Uncertainty Quantification, Verification & Validation, and predictions in Pionless EFT.

Doron Gazit – Racah Institute of Physics

ISRAEL SCIENCE FOUNDATION

EMMI Workshop and International Workshop XLIX on Gross Properties of Nuclei and Nuclear Excitations

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Thanks to my collaborators: Hilla De Leon and Lucas Platter

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Introduction

- Making accurate predictions is a herald of any theory, and nuclear theory is no different.
- Quantitative uncertainty estimate is essential for predictions.
- Verification and validation of the theory is at least nice to have.

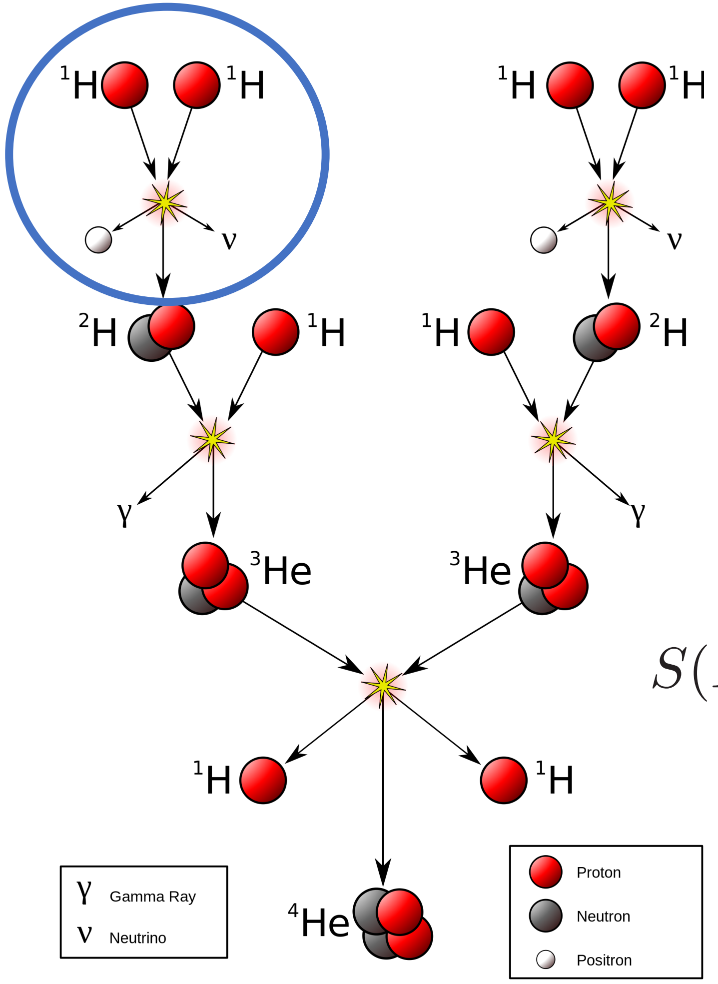
“A theory is something nobody believes, except the person who made it.
An experiment is something everybody believes, except the person who made it”

Introduction

- Making accurate predictions is a herald of any theory, and nuclear theory is no different.
- Quantitative uncertainty estimate is essential for predictions.
- Verification and validation of the theory is at least nice to have.
- The current work is intented to show that pionless EFT, at next-to-leading order, can achieve high accuracy and precision$\approx 1\%$, for M_1 observables of the deuteron, triton and ^{3}He at vanishing momentum transfer.
- We use this to predict the analogue proton-proton fusion at solar conditions and its theoretical uncertainty.

De-Leon, PhD thesis (2020). De-Leon, DG, arXiv: 2004.11670 (2020) De-Leon, Platter, DG, PRC 100, 055502 (2019) De-Leon, DG, arXiv: 2207.10176 (2022)

Weak proton-proton fusion in the Sun



Cannot be measured terrestrially – depends on theory

Very low proton-proton relative momentum (*E_{rel}~6 keV*).

Needed accuracy: ~1%.

$$\sigma(E) = \frac{S(E)}{E} \exp[-2\pi\eta(E)]$$

$$S(E) = S(0) + S'(0)E + S''(0)E^2/2 + \cdots$$

Theory challenge: accuracy and precision

Weak proton-proton fusion in the Sun – theory standards

SFII – Adelberger et al., Rev. Mod. Phys. 83, 195 (2011)

$$4.01(1 \pm 0.009) \times 10^{-25}\ \mathrm{MeV\,b} \quad \text{potential models},$$
$$4.01(1 \pm 0.009) \times 10^{-25}\ \mathrm{MeV\,b} \quad \mathrm{EFT}^*,$$
$$3.99(1 \pm 0.030) \times 10^{-25}\ \mathrm{MeV\,b} \quad \text{pionless EFT}.$$

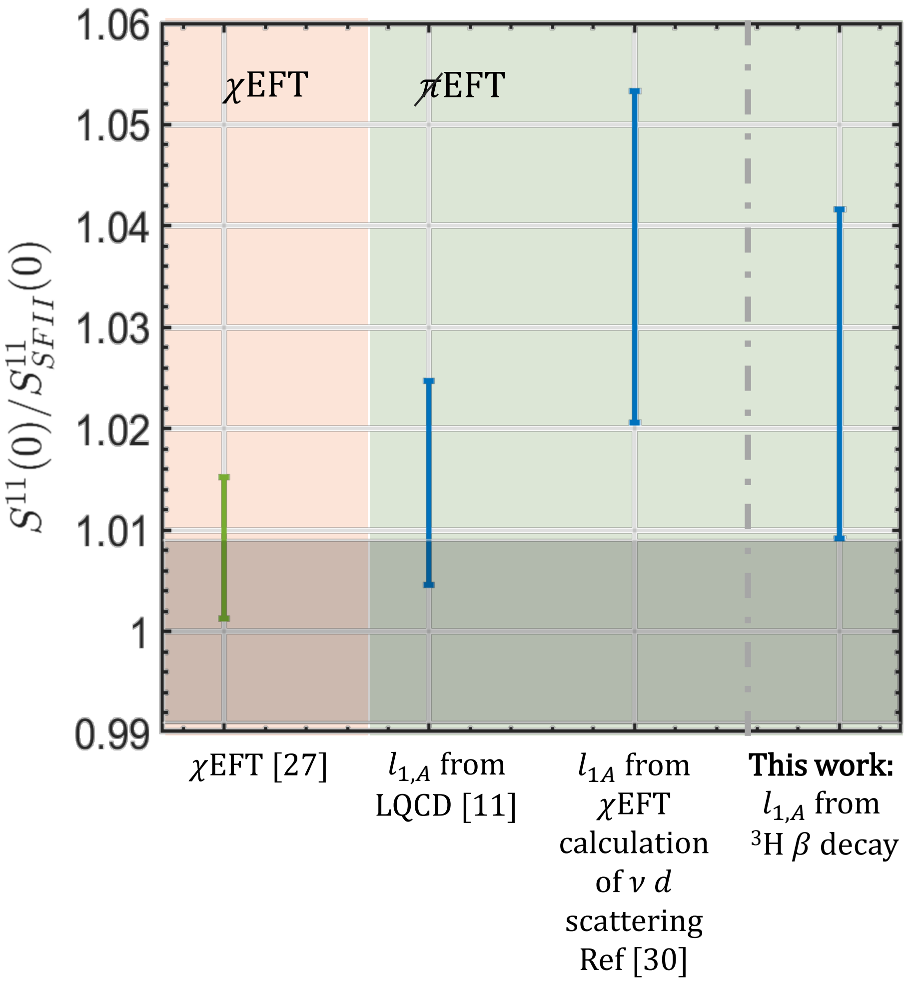
2011

SFII recommended value (2011): $S_{11}(0) = 4.01(1 \pm 0.009) \times 10^{-25}\ \mathrm{MeV\,b}.$

Marcucci et al. $S(0) = (4.030 \pm 0.006) \times 10^{-23}\ \mathrm{MeV\ fm}^2$ **2013**

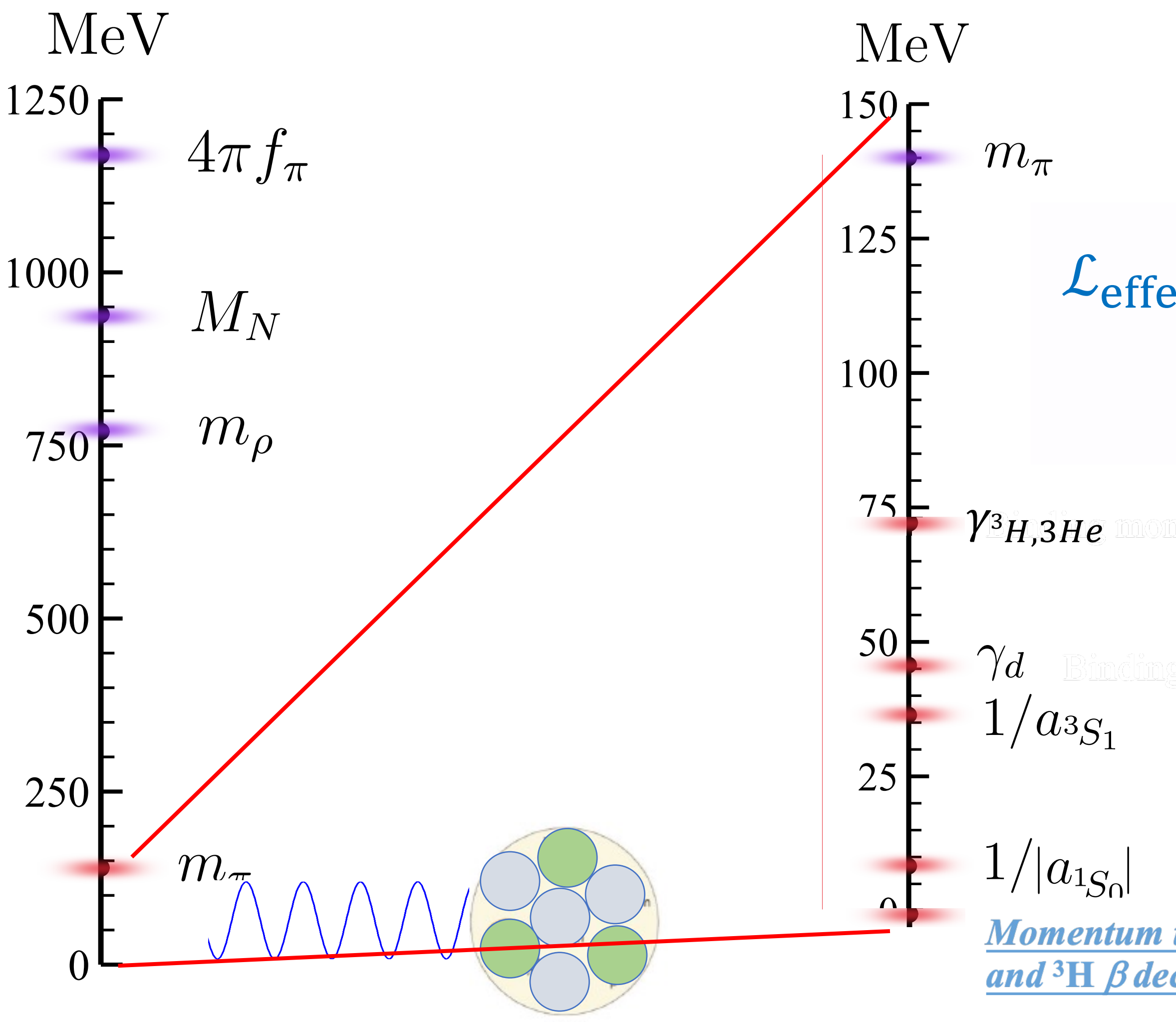
Acharya et al (1603.01593) *χEFT*:: $S(0) = (4.081^{+0.024}_{-0.032}) \times 10^{-23}\ \mathrm{MeV\ fm}^2$ **2016**

Weak proton-proton fusion in the Sun – theory standards



QCD scales

Pionless EFT scales



$$\mathcal{L}_{\text{effective}} = \underbrace{\mathcal{O}(1)}_{LO} + \underbrace{\mathcal{O}\left(\frac{q}{m_\pi}, \frac{r}{a}\right)}_{NLO} + \cdots +$$

Pionless EFT can be applied to reactions in A=2, 3 systems

Momentum transfer in solar pp-fusion and ^{3}H β decay

- $a_{^3S_1} \approx 5.4$ fm, $a_{^1S_0} \approx -23.7$ fm $\gg 1/m_\pi \approx 1.4$ fm
- effective ranges (1.8 fm, 2.7 fm) are natural

$$\gamma_{typical} = \sqrt{2M_N E/A}$$

From S. König

QCD scales

Pionless EFT scales

EMMI Rapid Reaction Task Forces

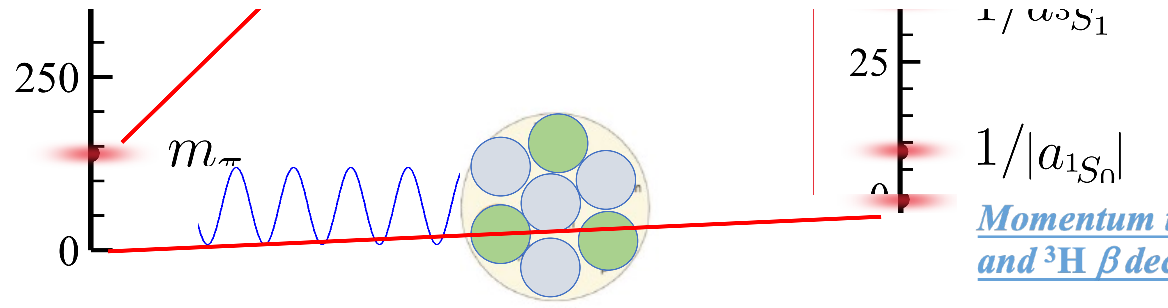
$$\mathcal{L}_{\text{effective}} = \mathcal{O}(1) + \mathcal{O}\left(\frac{q}{m}, \frac{r}{a}\right) + \cdots +$$

The systematic treatment of the Coulomb interaction in few-body systems

Part I: Jan 11-15, 2016, TU Darmstadt

Part II: May 30 - Jun 03, 2016, GSI, Darmstadt

Organizers: S. Koenig, D. Gazit, H. Grießhammer, J. Vanasse



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$$\gamma_{typical} = \sqrt{2M_N E/A}$$

From S. König

The pionless EFT expansion parameter

For any observable $\hat{T}$:

$$T = T_{LO} \times \left(1 + \underbrace{\frac{T_{NLO}}{T_{LO}}}_{order\ O(\epsilon)} + O(\epsilon^2) \right)$$

- Observables may differ in their convergence pattern.
- There can be several expansions, that differ by the two-body experimental observables that are chosen to be reproduced at each order:
  - **Effective range parameterization**: effective ranges are fully reproduced at NLO

$$\rho = \underbrace{0}_{LO} + \underbrace{\rho_{exp}}_{NLO}$$

  - **Z-parameterization**: deuteron residue is fully reproduced at NLO

$$Z_d = \underbrace{1}_{LO} + \underbrace{\left(Z_d^{exp} - 1\right)}_{NLO}$$

Phillips; Grießhammer

The pionless EFT expansion parameter

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  - **Effective range parameterization**: effective ranges are fully reproduced at NLO

$$\rho = \underbrace{0}_{LO} + \underbrace{\rho_{exp}}_{NLO} \Longrightarrow Z_d = \frac{1}{1-\gamma_t \rho_t} = 1 + \gamma_t \rho_t + O((\gamma_t \rho_t)^2) \approx 1.4$$ (i.e., 17% deviation from exp)

  - **Z-parameterization**: deuteron pole residue is fully reproduced at NLO

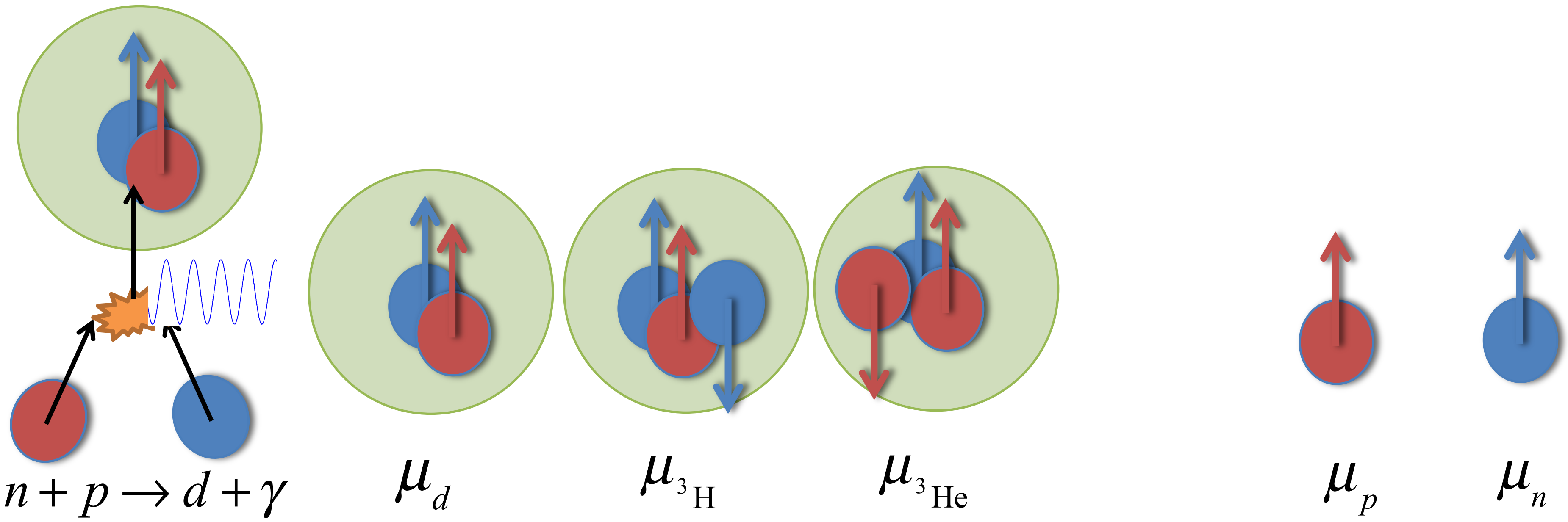
$$Z_d = \underbrace{1}_{LO} + \underbrace{(Z_d^{exp} - 1)}_{NLO} \Longrightarrow \rho_t = \frac{Z_d - 1}{\gamma_t} \approx 2.96\ \mathrm{fm}$$ (i.e., 40% deviation from exp)

The strong sector of pionless EFT A=2, 3 next-to-leading order expansion

- **5** Leading Order Parameters
  - nn and 2-np Scattering lengths: $^3S_1$, $^1S_0$.
  - pp scattering length.
  - Three body force strength renormalizing the three body system. (introduces cutoff Λ)
- **5** Next-to Leading Order parameters:
  - 2 effective ranges (or 1 effective range and Z_d)
  - Renormalizations of pp scattering length and LO-3NF.
  - isospin dependent 3NF to prevent logarithmic divergence in the binding energy of ^{3}He.
- Use ^{3}H and ^{3}He binding energies to fix the 3NF.
- For observables the cutoff dependence vanishes at momenta of the order of the pion-momentum. This allows to take the physical value at infinite cutoff. Rev. Mod. Phys. 92, 025004 (2020)

König; Vanasse; Hammer; van Kolck; De Leon, Platter, DG

M_1 $(q \rightarrow 0)$ observables at the A<4 systems:



The magnetic probe lagrangian

- The M_1 opearator is given by: $\hat{\mu} = -\frac{i}{2}\vec{\nabla}_q \times \hat{\mathcal{J}}(\vec{q})\big|_{q=0}$

- The interaction is expanded in clusters of nucleons:

$$\mathcal{L}^{\text{1-B}}_{\text{magnetic}} = \frac{e}{2M} N^\dagger \left(\kappa_0 + \kappa_1 \tau_3\right) \vec{\sigma} \cdot \vec{B} N$$

$$\begin{aligned}\mathcal{L}^{\text{2-B}}_{\text{magnetic}} =& e\Big[L_1' \left(N^T P_s^A N\right)^\dagger \left(N^T P_t^i N\right) B_i \\ &- L_2' \left(N^T P_t^i N\right)^\dagger \left(N^T P_t^j N\right) B_k + h.c\Big]\end{aligned}$$

EFT reordering of the interaction Lagrangian of 2-nucleon cluster and the magnetic probe

- Applying a Hubbard-Stratanovich transformation allows to write the 2-nucleon cluster as spin-singlet and spin-triplet states.
- The resulting 2-nucleon magnetic interaction Lagrangian is then naturally written as an effective range expansion:

$$\mathcal{L}^{2\text{-B}}_{\text{magnetic}} = \frac{e}{2M}\left[\kappa_1 L_1 (t^\dagger s + s^\dagger t)\cdot \vec{B} - i\epsilon^{ijk}\kappa_0 L_2((t^i)^\dagger t^j)\cdot B_k\right]$$

$$L_1(\mu) = \underbrace{-\frac{\rho_t+\rho_s}{\sqrt{\rho_t\rho_s}}}_{\text{LO}} + \frac{4}{\gamma_t\sqrt{\rho_t\rho_s}}\underbrace{l_1'(\mu)}_{\text{NLO}}$$

$$L_2(\mu) = -\underbrace{\frac{2}{\rho_t}}_{\text{LO}} + \frac{2}{\gamma_t\rho_t}\underbrace{l_2'(\mu)}_{\text{NLO}}\ ,$$

- The H-S transformation introduces a cutoff dependence. We choose to work with the same cutoffs and take them to infinity, $\mu = \Lambda \to \infty$.
- In previous studies μ was fixed arbitrarily at $\mu = m_\pi$.

Rev. Mod. Phys. 92, 025004 (2020)

A consistent perturbative calculation of M_1 observable

$$\langle\hat{\mu}\rangle = \langle\hat{\mu}\rangle^{\text{1-B}}_{\text{LO}} \times \left(\underbrace{1}_{\text{LO}} + \underbrace{\delta\langle\hat{\mu}\rangle^{\text{1-B}}_{\text{ERE}} + \delta\langle\hat{\mu}\rangle^{\text{2-B}}_{\text{ERE}}}_{\substack{\text{LO magntic opert.}\\ \text{NLO storng inter.}}} + \underbrace{\delta\langle\hat{\mu}\rangle^{\text{2-B}}}_{\substack{\text{NLO magntic opert.}\\ \text{LO storng inter.}}} \right)$$

A=2 M_1 observables (A=3 are less transparent):

Deuteron magnetic moment:

$$\langle\hat{\mu}_d\rangle = \kappa_0\left\{2Z_d^{\mathrm{NLO}} + Z_d^{\mathrm{LO}}\left[\gamma_t\rho_t L_2(\mu)\right]\right\} =$$

$$= 2\kappa_0\left[1 + \underbrace{0}_{\text{NLO strong inter.}} + \underbrace{l_2'(\mu)}_{\substack{\text{NLO magnetic opert.}\\ \text{LO strong inter.}}}\right]$$

Radiative capture of thermal neutron on proton $n + p \rightarrow d + \gamma$:

$$\sigma_{np} = 2\alpha\pi\frac{\left(\gamma_t^2 + q^2/4\right)^3 a_s^2}{M^4 q\gamma_t}Y_{np}^2 \equiv 2\alpha\pi\frac{\gamma_t^5 a_s^2}{M^4 q}(2\kappa_1)^2(Y_{np}')^2$$

$$Y_{np}' = \left(1 - \frac{1}{\gamma_t a_s}\right)\times\left[1 + \underbrace{\sqrt{Z_d^{\mathrm{NLO}}} - 1 - \frac{\gamma_t a_s}{\gamma_t a_s - 1}\frac{\gamma_t\left(\rho_t + \rho_s\right)}{4}}_{\substack{\text{NLO storng inter. corrections}\\ \text{LO magnetic op.}}} + \underbrace{\frac{\gamma_t a_s}{\gamma_t a_s - 1}l_1'(\mu)}_{\substack{\text{NLO magnetic}\\ \text{op. corrections}\\ \text{LO strong inter.}}}\right]$$

Cutoff dependence in the A=3 system

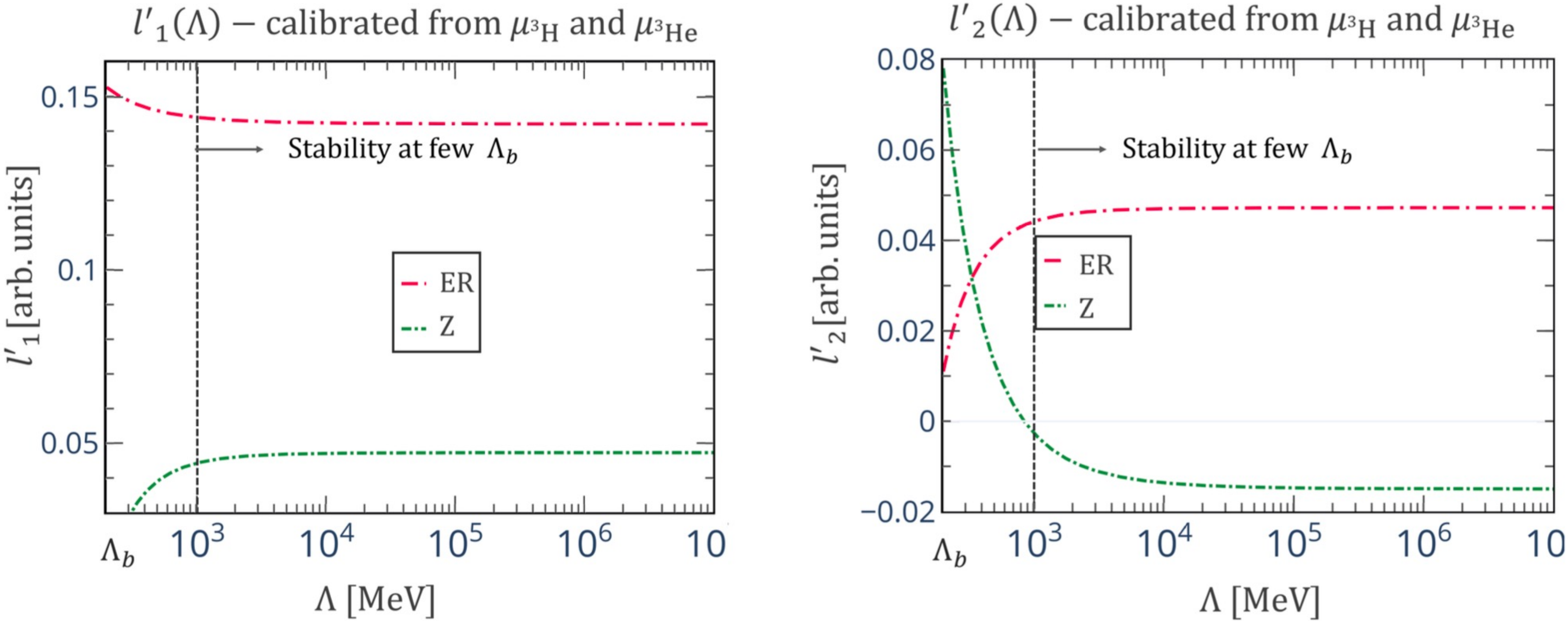


FIG. 2: Numerical results for the LECs $l'_1(\Lambda)$ (left panel) and $l'_2(\Lambda)$ (right panel), calibrated from the $M_1 = 3$ observables as a function of the cutoff Λ. The long (short) dotted-dashed lines are the numerical results for the ER-(Z-) parameterization.

Observables dependence on different fixing of l'_1 and l'_2:

	$l_1'^{\infty}/10^{-2}$	$l_2'^{\infty}/10^{-2}$	$\langle\hat{\mu}_{^3\mathrm{H}}\rangle$[NM]	$\lvert\langle\hat{\mu}_{^3\mathrm{He}}\rangle\rvert$[NM]	$\langle\hat{\mu}_d\rangle$[NM]	Y'_{np}
LO	0 (0)	0 (0)	2.76 (2.78)	1.84 (1.84)	0.88 (0.88)	1.18 (1.18)
NLO	4.72 (14.2)	-1.6 (4.1)	$\star$	$\star$	0.87 (0.92)	1.253 (1.31)
	4.66 (9.0)	-2.6 (-2.6)	2.978 (2.76)	2.145 (1.89)	$\star$	$\star$
	4.66 (9.0)	-2.4 (29)	$\star$	2.144 (1.66)	0.86 (1.17)	$\star$
	4.66 (9.0)	-0.13 (-31)	2.996 (2.59)	$\star$	0.88 (0.61)	$\star$
	4.92 (15.2)	-2.6 (-2.6)	$\star$	2.143 (2.23)	$\star$	1.255 (1.32)
	4.60 (13.4)	-2.6 (-2.6)	2.967 (2.91)	$\star$	$\star$	1.253 (1.30)
Mean	4.73 (13.0)	-1.7 (-0.04)	2.98 (2.75)	2.144 (1.93)	0.87 (0.89)	1.253 (1.31)
std	0.2 (2.8)	1.1 (25)	0.015 (0.16)	0.001 (0.28)	0.01 (0.26)	0.001 (0.01)
Exp data			2.979 [47]	2.128 [47]	0.857 [17]	1.253 [18]

Nominal numbers – Z parameterization

In brackets – ER parameterization.

NLO contribution to observables –
significantly smaller than naïve pionless EFT expansion parameter

M_1	$\delta\langle\hat{\mu}\rangle_{\text{total}}$	$\delta\langle\hat{\mu}\rangle_{\substack{\text{NLO}\\\text{strong}\\\text{inter.}}}$	$\delta\langle\hat{\mu}\rangle^{\text{2-B}}_{\substack{\text{NLO}\\\text{magnetic}\\\text{opert.}}}$
$\langle\hat{\mu}_{^3\text{H}}\rangle$	7% (1%)	3% (11%)	5% (10%)
$\langle\hat{\mu}_{^3\text{He}}\rangle$	13% (4%)	3% (25%)	10% (29%)
$\langle\hat{\mu}_{d}\rangle$	1% (1%)	0% (0%)	1% (1%)
Y'_{np}	6% (9%)	2% (2%)	4% (12%)

Nominal numbers – Z parameterization
In brackets – ER parameterization.

Intermittent results:

(1) Z-parameterization has a more natural convergence pattern compared to the ER-parameterization at NLO:

- ER has larger fluctuations between different NLO contributions.
- ER has large fluctuations in values of LECs

(2) Isoscalar two-body coupling is consistent with zero:

- The isoscalar coupling is basically consistent with zero.
- The deuteron NLO contribution almost vanishes (and, we are not supposed to look at this now, but the LO result is very close to the experimental result).
- Huge fluctuations in size of l'_2 compared to l'_1

- We take this as a numerical evidence that l'_2 is higher than NLO.
- We continue only with Z-parameterization.

Intermittent results (cont'd):

- Z parameterization results with $l'_2=0$:

	$l_1'^{\infty}/10^{-2}$	$\langle\hat{\mu}_{^3\mathrm{H}}\rangle$[NM]	$\langle\hat{\mu}_{^3\mathrm{He}}\rangle$[NM]	Y'_{np}
	4.36	$\star$	-2.10	1.250
	4.97	3.00	$\star$	1.256
	4.66	2.99	-2.11	$\star$
Mean	4.7	2.99	-2.11	1.253
Standard deviation	0.6	0.01	0.01	0.006
%NLO/LO		8%	14%	6%
Exp. data		2.979	-2.128	1.253

(3) NLO contribution is smaller than the Naïve pionless EFT estimate.

Order-by-order Bayesian uncertainty estimate

- The BUQEYE collaboration (and other approaches) have nicely established a way to infer a truncation error in an EFT expansion of the form:
  - $\langle M_1 \rangle = \langle M_1 \rangle_{LO} \cdot \left(1 + c_{M_1}^{NLO} \cdot \delta + c_{M_1}^{N^2LO} \cdot \delta^2\right) + \cdots$
- However, in the current case, the value of the expansion parameter is unclear.
- We thus first use a Bayesian approach estimate the p.d.f ot the expansion parameter.
- The objective, maximal entropy, form of the distribution is *log-normal*.
- We use our different observables as "independent" measurements of the expansion parameter.
- The result is *a Student's-t distribution* for the expansion parameter.

Estimating the expansion parameter

- We find that at a 95% degree of belief, the expansion parameter is within the range of 0.05 < **δ** < 0.13.

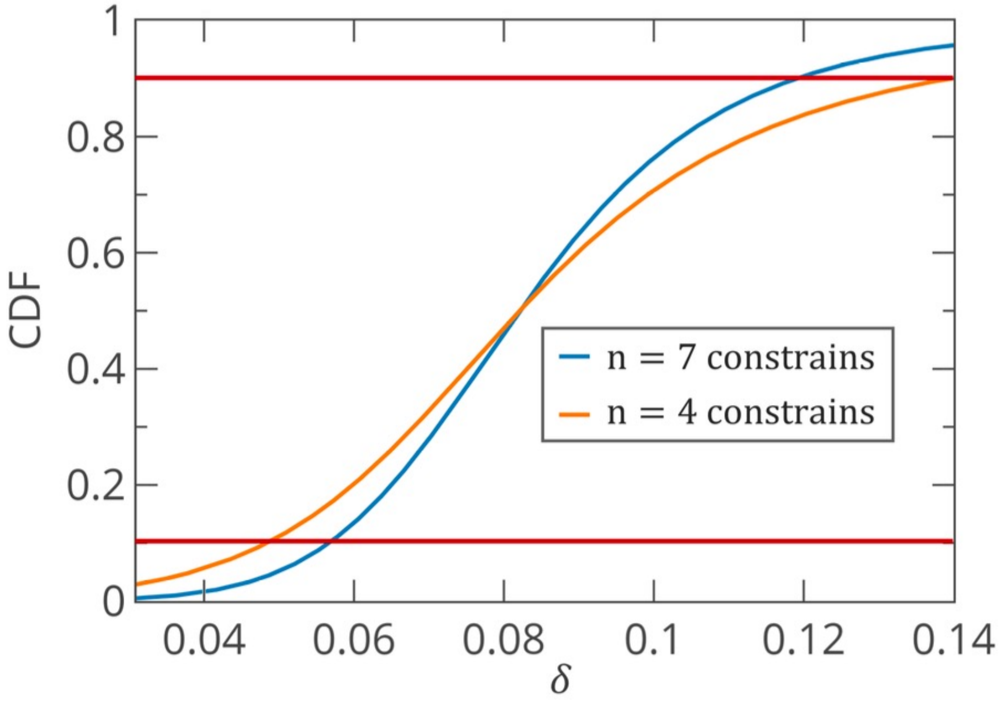


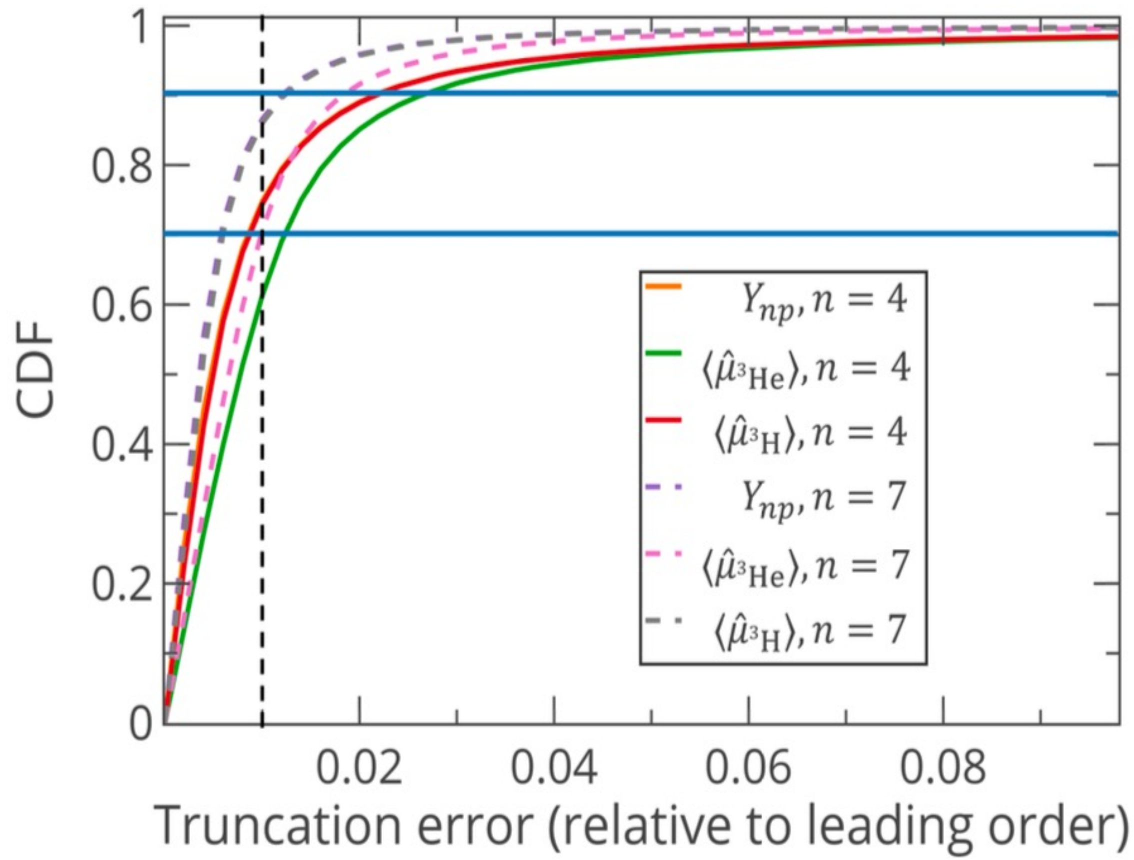
FIG. 3: Cumulative Density Functions (CDFs) of δ, the expansion parameter. The blue curve represents a calculation that takes into account the constraints of the NLO contributions of $\langle \hat{\mu}_{^3\mathrm{H}} \rangle$, $\langle \hat{\mu}_{^3\mathrm{He}} \rangle$, Y_{np}, the N^{2}LO contribution of $\langle \hat{\mu}_d \rangle$, and the variation of $l_1'^{\infty}$. The orange curve takes into account only the first four constraints. The red lines limit the $10\% - 90\%$ probability range.

Estimating the truncation error

$$pr\left(\Delta\middle|\left\{a^{\mathrm{NLO}}_{M_1^k}\right\}_{k=1}^{n}\right) = \int d\delta\, pr\left(\Delta\middle|\left\{c^{\mathrm{NLO}}_{M_1^k}\right\}_{k=1}^{n},\delta\right)\cdot pr\left(\delta\middle|\left\{a^{\mathrm{NLO}}_{M_1^k}\right\}_{k=1}^{n}\right). \quad \text{(A-2)}$$

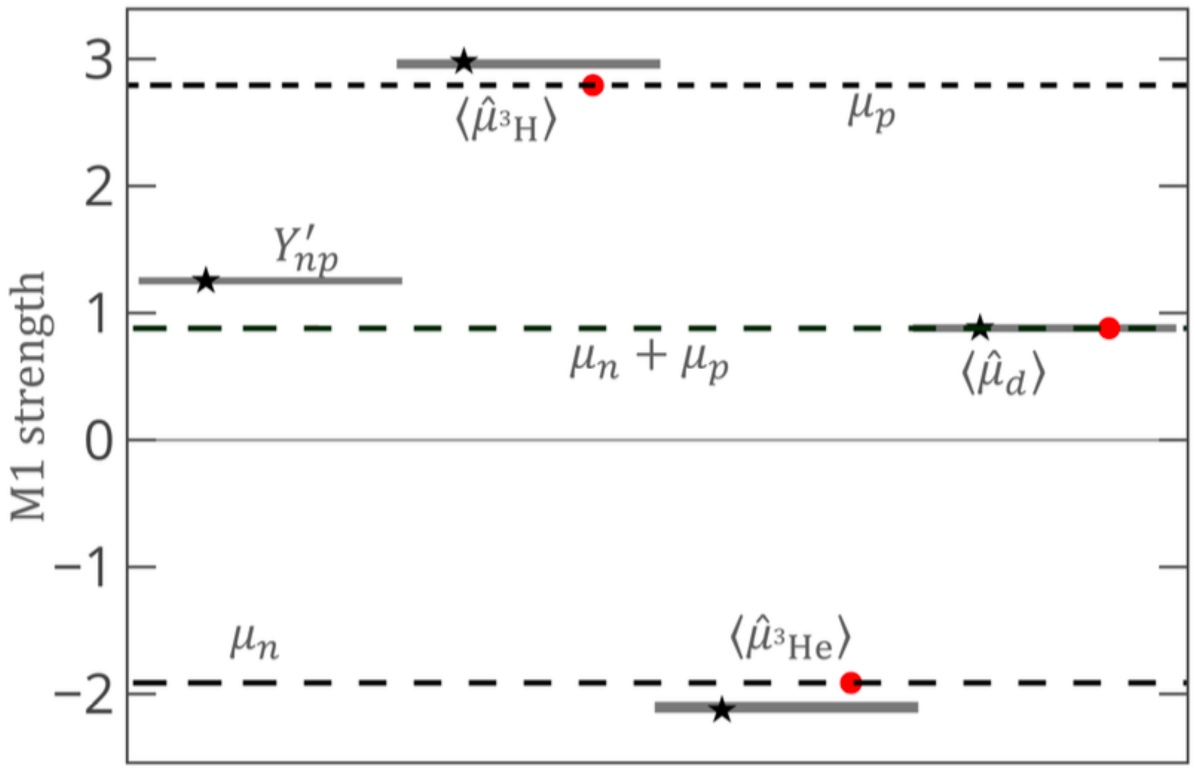
From BUQEYE formalism

our approach

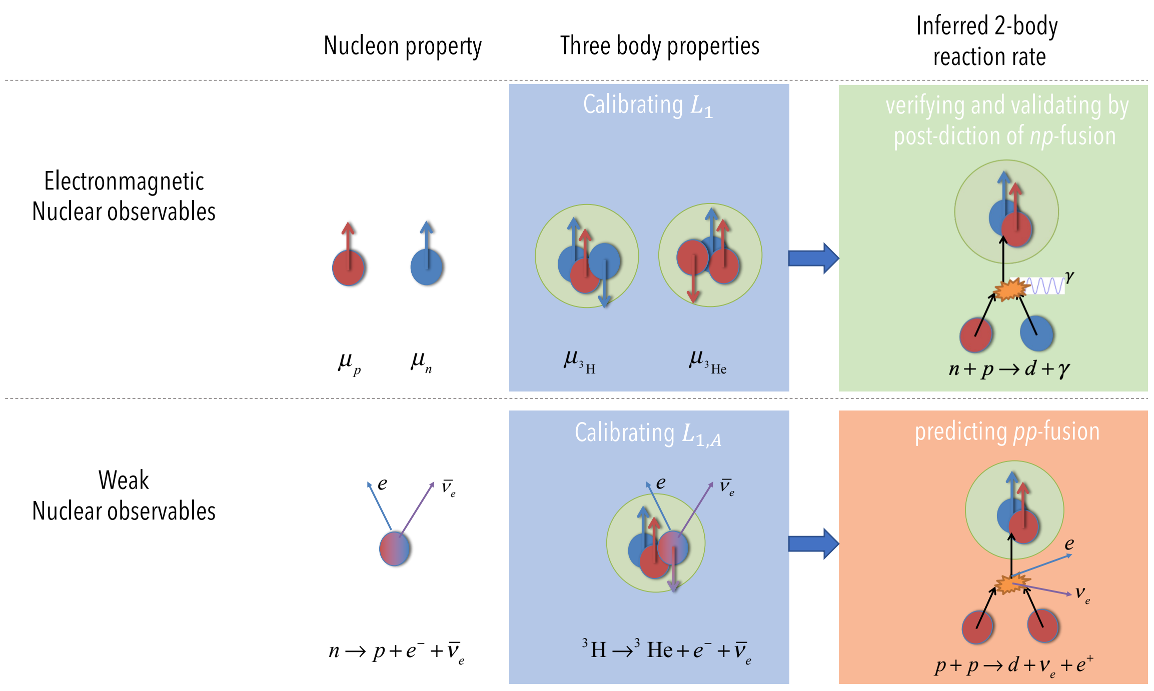


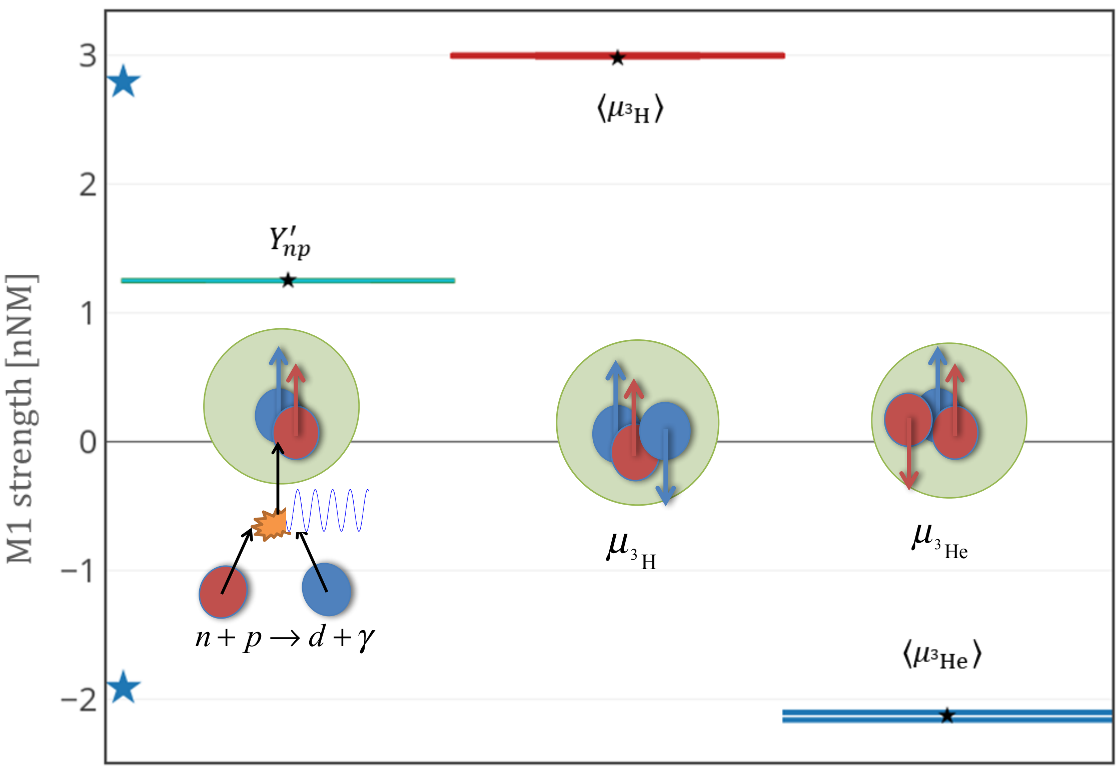
Final result for M_1 observables

		This work [NM]	Experiment [NM]	
Y'_{np}	=	1.253 ± 0.006	1.2532 ± 0.0019	[18]
$\langle \hat{\mu}_{^3\mathrm{H}} \rangle$	=	2.99 ± 0.015	2.97896...	[16]
$\langle \hat{\mu}_{^3\mathrm{He}} \rangle$	=	-2.11 ± 0.02	$-2.12750...$	[16]
$\langle \hat{\mu}_d \rangle$	=	0.88 ± 0.01	0.857	[17] ,



Take these results to predict proton-proton fusion





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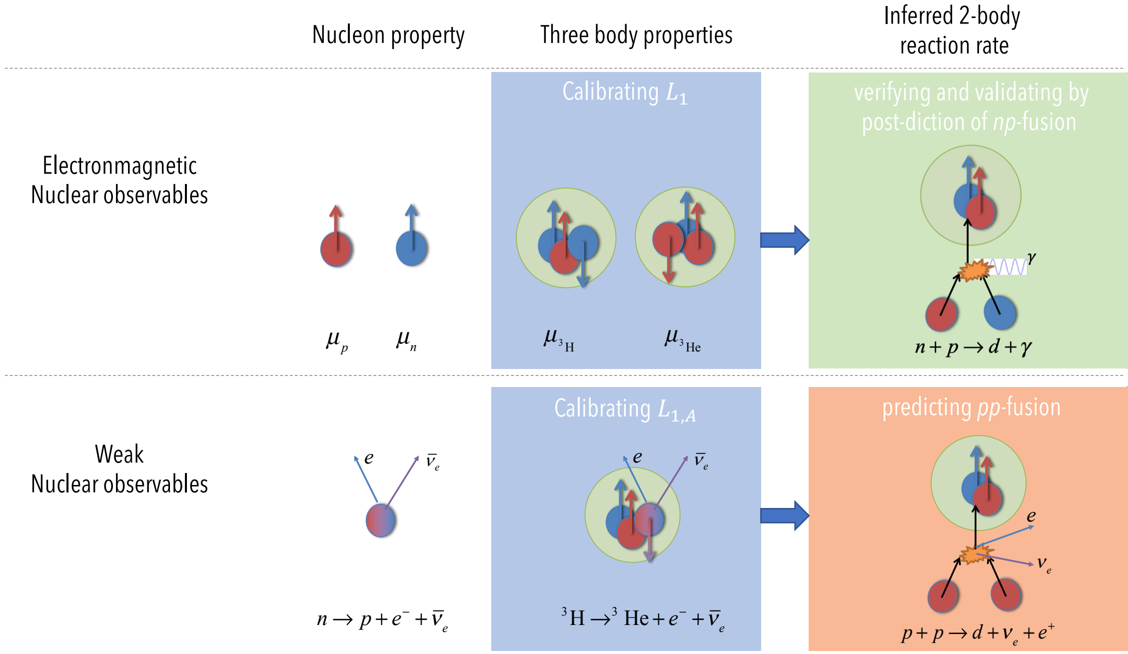
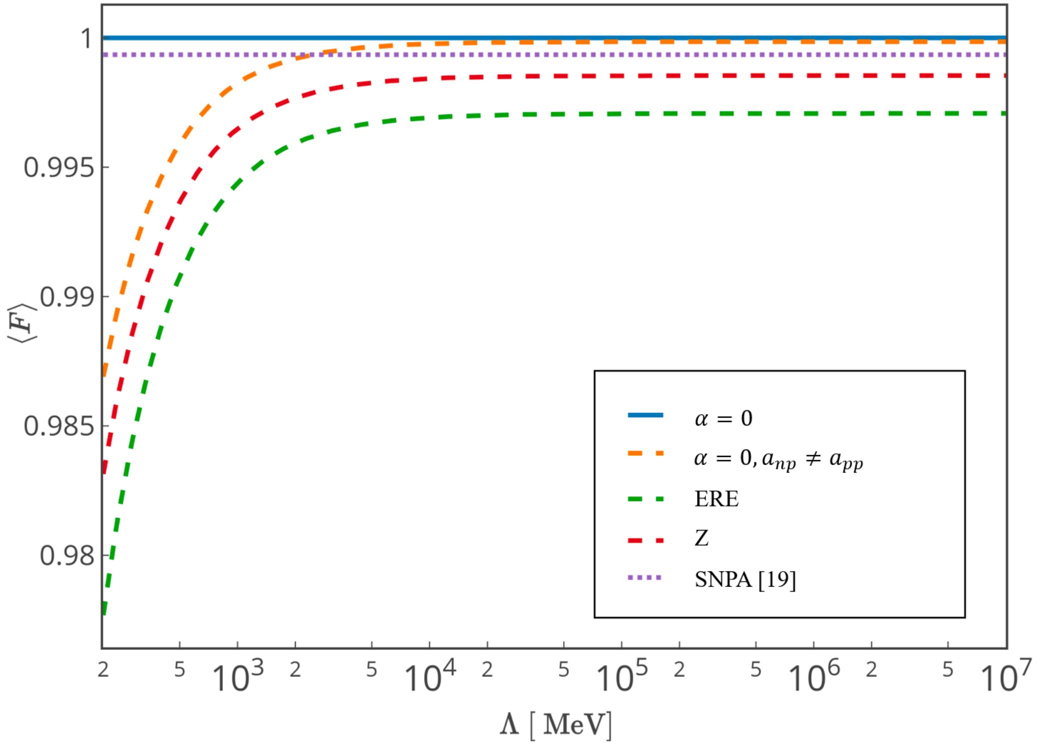


$$Y'_{np} = \left(1 - \frac{1}{\gamma_d a_s}\right) \cdot \sqrt{Z_d^{\mathrm{NLO}}} - \frac{\gamma_d}{4}\left[\rho_t + \rho_s + \frac{\sqrt{\rho_t \rho_s}}{\kappa_1} l_1(\mu)\right]$$
$$\approx 1.206 + 0.07 \times l_1 \ , \qquad (3)$$

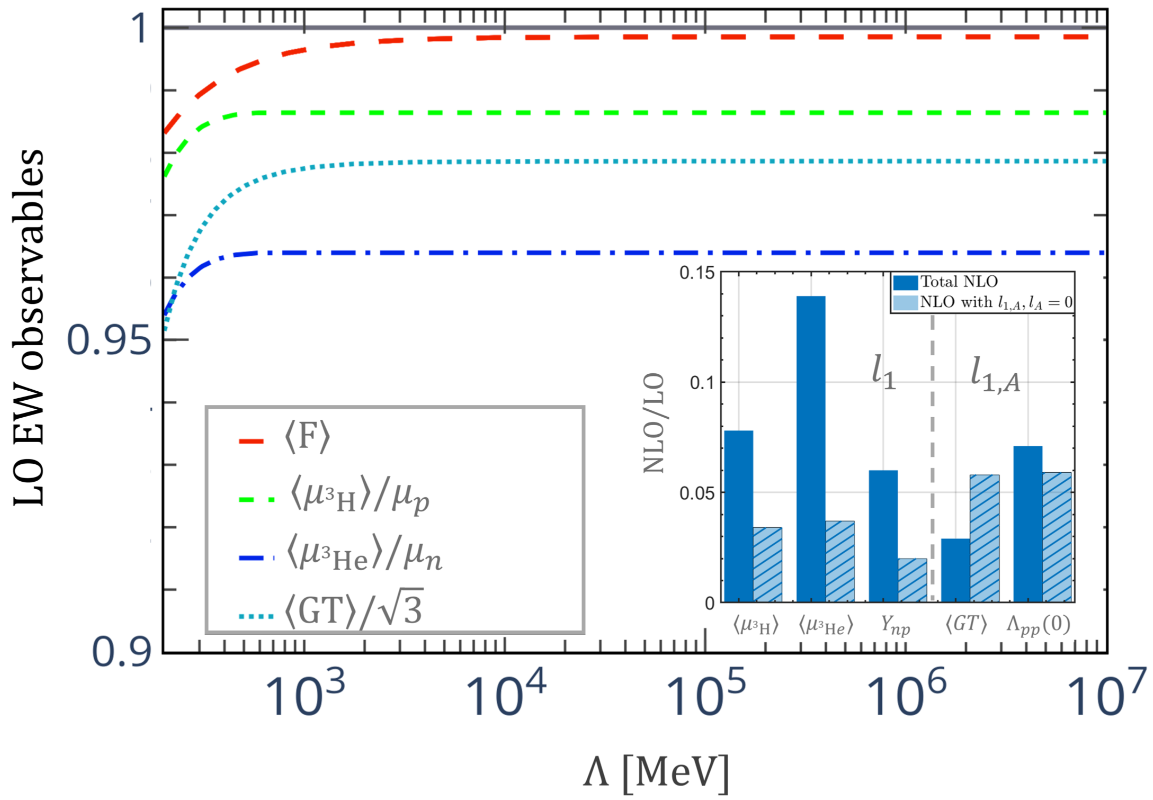
$$|\Lambda_{pp}(0)| = \sqrt{Z_d^{NLO}}\,[e^{\chi} - M\alpha a_C I(\chi)] +$$
$$+ \sqrt{Z_d^{LO}} \frac{a_C \gamma_d^2}{2} \sqrt{\rho_t \rho_s}\left(\frac{\rho_t + \rho_s}{2\sqrt{\rho_t \rho_s}} - l_{1,A}\right) \approx$$
$$\approx 2.655 + 0.6 \times l_{1,A} \approx 2.685$$

	Nuclear non-conserved current	two-body contact strength
Electromagnetic nuclear observables	$A_i = \frac{e}{2M}\Big\{ \underbrace{N^\dagger [(\kappa_0 + \kappa_1 \tau_3)\sigma_i]\ N}_{\mathrm{LO}} - \underbrace{2\kappa_0 (\vec{t}^\dagger \times \vec{t})_i}_{\mathrm{NLO}} - \underbrace{L'_1 (t_i^\dagger s + s^\dagger t_i)}_{\mathrm{NLO}} \Big\}$	$L'_1(\mu) = -\frac{\rho_t + \rho_s}{\sqrt{\rho_t \rho_s}}\kappa_1 + \underbrace{\frac{M}{\pi\sqrt{\rho_t \rho_s}} L_1 (\mu - \gamma_d)\left(\mu - \frac{1}{a_s}\right)}_{l_1,\ \text{RG invariant combinations}}$
Weak nuclear observables	$A_i^{\pm} = \underbrace{\frac{g_A}{2} N^\dagger \sigma_i \tau^{\pm} N}_{\mathrm{LO}} - \underbrace{L'_{1,A}\left(t_i^\dagger s + s^\dagger t_i\right)}_{\mathrm{NLO}}$	$L'_{1,A}(\mu) = -\frac{\rho_t + \rho_s}{2\sqrt{\rho_s \rho_t}} g_A + \underbrace{\frac{1}{2\pi\sqrt{\rho_s \rho_t}} L_{1,A} (\mu - \gamma_d)\left(\mu - \frac{1}{a_s}\right)}_{l_{1,A},\ \text{RG invariant combinations}}$

Bayesian uncertainty estimate using NLO/LO values



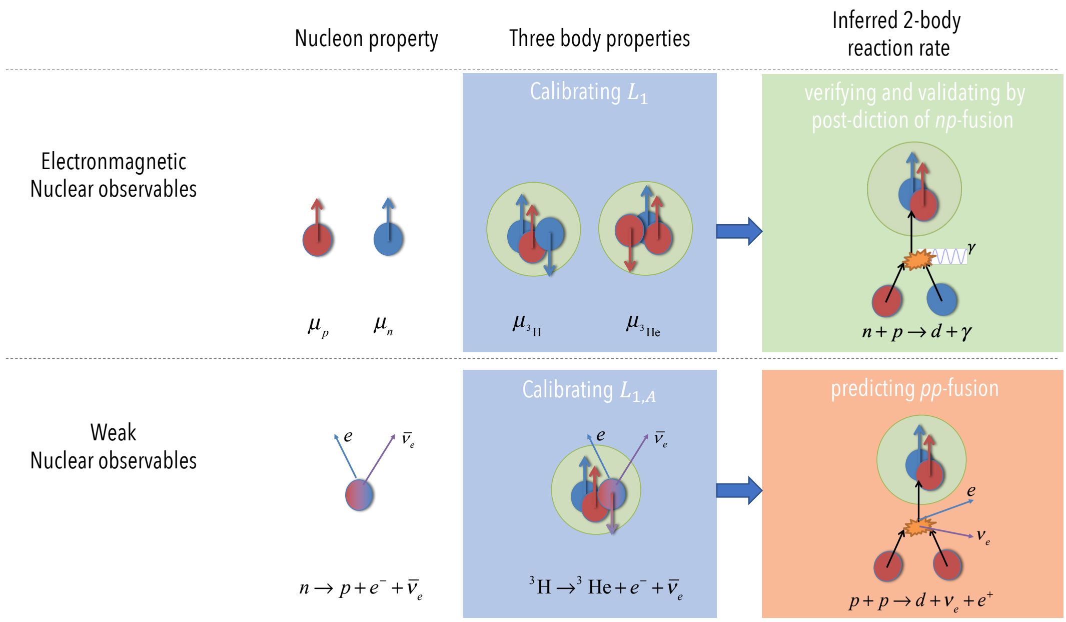
3H and 3He have almost the same wave function



RG invariance of all three-body observables.
The value is taken at infinity.

Arbitrarily choosing LECs values at m_π is problematic

$S^{11}(0)$ prediction

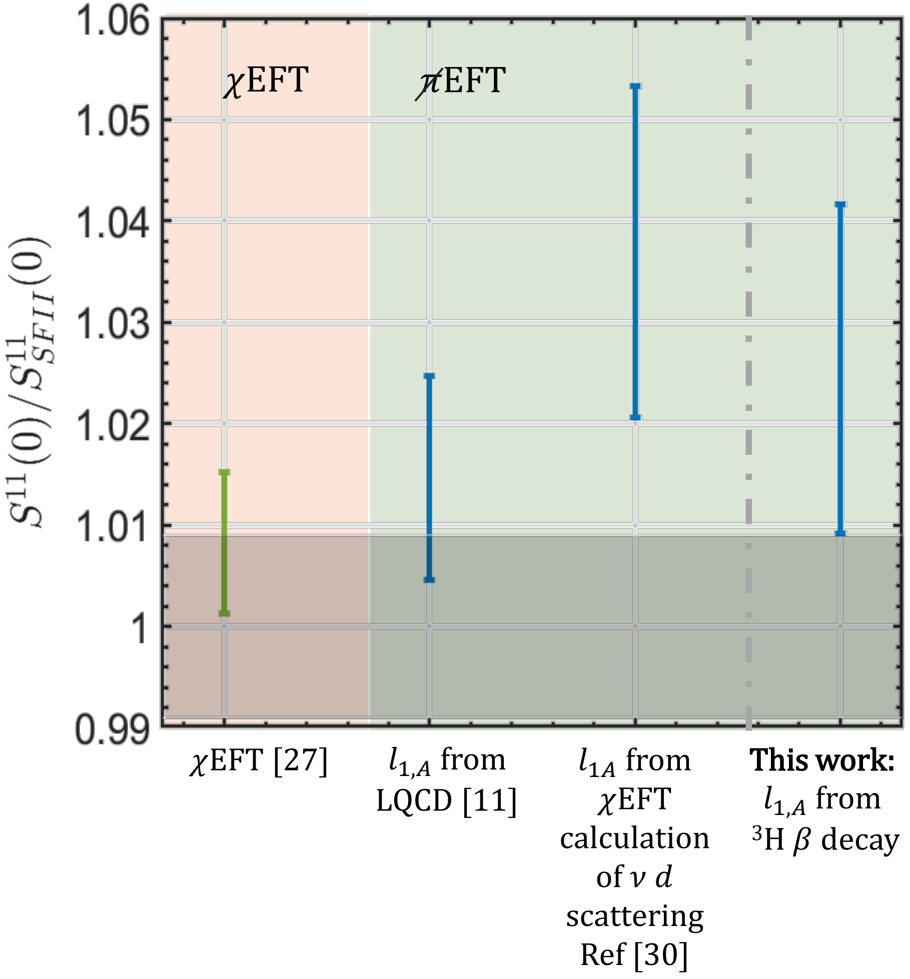


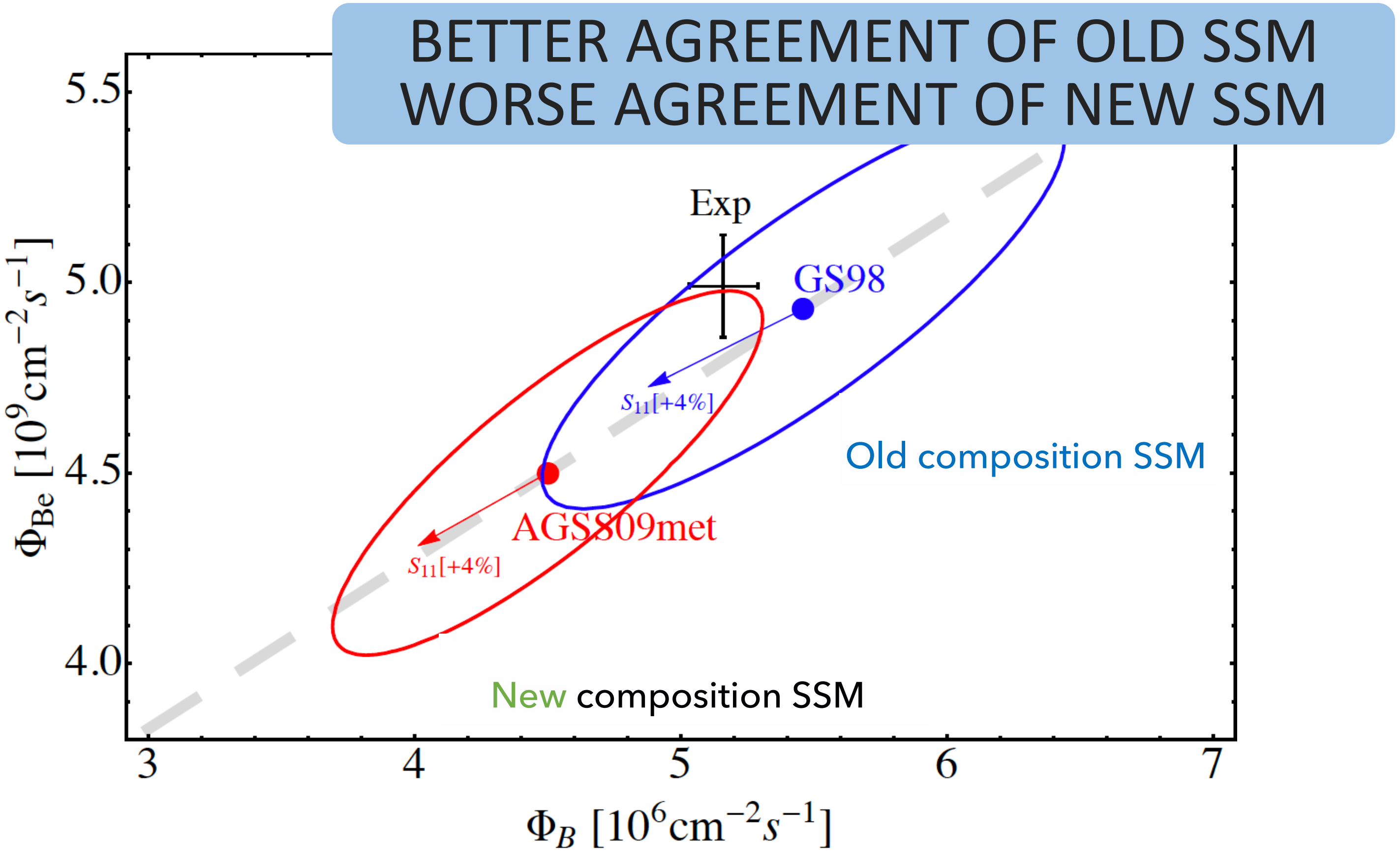
$$S^{11}(0) = (4.14 \pm 0.01 \pm 0.005 \pm 0.06) \cdot 10^{-23} \text{ MeV fm}^2.$$

g_A | ^{3}H halflife | theoretical uncert.

$$S^{11}_{corr}(0) = 4.11 \text{ MeV fm}^2.$$

Enhanced pp-fusion rate





Enhanced "Solar composition problem"

Discussion and results

In this case

- Pionless EFT has a predictive power, combining accuracy and precision.
- The theory is renormalizable.
- Small number of parameters, with concrete experimental origin (except 3NF).
- The agreement of the theory with experiment in the electromagnetic sector validates it and verifies the theory.
- Surprising EFT results:
    - The isoscalar coupling constant is found numerically to be consistent with orders higher than NLO:
        - This is consistent with chiral EFT counting! Is this a remnant of chiral symmetry?
    - Expansion parameter smaller than expected by naïve pionless estimate:
        - Does this originate in a unitary expansion or is it an emergence of Wigner SU(4) symmetry.
        - A small expansion parameter is needed for a "shell model" structure of the lightest nuclei magnetic moments.
        - Consistent with the small NLO contribution in triton beta decay.
- N2LO – not so elegant verification anymore due to three body electroweak current.