

- **HH method**: systematic study of  $A \geq 4$  bound- and scattering states
- **Further *ab-initio* predictions in  $\chi$ EFT** for
  - Reactions involved in the BBN network or stellar evolution
  - $e^+e^-$  production in  $p+{}^7\text{Li}$  (ATOMKI) (**but also in  $p+{}^2\text{H}$** )
  - Muon capture on  $A = 3, 4, 6$  nuclei (work in progress)
  - $\beta$ -decay of  $6 \leq A \leq 8$  systems
- **Low energies**  $\rightarrow$  “new” framework:  $\not\chi$ EFT

## Pionless EFT ( $\not\chi$ EFT): going lower in energy ...

### Advantages

- **drastic simplification in the operatorial structure** for both potentials and currents
- **faster convergence** in the HH expansion
- more direct match with lattice QCD calculations (performed at large  $m_\pi$ )
- large  $a_{NN} \Rightarrow$  short-range  $NN$  dynamics does not decouple in the  $NNN$  sector  $\Rightarrow V_{NNN}$  at LO



# Local $V_{NN} + V_{NNN}$ in $\not\{EFT$

- $V_{NN} \rightarrow$  contact terms up to  $Q^4$  (N3LO)

$$C(r) = C_0(r)P_0^\tau + C_1(r)P_1^\tau$$

$$C_\alpha(r) = \frac{e^{-(r/R_\alpha)^2}}{\pi^{3/2} R_\alpha^3}$$

Model	a	b	c	d	o
$R_0$ (fm)	1.7	1.9	2.1	2.3	1.54592984
$R_1$ (fm)	1.5	2.0	2.5	3.0	1.83039397

Model	Order	$T_{\text{lab}}$ (MeV)	$N_{np}$	$\chi^2(np)/\text{datum}$	$N_{pp}$	$\chi^2(pp)/\text{datum}$	$N$	$\chi^2/\text{datum}$
a	LO	0-1	91	5.54	157		248	
	NLO	0-15	381	1.83	394	1.53	776	1.67
	N3LO	0-25	643	1.60	451	1.24	1096	1.45
b	LO	0-1	91	37.6	157		248	
	NLO	0-15	382	1.39	395	1.09	778	1.24
	N3LO	0-25	646	1.42	452	1.06	1099	1.27
c	LO	0-1	91	24.8	157		248	
	NLO	0-15	378	2.34	392	1.97	771	2.15
	N3LO	0-25	645	1.83	453	1.33	1099	1.62
d	LO	0-1	91	41.2	157		248	
	NLO	0-15	377	10.2	392	6.88	770	8.51
	N3LO	0-25	638	2.03	446	8.09	1085	4.52
o	LO	0-1	91	2.16	157		248	
	NLO	0-15	382	1.27	394	1.08	777	1.17
	N3LO	0-25	650	1.25	452	1.10	1103	1.19

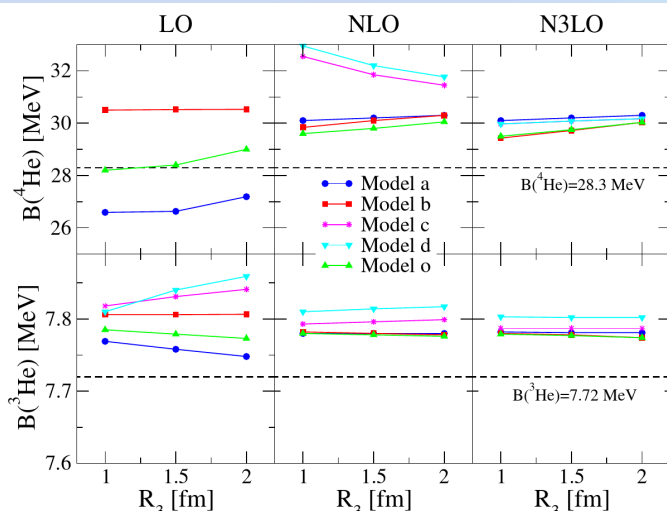
- $V_{NNN}$  up to LO  $\rightarrow c_E$  fitted to  $B(^3\text{H})$

R. Schiavilla *et al.*, Phys. Rev. C **103**, 054003 (2021)

# $\not\equiv$ EFT: from few- to many-body systems (I)

R. Schiavilla *et al.*, Phys. Rev. C **103**, 054003 (2021)

- $V_{NN}$  LO-N3LO fitted to  $NN$  systems
- $V_{NNN}$  only at LO fitted to  $B(^3\text{H}) \Rightarrow B(^3\text{He}), B(^4\text{He}), \dots =$  predictions

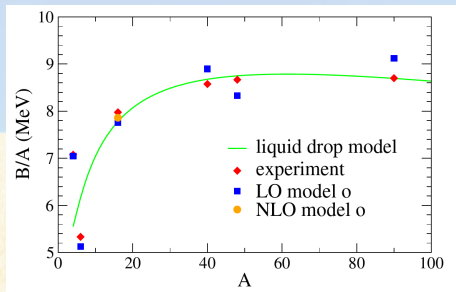


# $\neq$ EFT: from few- to many-body systems (II)

R. Schiavilla *et al.*, Phys. Rev. C **103**, 054003 (2021)

$V_{NN} + V_{NNN}$  applied to

- ${}^4\text{He}$ ,  ${}^6\text{Li}$ ,  ${}^6\text{He} \rightarrow \text{HH} + \text{AFDMC}$  (benchmark)
- ${}^{16}\text{O}$ ,  ${}^{40}\text{Ca}$ ,  ${}^{48}\text{Ca}$ ,  ${}^{90}\text{Zr} \rightarrow \text{AFDMC}$



Outlook:

- 1 Go beyond  $V_{NNN}(\text{LO}) \rightarrow V_{NNN}(\text{N3LO})$  ( $A_y$ -puzzle)
- 2 Develop the **consistent electroweak transition operators**



## In collaboration with

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- D. Logoteta (Univ. Pisa)
- L. Girlanda (Univ. del Salento)
- A. Gnech (ECT\*)
- R. Schiavilla (JLab-ODU)
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**Thank you, Pierre, for all your inspiring work!**

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Thank you All for your attention!