Chiral EFT for *ab initio* nuclear physics

Hopes, Highlights, and Headaches...

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Chiral EFT: New Perspectives, INT Seattle, March 17-21, 2025

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Swedish Research Council

What is *ab initio* in nuclear theory?

Why uncertainty quantification and Bayesian inference?

Inferring the breakdown scale of pionless EFT

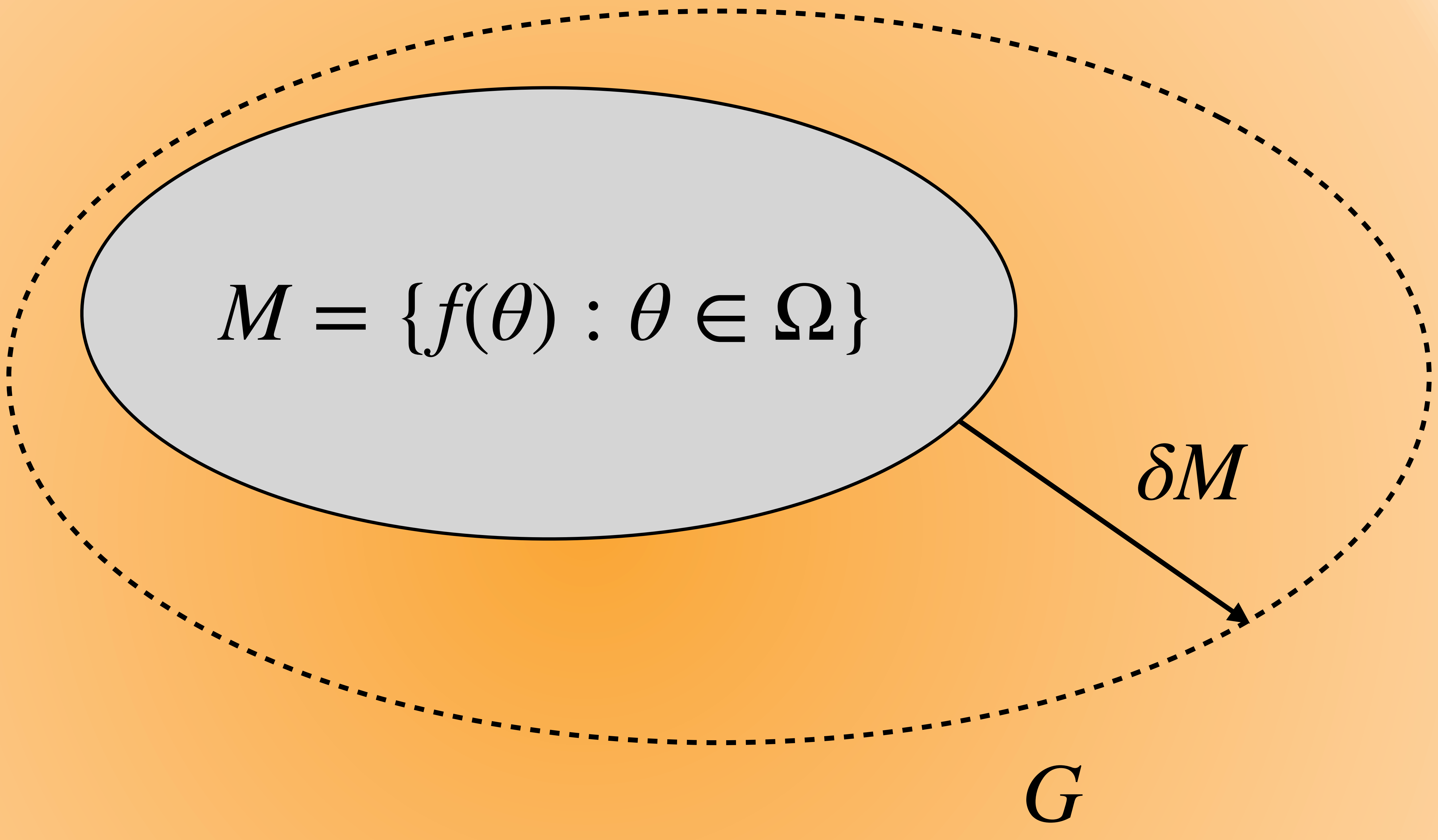
Calibrating renormalizable chiral EFT

$\mathbf{N3LO_{Texas}(394)}$: a chiral potential for accurate predictions

Remember: models are not reality

- we simplify and/or do not know the full story

We consider a **model** of some nuclear observable as a function
$y = f(\theta),\ \theta \in \Omega \subset \mathbb{C}^d$, where Ω is some specified parameter space

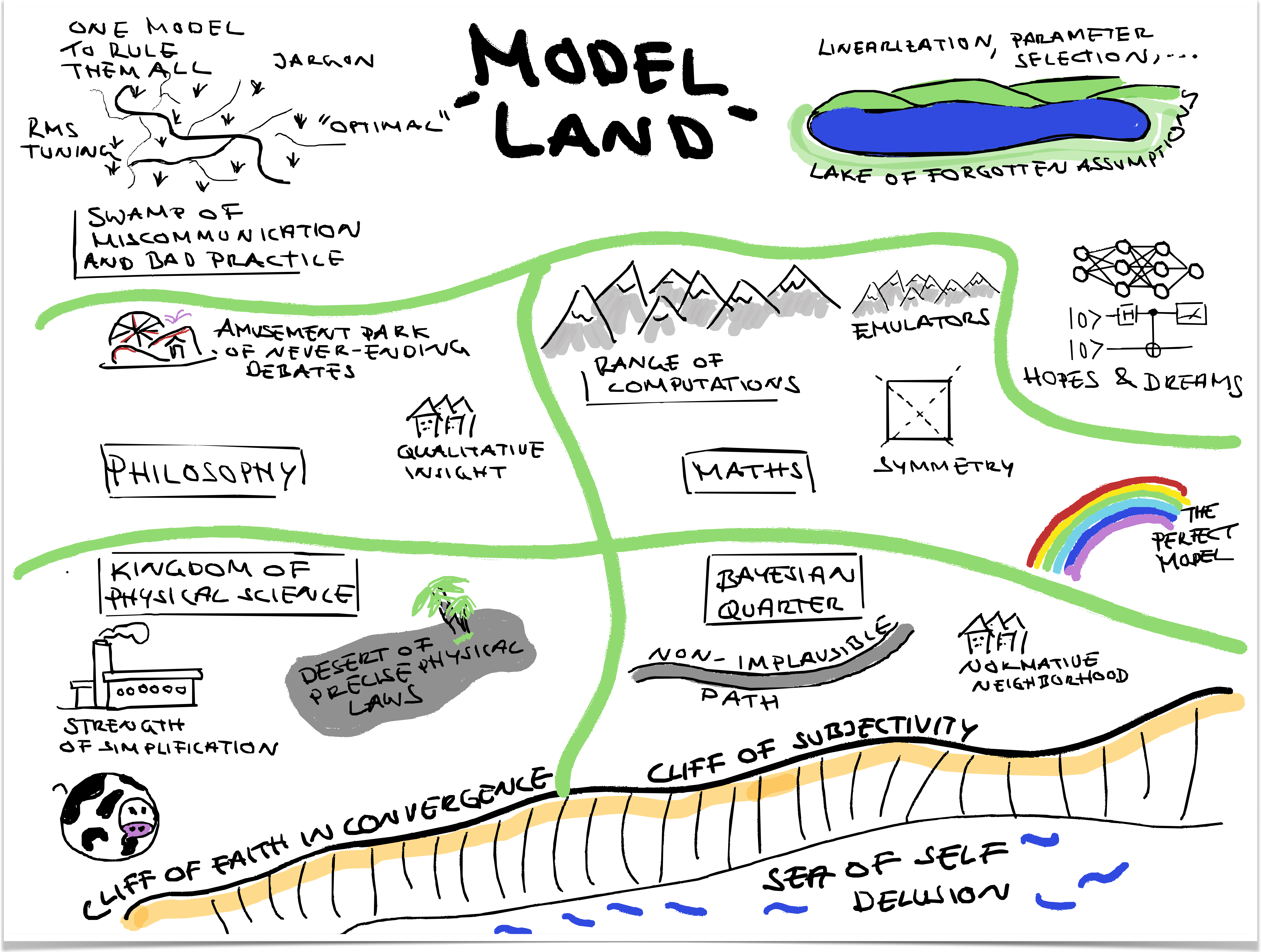


"All models are wrong"
i.e., data $D \sim G$ where $G \notin M$

G. E. P. Box (1976)

We should include an estimate of the model discrepancy δM to (hopefully) make more meaningful inferences and predictions.

Kennedy and O'Hagan (2001)
Brynjarsdóttir and O'Hagan (2014)



Inspiration: Thomson & Smith, Economics 13 (2019) *Escape from model-land*

Ab initio offers an inferential advantage

Nuclear *ab initio:* a *systematically improvable* approach for quantitatively describing nuclei using the finest resolution scale possible while maximizing its predictive capabilities.

$$H(\vec{\alpha})|\Psi\rangle = E|\Psi\rangle$$

χ*EFT* **to approximate low-energy QCD**

***A*-body methods with controllable approximation**

$$H(\vec{\alpha}) = T + V^{(0)}(\vec{\alpha}_{(0)}) + V^{(1)}(\vec{\alpha}_{(1)}) + V^{(2)}(\vec{\alpha}_{(2)}) + \ldots \qquad |\Psi\rangle = |\Phi^{(0)}\rangle + |\Phi^{(1)}\rangle + |\Phi^{(2)}\rangle + \ldots$$

This systematicity creates an *inferential advantage*. We can test our assumptions about the model as we increase its the fidelity.

$$y_{\text{exp}}(\vec{x}) = \underbrace{y_{\text{th}}(\vec{\alpha};\vec{x}) + \delta y_{\text{th}}(\vec{\alpha};\vec{x})}_{\text{'Model'}} + \delta y_{\text{exp}}(\vec{x})$$

A. Ekström, C.Forssen, G.Hagen, G. R. Jansen, W. Jiang, and T. Papenbrock, Frontiers (2022)

Why uncertainty quantification?

- Predicting future data $\widetilde{y}$ from past data y is an uncertain process.
- Quantifying this uncertainty with probability:
  - enhances transparency and communication of results
  - helps improve decision-making and model assessment

Why Bayesian inference?

The probability for $\widetilde{y}$ given y is called the *posterior predictive distribution*, and this quantity is fundamental to Bayesian inference.

$$p(\widetilde{y}\,|\,y, I)$$

Here, I denotes *your* background knowledge. To enable quantitative statements, we construct a *model* M. Any model comes with uncertain parameters $\vec{\alpha}$.

$$p(\widetilde{y}\,|\,y, M, I) = \int p(\widetilde{y}\,|\,\vec{\alpha}, M, I)\, p(\vec{\alpha}\,|\,y, M, I)\, d\vec{\alpha}$$

D. V. Lindley, The Statistician (2000)
Bernardo and Smith, Wiley (1994)

What is the breakdown scale M_{hi} of pionless EFT?

Inferring the breakdown scale of pionless EFT: $p(M_{\rm hi} | \sigma_{np}, I)$

an example of how to use Bayes to test your assumptions

Pionless EFT is a short-range and non-relativistic EFT built from contact interactions.

The breakdown scale $M_{\rm hi}$ is due to excluded massive degrees of freedom. **Expectation**: pion mass.

We explore pionless EFT up to NNLO, and calibrate the LECs to Nijmegen effective range parameters.

We compute np total cross section from spin-averaged singlet (s) and triplet (t) S-wave t-matrix amplitudes

$$\sigma_{np}(k) = 4\pi \left(\frac{1}{4} |t_s(k)|^2 + \frac{3}{4} |t_t(k)|^2 \right)$$

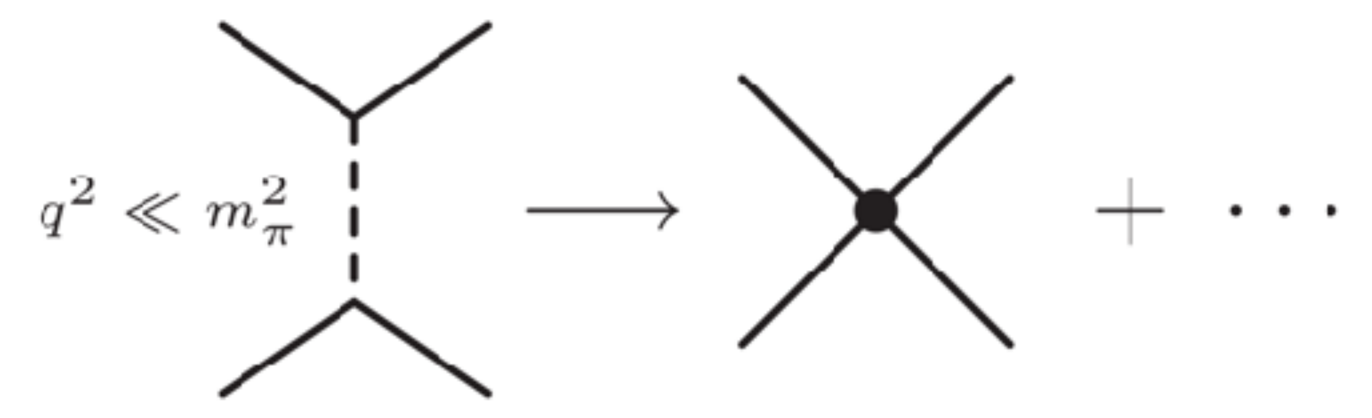


FIG. 2. Reduction of pion exchange (dashed line) to a series of contact interactions between nucleons (solid lines) for $q^2 \ll m_\pi^2$.

Hammer, König, Kolck Rev. Mod. Phys **92** (2020)

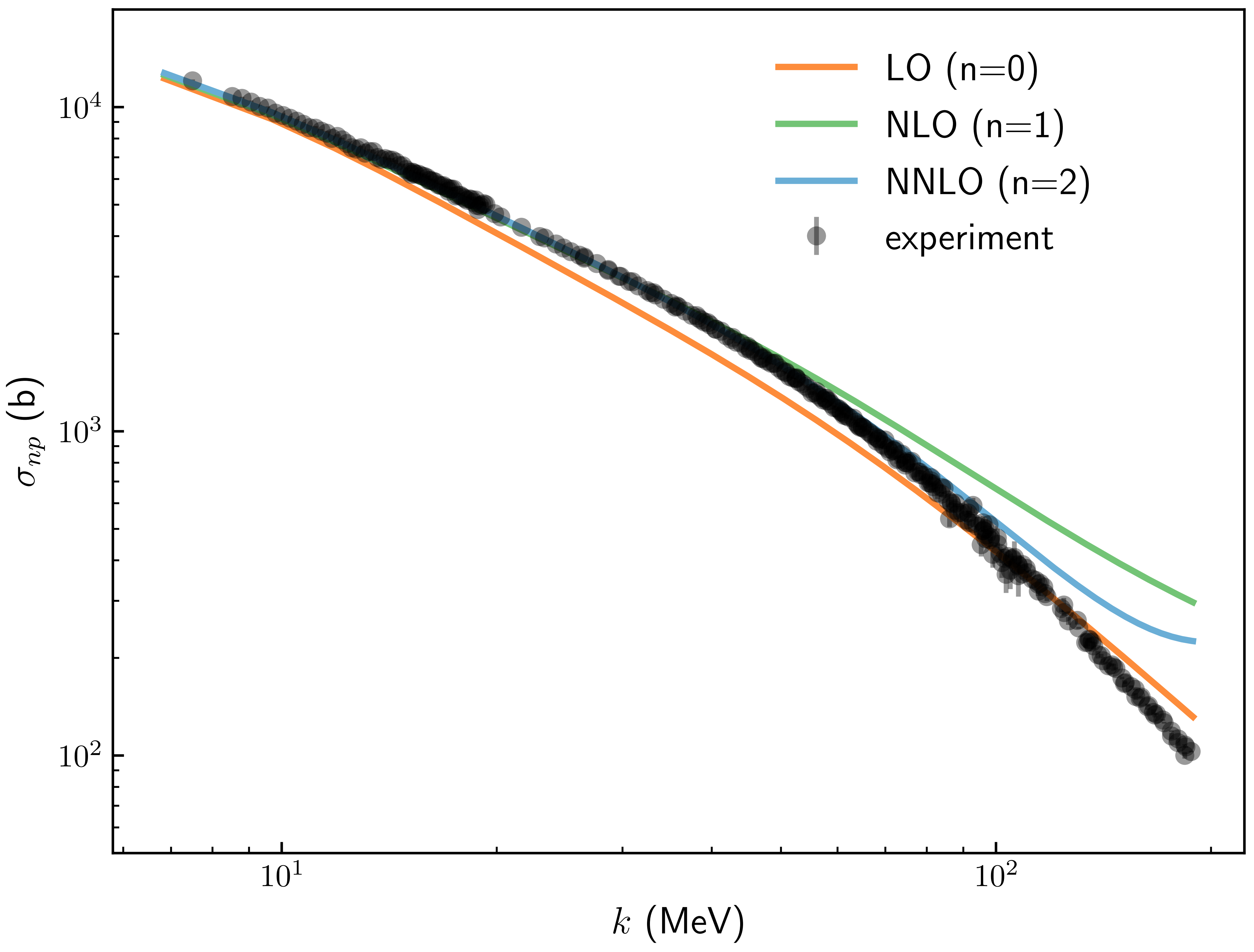
We assume order-by-order convergence of $\sigma_{np}^{(n)} = \sigma_{\rm ref}(k) \sum_{i=0}^{n} c_i(k)[Q(k)]^i$ and use Bayesian inference to quantify $p(M_{\rm hi} | \sigma_{np}^{(n)}, I)$. The expansion parameter $Q(k) = \dfrac{f(k)}{M_{\rm hi}}$ with $f(k)$ interpolating over $1/a_t$

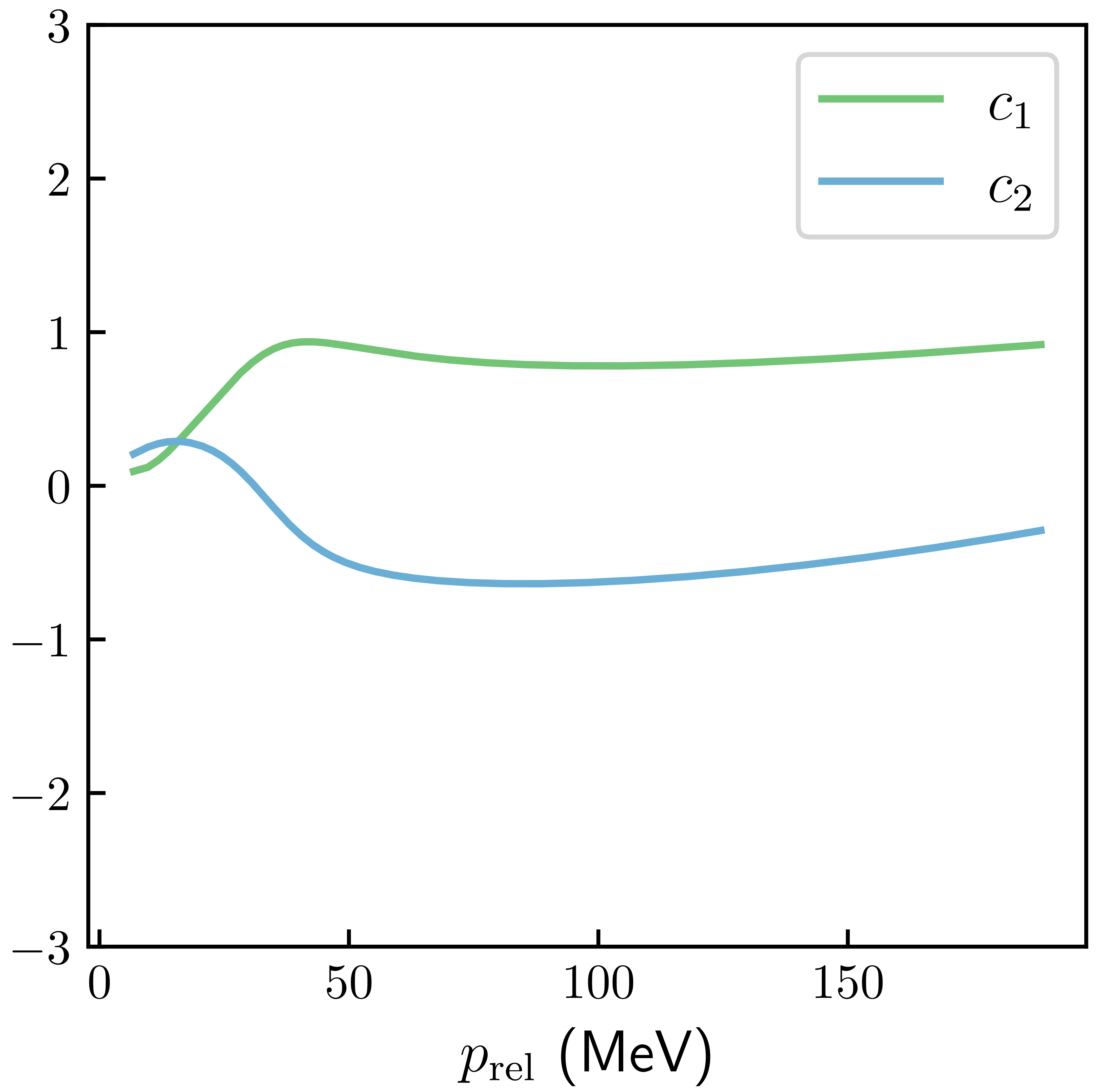
Ekström and Platter, Phys. Lett. **B (2025)**

Order-by-order convergence

Here, assuming $M_{\text{hi}} = m_\pi$

$$c_j(k) = \frac{\sigma^{(j)}(k) - \sigma^{(j-1)}(k)}{\sigma_{\text{ref}}[Q(k)]^j}$$





Ekström and Platter, Phys. Lett. **B (2025)**

Inferring the breakdown scale of pionless EFT

Bayes rule, and our assumptions

We use Bayes rule to 'invert' the quantity of interest as

$$p(M_{\text{hi}} \,|\, \sigma_{np}, I) \propto p(\sigma_{np} \,|\, M_{\text{hi}}) \cdot p(M_{\text{hi}} \,|\, I)$$

We assume...

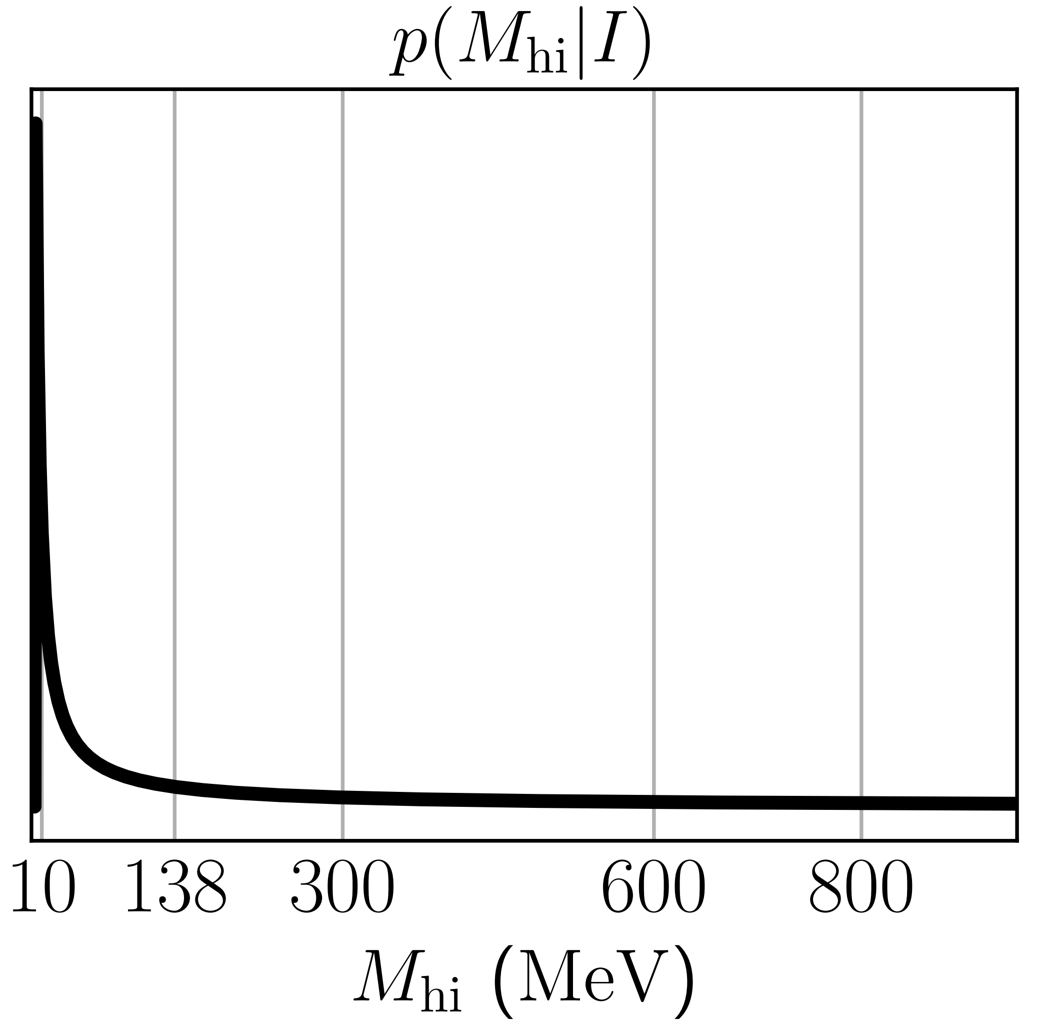
- ... $\mathcal{O}(1)$, independent, and normally distributed EFT expansion coefficients $c_i(k)$ via $c_i \,|\, \bar{c}^2 \sim \mathcal{N}(0, \bar{c}^2)$ with an inverse gamma prior $\bar{c}^2 \sim \mathcal{IG}(a_0 = 1, b_0 = 1)$. Yields $\mathbb{P}(\bar{c}^2 \in [1/3, 3]) \approx 0.67$
- ... a reference scale σ_{ref} set by LO, i.e., $\sigma_{np}^{(n=0)}$
- ... a scale invariant log-uniform prior $p(M_{\text{hi}} \,|\, I)$ over a large interval $M_{\text{hi}} \in (m_\pi/40, 40 m_\pi)$

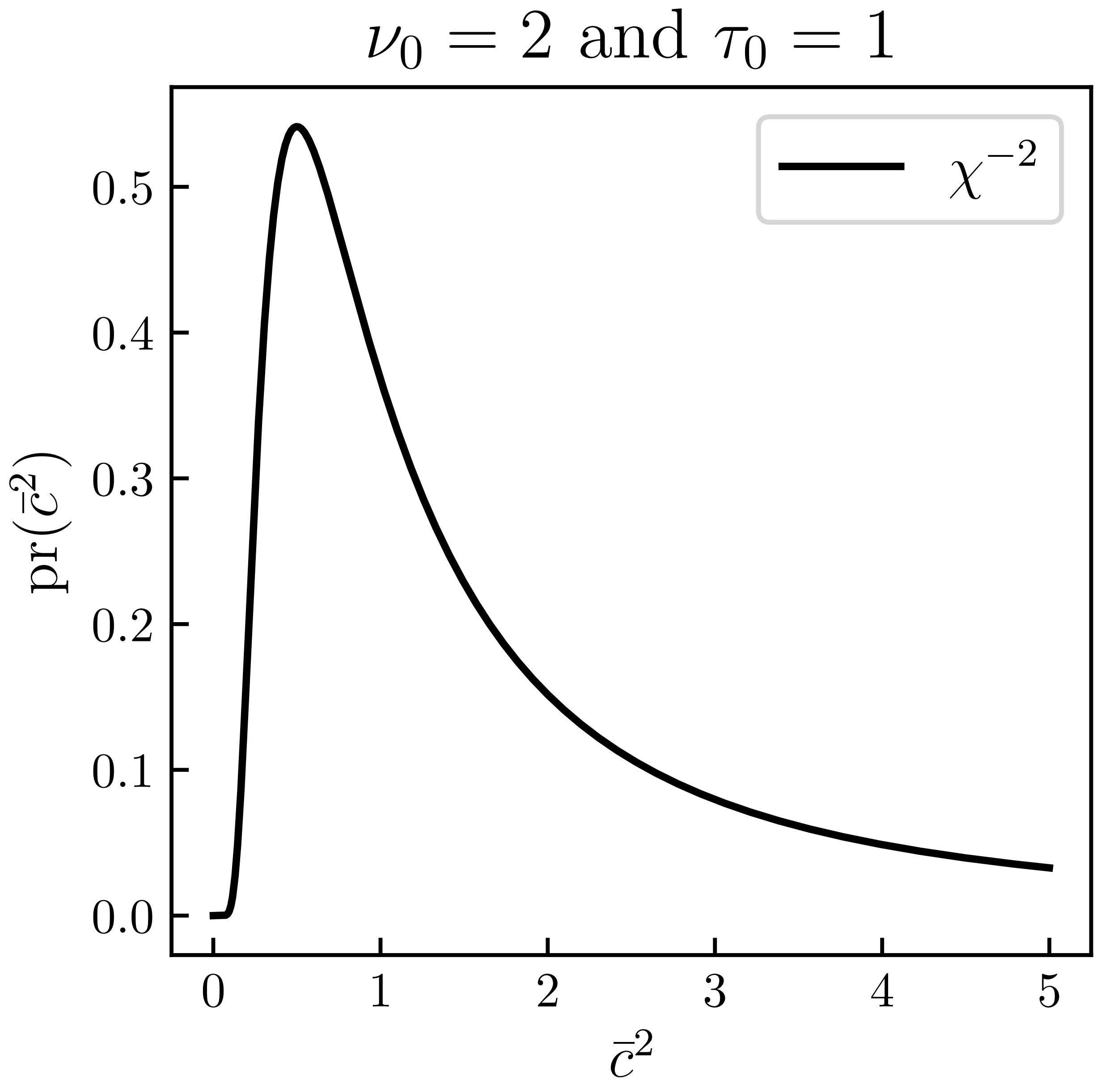
Independence enables factorization of the likelihood $p(\sigma_{np} \,|\, M_{\text{hi}}) = \prod_{i=1}^{K} p(\sigma_{np}(k_i) \,|\, M_{\text{hi}})$

We choose $K = 3$ scattering momenta k=69, 137, 181 MeV ($T_{\text{lab}} = 10, 40, 70$ MeV).

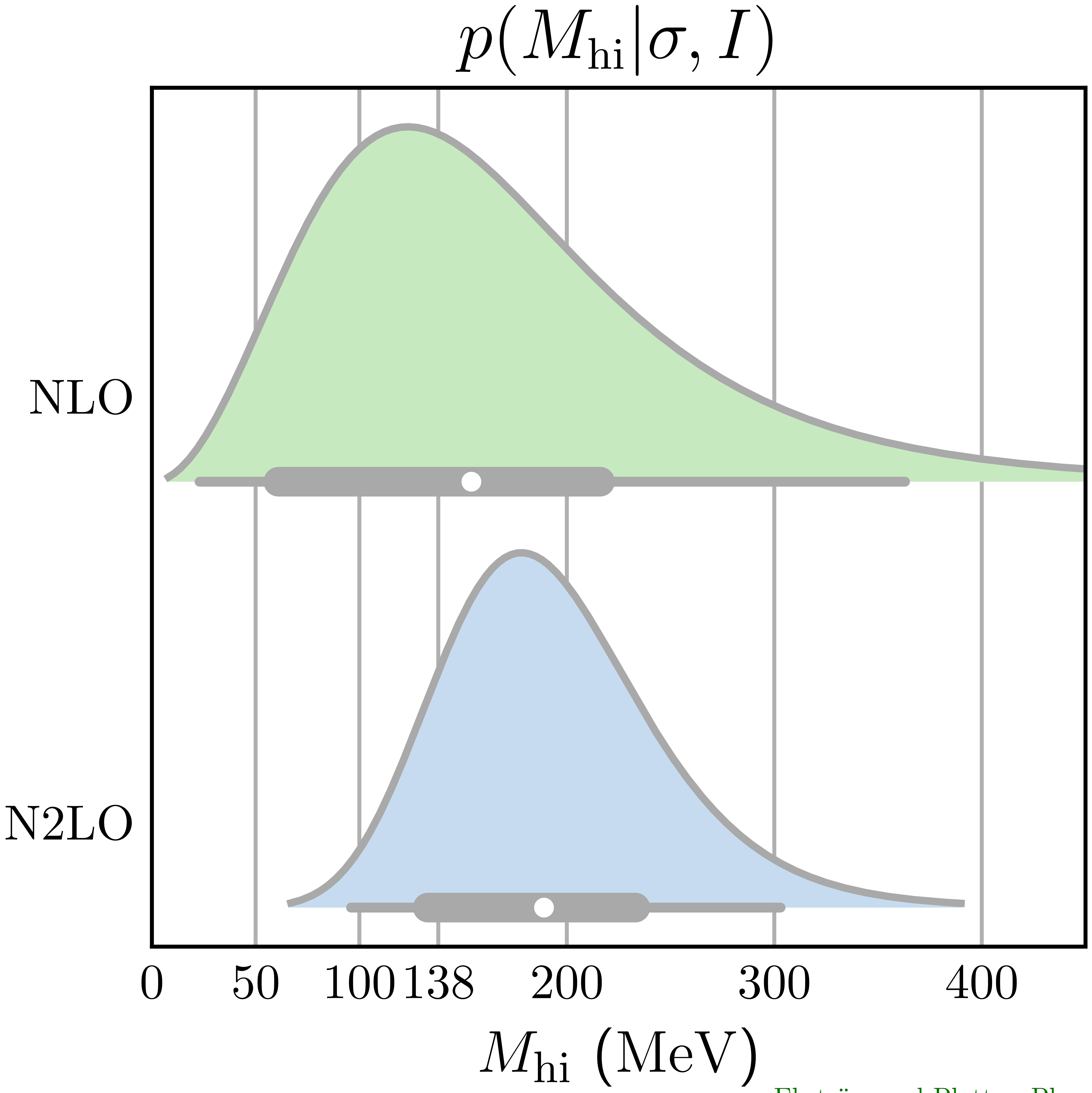
Melendez et al Phys Rev C (2019)

prior



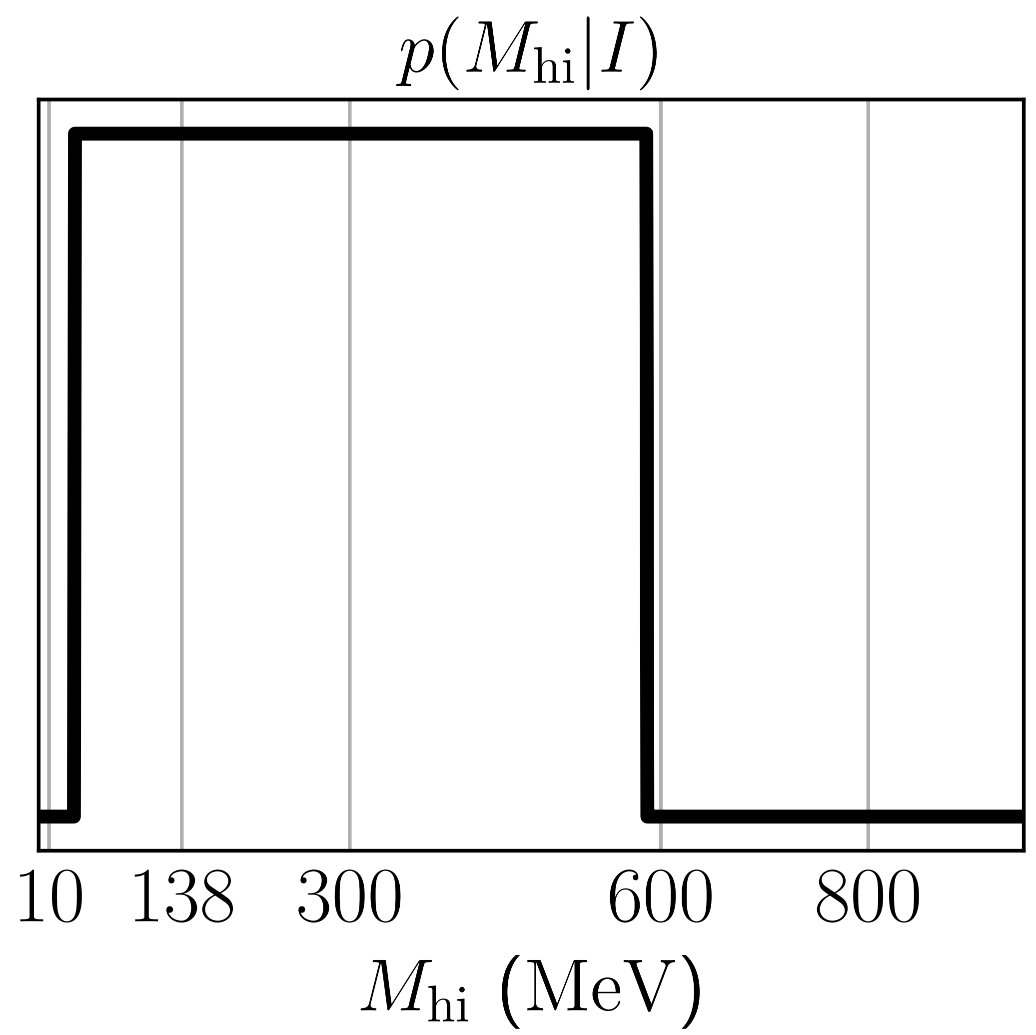


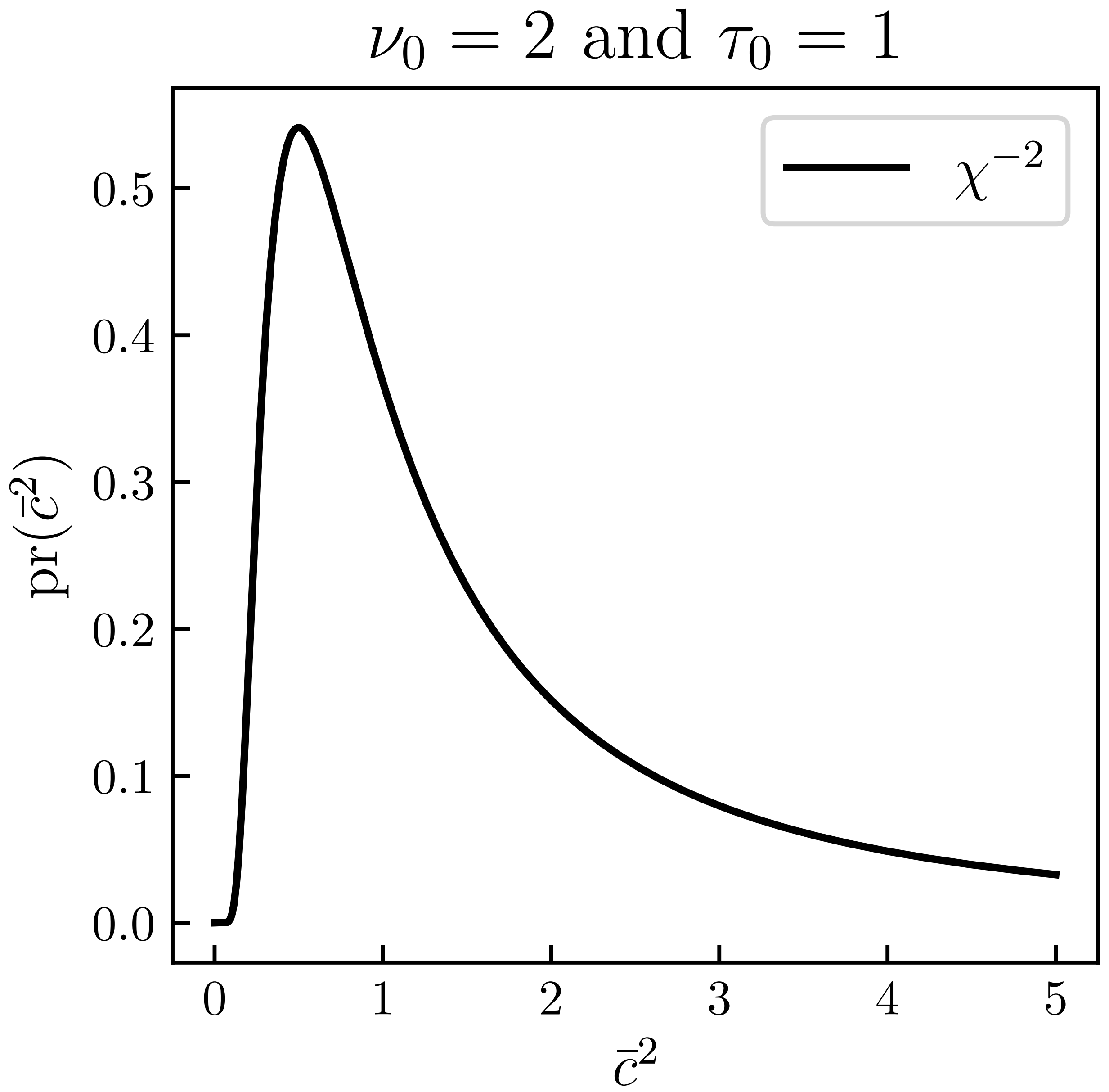
posterior



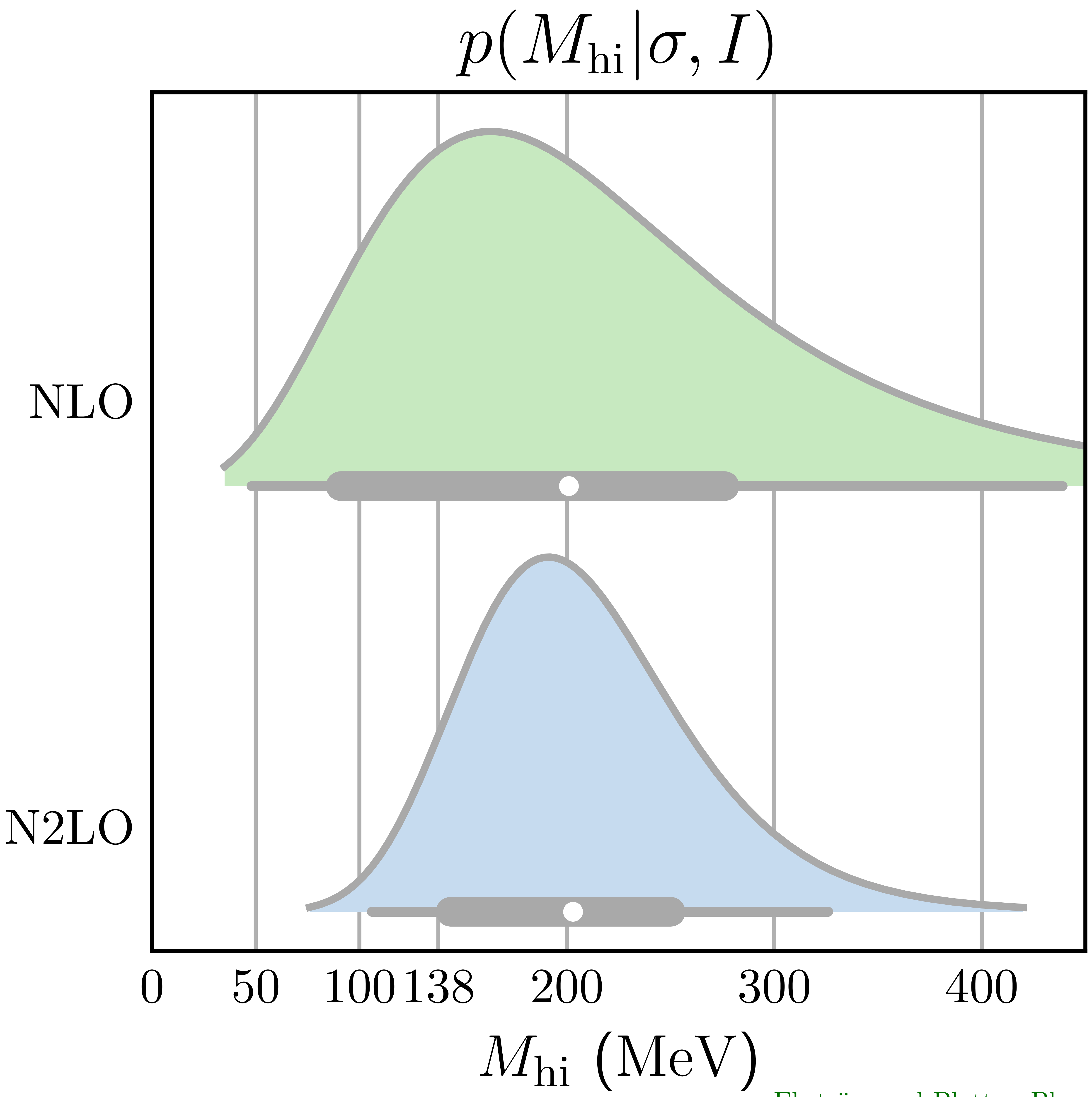
Ekström and Platter, Phys. Lett. **B (2025)**

prior





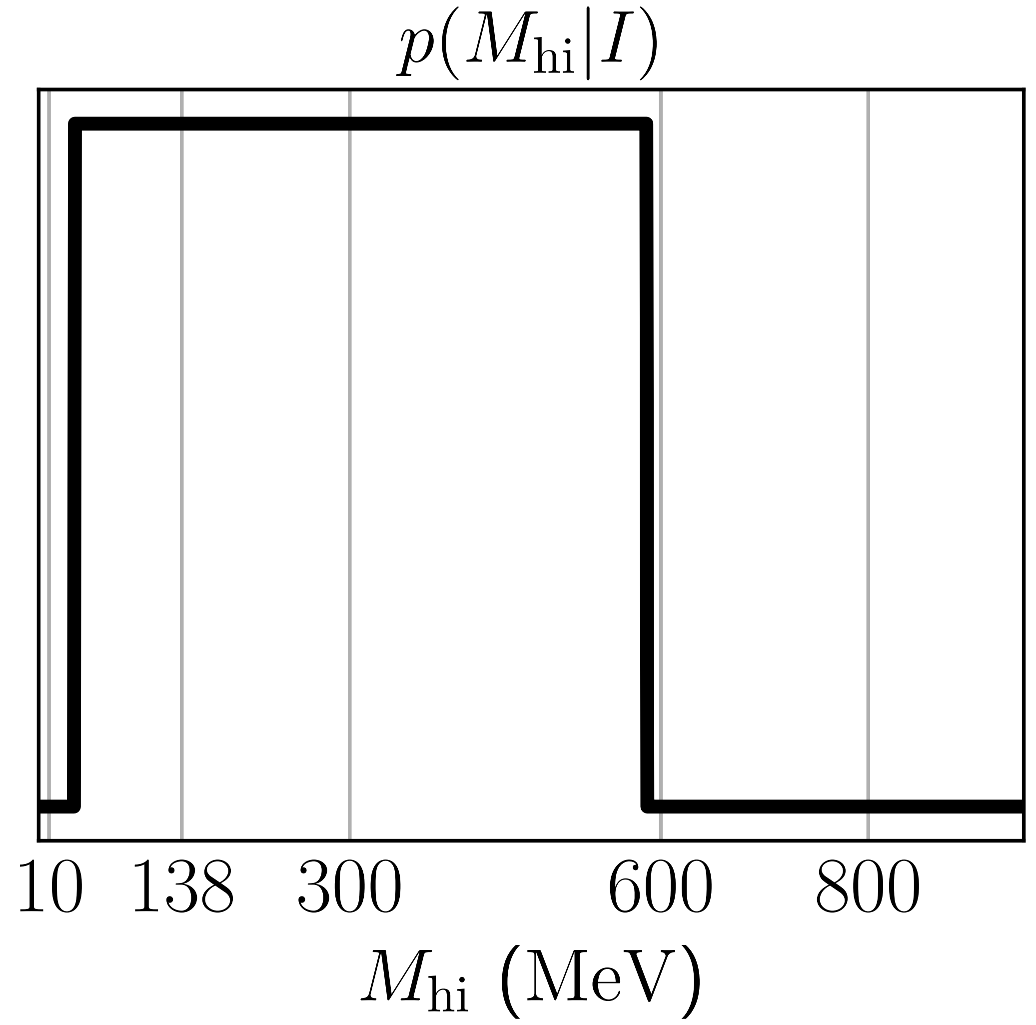
posterior

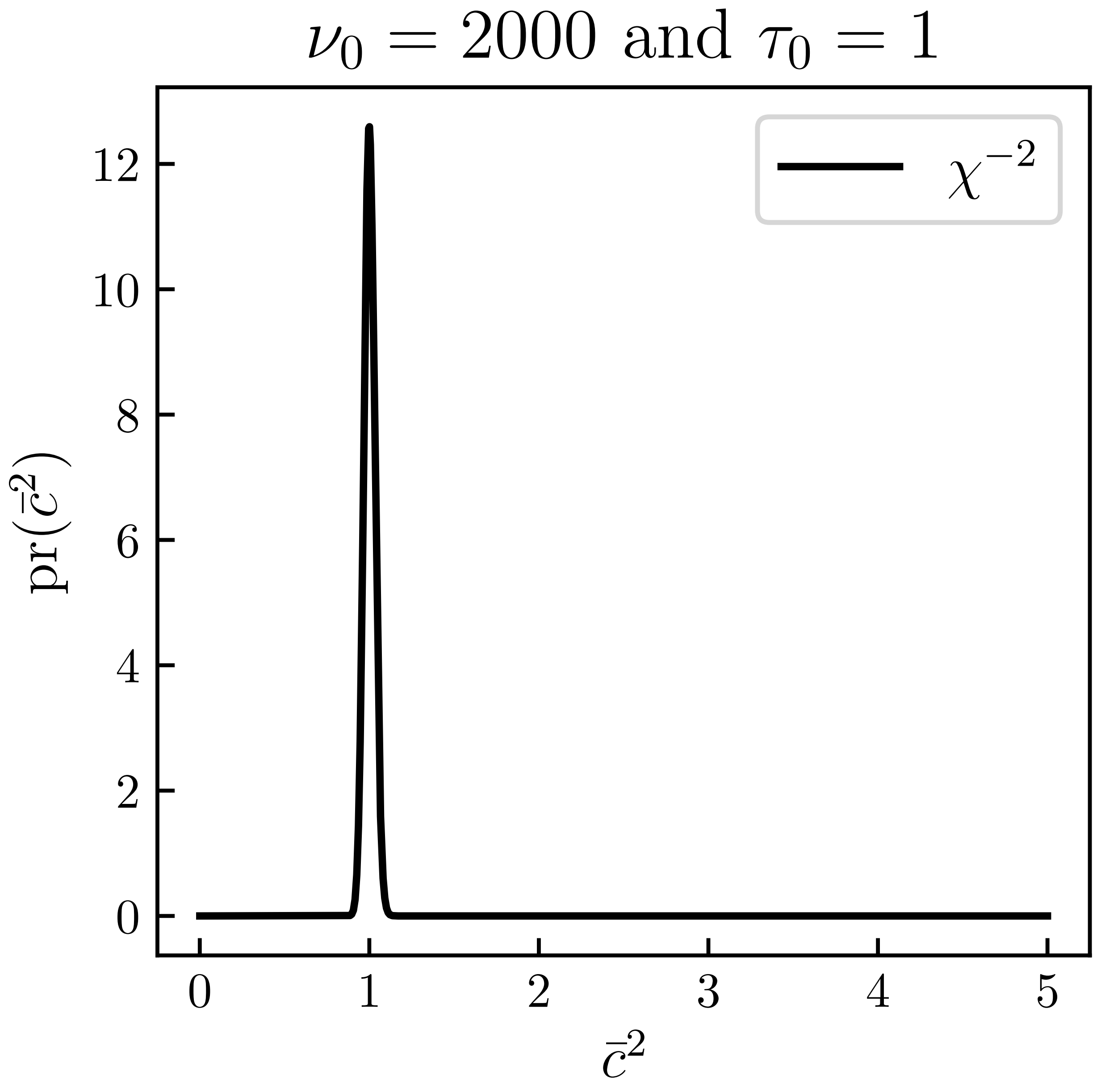


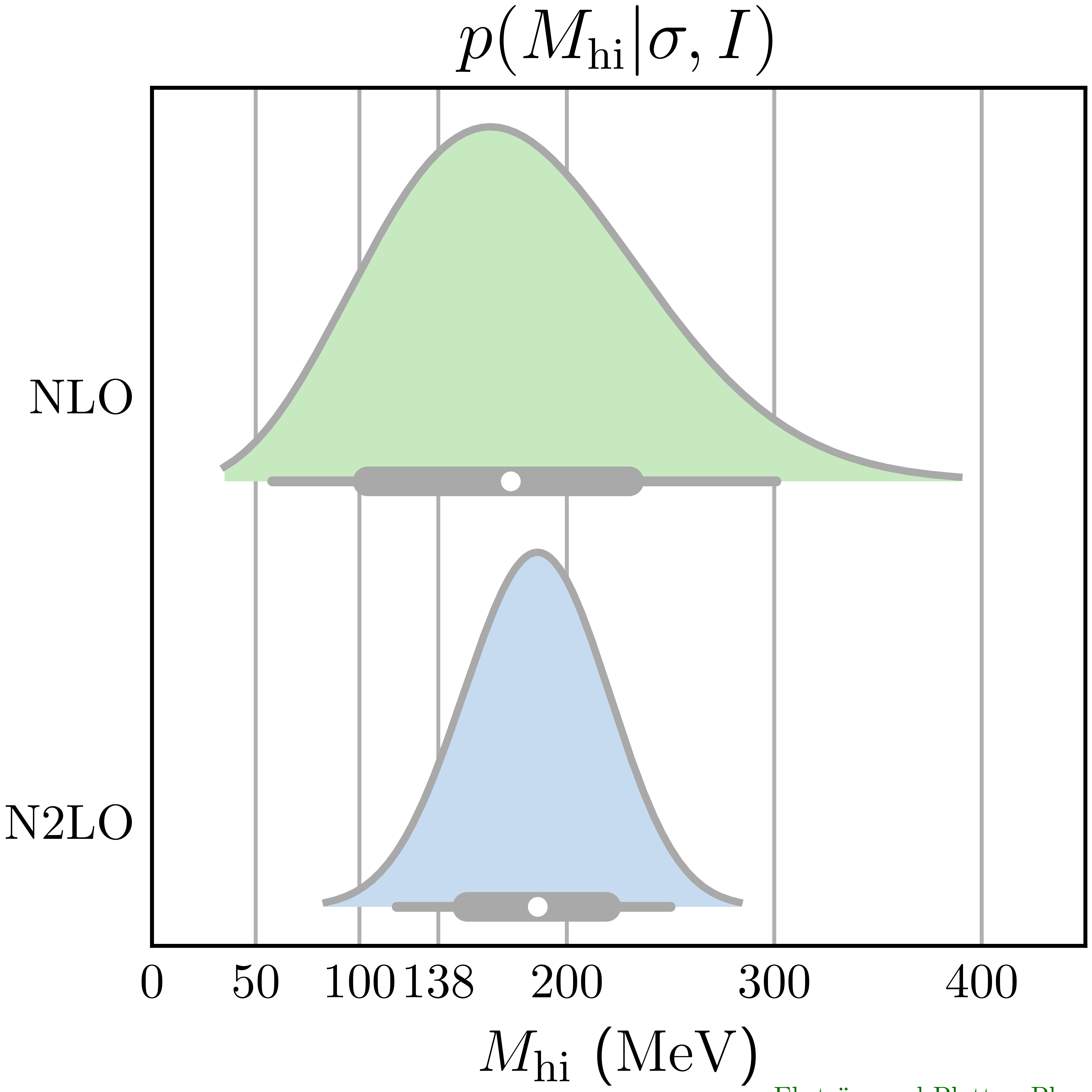
Ekström and Platter, Phys. Lett. **B (2025)**

prior

posterior



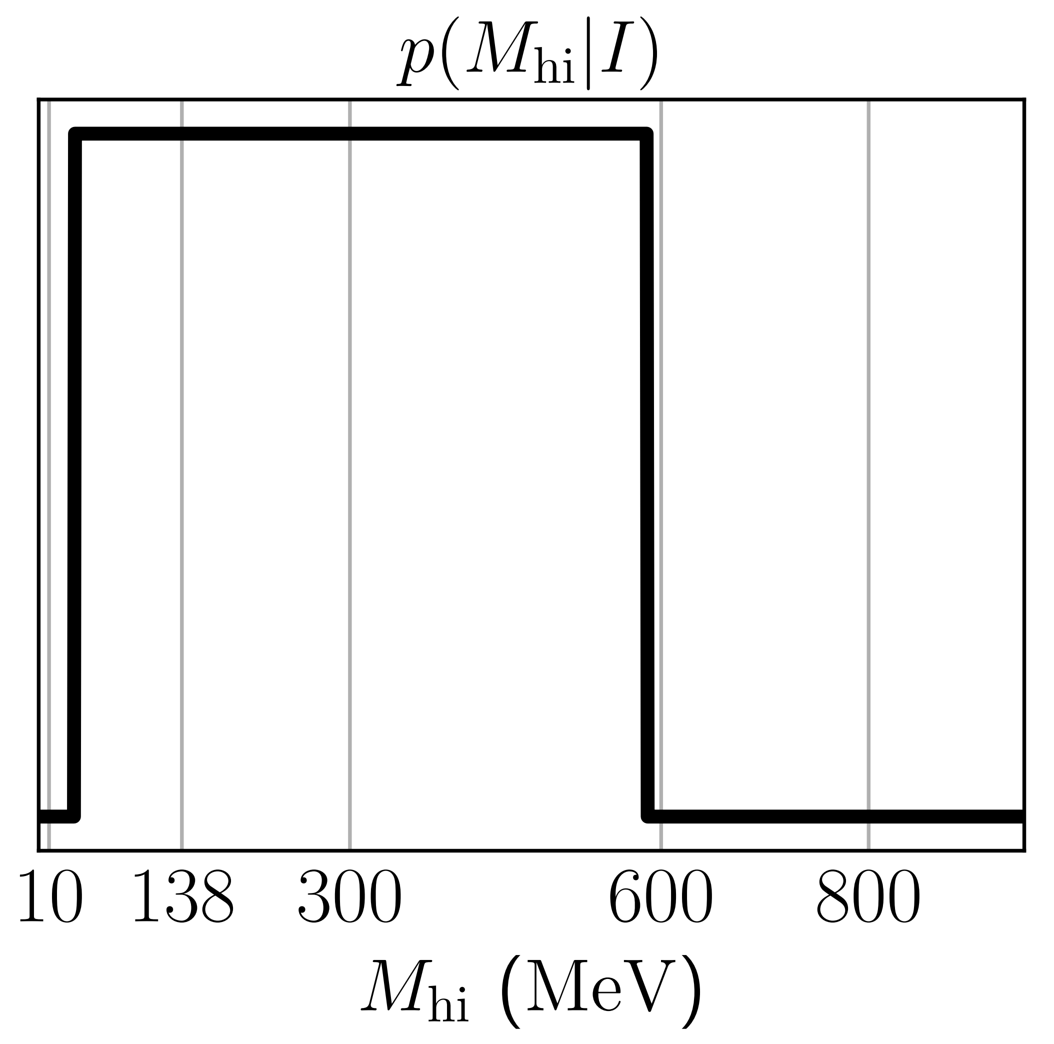


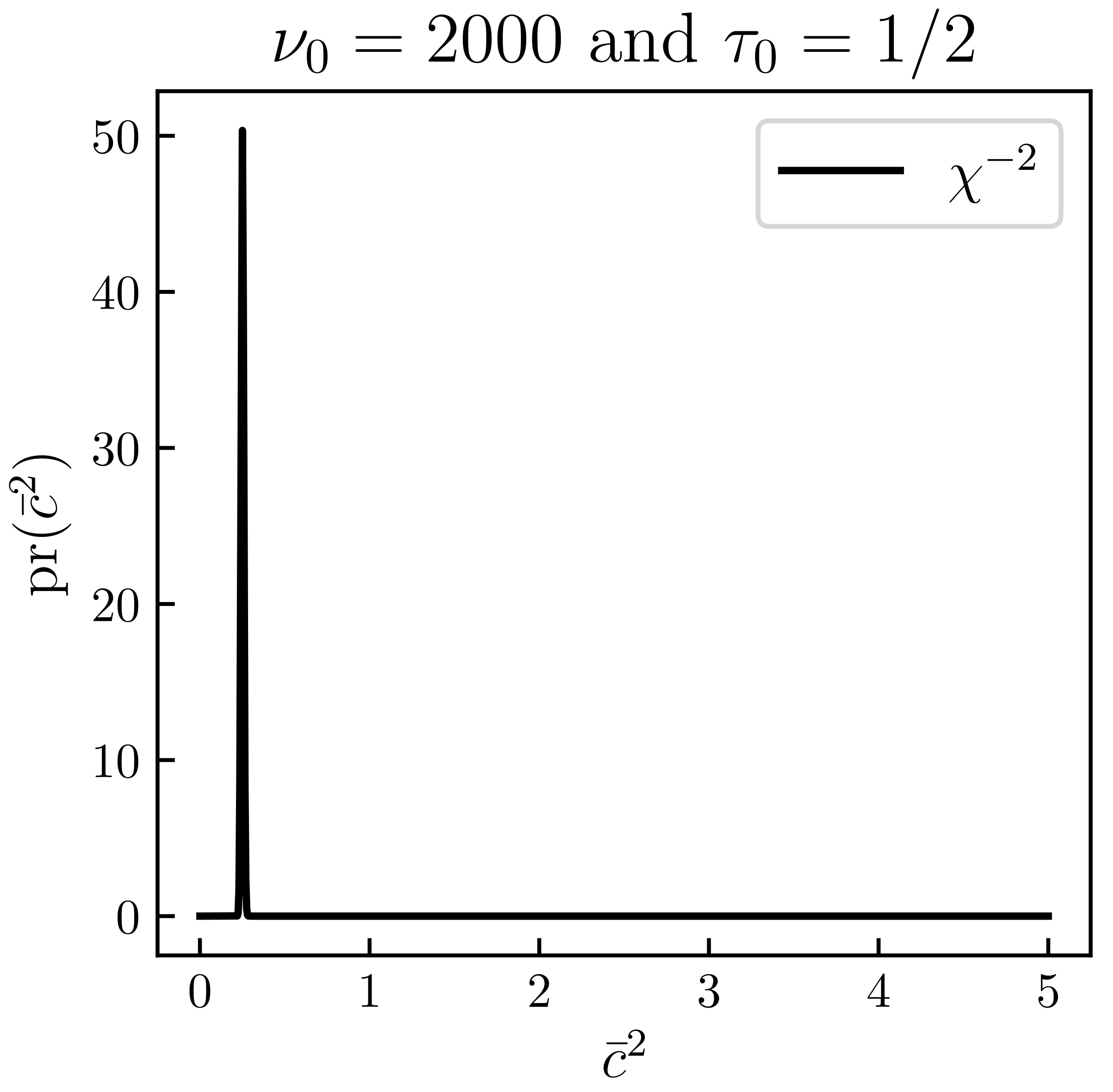


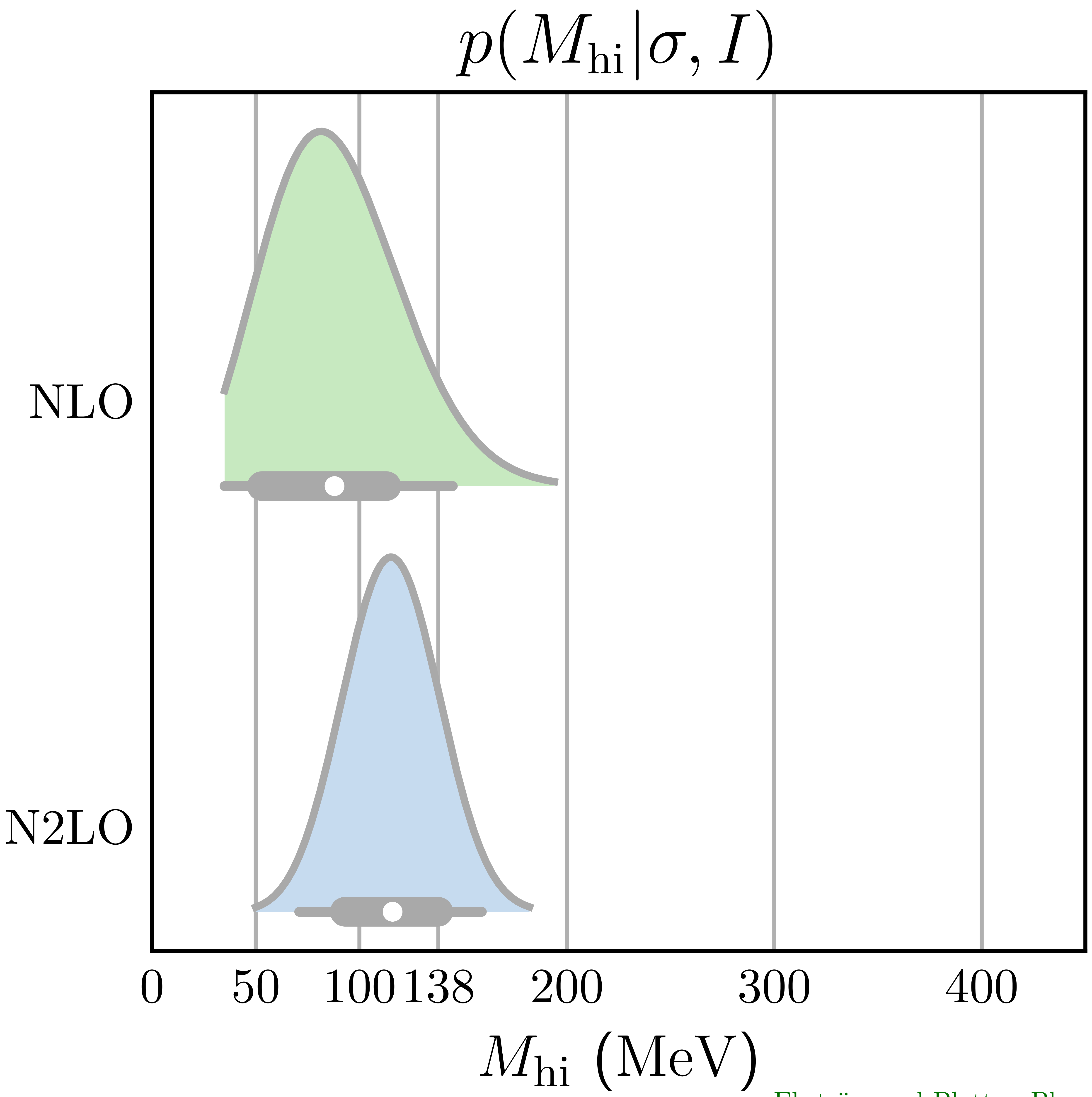
Ekström and Platter, Phys. Lett. **B (2025)**

prior

posterior







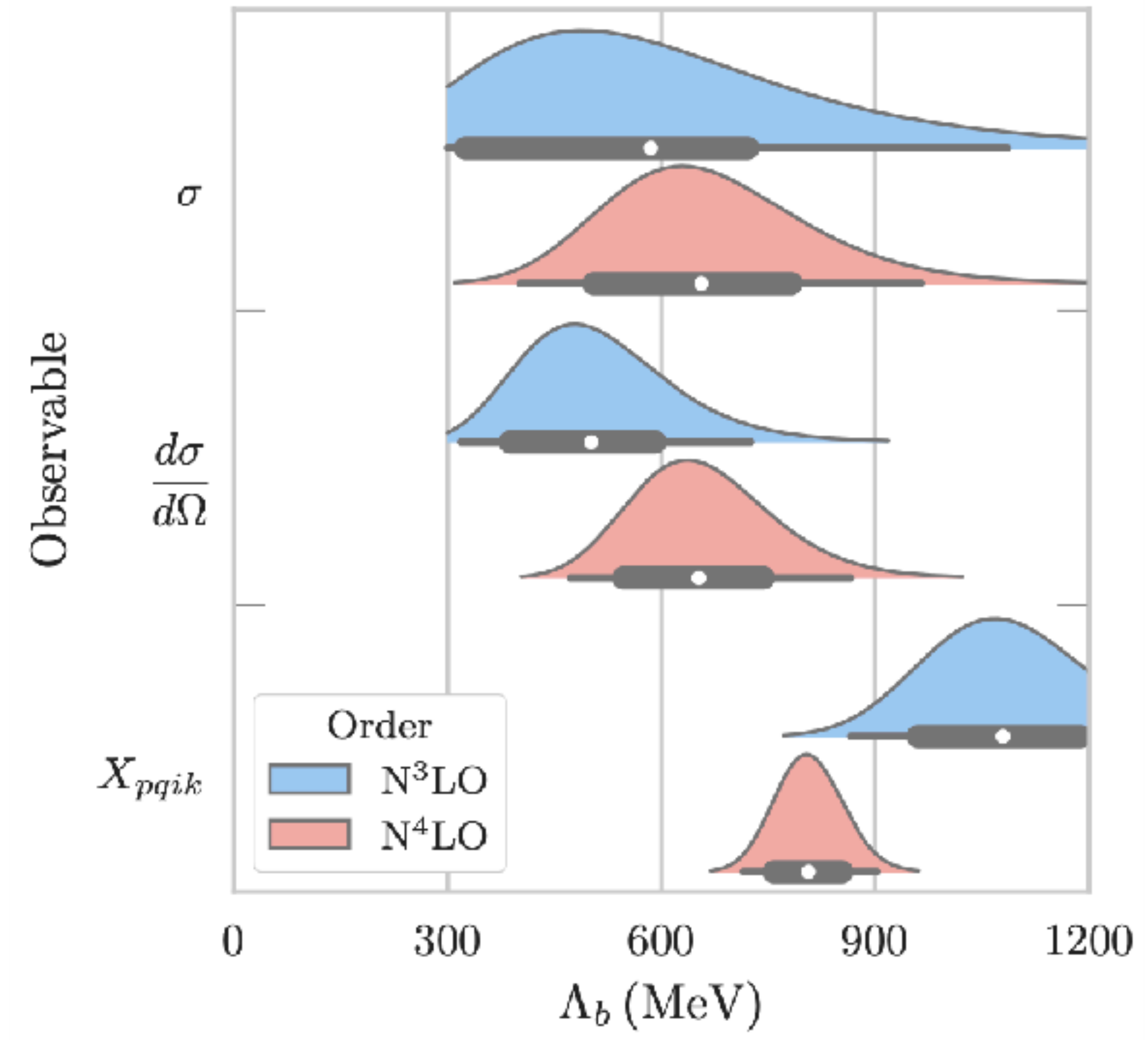
Ekström and Platter, Phys. Lett. **B (2025)**

Other examples, all conditional on assumptions

Millican et al Phys. Rev. C (2024)

	Extracted Values of Λ_b and m_{eff} in MeV for different parar					
Q	p	x_E	x_θ	Λ_b	m_{eff}	Observable(s)
Q_{sum}	p_{rel}	p_{rel}	$-\cos(\theta)$	570 ± 10	138 ± 3	All 2D obs.
Q_{smax}	p_{rel}	p_{rel}	$-\cos(\theta)$	378 ± 5	106 ± 0	All 2D obs.
Q_{sum}	p_{rel}	E_{lab}	$-\cos(\theta)$	610 ± 10	186 ± 4	All 2D obs.
Q_{smax}	p_{rel}	E_{lab}	$-\cos(\theta)$	459 ± 6	155 ± 1	All 2D obs.
Q_{sum}	$p_{\text{smax}}(p_{\text{rel}}, q_{\text{CM}})$	p_{rel}	$-\cos(\theta)$	660 ± 10	172 ± 4	All 2D obs.
Q_{sum}	p_{rel}	p_{rel}	q_{CM}	650 ± 10	184 ± 5	All 2D obs.
Q_{sum}	p_{rel}	p_{rel}	θ	590 ± 10	144 ± 2	All 2D obs.
Q_{sum}	p_{rel}	p_{rel}	$-\cos(\theta)$	530 ± 10	120 ± 3	All 2D obs.
Q_{sum}	p_{rel}	p_{rel}		990 ± 90	350 ± 40	σ_{tot}
Q_{smax}	p_{rel}	p_{rel}		670 ± 70	250 ± 40	σ_{tot}

Melendez et al Phys Rev C (2019)



Pionless EFT in analysis based on WPC (minus pions) yields $M_{\text{hi}} \in [50.11, 63.03]$ MeV
"Bayesian inference as a useful too to identify inconsistent PC" Bub et al Phys. Rev. C (2025) *accepted*

Calibrating of renormalizable chiral EFT

RG-invariant χEFT: proposal by Long & Yang

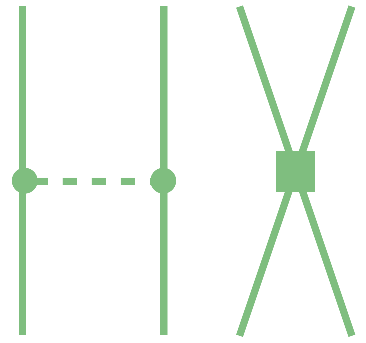
non-perturbative one-pion-exchange

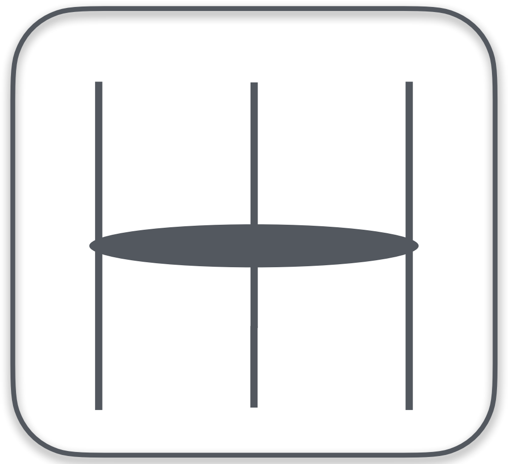
$^3S_0, ^3S_1 - ^3D_1, ^3P_{0,1}, ^3P_2 - ^3F_2, ^1P_1$

All other partial waves

amplitude expanded in (Q/Λ_χ)

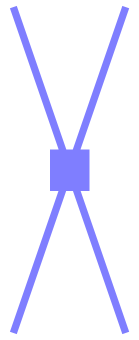
perturbative contriutions

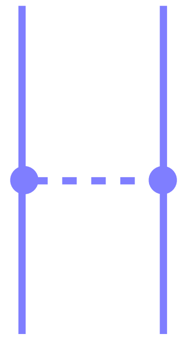
LO g_A  $C_{^1S_0}, C_{^3S_1}, D_{^3P_0}, D_{^3P_2}$



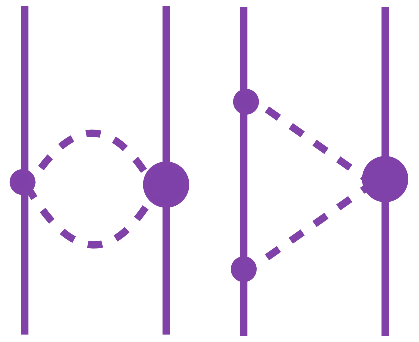
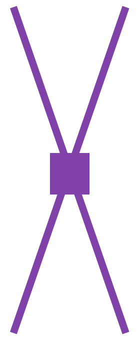
promote?

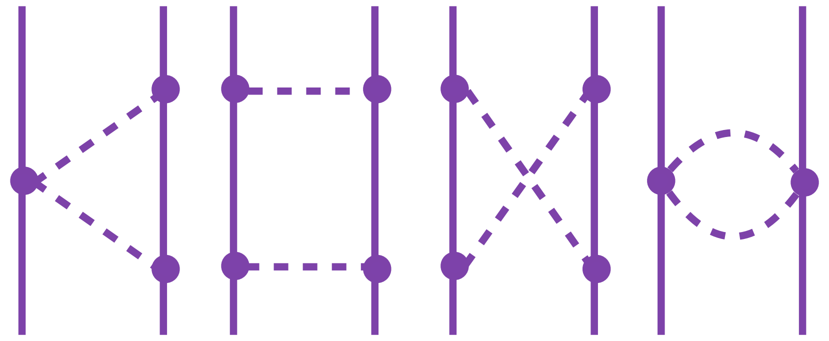
See C.-J. Yang Talk

NLO  $D_{^1S_0}$

g_A 

N²LO $E_{^1S_0}, D_{^3S_1}, D_{^3S_1-^3D_1}, D_{^1P_1},$
$D_{^3P_1}, E_{^3P_0}, E_{^3P_2}, E_{^3P_2-^3F_2}$

N³LO  $c_{1,3,4}$  $F_{^1S_0}$

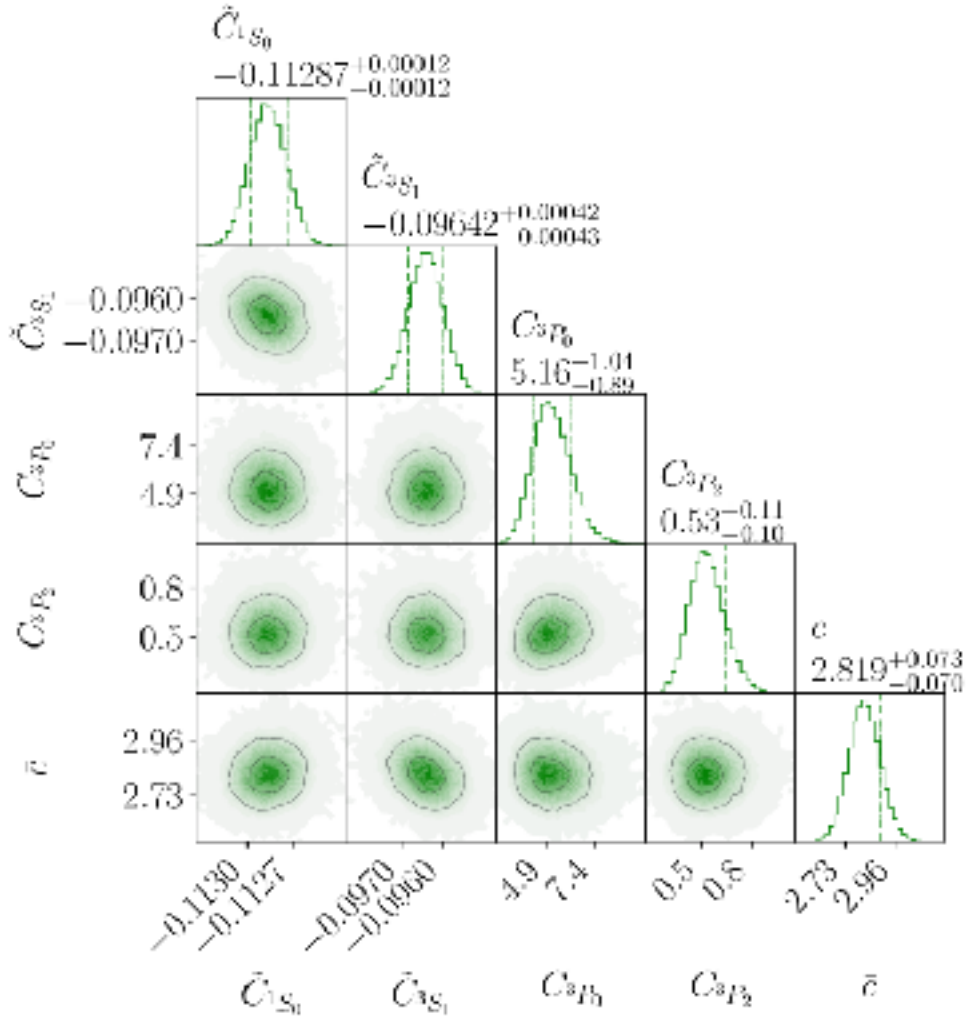


Long & Yang, Phys. Rev. C **84**, 057001 (2011), Phys. Rev. C **85**, 034002 (2012), Phys. Rev. C **86**, 024001 (2012), Yang et al, Eur. Phys. Jour. A **59**, 233 (2023)

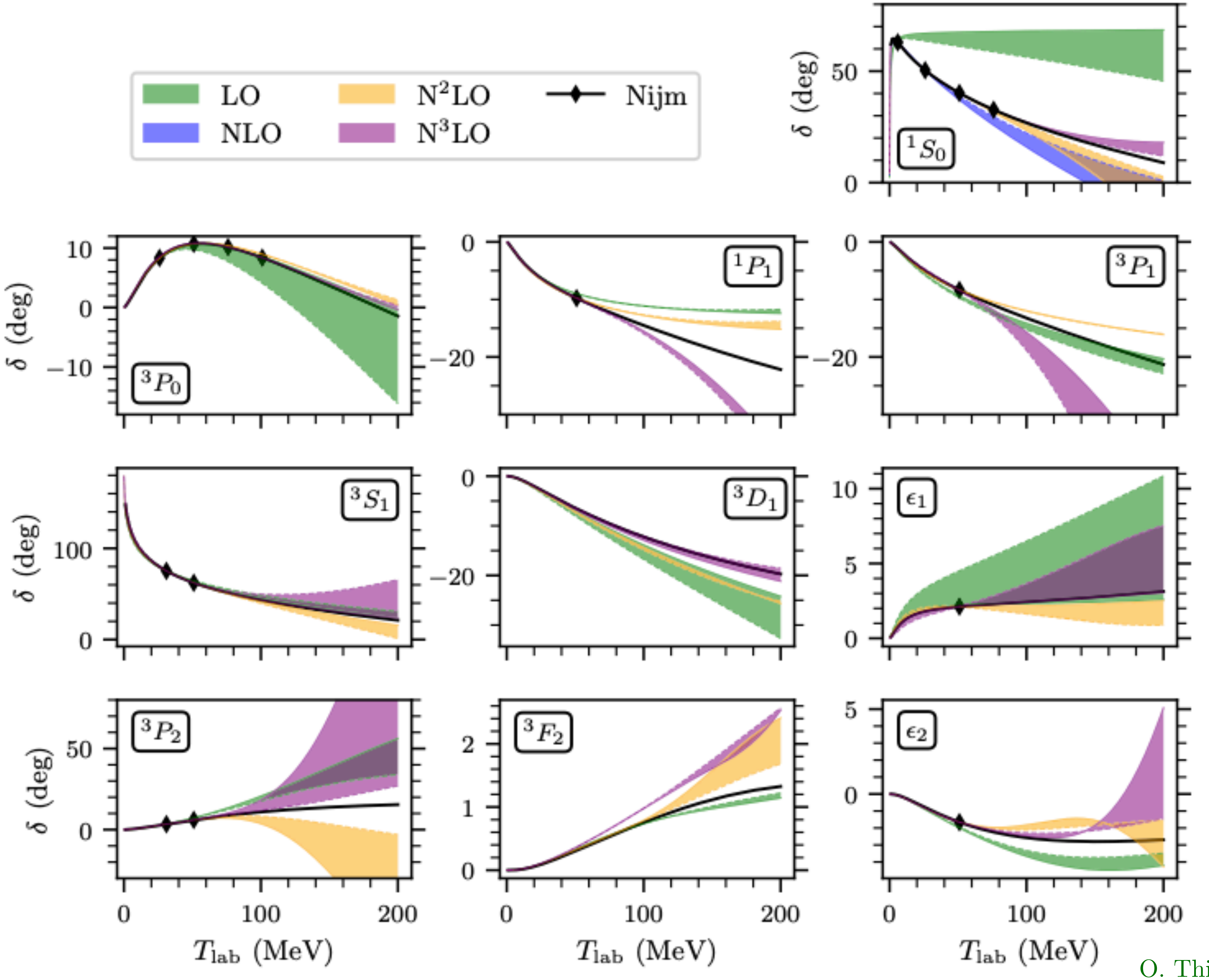
Calibrated up to N3LO using *np* phase shifts

Bands are from cutoff variation 500 MeV+2500 MeV

Perturbative computation of NLO, N2LO, N3LO phase shifts. Calibrated to Nijmegen phase shift database (black diamonds)



O. Thim, et al, Phys. Rev. C (2023)

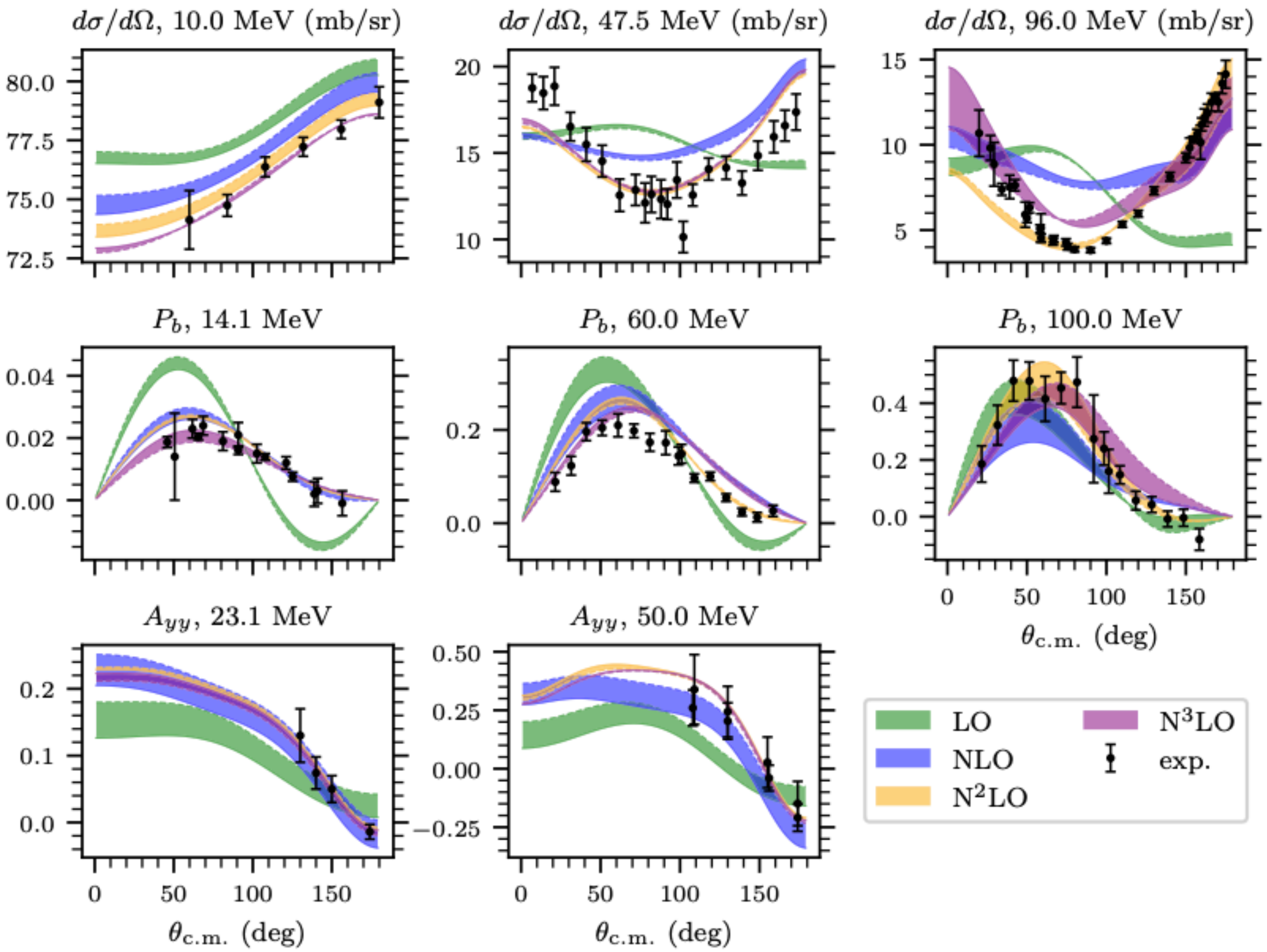


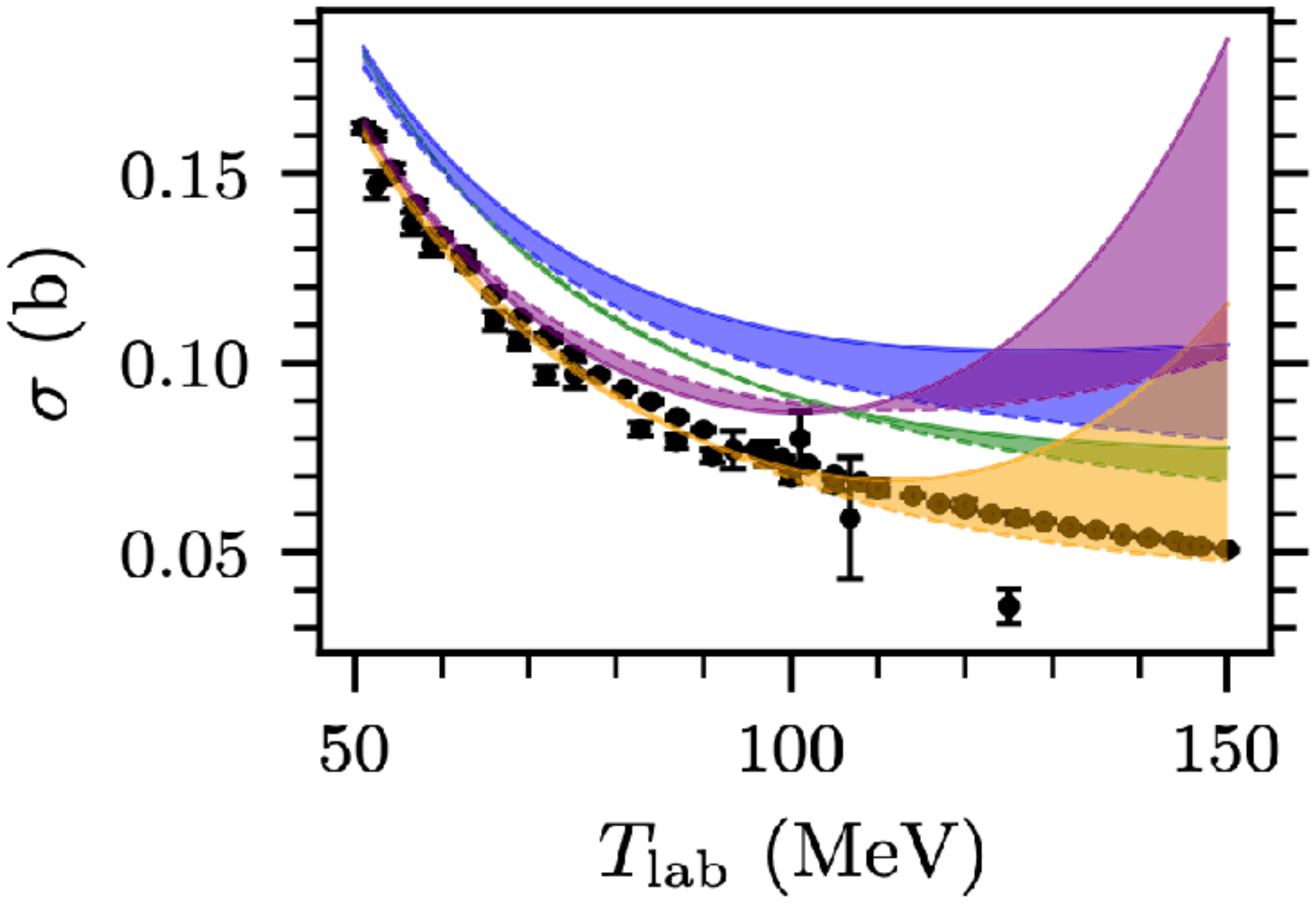
Oliver Thim
Chalmers PhD student

O. Thim, et al, Phys. Rev. C (2024)

Predicting *np* scattering cross sections

Bands from cutoff variation 500-2500 MeV





$\Lambda_b \approx 220\,\text{MeV} \approx m_\Delta - m_N$

$p(\Lambda_b | \sigma, I)$?

O. Thim, et al, Phys. Rev. C (2024)

Exceptional cutoff value in $^3P_0$

$$V_{\rm LO} = V_{1\pi} + C^{(0)}_{^1S_0} + C^{(0)}_{^3S_1} + D^{(0)}_{^3P_0} p'p + D^{(0)}_{^3P_2} p'p$$

$$V_{\rm NLO} = C^{(1)}_{^1S_0} + D^{(0)}_{^1S_0}(p'^2 + p^2)$$

$$V_{\rm NNLO} = V^{(0)}_{2\pi} + \ldots + D^{(1)}_{^3P_0} p'p + E^{(0)}_{^3P_0} p'p(p'^2 + p^2)$$

When $V_{1\pi}$ is singular and attractive, it strongly affects the scattering amplitude and necessitates the inclusion of short-range counterterms to achieve RG invariance.

Perturbative N2LO amplitude: $T_{\rm NNLO} = (1 + T_{\rm LO}G_0)V_{\rm NNLO}(1 + G_0 T_{\rm LO})$

$$\delta_{\rm NNLO}(k_1) = D \cdot \delta^D_{\rm NNLO}(k_1) + E \cdot \delta^E_{\rm NNLO}(k_1) + \delta^{2\pi}_{\rm NNLO}(k_1)$$

$$\delta_{\rm NNLO}(k_2) = D \cdot \delta^D_{\rm NNLO}(k_2) + E \cdot \delta^E_{\rm NNLO}(k_2) + \delta^{2\pi}_{\rm NNLO}(k_2)$$

See B. Long Talk

At certain (exceptional) cutoff values Λ_E the NNLO LECs $D^{(1)}_{^3P_0}, E^{(0)}_{^3P_0}$ are proportional to linearly dependent contributions to the perturbative phase shift. This yields a zero-determinant for the linear equations matching to phase shifts at on-shell kinematical points k_1 & k_2. (fairly independently of k_1 & k_2)

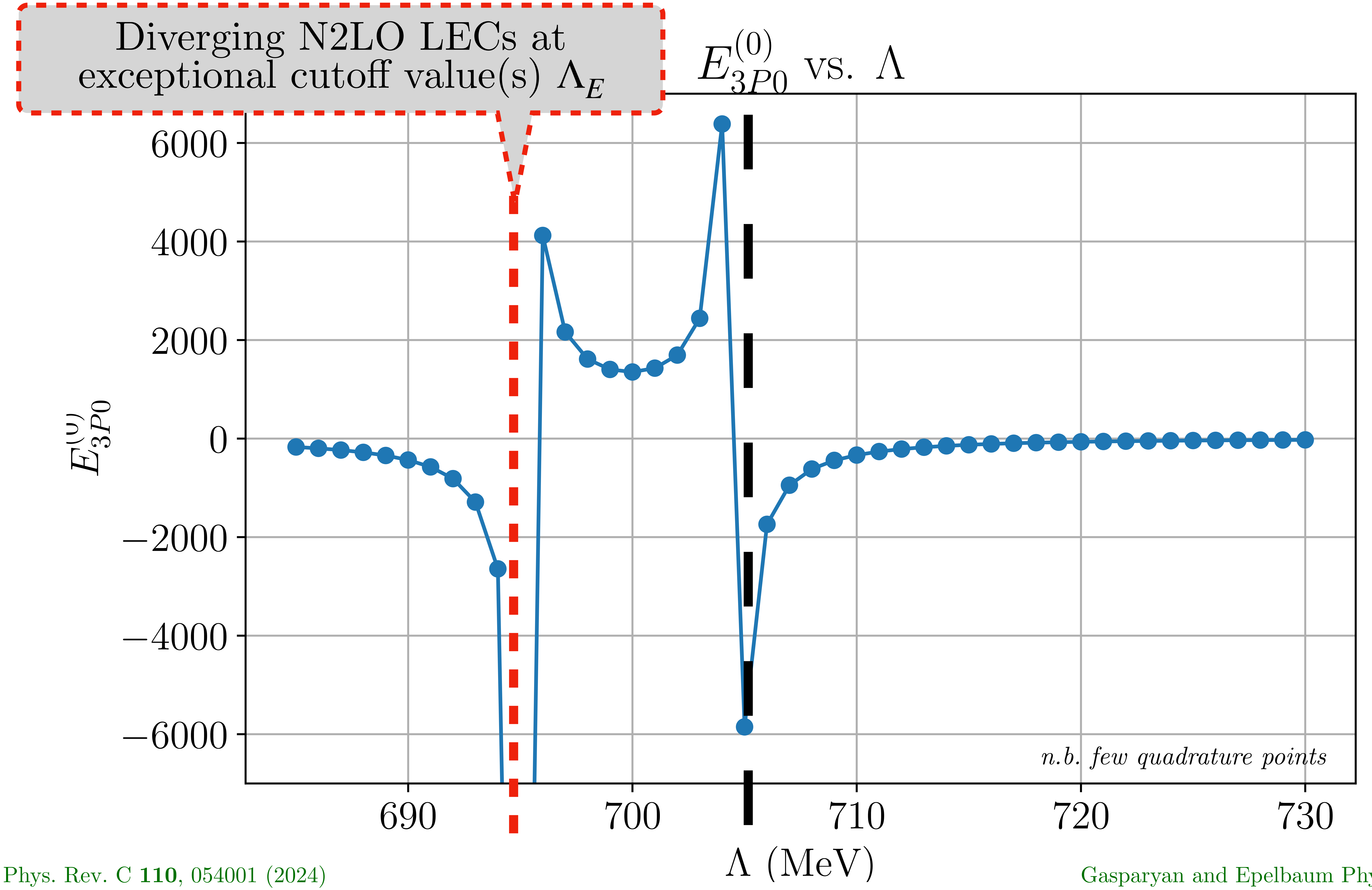
Possible to break linear dependence at NNLO by shifting the LO calibration phase shift by some value (a ‘nugget’) and thereby alter the short-range distorted LO wave.

Peng, Long, Xu Phys. Rev. C **110**, 054001 (2024)

Gasparyan and Epelbaum Phys. Rev. C **107**, 034001 (2023)

Shi, Peng, Liu, Lyu, Long, Phys. Rev. C **106,** 015505 (2022)

Cutoff variation: limit cycle and exceptional cutoffs Λ_E

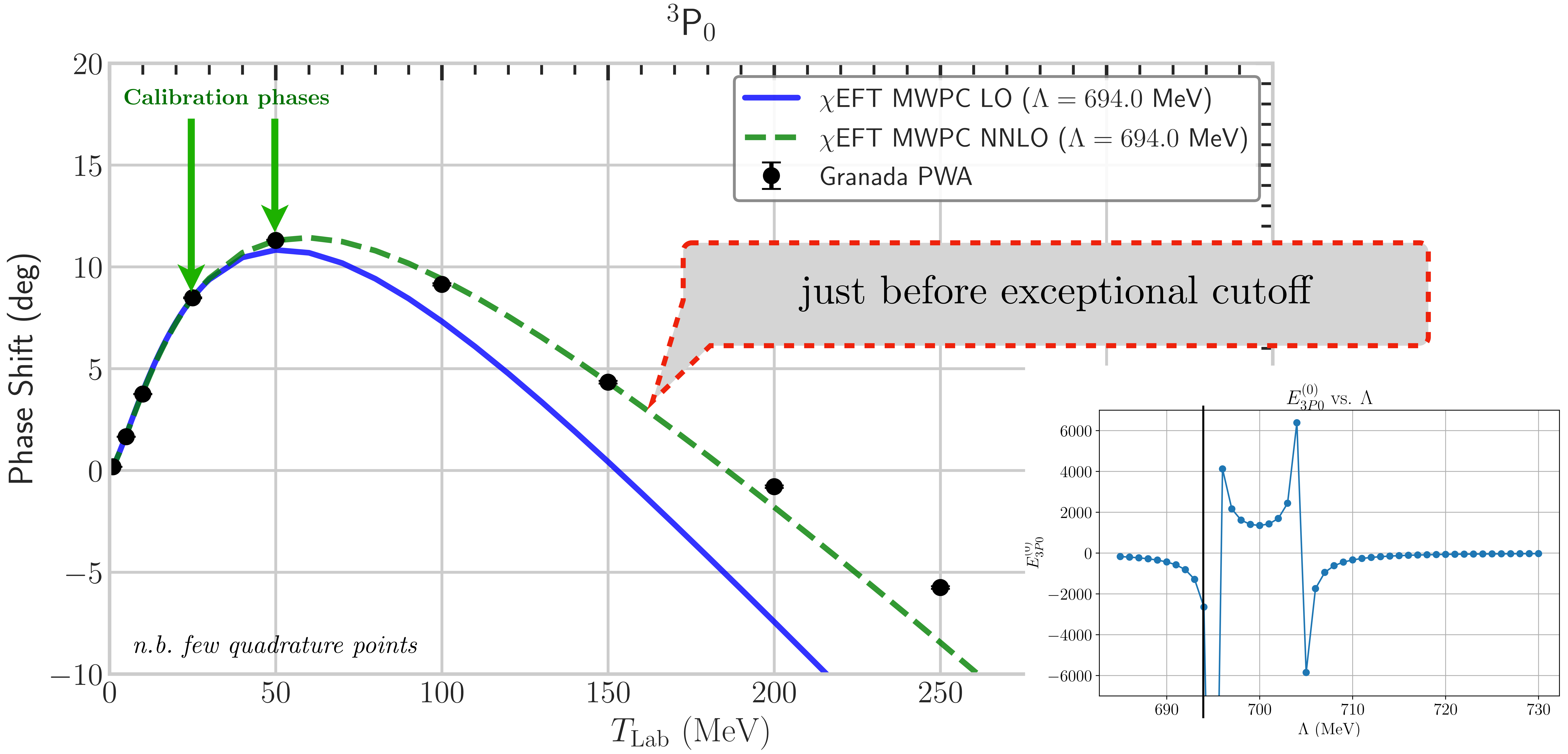


Peng, Long, Xu Phys. Rev. C **110**, 054001 (2024)

Gasparyan and Epelbaum Phys. Rev. C **107**, 034001 (2023)]

Exceptional cutoffs

At $\Lambda = \Lambda_E$ we have linearly dependent equations for $D^{(1)}$ and $E^{(0)}$



Peng, Long, Xu Phys. Rev. C **110**, 054001 (2024)

Gasparyan and Epelbaum Phys. Rev. C **107**, 034001 (2023)]

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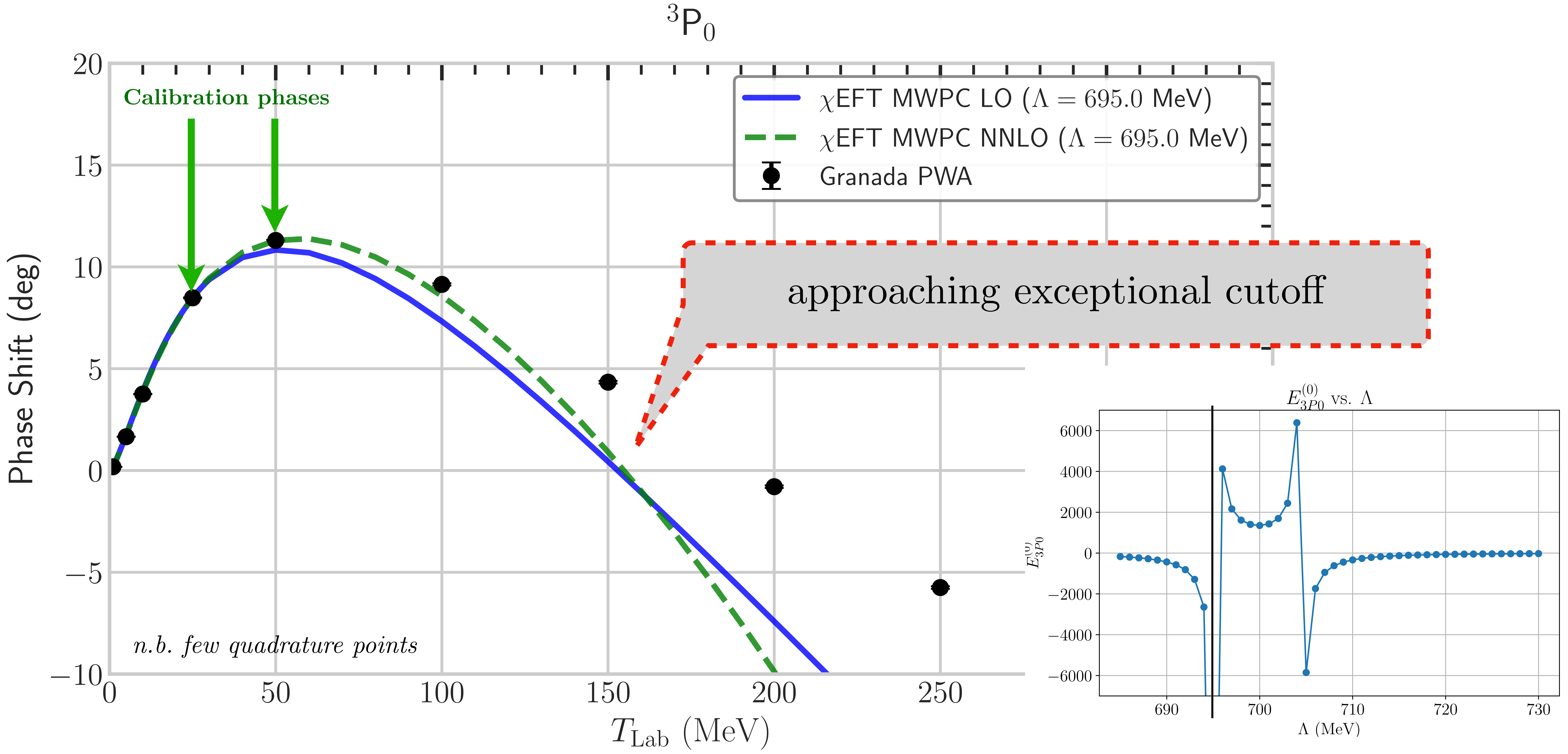

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Gasparyan and Epelbaum Phys. Rev. C **107**, 034001 (2023)]

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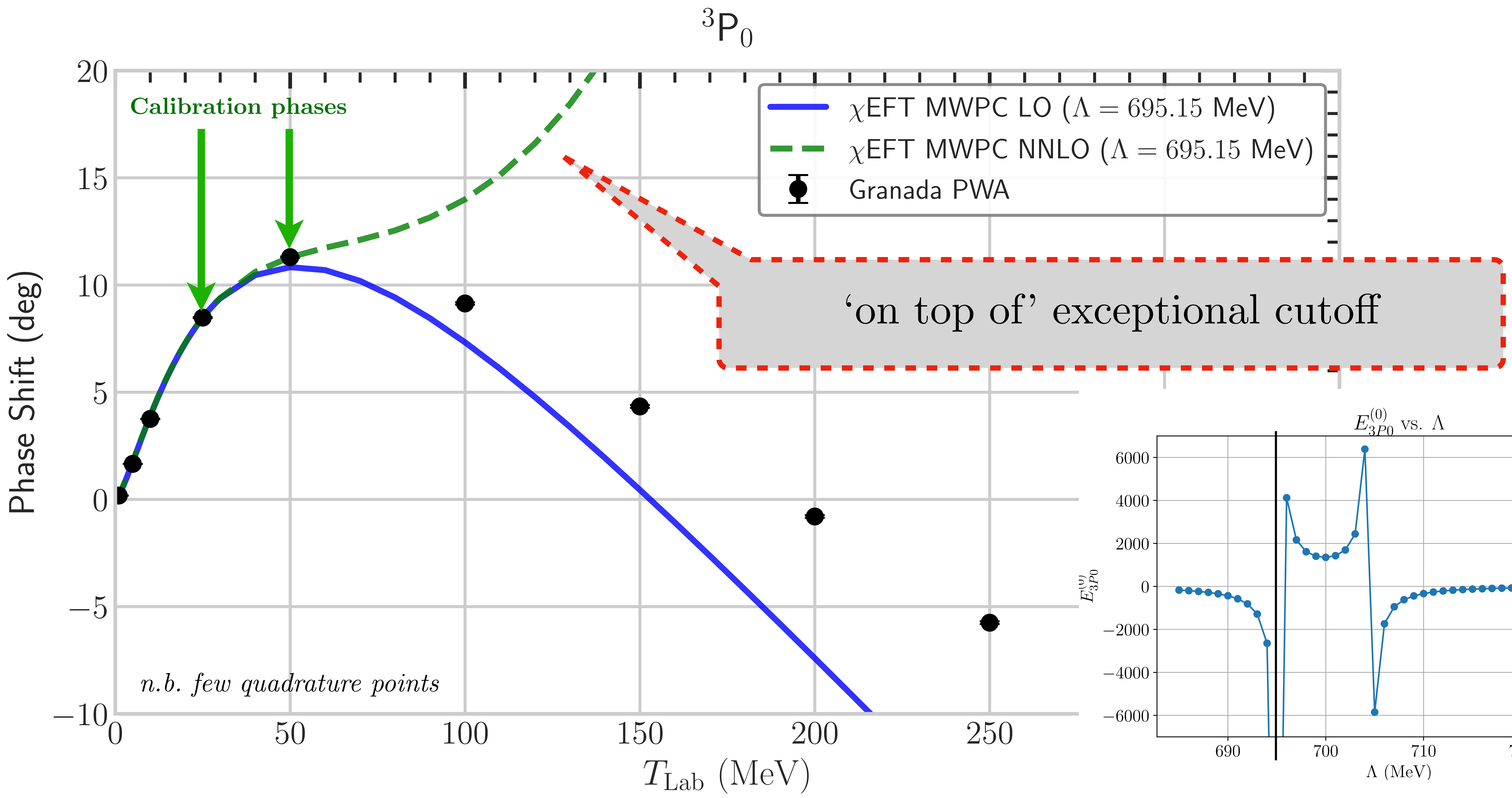

Peng, Long, Xu Phys. Rev. C **110**, 054001 (2024)

Gasparyan and Epelbaum Phys. Rev. C **107**, 034001 (2023)]

Exceptional cutoffs

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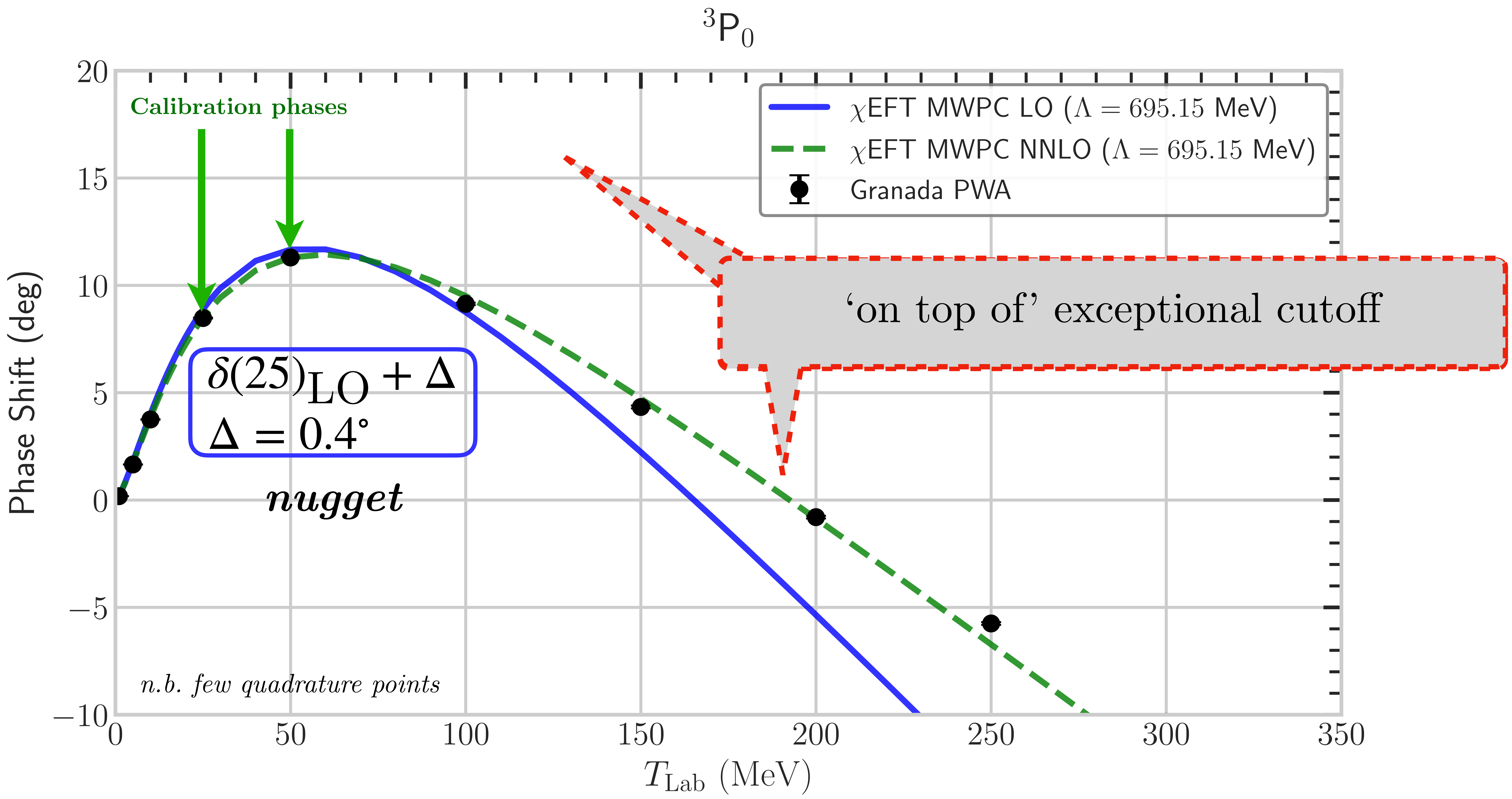
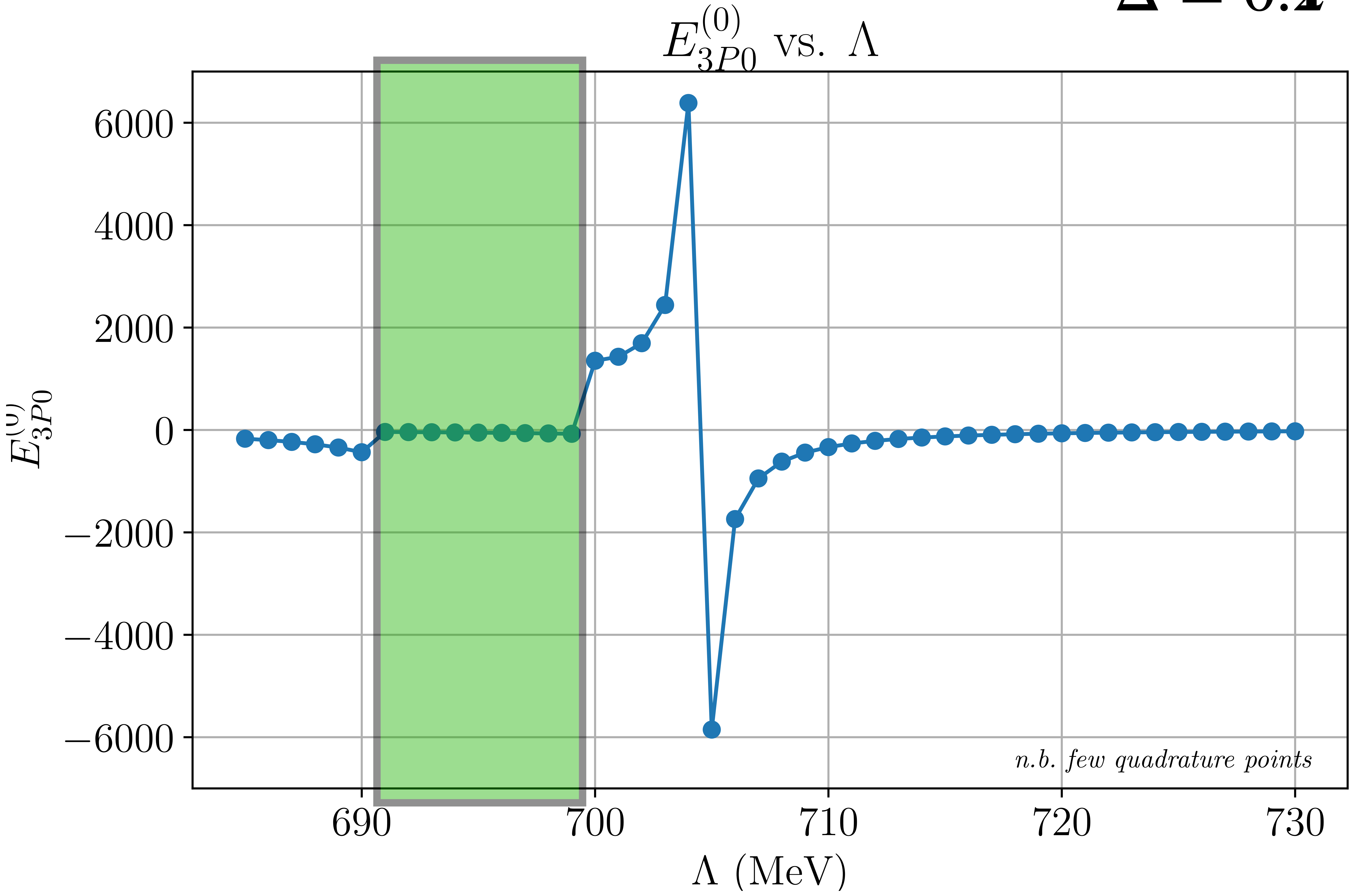
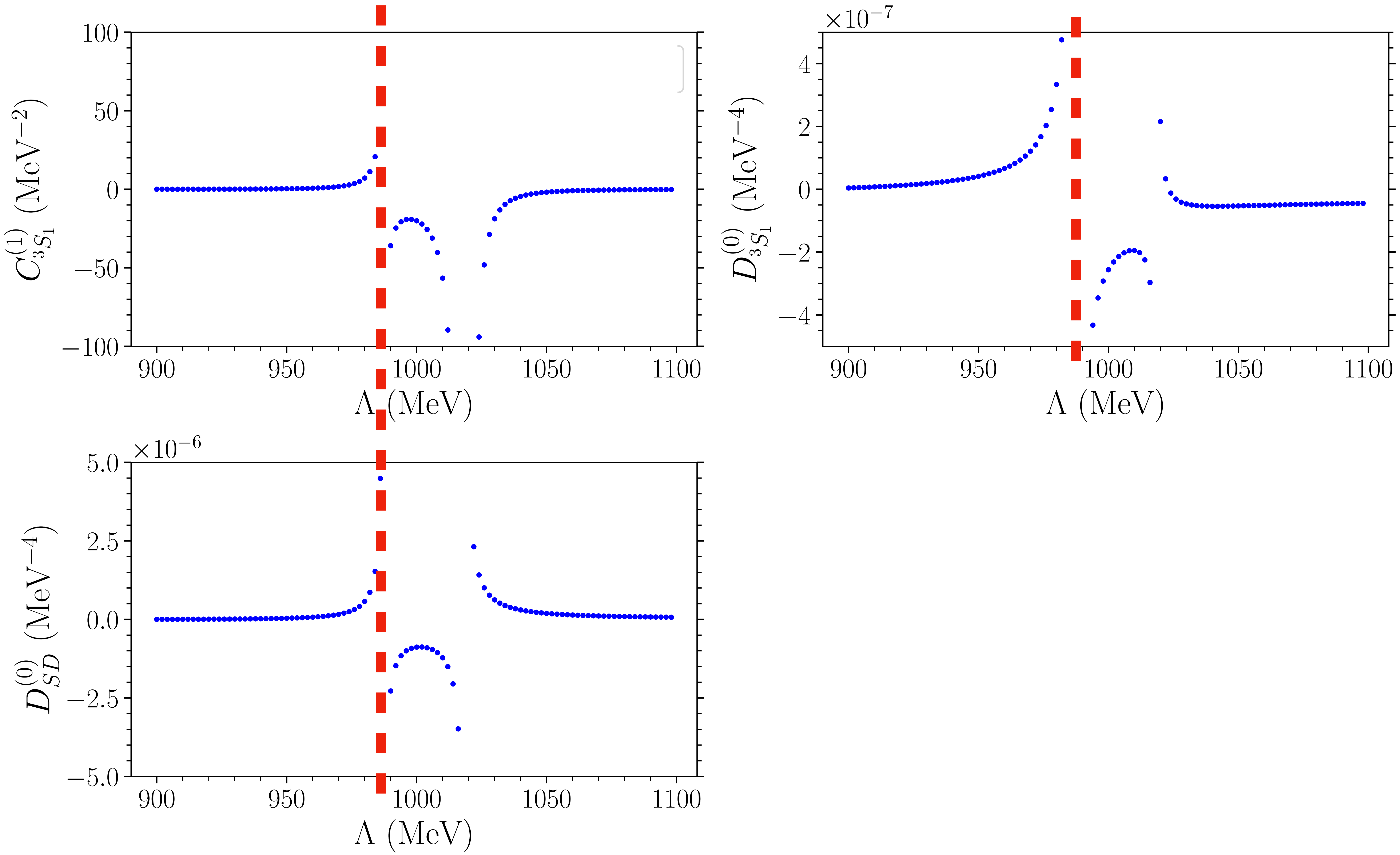


$\Delta = 0.4^\circ$



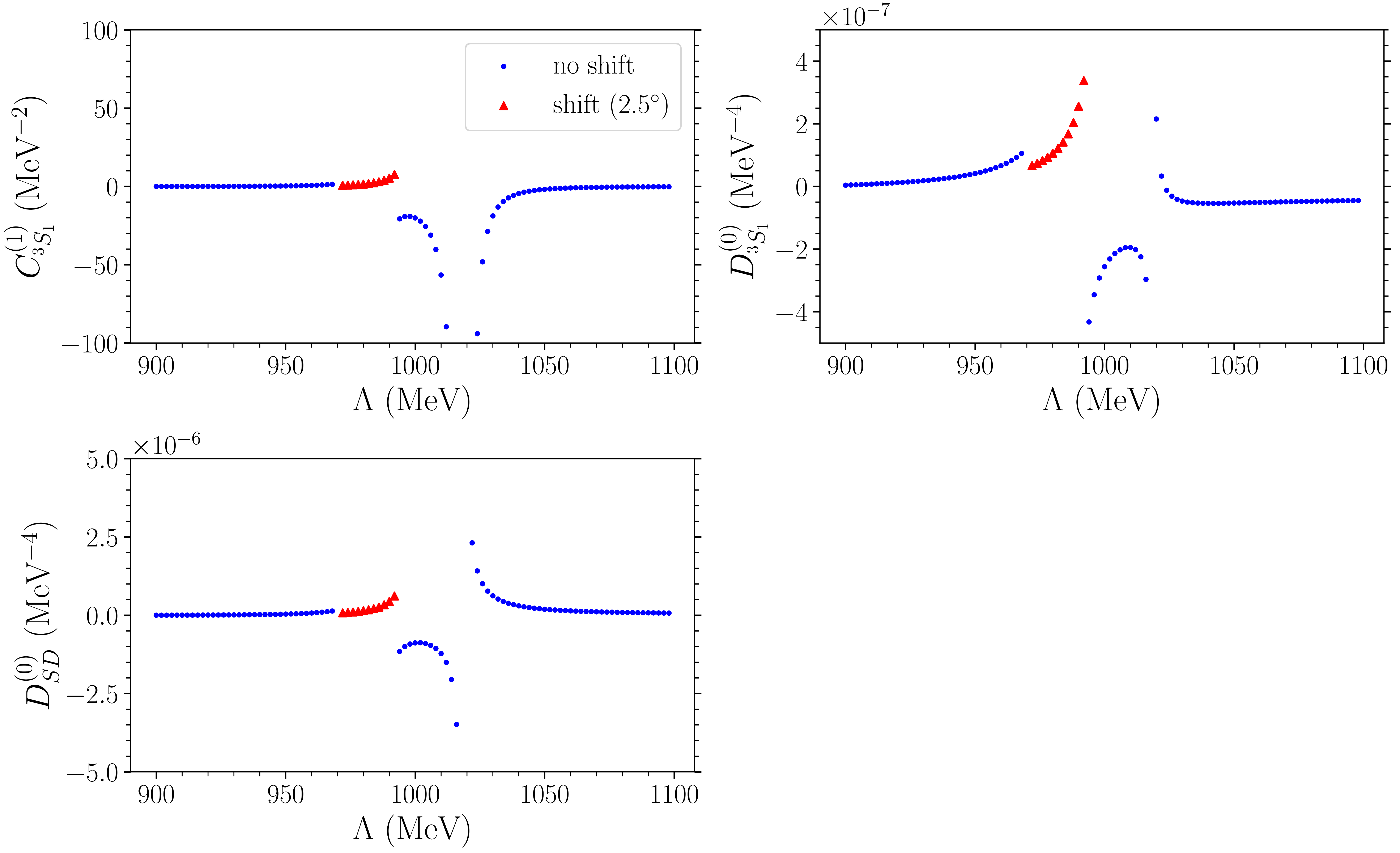
Deuteron channel ($^3S_1 - ^3D_1$) at N2LO

Exceptional cutoff LEC value divergences



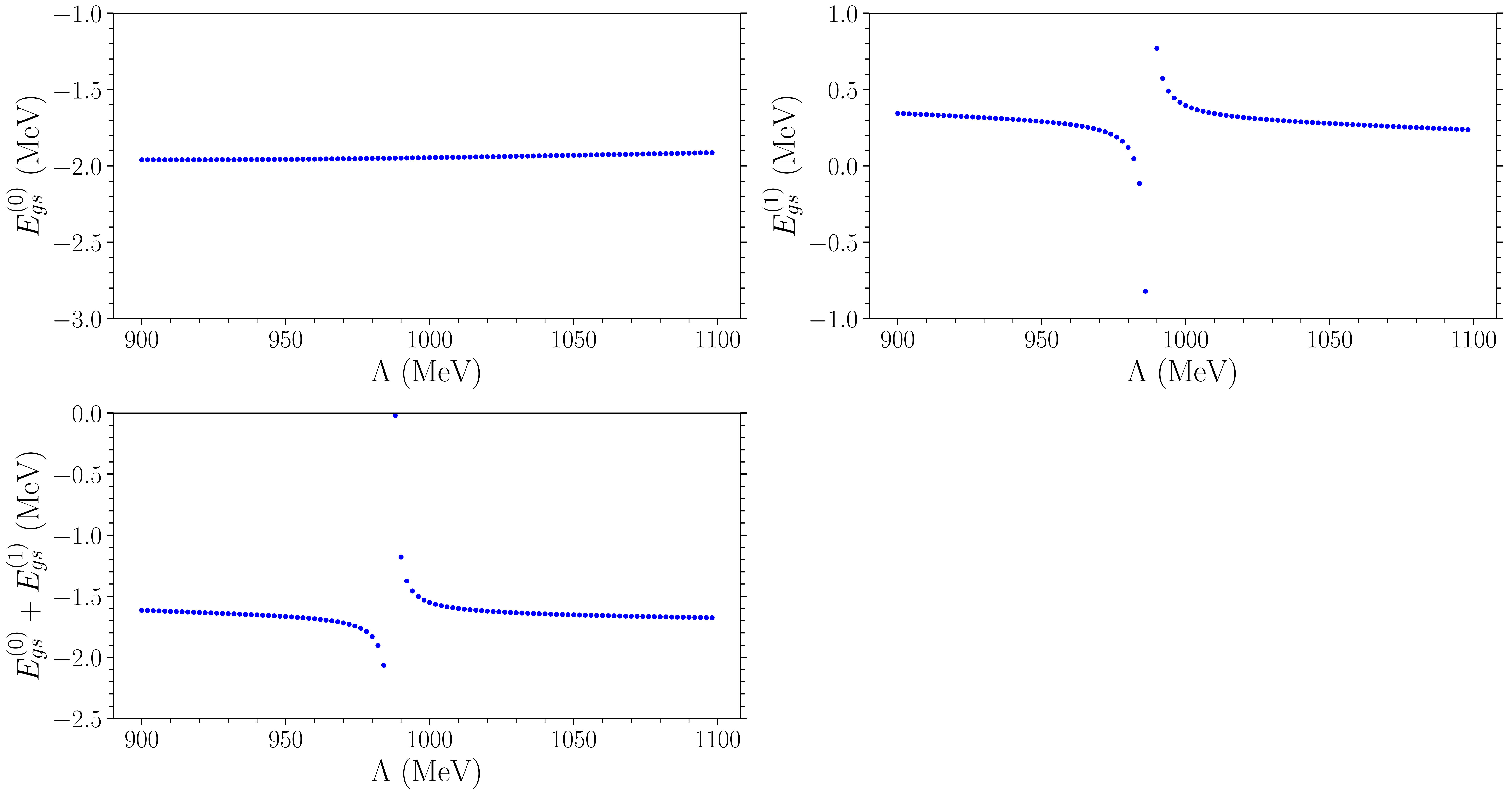
Deuteron channel ($^3S_1 - ^3D_1$) at N2LO

adding a small nugget $\Delta = 2.5°$



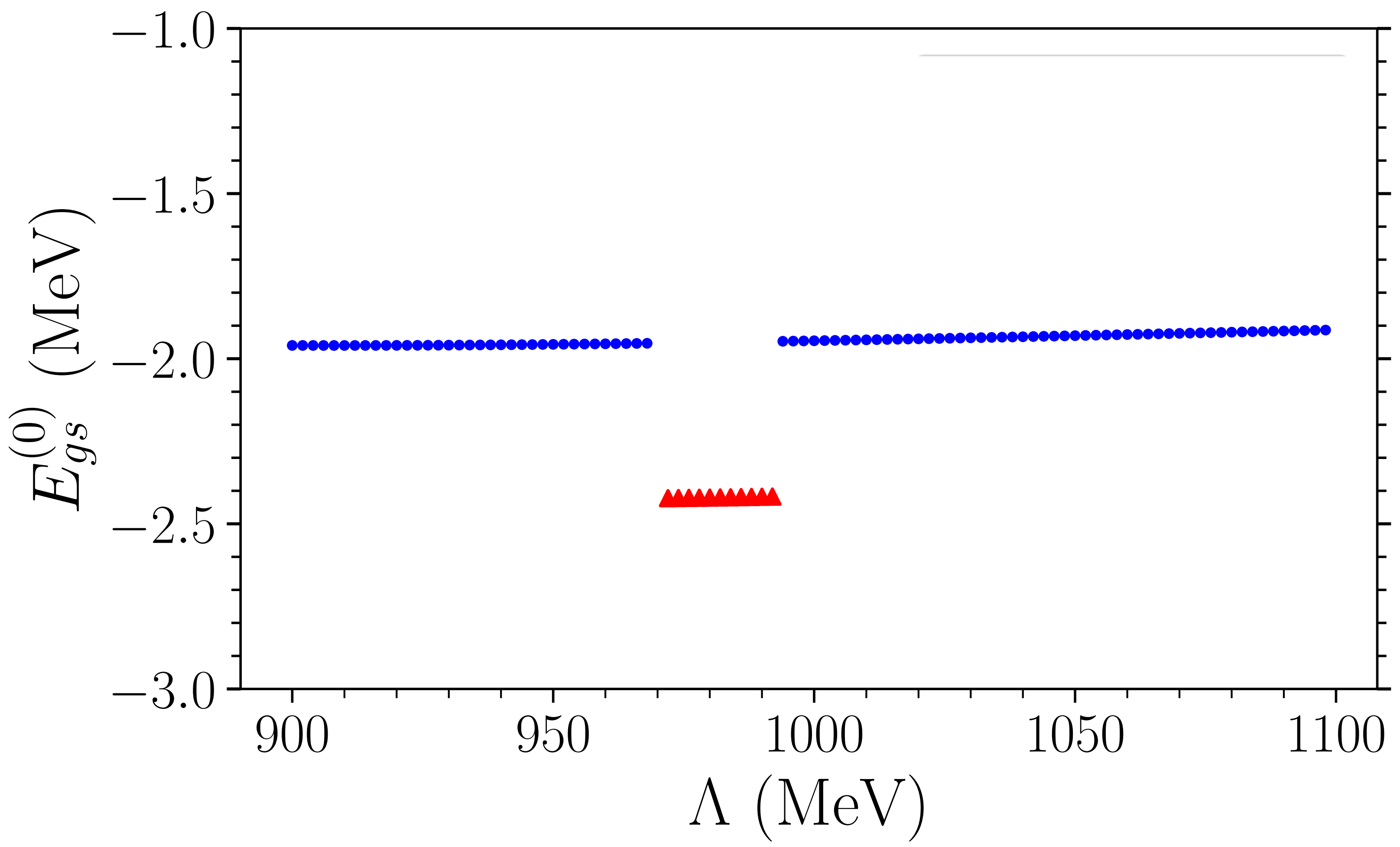
Deuteron energy at N2LO

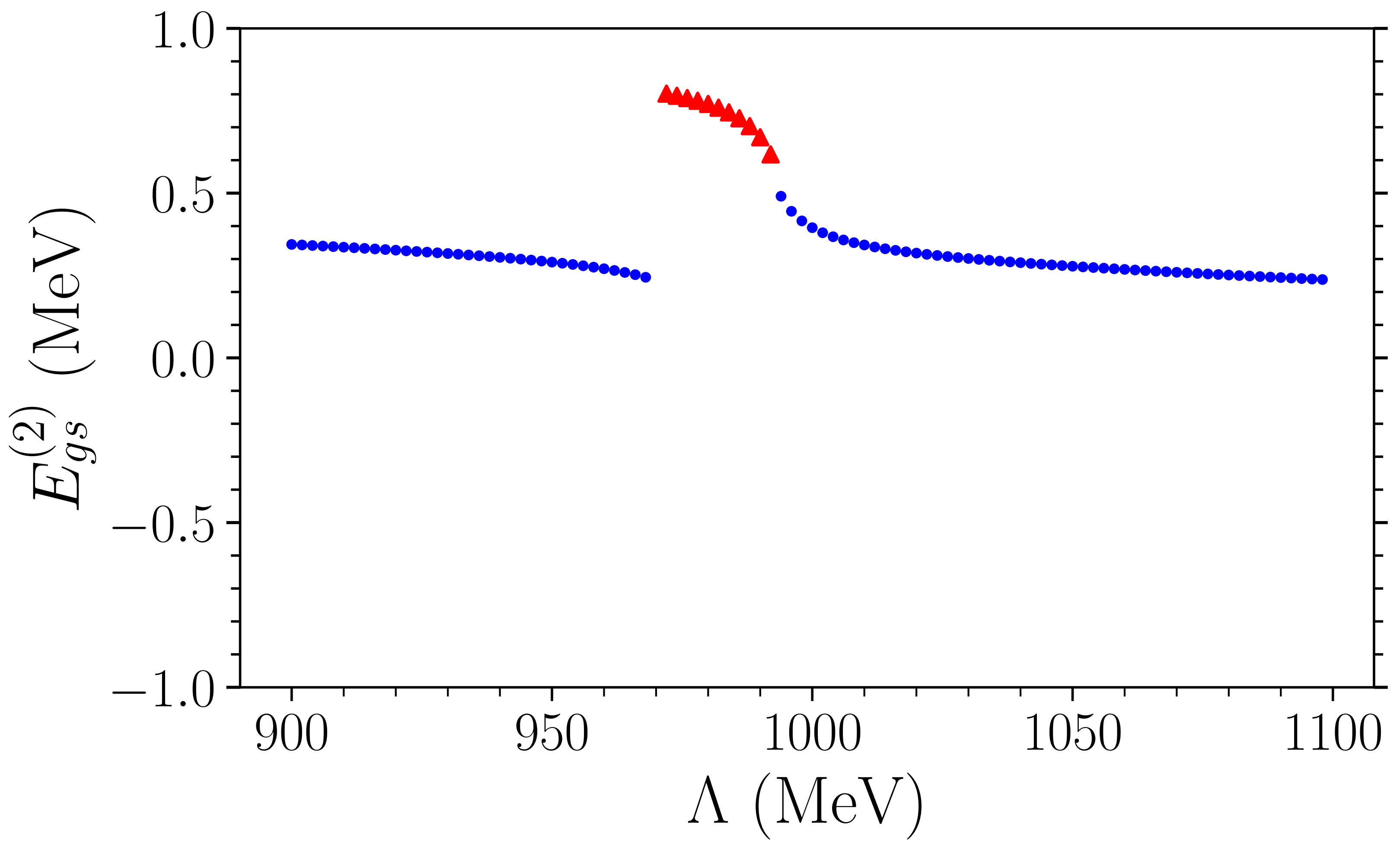
Divergence at exceptional cutoff

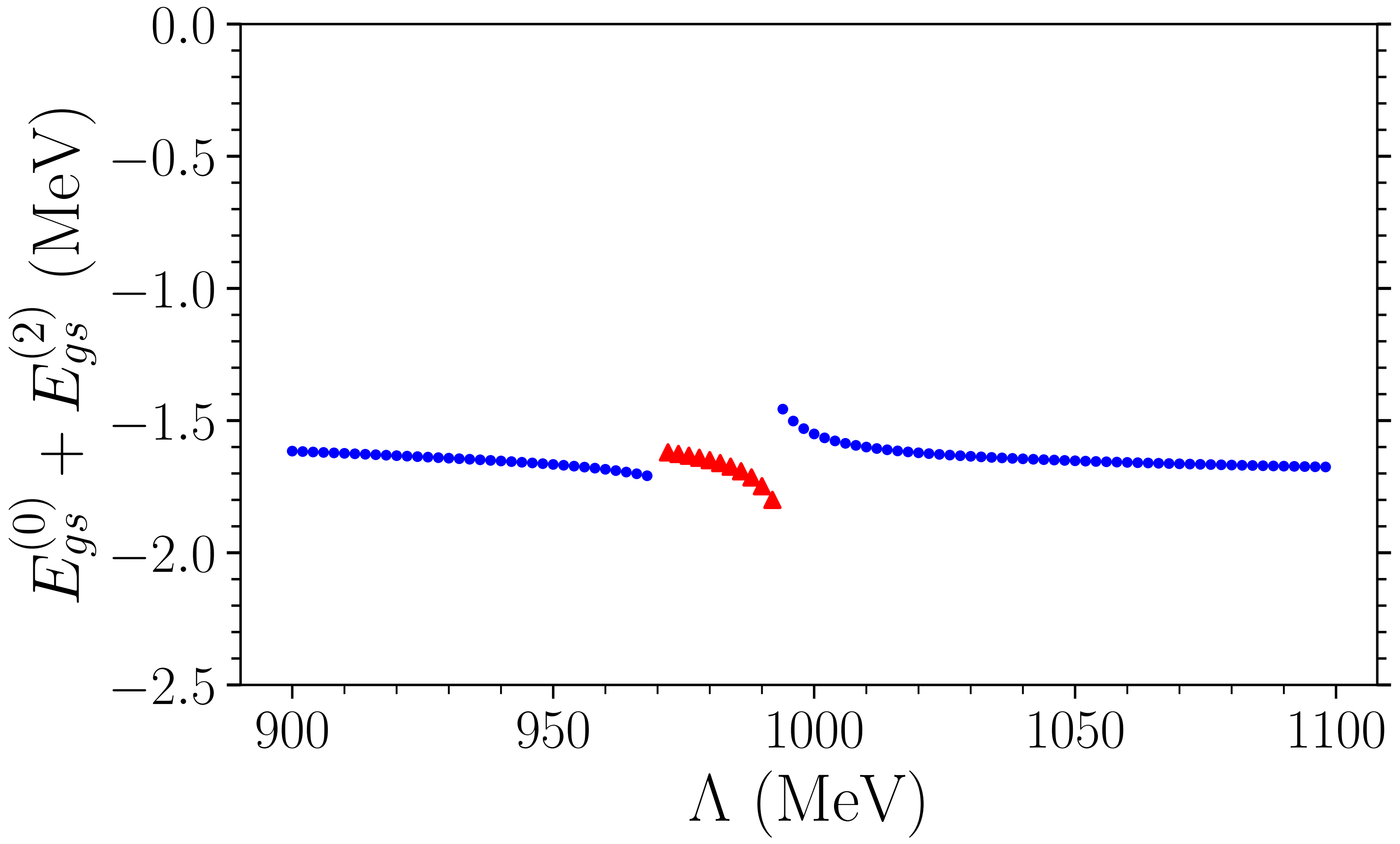


Deuteron energy at N2LO

adding a small nugget $\Delta = 2.5^\circ$





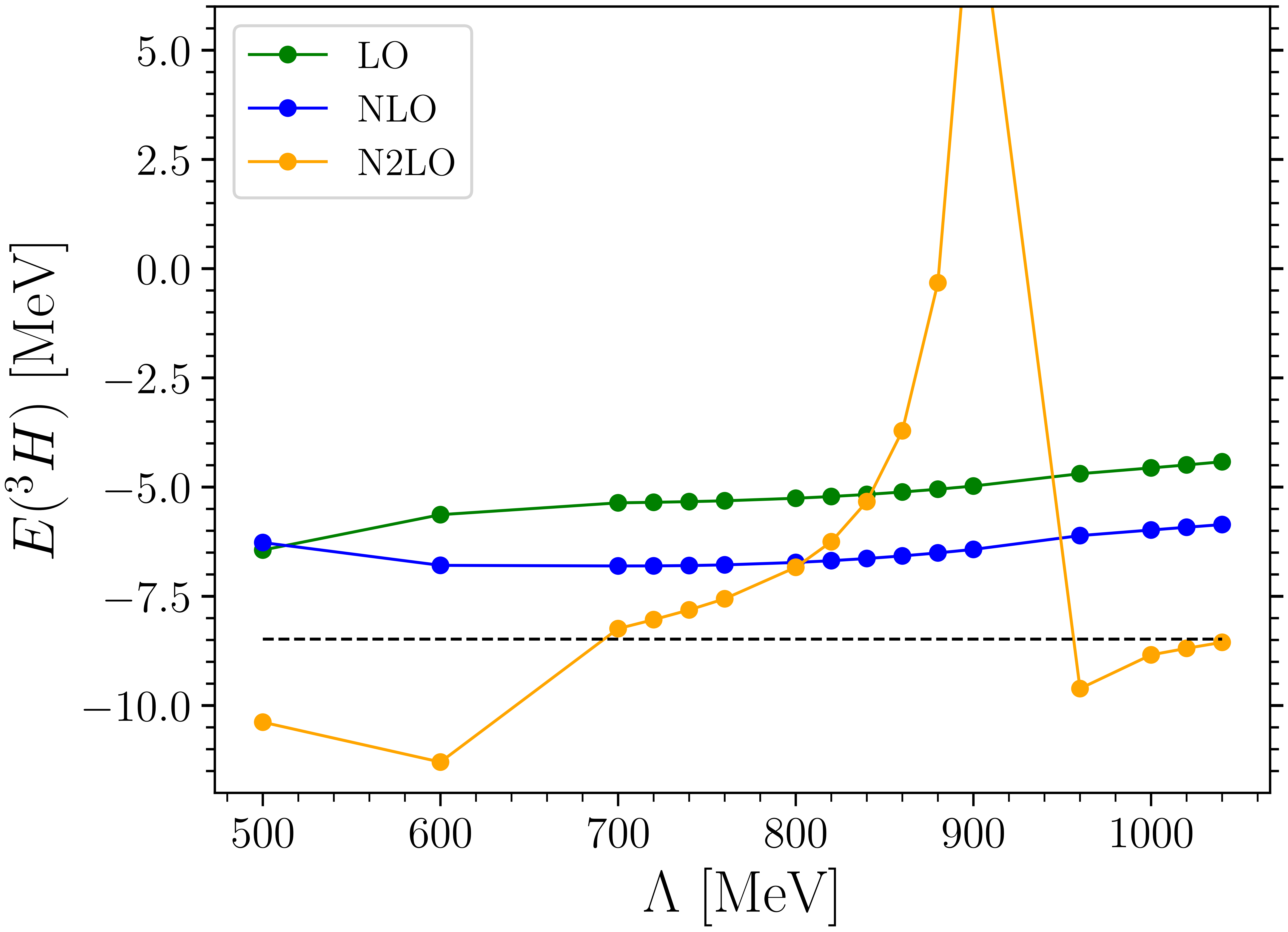


We can correct the effect of Λ_E in the deuteron energy

The colinearity increases continuously as we approach Λ_E.
What is the relevant range of cutoffs for adding a nugget term?

Is the N2LO correction still perturbatively small?

Triton NCSM predictions up to N2LO



Approaching Λ_E yields ill-conditioned design matrices.

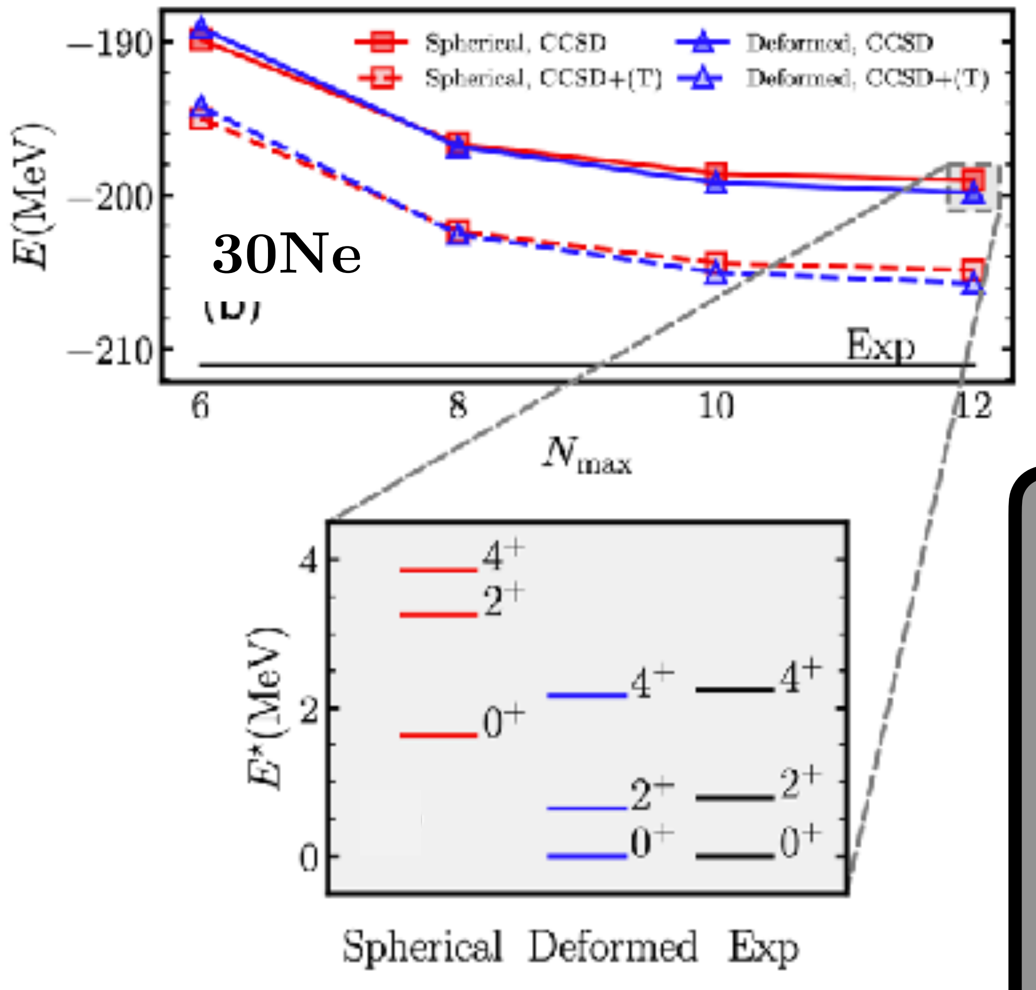
Not a problem away from Λ_E, e.g., for small cutoffs ~ 500 MeV in this PC.

Exceptional cutoff regions and large values of LECs to blame? Numerical inaccuracy?

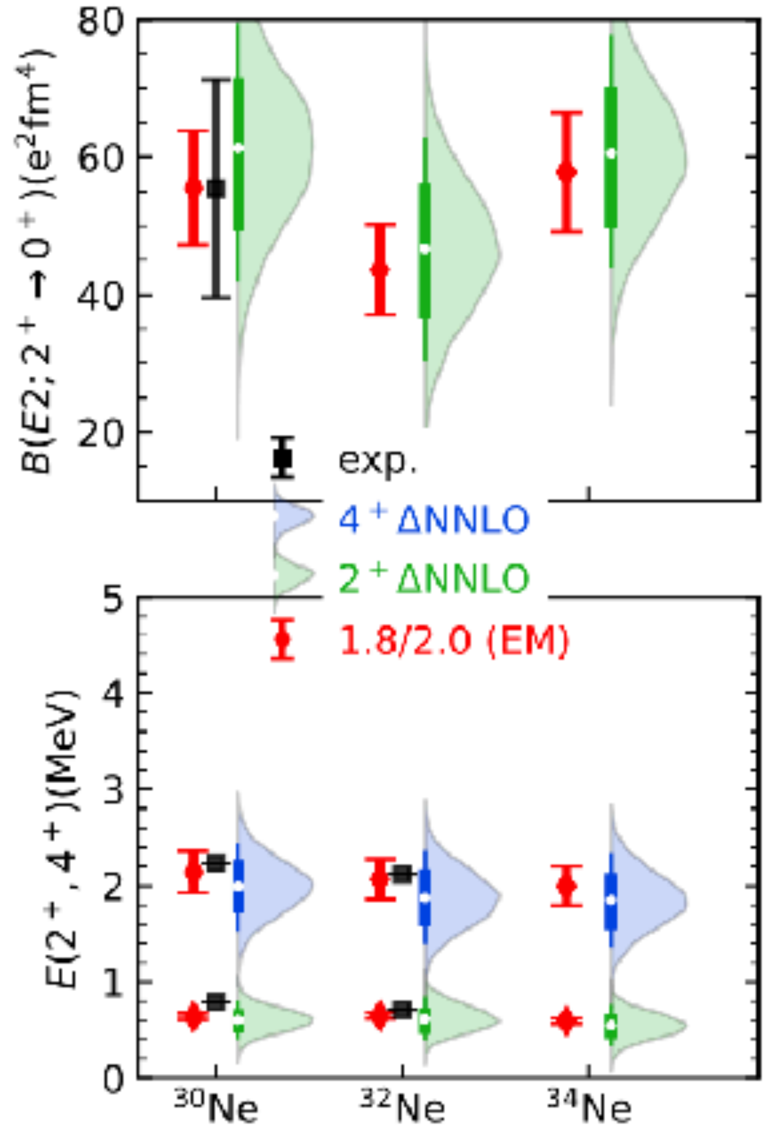
NCSM $N_{max}=44$ $\hbar\omega = 35$ MeV
(not converged at large Λ-values)

Why do some WPC interactions work better than others?

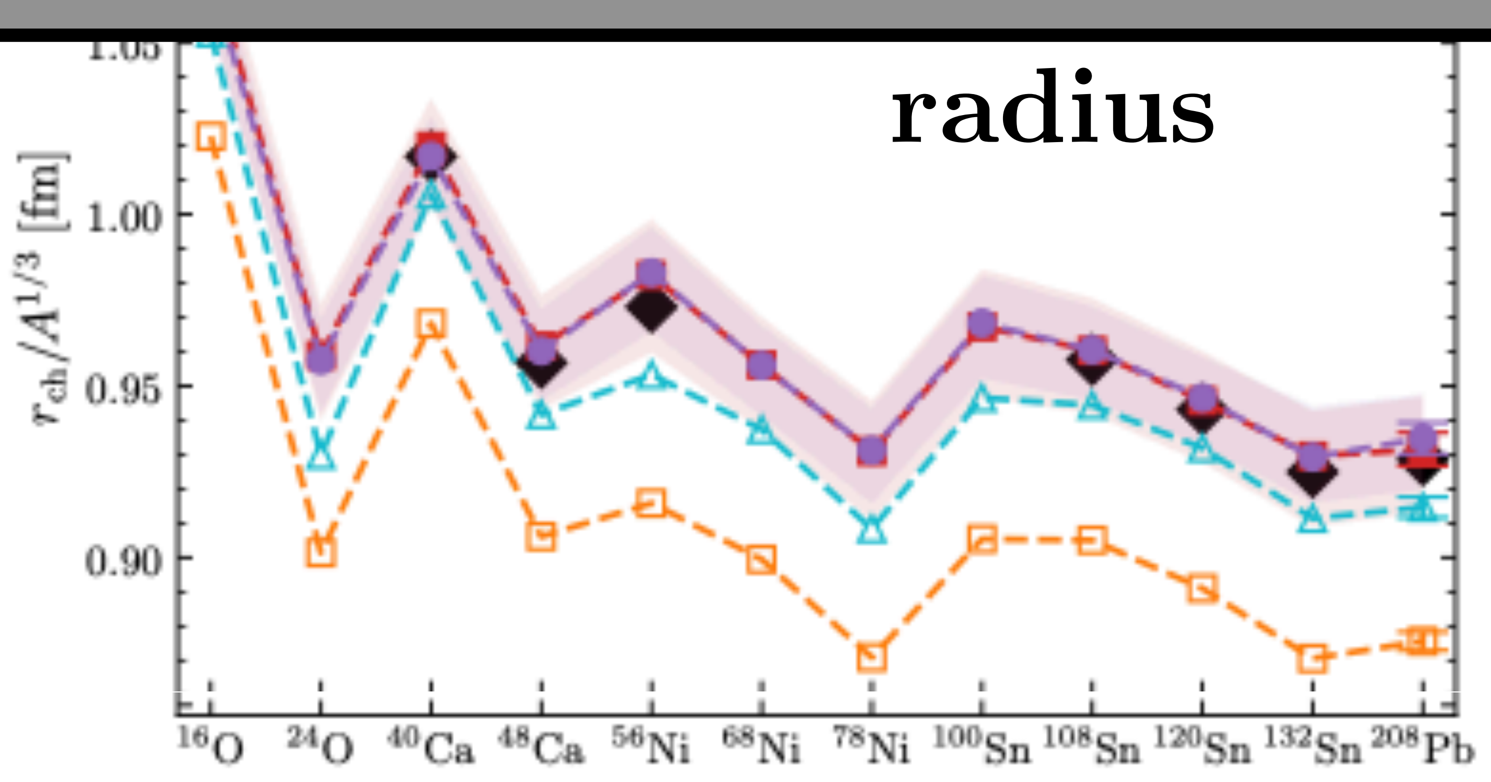
"magic"



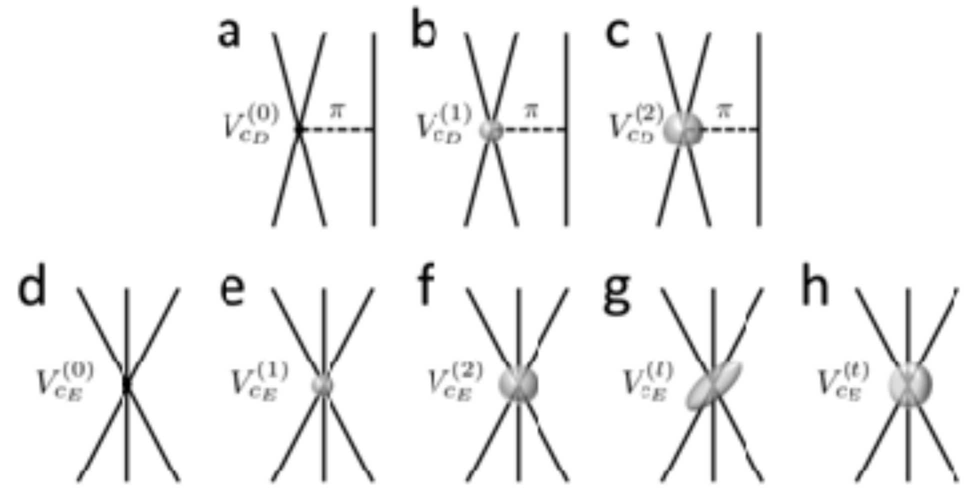
$$\{y_k(\boldsymbol{\alpha}) + \varepsilon_{\mathrm{MB}} + \varepsilon_{\mathrm{EFT}} : \boldsymbol{\alpha} \sim p(\boldsymbol{\alpha}|\mathcal{D}_{\mathrm{cal}})\}$$

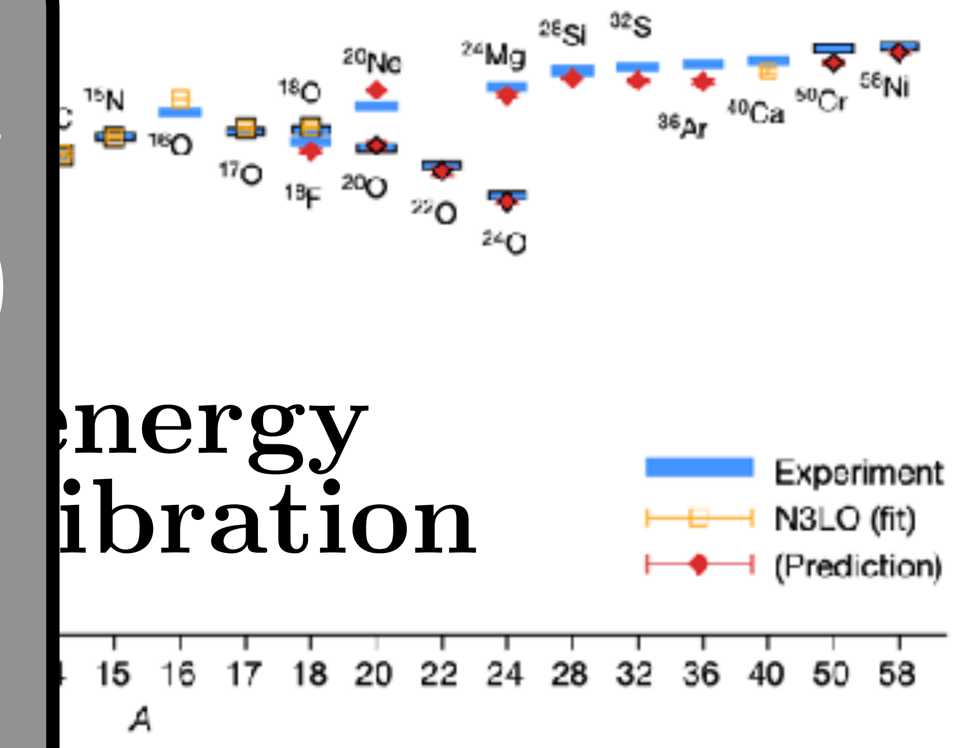


N3LO-NN+N2LO-3N
SRG evolved NN and
fit 3N LECs to A=2,4,16



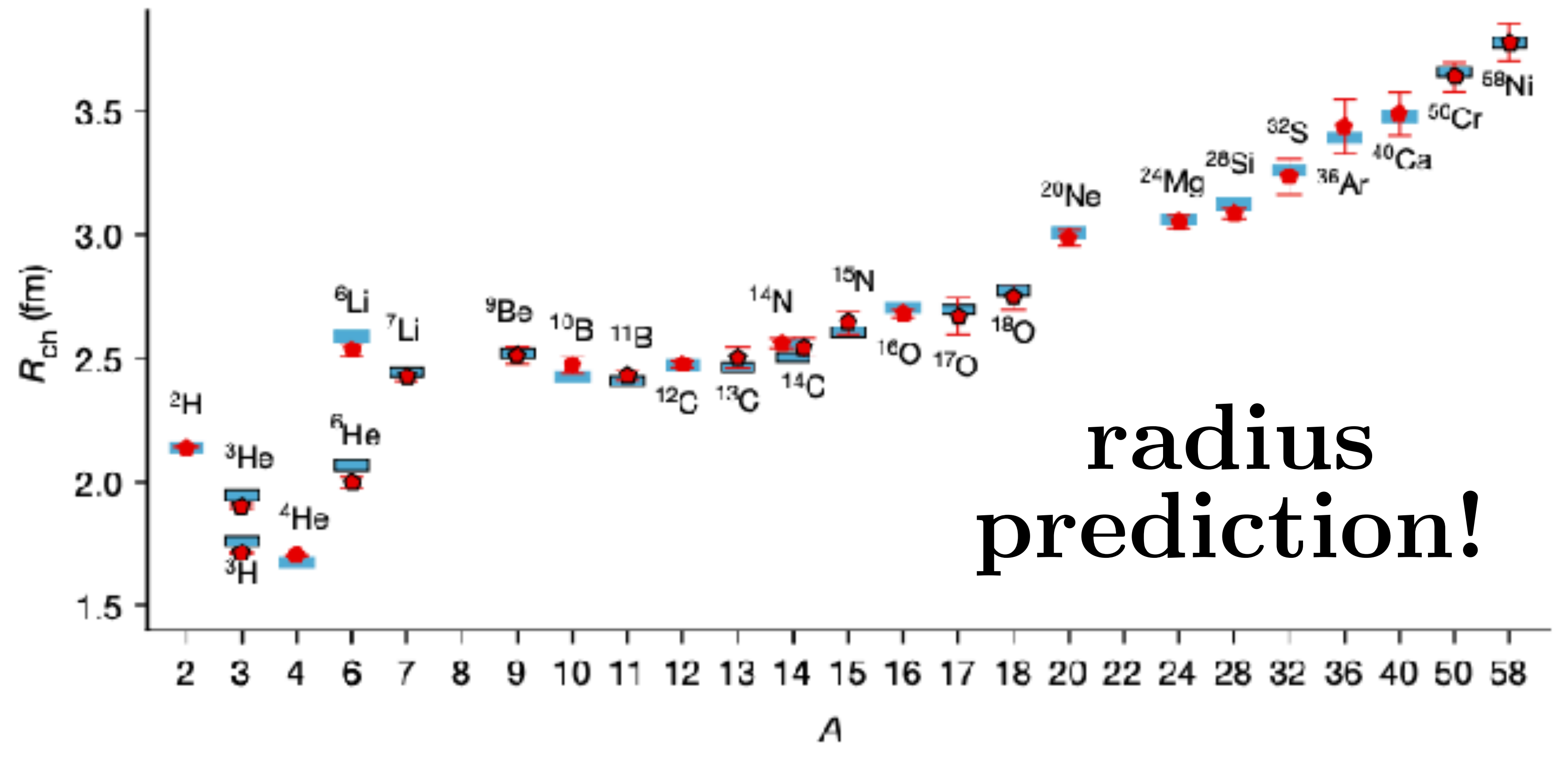
Lattice EFT





Can we construct an accurate chiral interaction beyond N2LO that is not SRG-tuned? ('magic')

(Lattice interactions are challenging for other many-body methods)

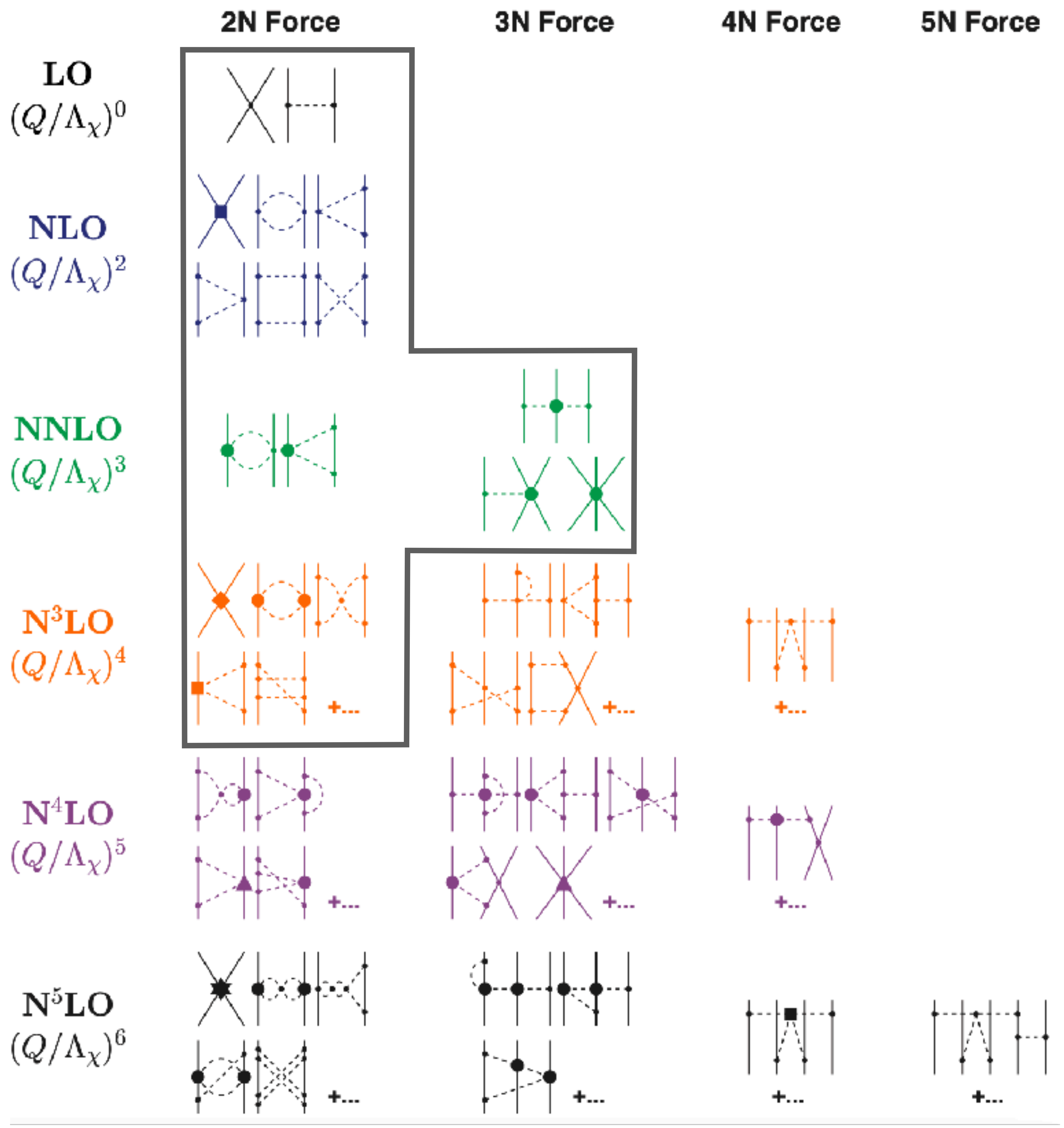


Sun. et al Phys Rev. X (2025)

Arthuis et al arXiv (2024)

Elhatisari et al Nature (2024)

N3LO$_{\text{Texas}}$(394)



Entem, Machleidt, Nosyk Phys Rev C **96** (2017)

$$\Lambda = 2\,\text{fm}^{-1} = 394\,\text{MeV}$$

$$f_\Lambda(p) = \exp\left[-\left(p^2/\Lambda^2\right)^{\{n=4\}}\right]$$

$$f_\Lambda(p,q) = \exp\left[-\left(\left(p^2 + 3/4q^2\right)/\Lambda^2\right)^{\{n=4\}}\right]$$

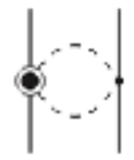
πN LECs according to Roy-Steiner analysis

c_1 [GeV^{-1}]	-1.07 ± 0.02	$\bar{d}_1 + \bar{d}_2$ [GeV^{-2}]	1.04 ± 0.06
c_2 [GeV^{-1}]	3.20 ± 0.03	$\bar{d}_3$ [GeV^{-2}]	-0.48 ± 0.02
c_3 [GeV^{-1}]	-5.32 ± 0.05	$\bar{d}_5$ [GeV^{-2}]	0.14 ± 0.05
c_4 [GeV^{-1}]	3.56 ± 0.03	$\bar{d}_{14} - \bar{d}_{15}$ [GeV^{-2}]	-1.90 ± 0.06

M. Hoferichter *et al.* Phys. Rev. Lett. **115**, 192301 (2015); Phys Rep. **625**, 1 (2016)

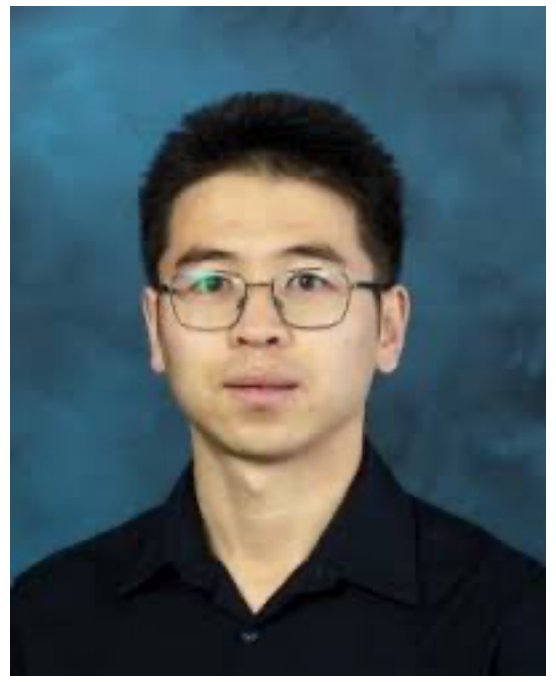
N3LO includes contacts $\widehat{D}_{^1S_0}, \widehat{D}_{^3S_1}, \widehat{D}_{^3S_1-^3D_1}$

N3LO 2π-exchange and "relativistic corrections"

$\frac{Q}{M_N} \sim \left(\frac{Q}{\Lambda_\chi}\right)^2$ We promote $V_{2\pi}^{(\text{N4LO})} \propto \frac{c_i}{M_N}$  ... to N3LO

Calibrating N3LO$_{\text{Texas}}$(394)

Our initial strategy

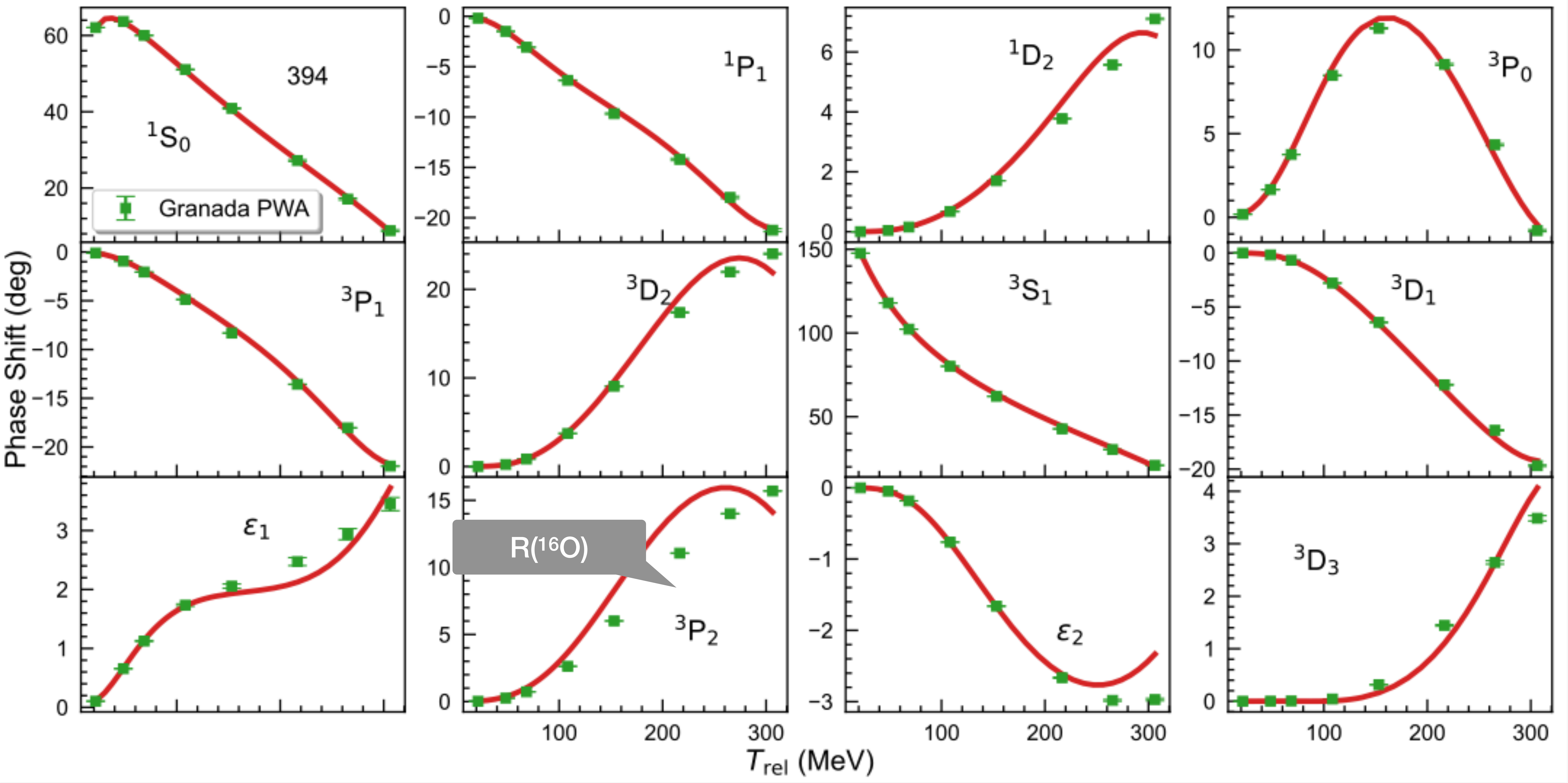


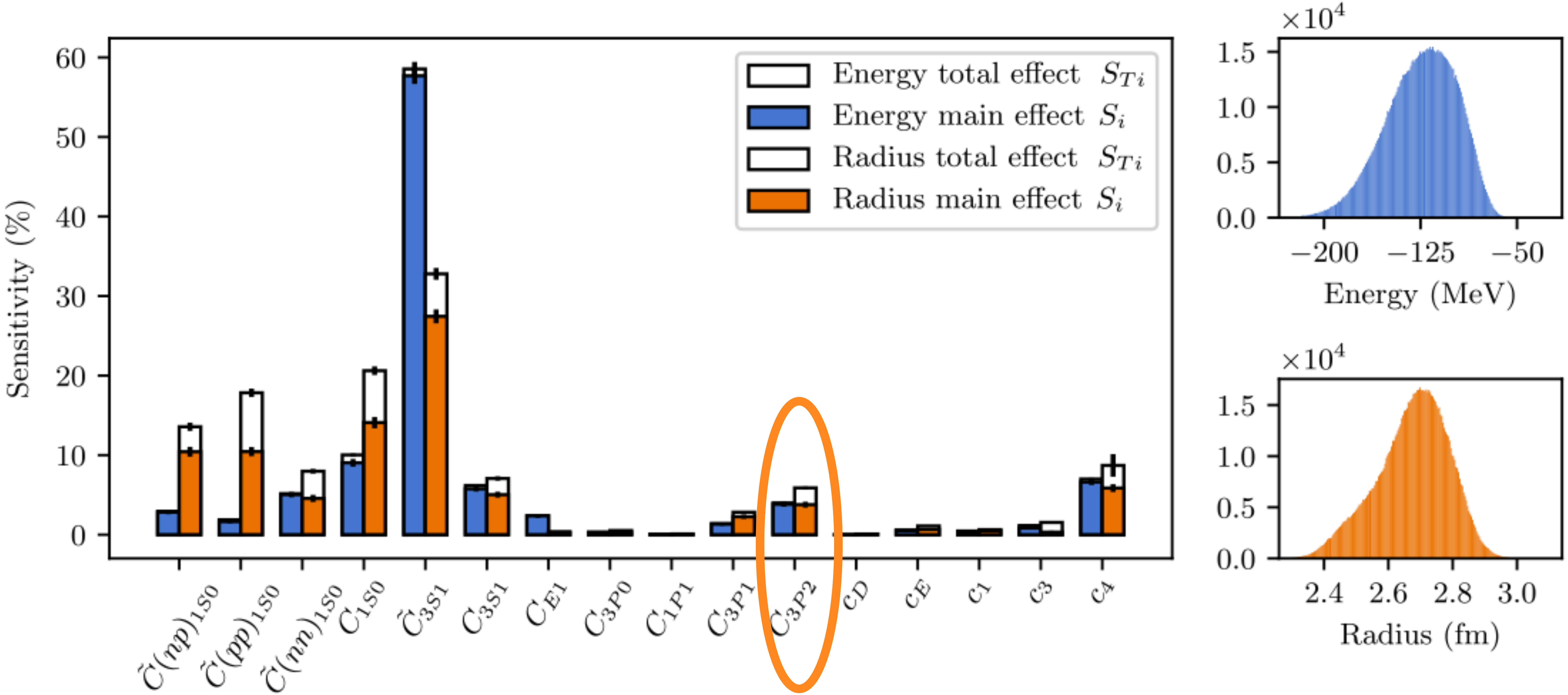
Baishan Hu
Texas A&M

```
'Ct_1S0pp':    [ -0.30  ,  -0.10  ]
'Ct_1S0np':    [ -0.30  ,  -0.10  ]
'Ct_1S0nn':    [ -0.30  ,  -0.10  ]
'Ct_3S1':      [ -0.30  ,  -0.10  ]
'C_1S0':       [ 2.30   ,  2.90   ]
'C_3P0':       [ 0.80   ,  1.40   ]
'C_1P1':       [ -1.00  ,  1.00   ]
'C_3P1':       [ -1.40  ,  1.50   ]
'C_3S1':       [ 0.10   ,  1.70   ]
'C_3S1-3D1':   [ 0.00   ,  1.20   ]
'C_3P2':       [ -2.10  ,  2.40   ]
'Dh_1S0':      [ -2.20  ,  4.50   ]
'D_1S0':       [ -28.00 ,  -18.00 ]
'D_3P0':       [ 3.90   ,  6.40   ]
'D_1P1':       [ 8.50   ,  18.00  ]
'D_3P1':       [ 2.00   ,  10.50  ]
'Dh_3S1':      [ -9.70  ,  9.30   ]
'D_3S1':       [ -38.60 ,  16.70  ]
'D_3D1':       [ -8.20  ,  4.50   ]
'Dh_3S1-3D1':  [ -10.00 ,  9.30   ]
'D_3S1-3D1':   [ -7.40  ,  10.00  ]
'D_1D2':       [ -2.60  ,  1.10   ]
'D_3D2':       [ -8.00  ,  -2.00  ]
'D_3P2':       [ -3.00  ,  15.30  ]
'D_3P2-3F2':   [ -2.60  ,  2.90   ]
'D_3D3':       [ -3.00  ,  1.00   ]
'cD':          [ -5.00  ,  5.00   ]
'cE':          [ -3.00  ,  3.00   ]
```

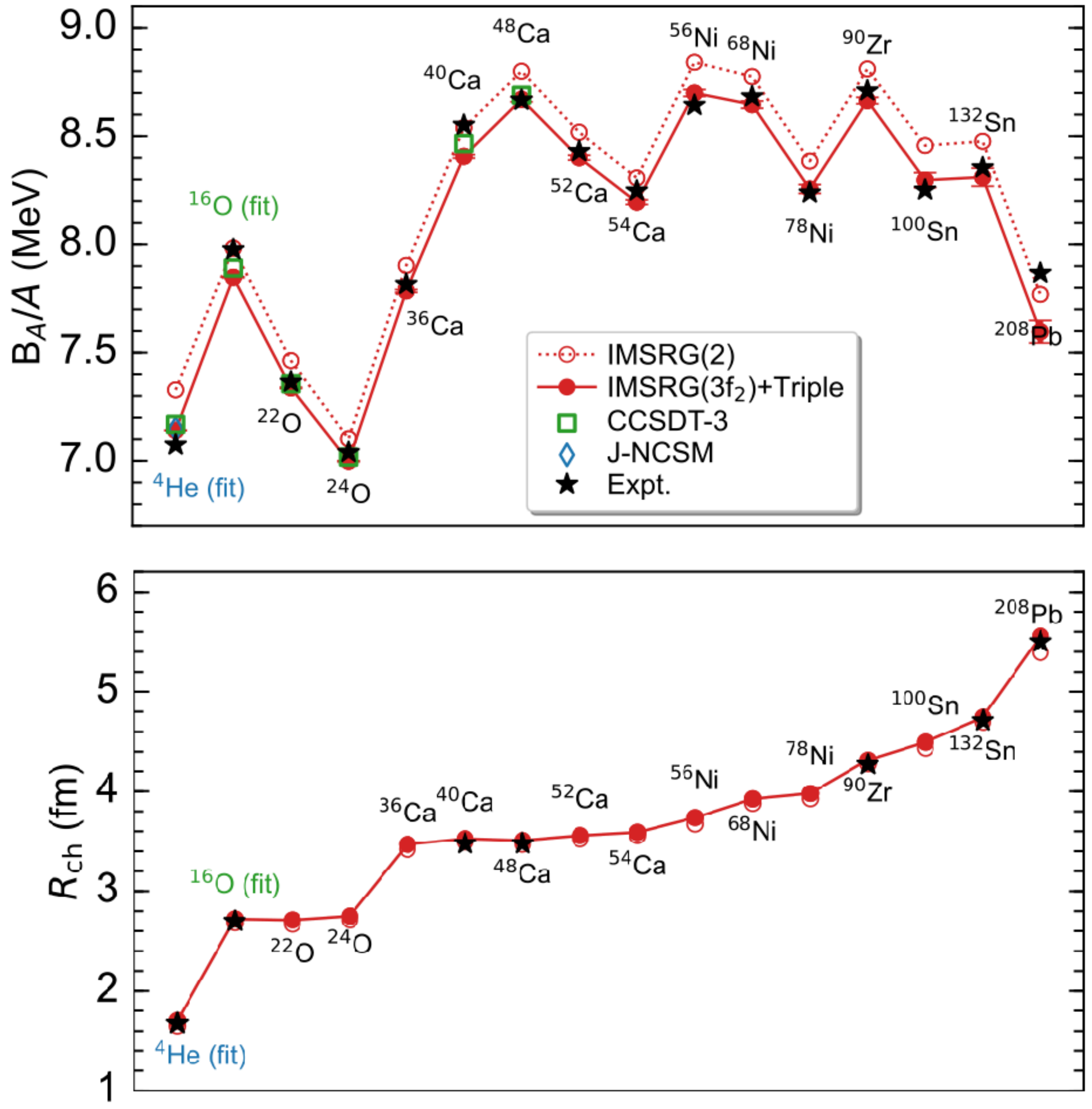
1. Setup emulators for *np* phase shifts, *nn/pp* ERE, and E/R(^{2}H,^{4}He,^{16}O)
2. Generate 2000 random (LHS) points in space of 28 contact LECs (including c_D,c_E)
3. Optimize wrt L_1 loss function (forgives outliers) for E<0 observables, heavy weight on R(^{16}O). L_2 loss function (penalizes outliers) for phase shifts.
4. Select subset of 20 interactions that yield good description of phase shifts and A=2,4,16 observables.
5. **'Best one': N3LO$_{\text{texas}}$**

N3LO$_{\text{Texas}}$(394): accurate predictions





Ekström, Hagen Phys. Rev. Lett. (2019)



See G. Hagen Talk

Summary

Nuclear *ab initio:* a *systematically improvable* approach for quantitatively describing nuclei using the finest resolution scale possible while maximizing its predictive capabilities.

Bayesian inference is useful for testing your assumptions, and of course model calibration and uncertainty quantifying uncertainties (not discussed in this talk)

The pionless EFT breakdown scale is $\sim 1.4 m_\pi$, *consistent* with EFT assumptions.

Exceptional cutoff *regions* can be numerically managed at the *NN* level.
What about A>2?

We can describe low-energy structure of several nuclei across the nuclear chart using Weinberg PC. However, realistic model parametrizations *hides* rather well in the vast parameter space of LECs.

Thank you for your attention