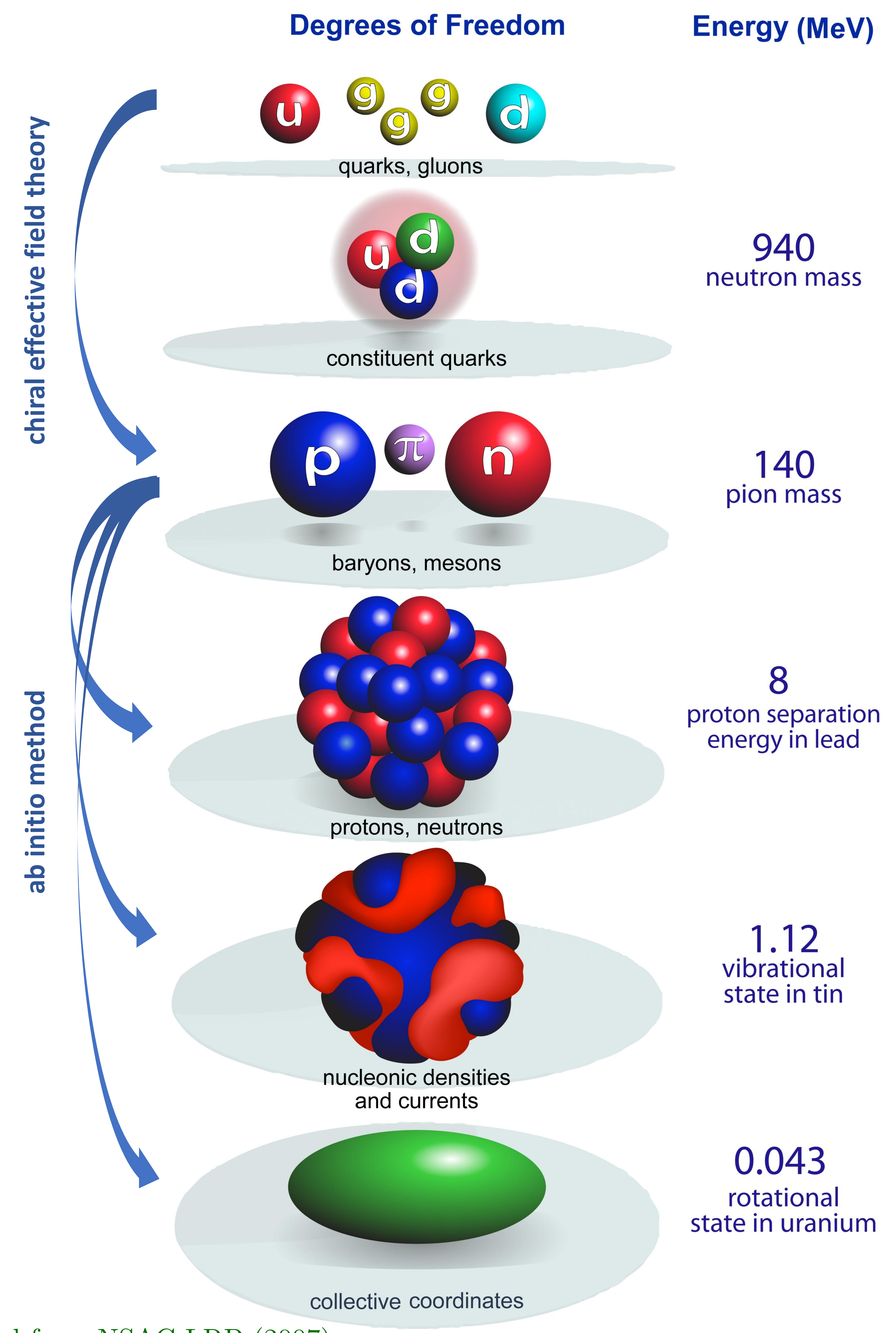
Recent advances in chiral forces and uncertainty quantification for nuclear structure

Andreas Ekström

Gogny Conference, Amphithéâtre Bilski Pasquier, Paris, December 10-13, 2024

CHALMERS UNIVERSITY OF TECHNOLOGY

Swedish Research Council



Adapted from NSAC LRP (2007)

Overview

Describing nuclear phenomena across a wide range of energy scales—remains a long-standing **challenge** in nuclear physics.

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

In this talk, I will highlight recent advances in *ab initio* nuclear structure calculations, focusing on developments in chiral nuclear forces and methods for estimating uncertainties in theoretical predictions.

Some parallels between Gogny's work and *ab initio* developments

A SMOOTH REALISTIC LOCAL NUCLEON-NUCLEON FORCE SUITABLE FOR NUCLEAR HARTREE-FOCK CALCULATIONS

D. GOGNY *, P. PIRES and R. DE TOURREIL
Institut de Physique Nucléaire, Division de Physique Théorique **. 91– *Orsay, France*

Received 1 July 1970

The aim of this work is to construct a smooth local potential giving an acceptable fit to two nucleon data up to 300 MeV and reasonable properties for finite nuclei, particularly the radii, in the H.F

multiscale challenge without overfitting

have little relation to basic two body data. It seems to us clear that in order to answer the question, whether an interaction can be found which fits two body data and works in H.F., one must fit it to the H.F. results directly, and not

valuable information in many-body systems

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Eur. Phys. J. A (2017) 53: 214
DOI 10.1140/epja/i2017-12403-6
The European Physical Journal A
Regular Article – Theoretical Physics

Daniel Gogny*

J.-F. Berger[1], J.-P. Blaizot[2], D. Bouche[1], P. Chaix[2], J.-P. Delaroche[1], M. Dupuis[1,a], M. Girod[1], J. Gogny[3], B. Grammaticos[4], D. Iracane[2], J. Lachkar[2], F. Mariotte[5], N. Pillet[1], and N. Van Giai[6]

nuclei. After the laborious and rather disappointing second order calculations of the G-matrix based on the GPT interaction performed along with M. Maire [2], Daniel convinced himself that the only possible "way out" was the "phenomenological effective force" allowing for mean-field calculations of Hartree

revisit the interaction model

He ingeniously used physics insights previously harvested from studies based on the GPT interaction to design an elaborate fitting procedure guided by both nuclear matter and

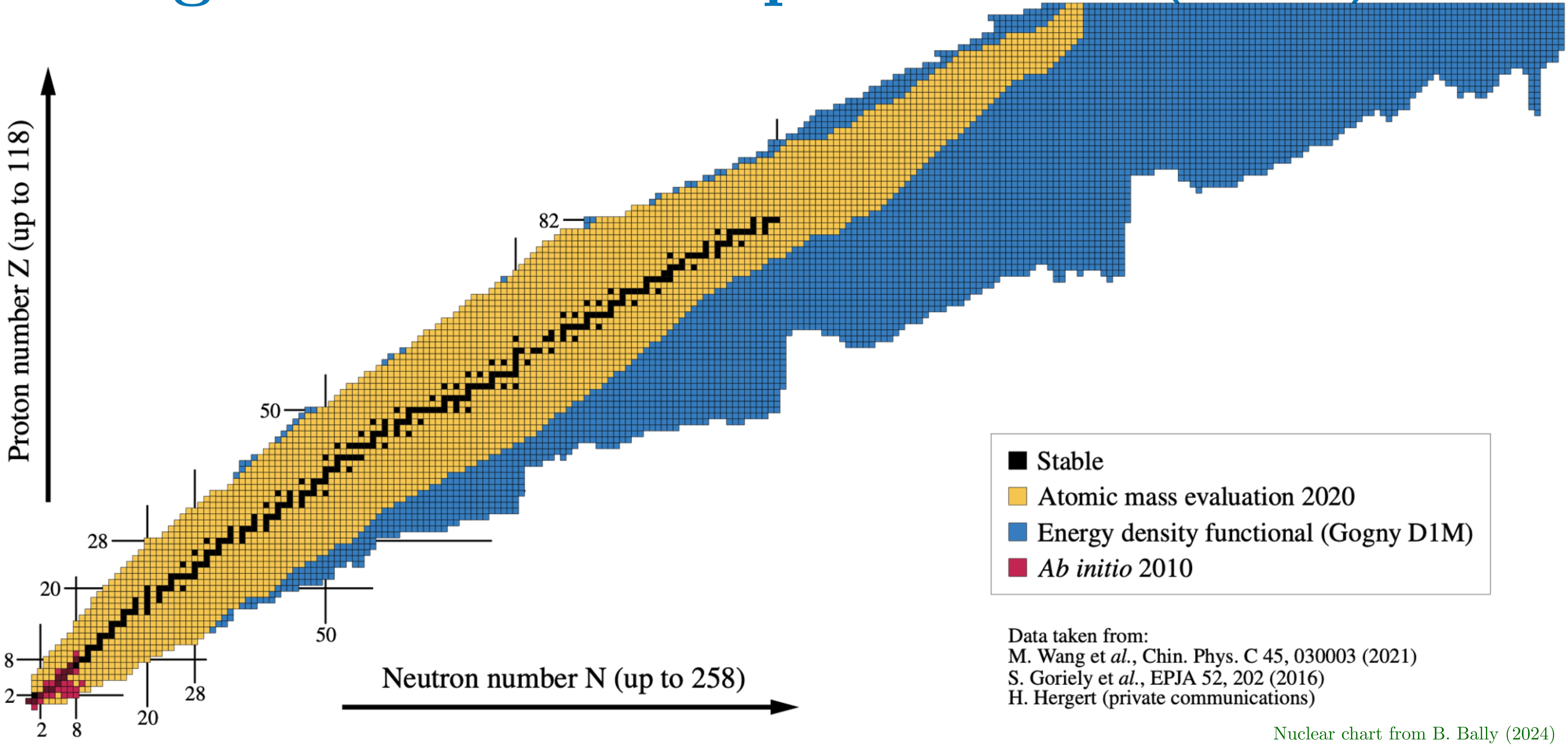
lations nece

effective interaction (D1 stands for Daniel 1) were conducted on weekends, when computers were more accessible. Finally the D1 pa

inference conditioned on experience

a computational challenge

Progress in *ab initio* predictions (2010)

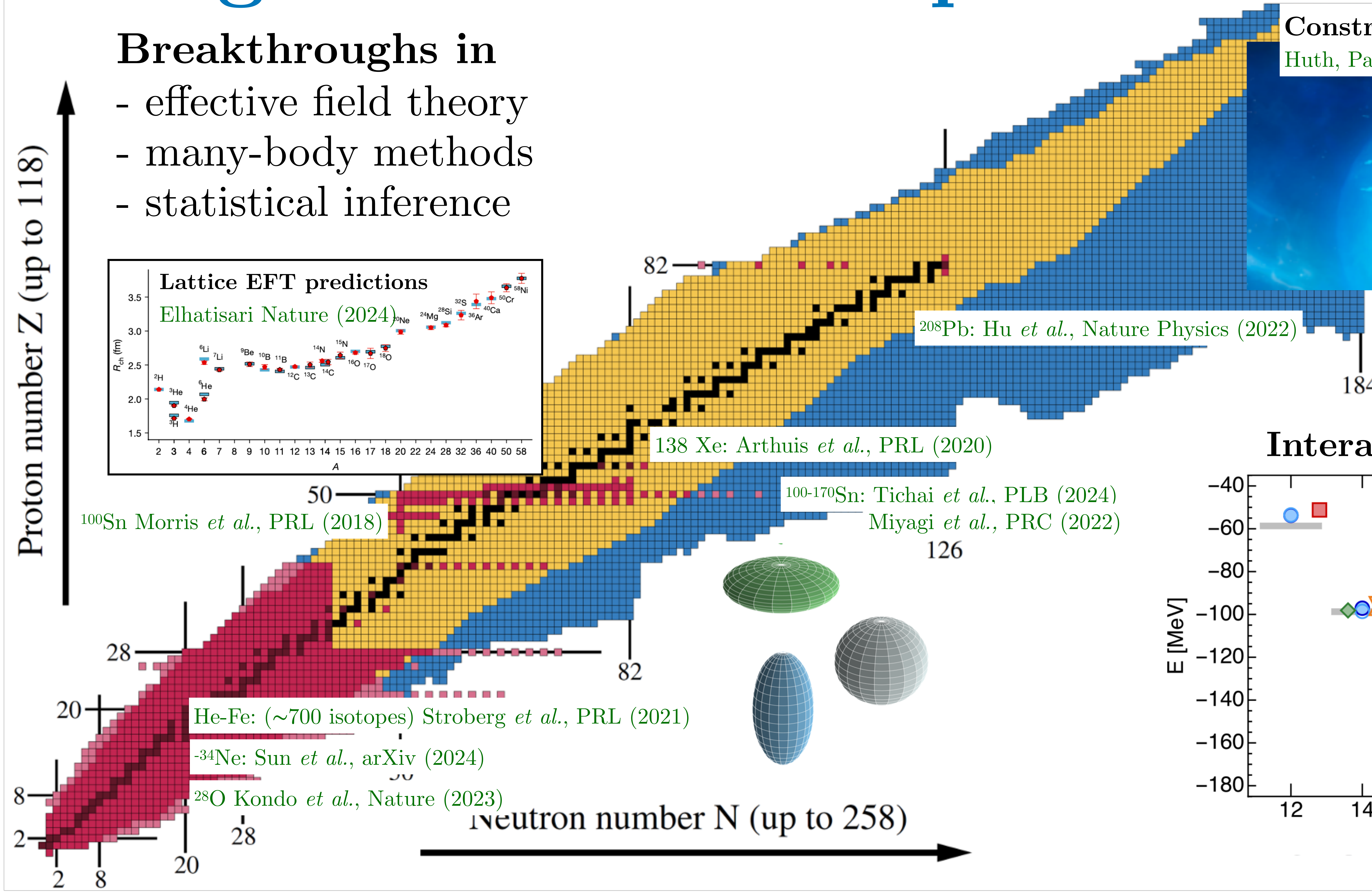


Data taken from:
M. Wang et *al.*, Chin. Phys. C 45, 030003 (2021)
S. Goriely et *al.*, EPJA 52, 202 (2016)
H. Hergert (private communications)

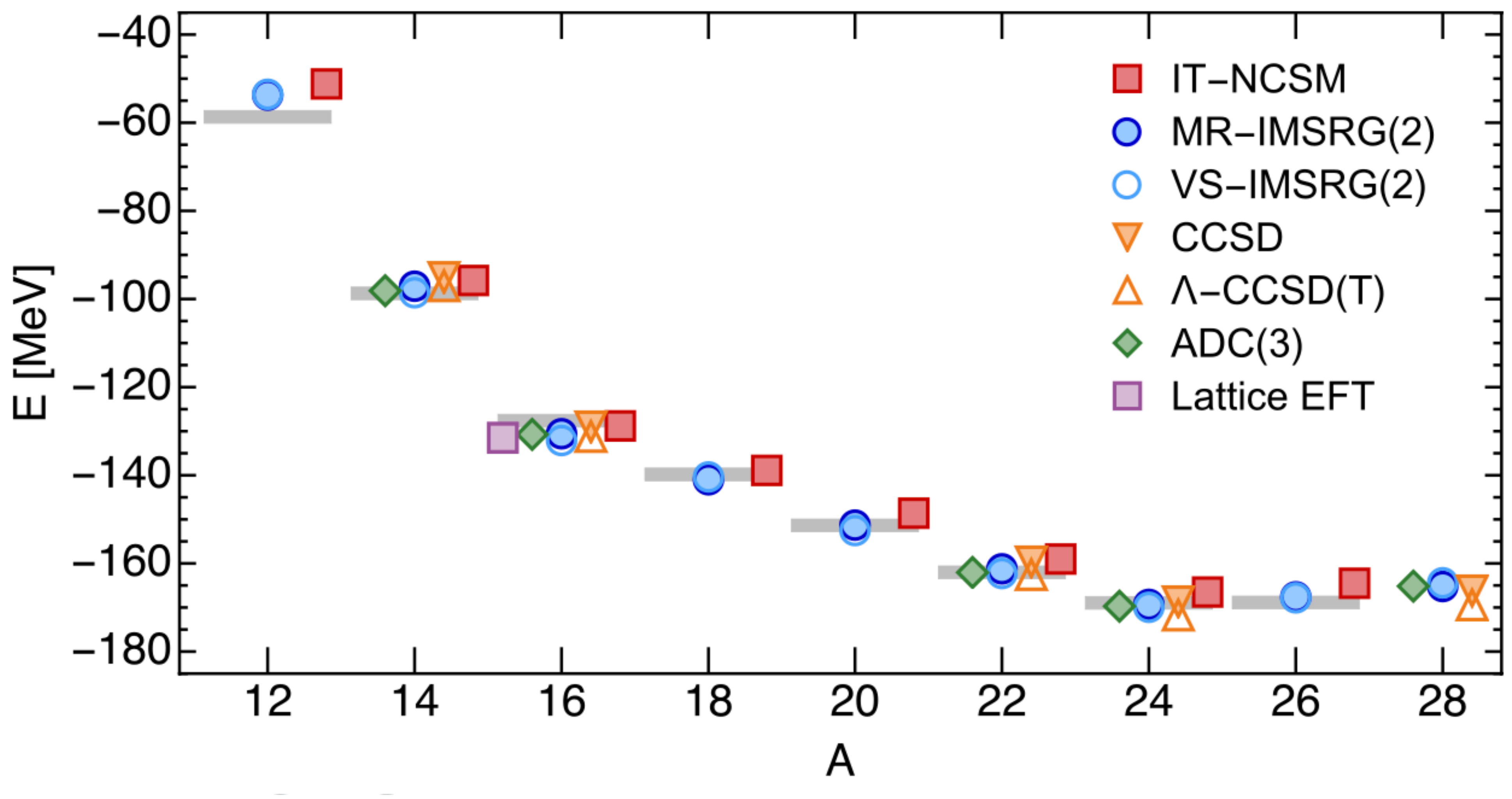
Nuclear chart from B. Bally (2024)

Progress in *ab initio* predictions (2024)

Breakthroughs in
- effective field theory
- many-body methods
- statistical inference



Interaction uncertainty dominates



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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.

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

***χEFT* 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)

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Challenge: quantifying *ab initio* many-body uncertainties, irregular convergence patterns, correlated predictions, multiple scales

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

Why uncertainty quantification?

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

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
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Challenge: how to measure probabilities?
cognitive biases, philosophical interpretations,
domain standards, real-world complexity,...

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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 $\vec{\alpha}$.

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

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Bayes' rule: from likelihood & prior to posterior

- Collect N data points that we gather in a data vector y
- To explain the data, propose some model M, depending on parameters $\vec{\alpha}$
- Apply Bayes' rule

Posterior **Likelihood** **Prior**

$$p(\vec{\alpha} \,|\, y, M, I) = \frac{p(y \,|\, \vec{\alpha}, M, I) \cdot p(\vec{\alpha} \,|\, M, I)}{p(y \,|\, M, I)}$$

Marginal likelihood

most likely not Rev. T. Bayes

- The **prior** encodes our knowledge about the parameter values before analyzing the data
- The **likelihood** is the probability of the data given a set of parameters
- The **marginal likelihood** (or model evidence) provides normalization of the posterior
- The **posterior** is the complete inference and resulting probability density for the parameters $\vec{\alpha}$

Bayes' rule: from likelihood & prior to posterior

Challenge: formulating the prior and likelihood. Computational costs

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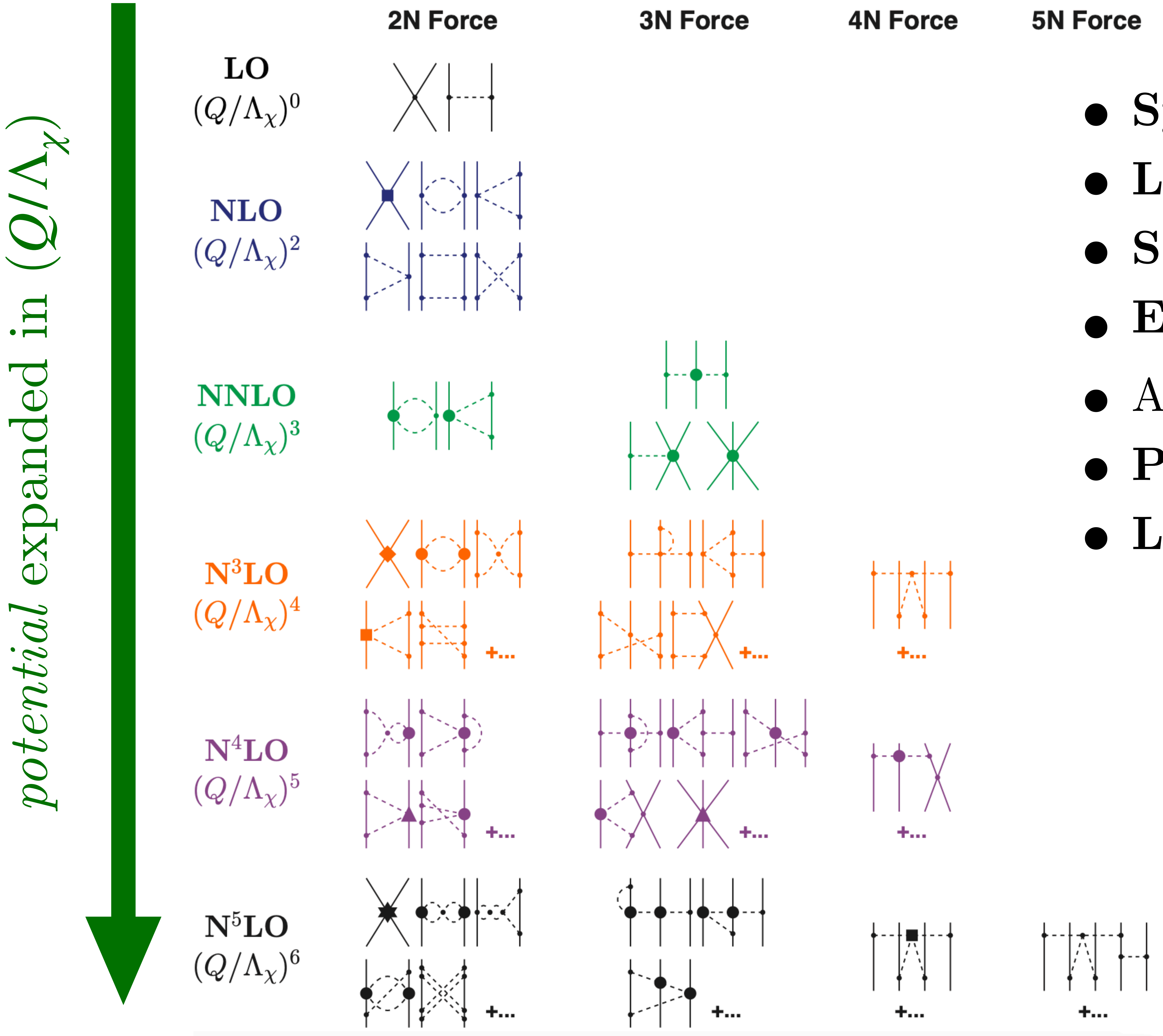
Chiral effective field theory (χEFT)

- Weinberg power counting (WPC)



- **Symmetries** of QCD dictate contents of effective Lagrangian
- **Long-ranged** physics governed by pion exchanges
- **Short-ranged** physics determined by a set of contact interactions
- **Expansion** in (Q/Λ_χ) [soft scale ($\sim m_\pi$) over hard scale ($\sim m_N$)]
- All operators must be regulated ⇒ **cutoff dependence**
- **Power counting** organizes contributions (diagrams) at each order
- **Low-energy** constants (LECs) must be fit from data once

Weinberg, van Kolck, Kaplan, Savage, Wise, Weise, Kaiser, Bernard, Meißner, Epelbaum, Machleidt, Entem, ...

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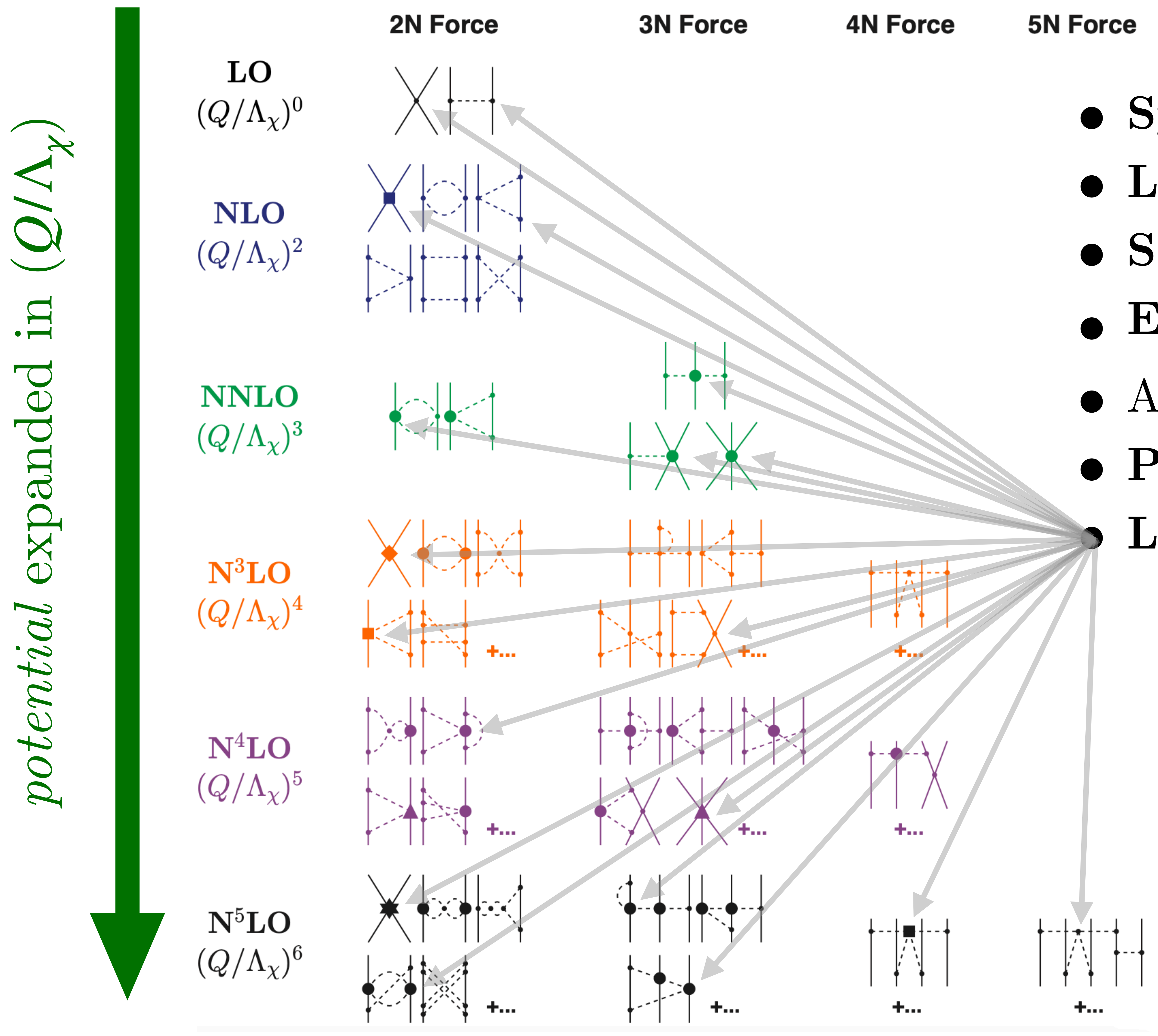

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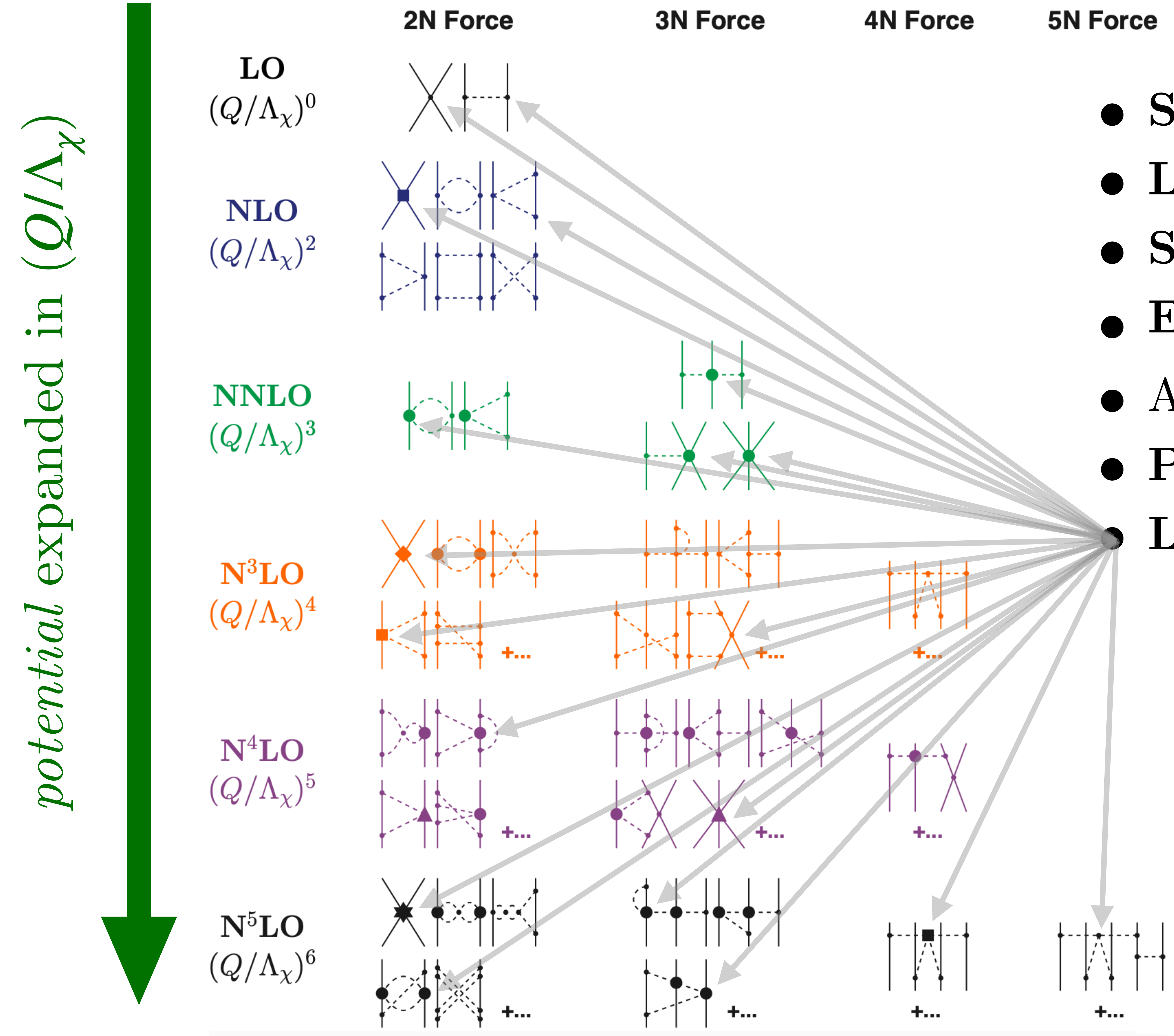

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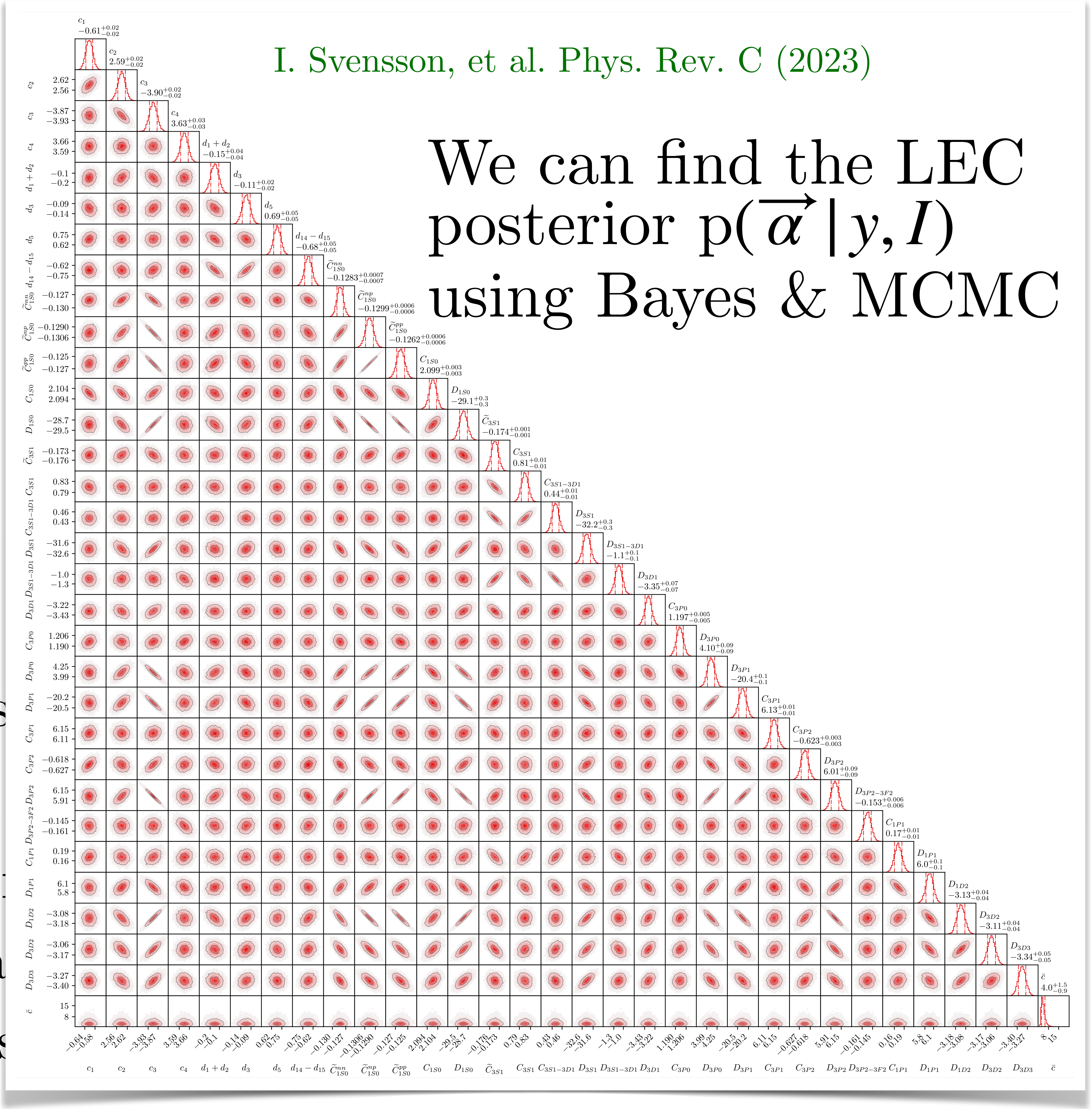

We can find the LEC posterior $p(\vec{\alpha}\,|\,y, I)$ using Bayes & MCMC

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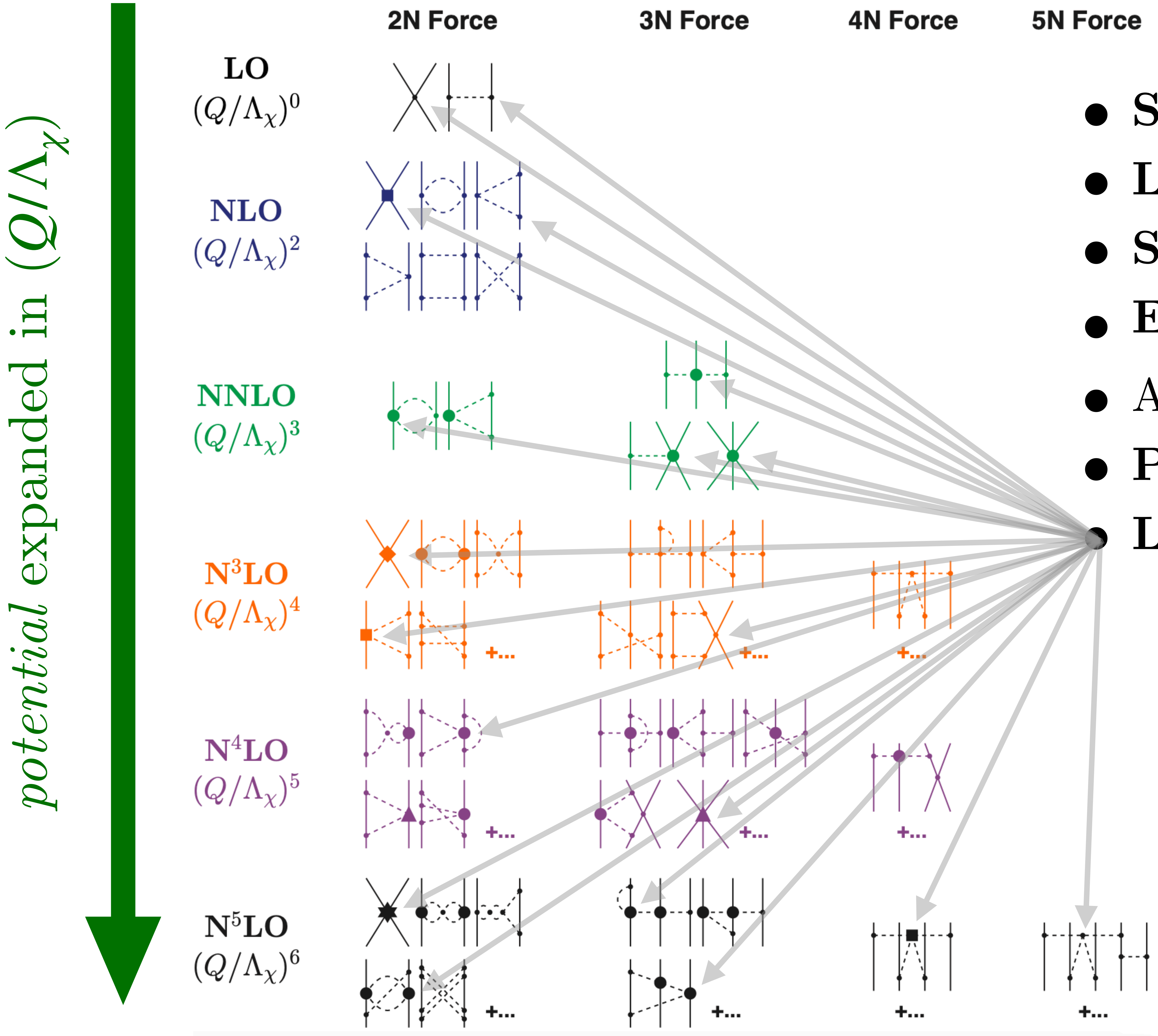

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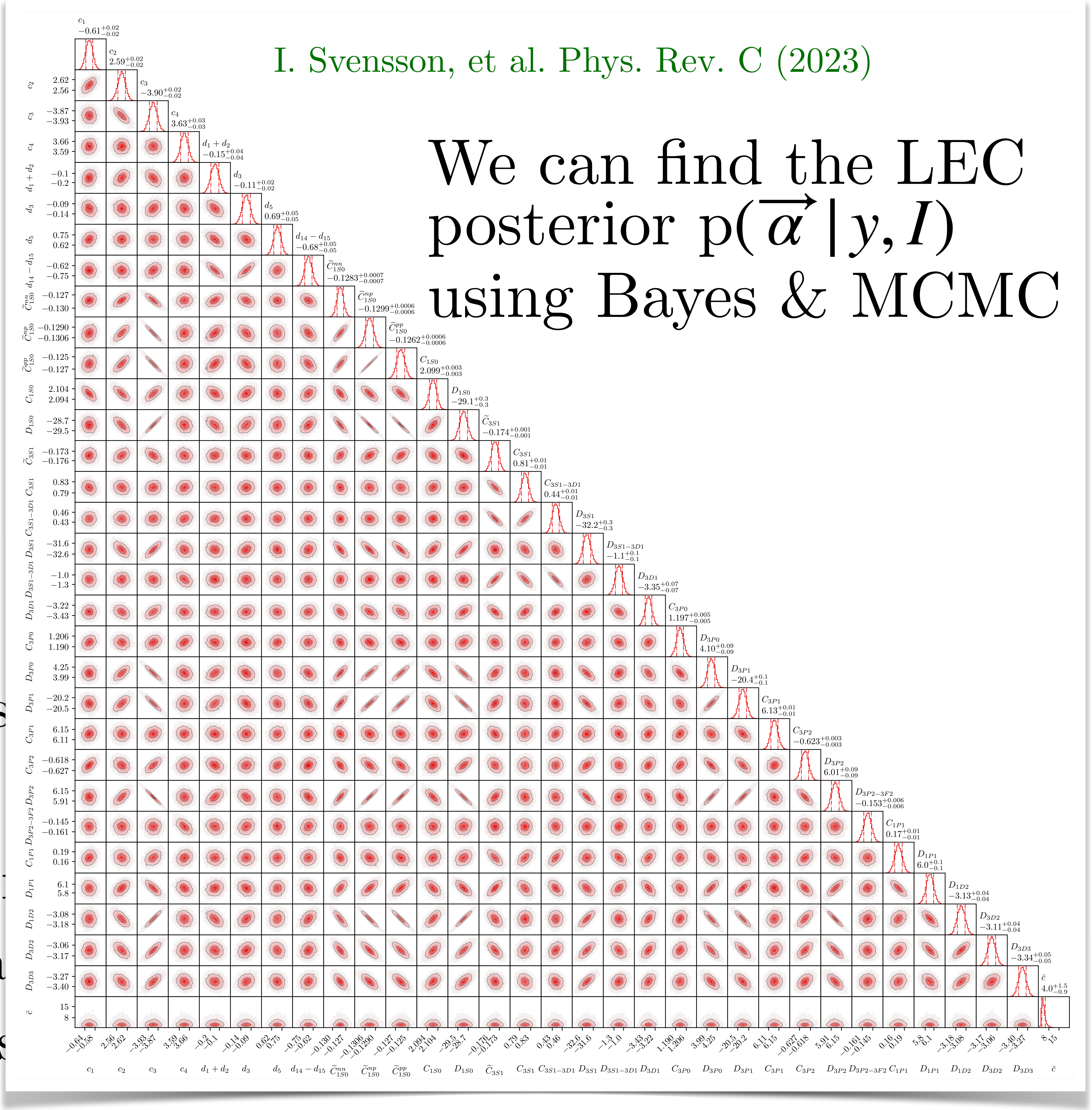

I. Svensson, et al. Phys. Rev. C (2023)

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$$y_{\text{th}}^{(k)} = y_{\text{ref}} \sum_{\nu=0}^{k} c_\nu \left(\frac{Q}{\Lambda_\chi}\right)^\nu \quad \text{and} \quad \delta y_{\text{th}}^{(k)} = y_{\text{ref}} \sum_{\nu=k+1}^{\infty} c_\nu \left(\frac{Q}{\Lambda_\chi}\right)^\nu$$

EFT prediction **EFT truncation error**

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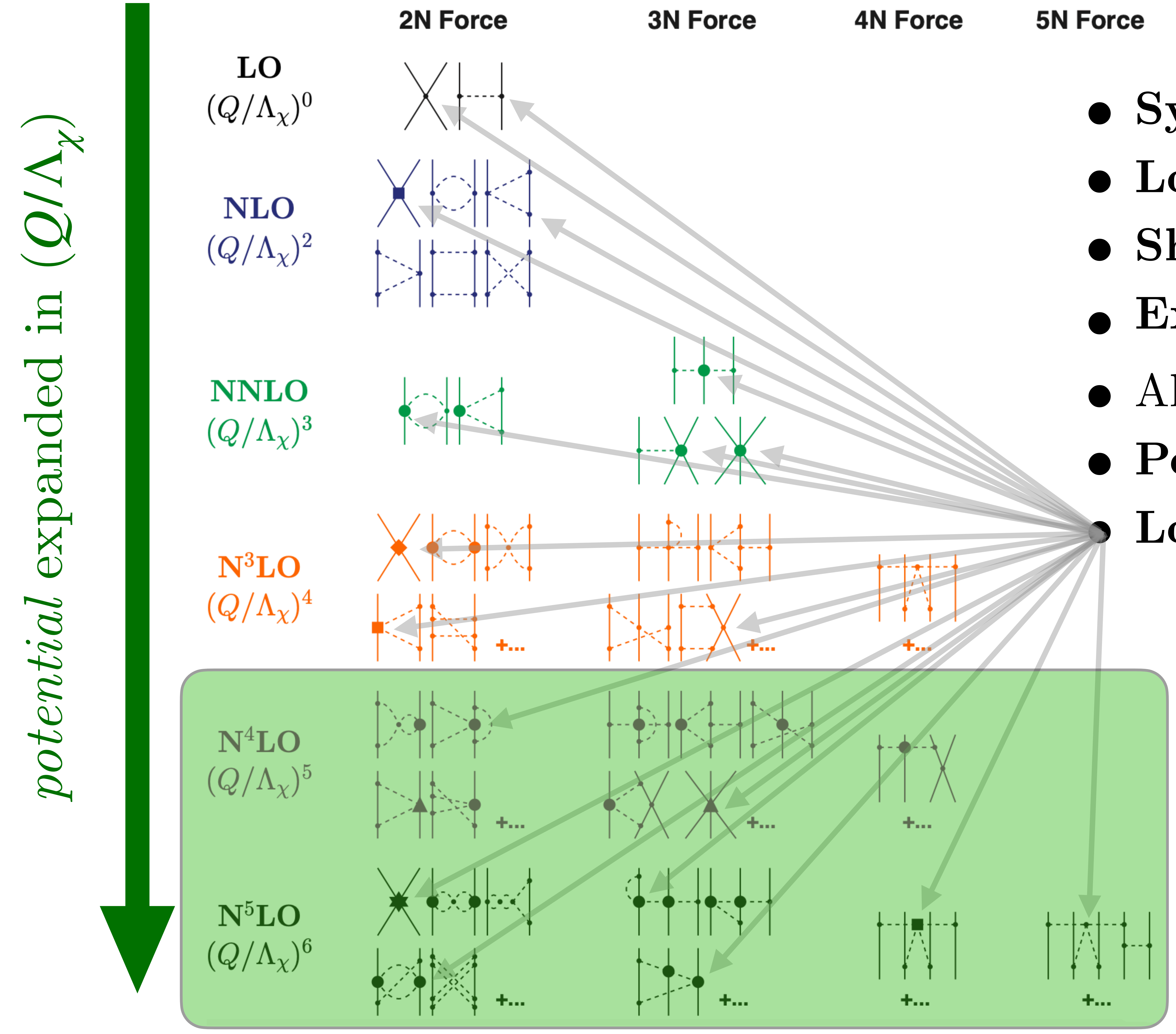

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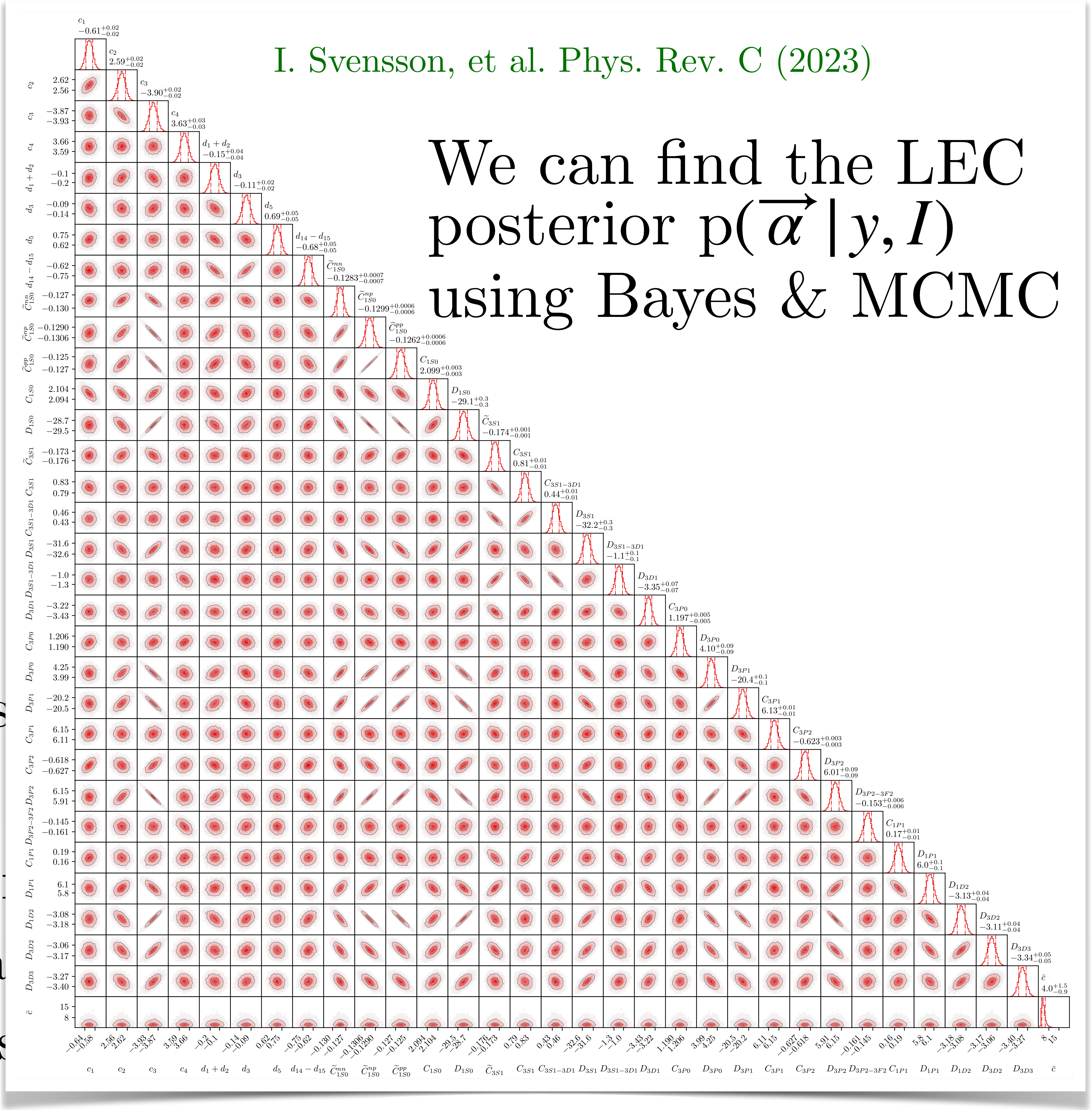

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EFT prediction

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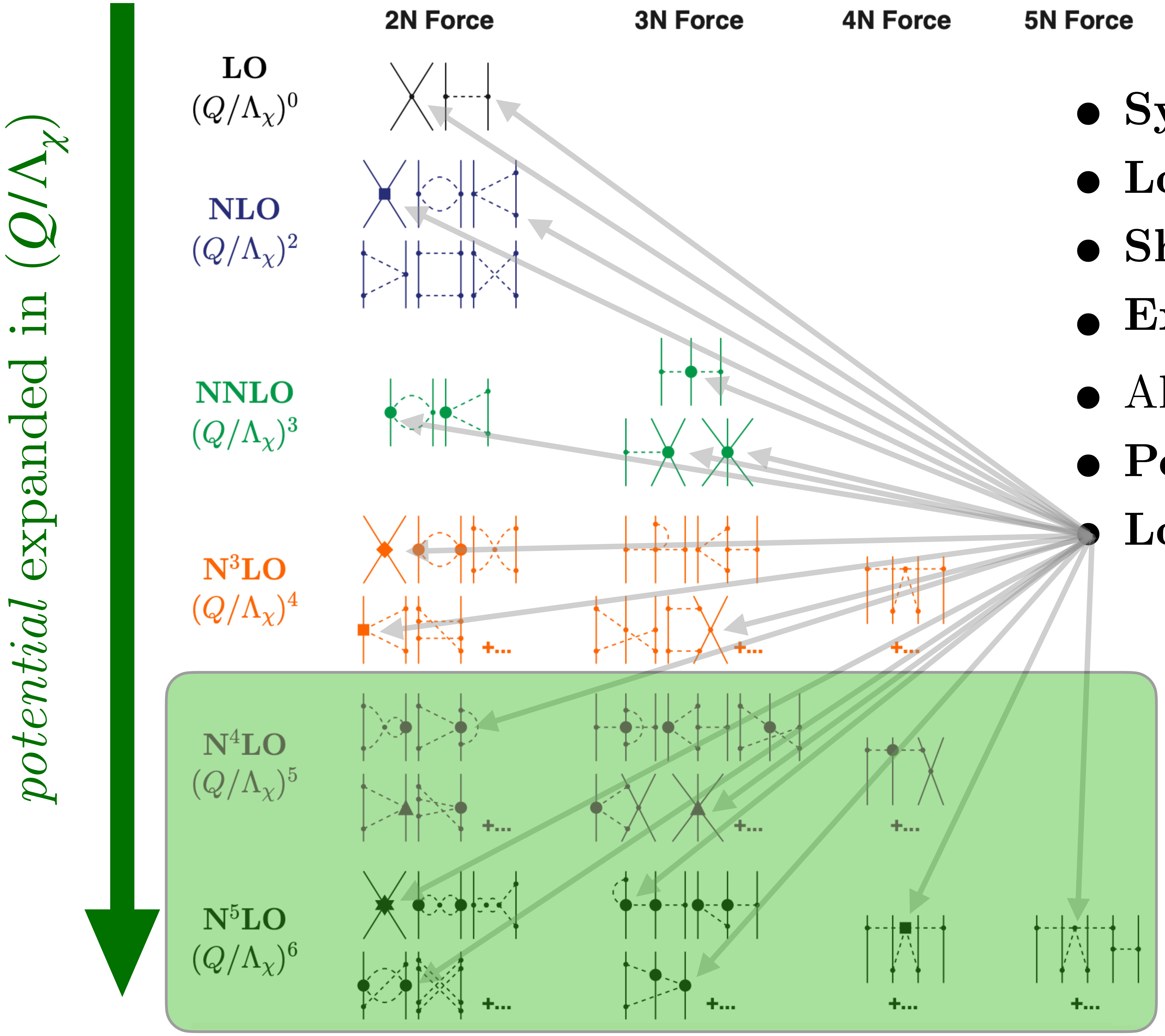

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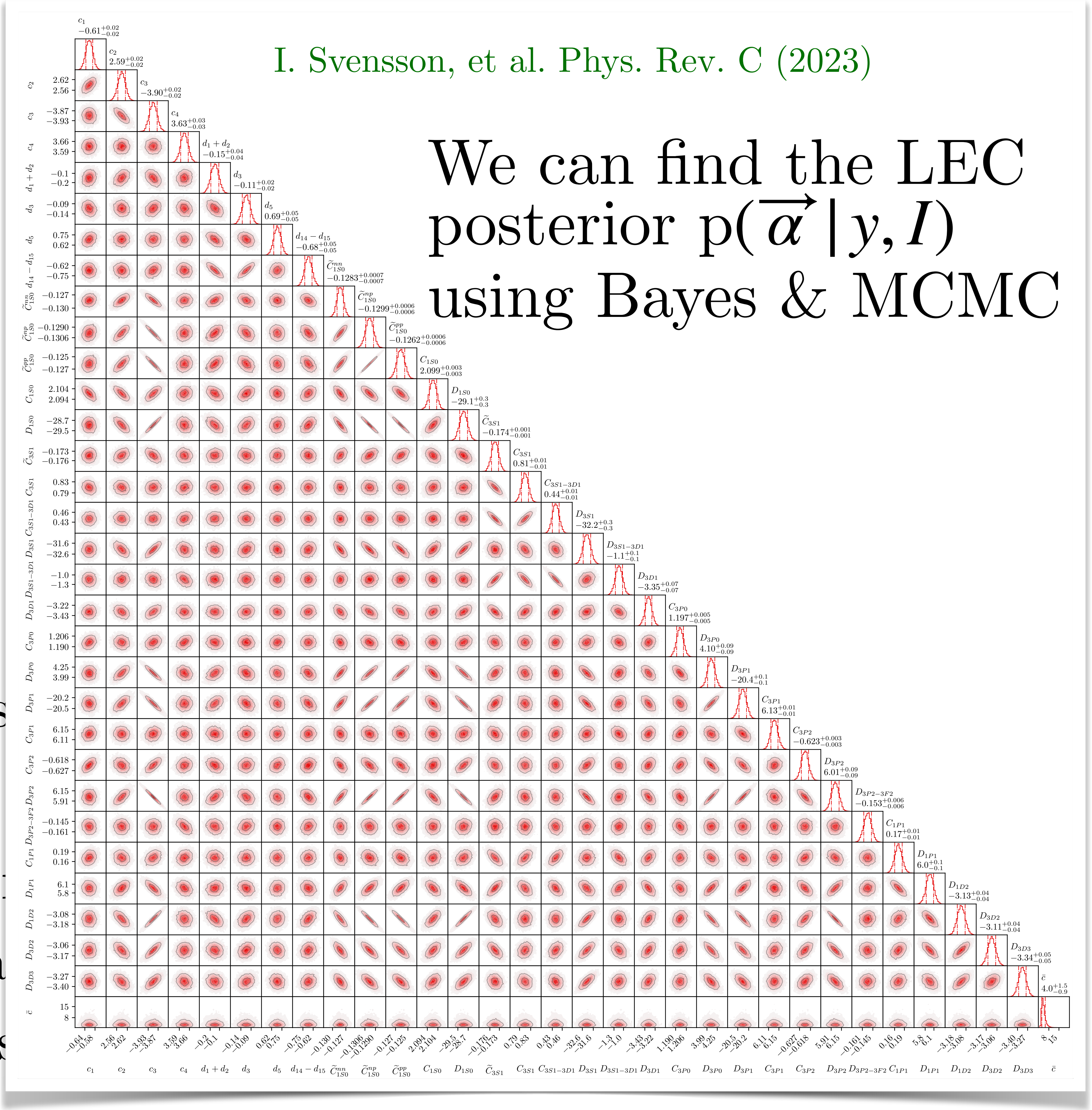

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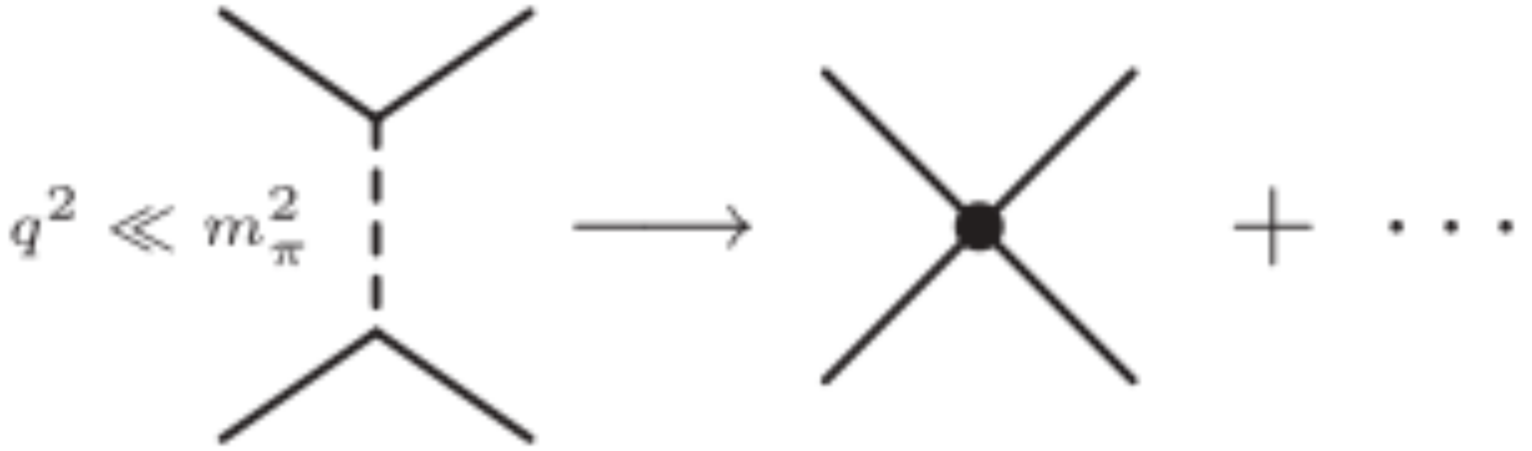
EFT prediction **EFT truncation error**

Challenge: which power counting (if any) will generate a pionfull EFT for the nuclear interaction?

Weinberg, van Kolck, Kaplan, Savage, Wise, Weise, Kaiser, Bernard, Meißner, Epelbaum, Machleidt, Entem, ...

Using Bayes to test your assumptions

- Inferring the breakdown scale of pionless EFT

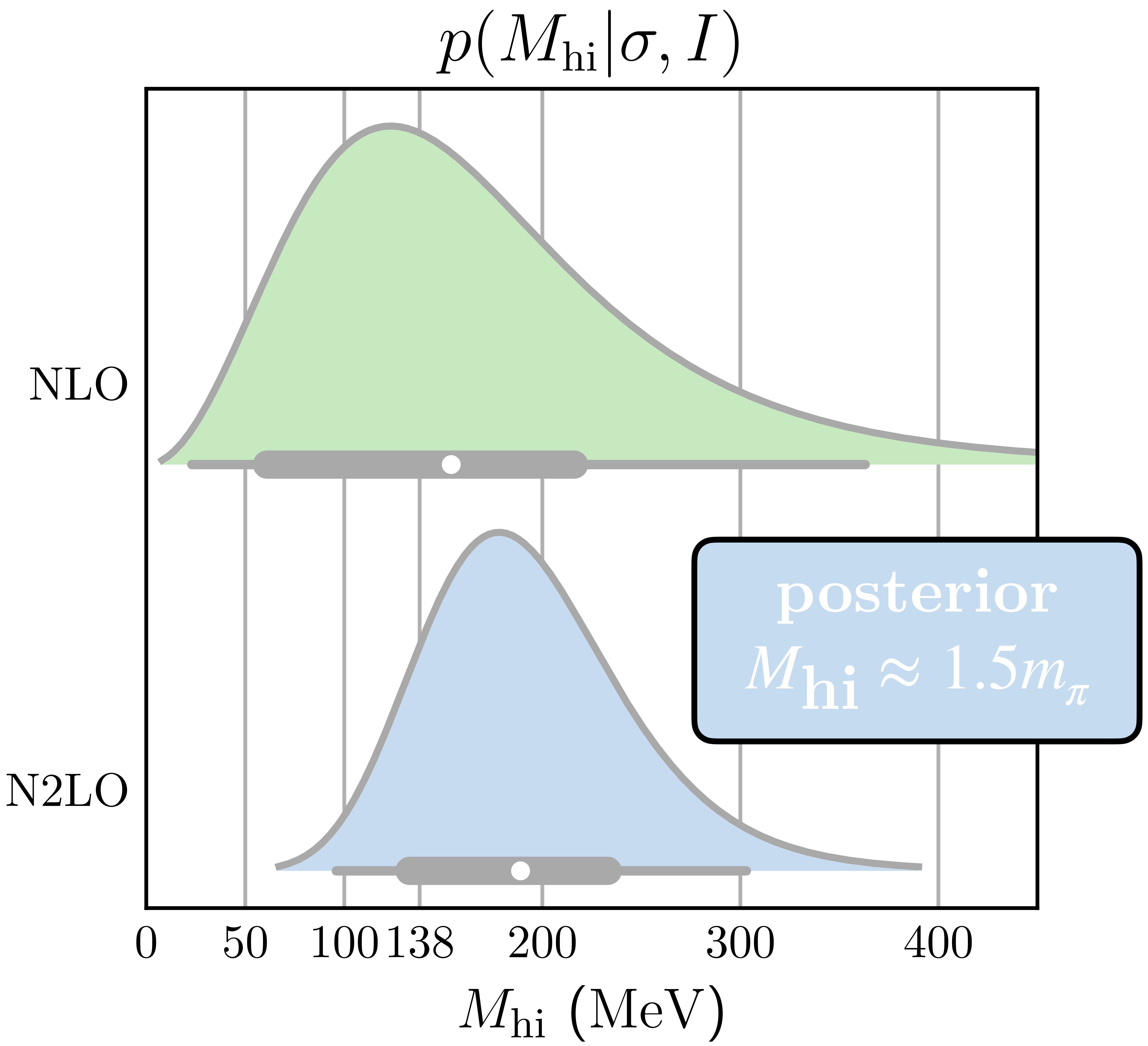


The breakdown scale is due to excluded massive degrees of freedom. The pion!

$$y_{\rm th}^{(n)} = y_{\rm ref} \sum_{\nu=0}^{n} c_\nu \left(\frac{Q}{M_{\rm hi}} \right)^\nu$$

$$p(M_{\rm hi}|\boldsymbol{\sigma}, I) \propto p(\boldsymbol{\sigma}|M_{\rm hi}, I)p(M_{\rm hi}|I)$$ log-uniform prior

$$p(M_{\rm hi}|\boldsymbol{\sigma}, I) \propto p(M_{\rm hi}|I) \prod_{i=1}^{K} \left(\tau_i^{\nu_i} \prod_{n\in[1,2]} Q(k_i)^n \right)^{-1}$$



A. Ekström and L. Platter, PLB (accepted; 2024)
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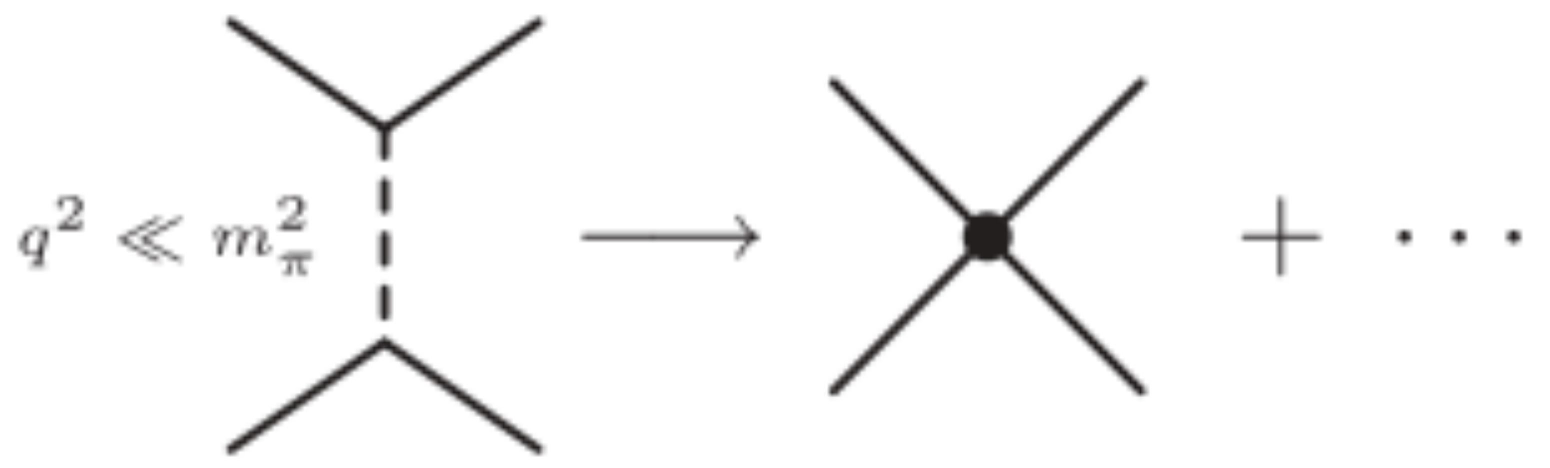

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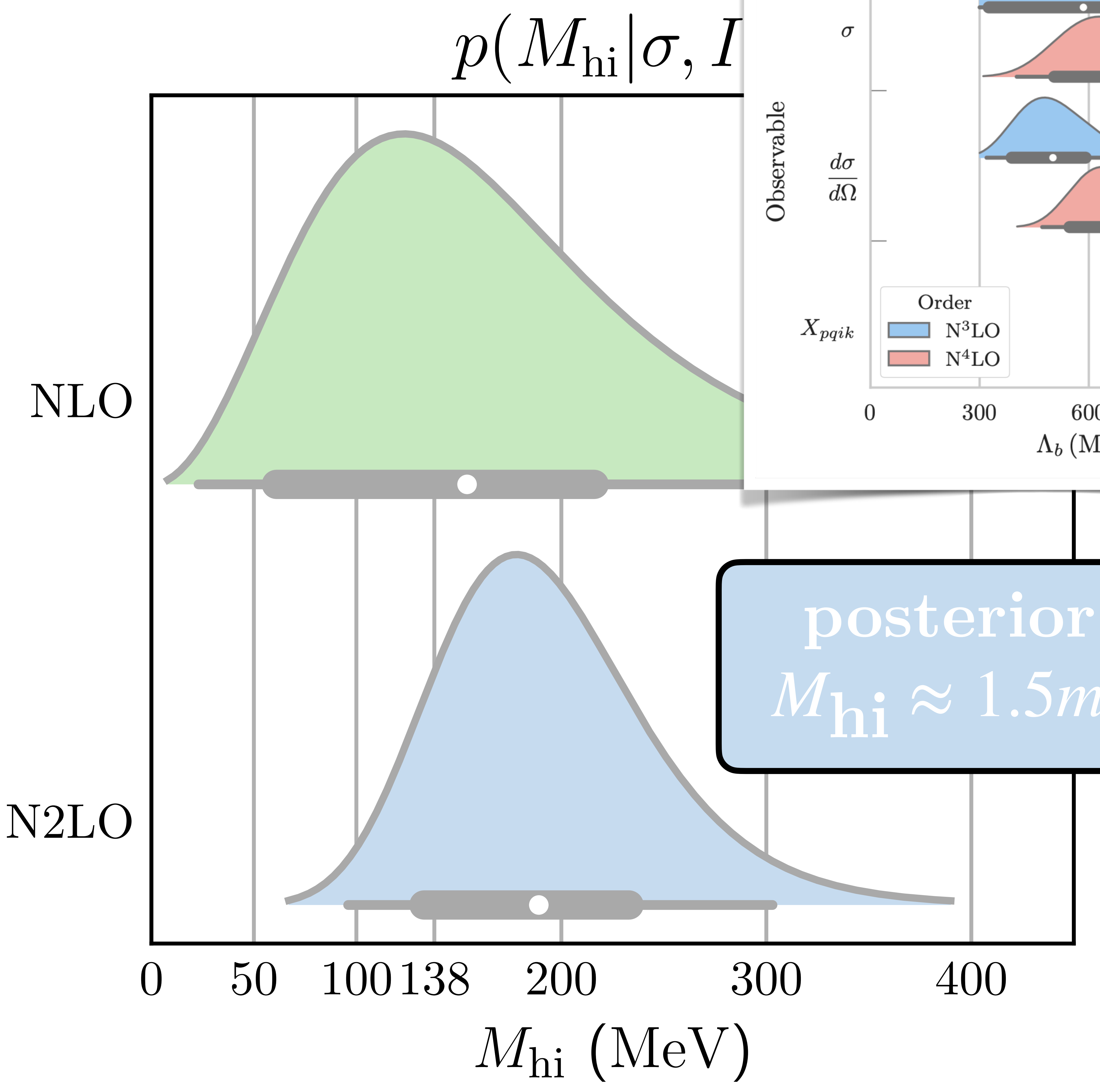

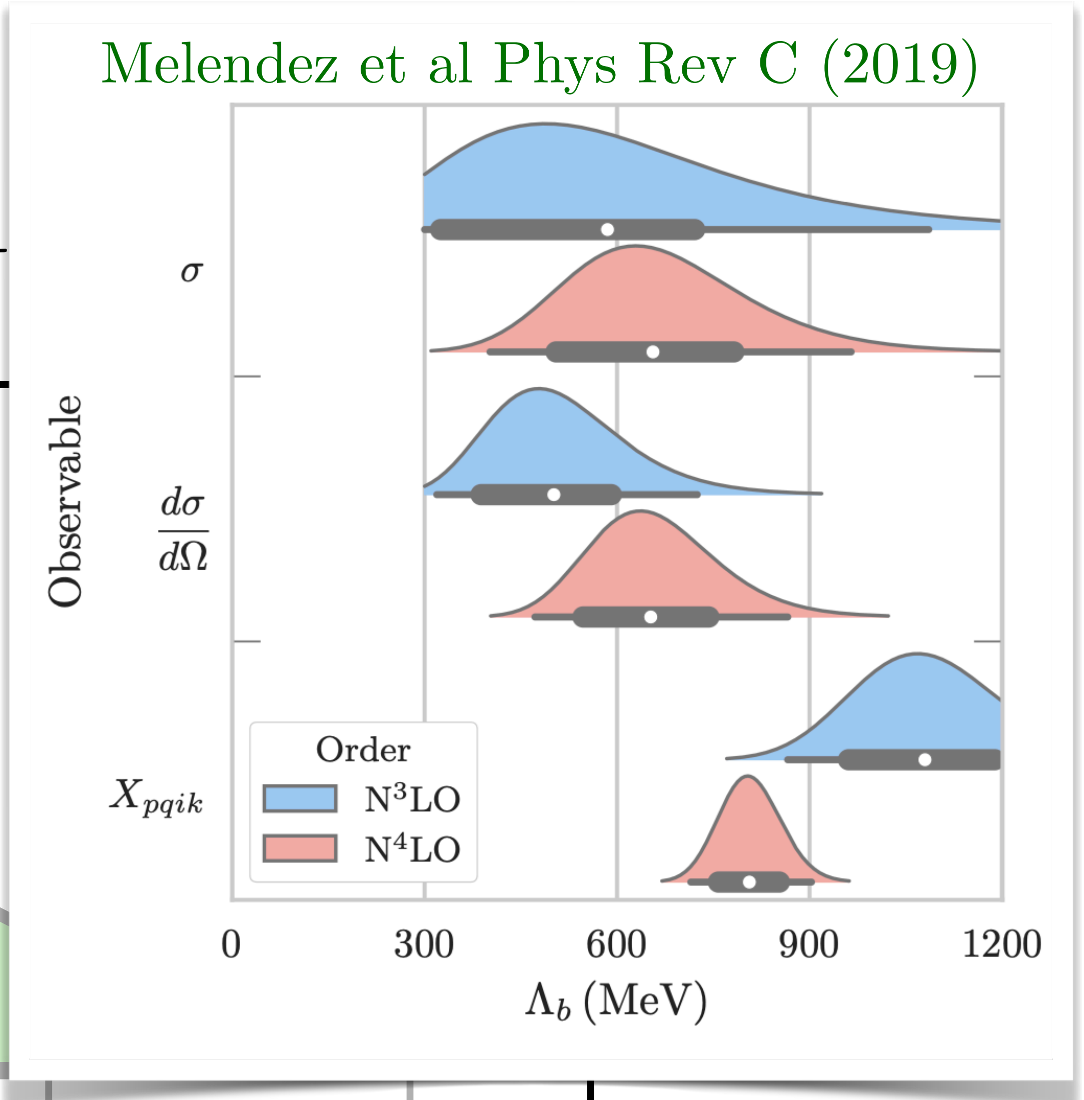

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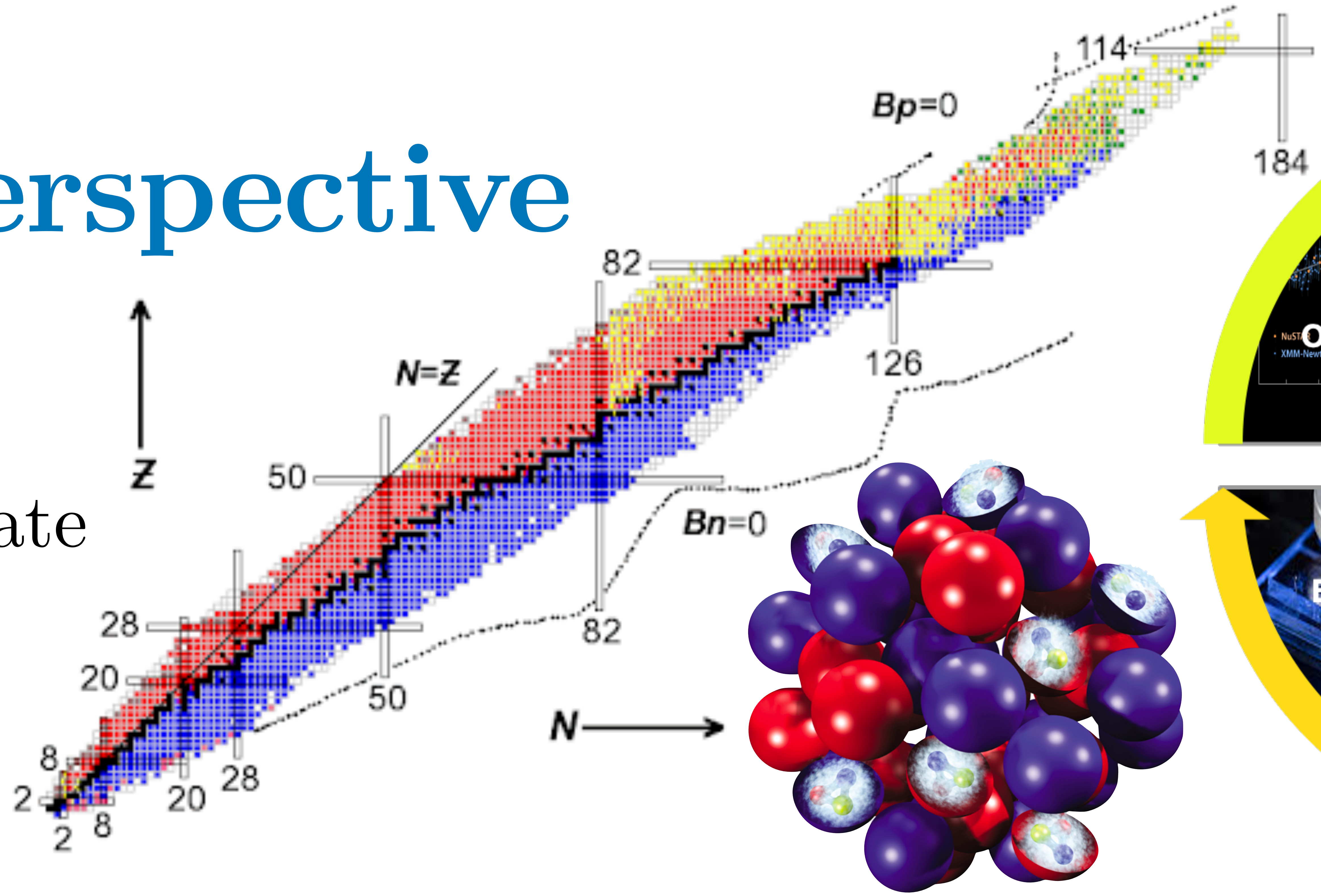
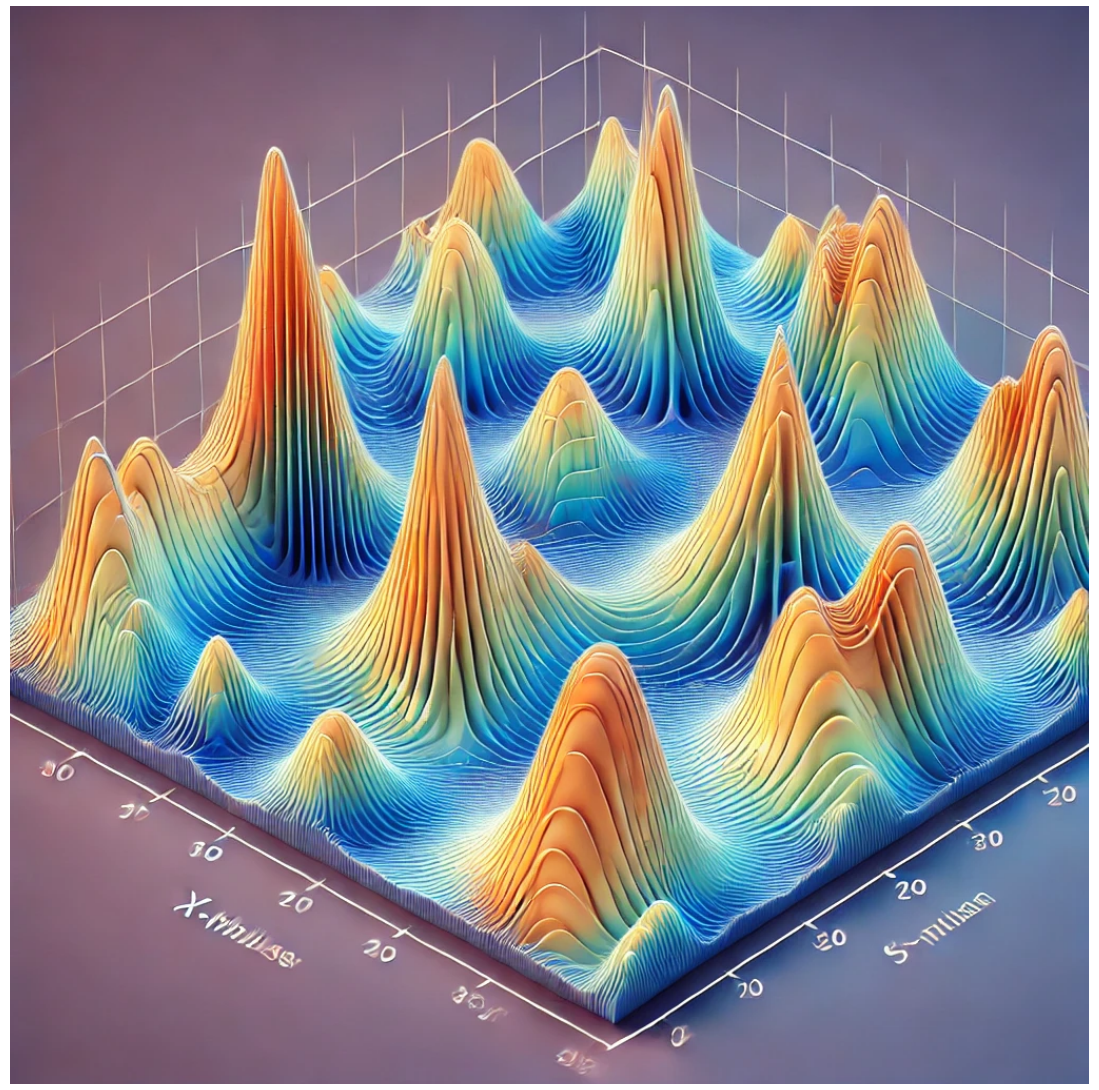
A bigger perspective

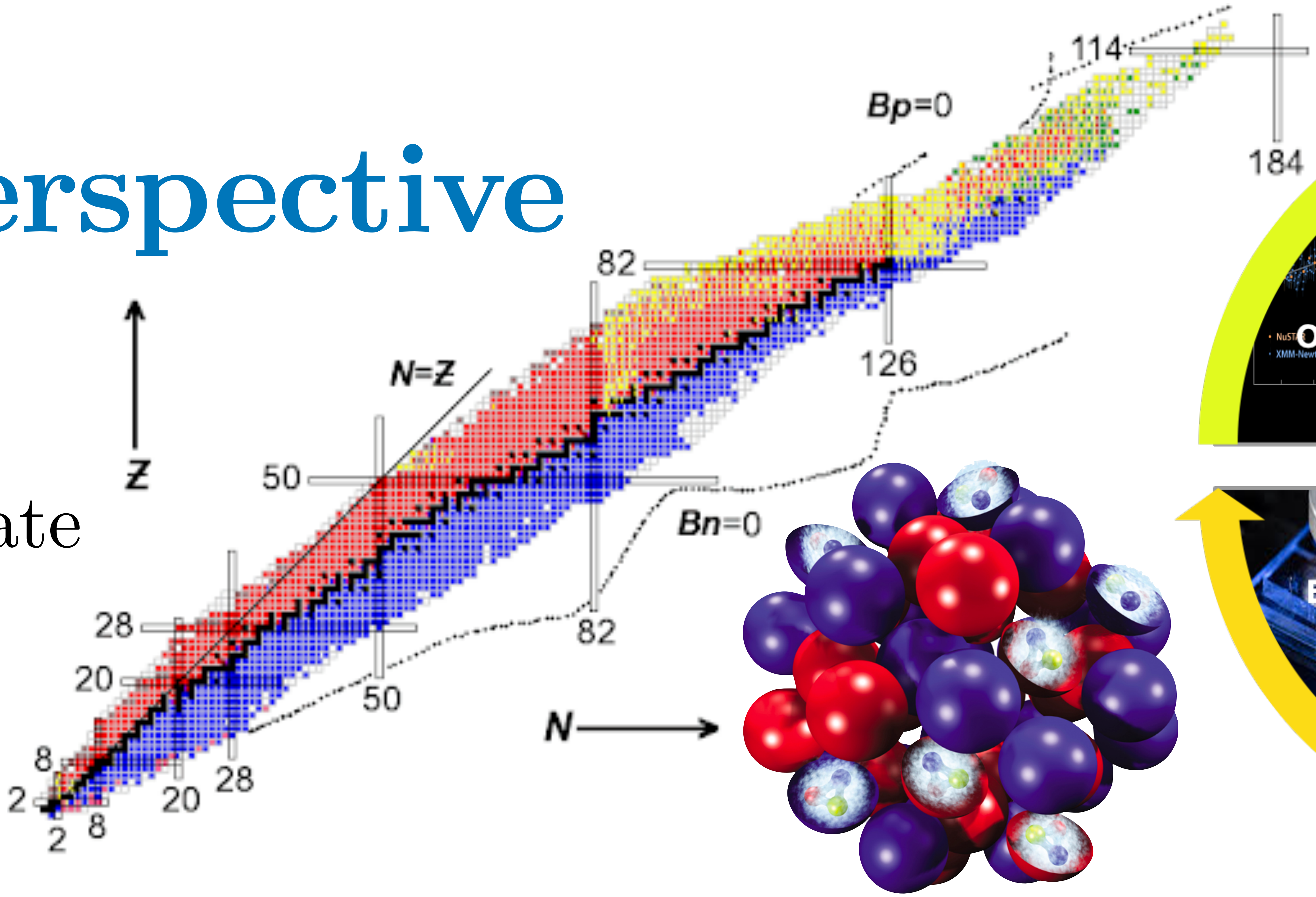


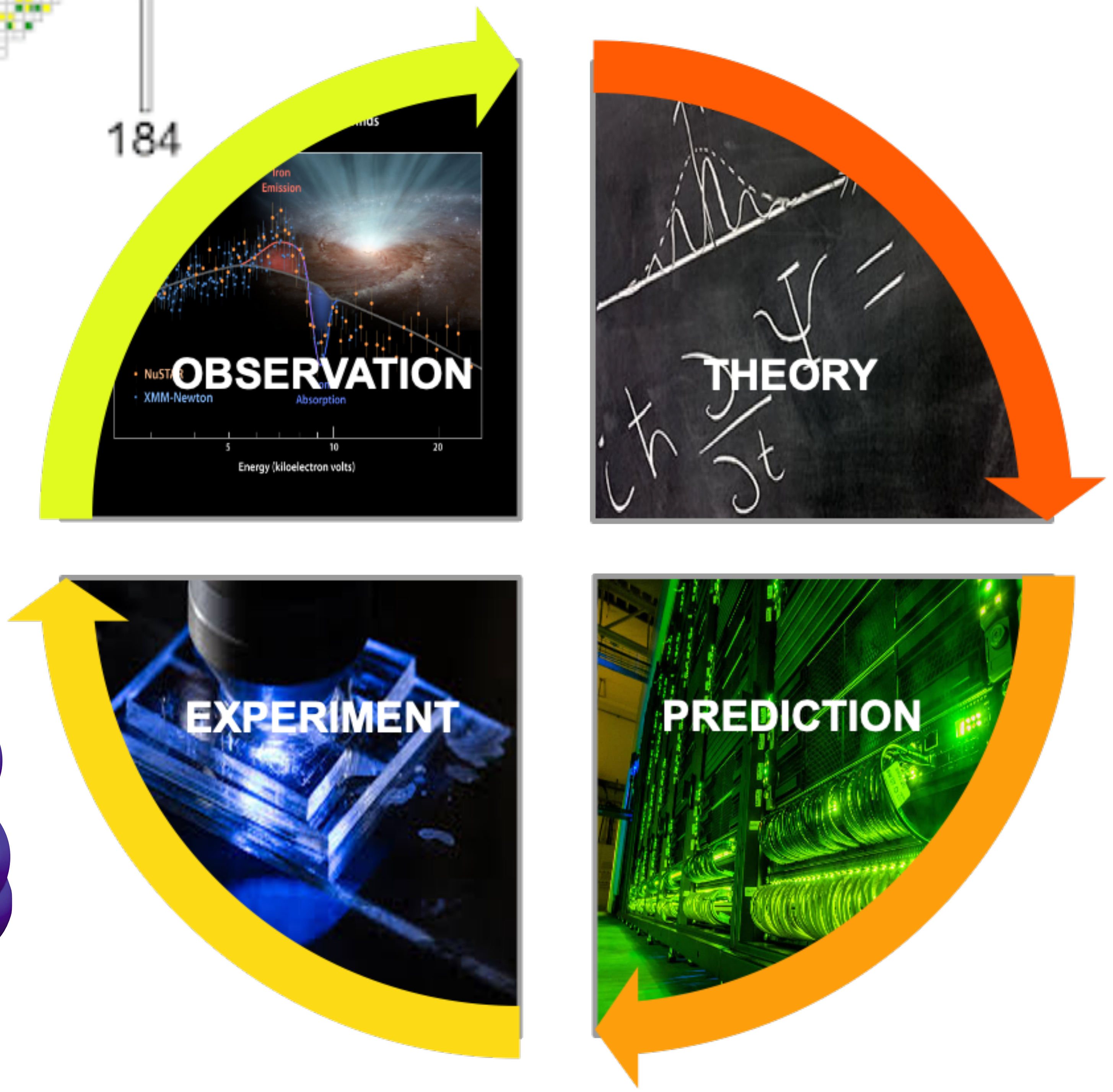
We need data from A>3 nuclei to calibrate chiral NN+3N interactions



We would like to test our *ab initio* model across the nuclear chart.
Can we find regions in the parameter space that reproduce seen data?

A bigger perspective





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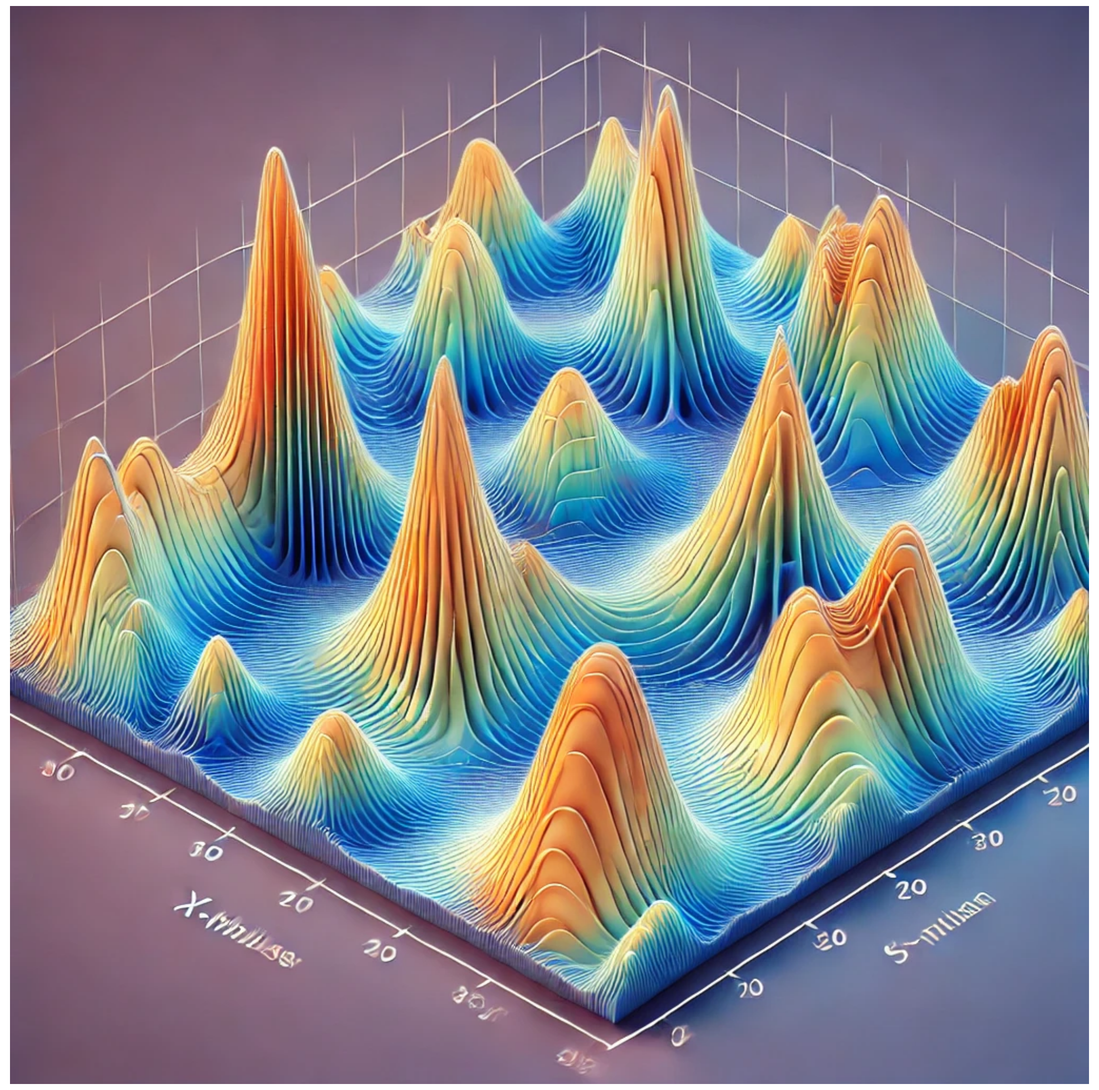

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- multimodal and high-D parameter space
- *ab initio* errors difficult to quantify

A bigger perspective

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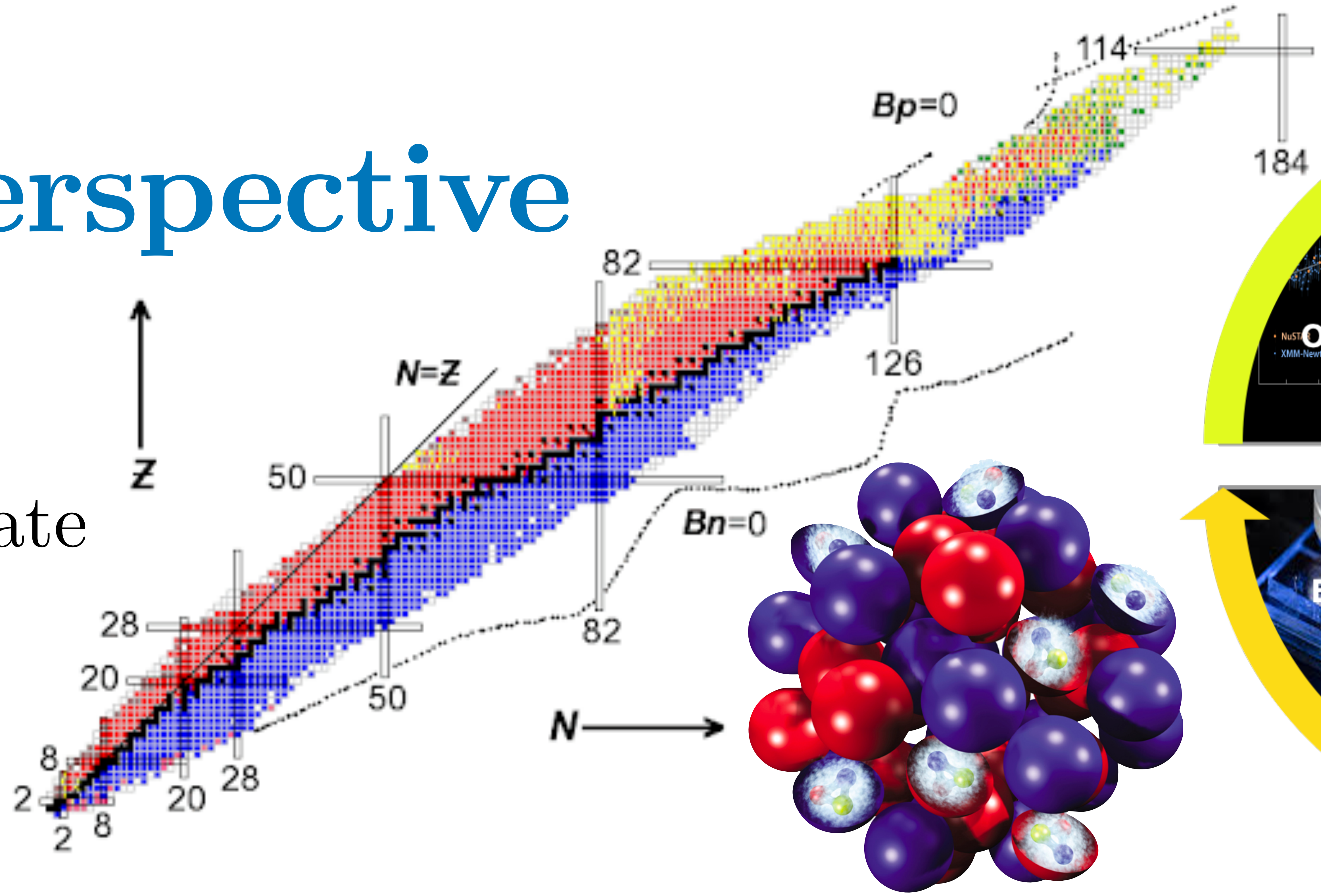

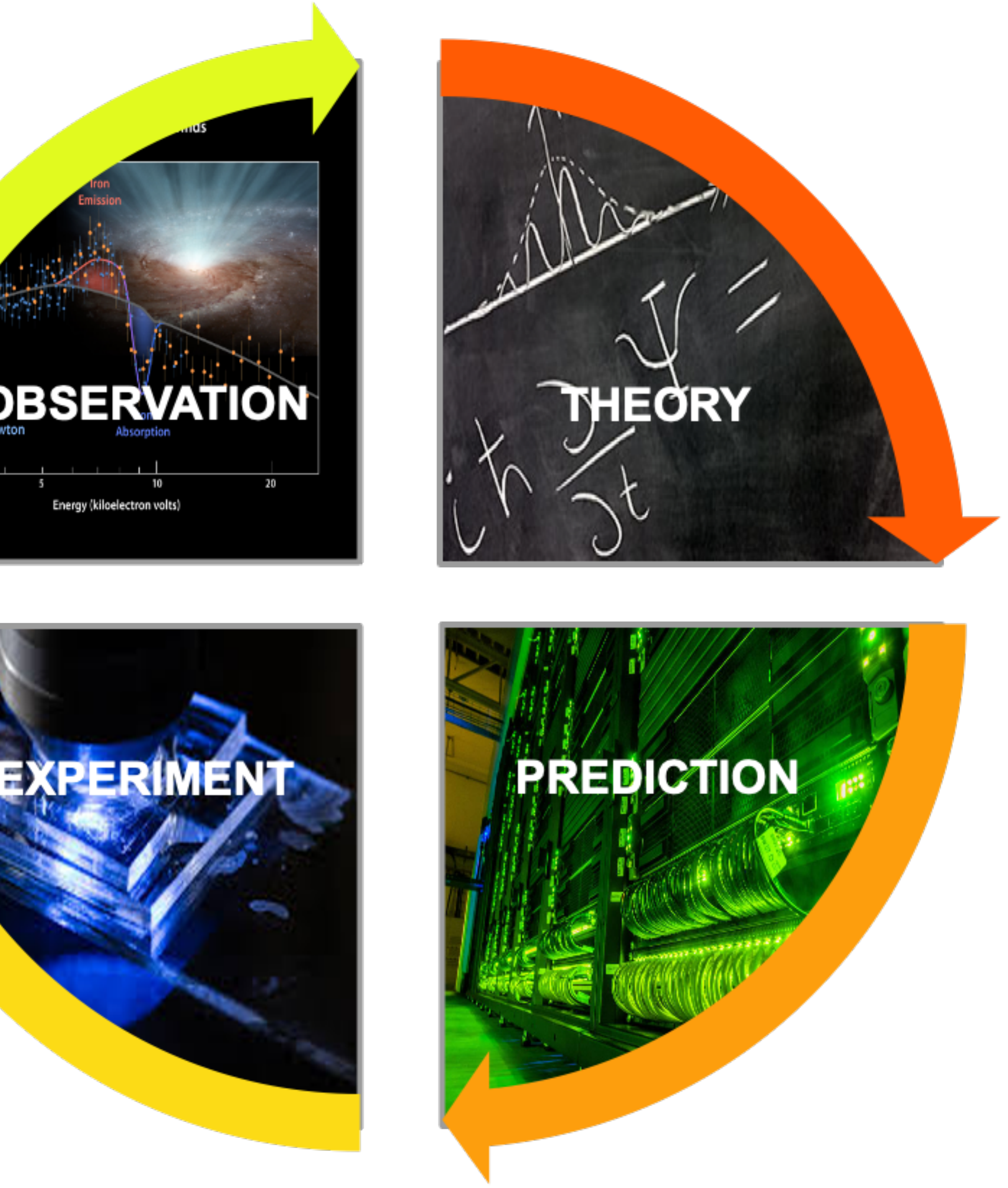

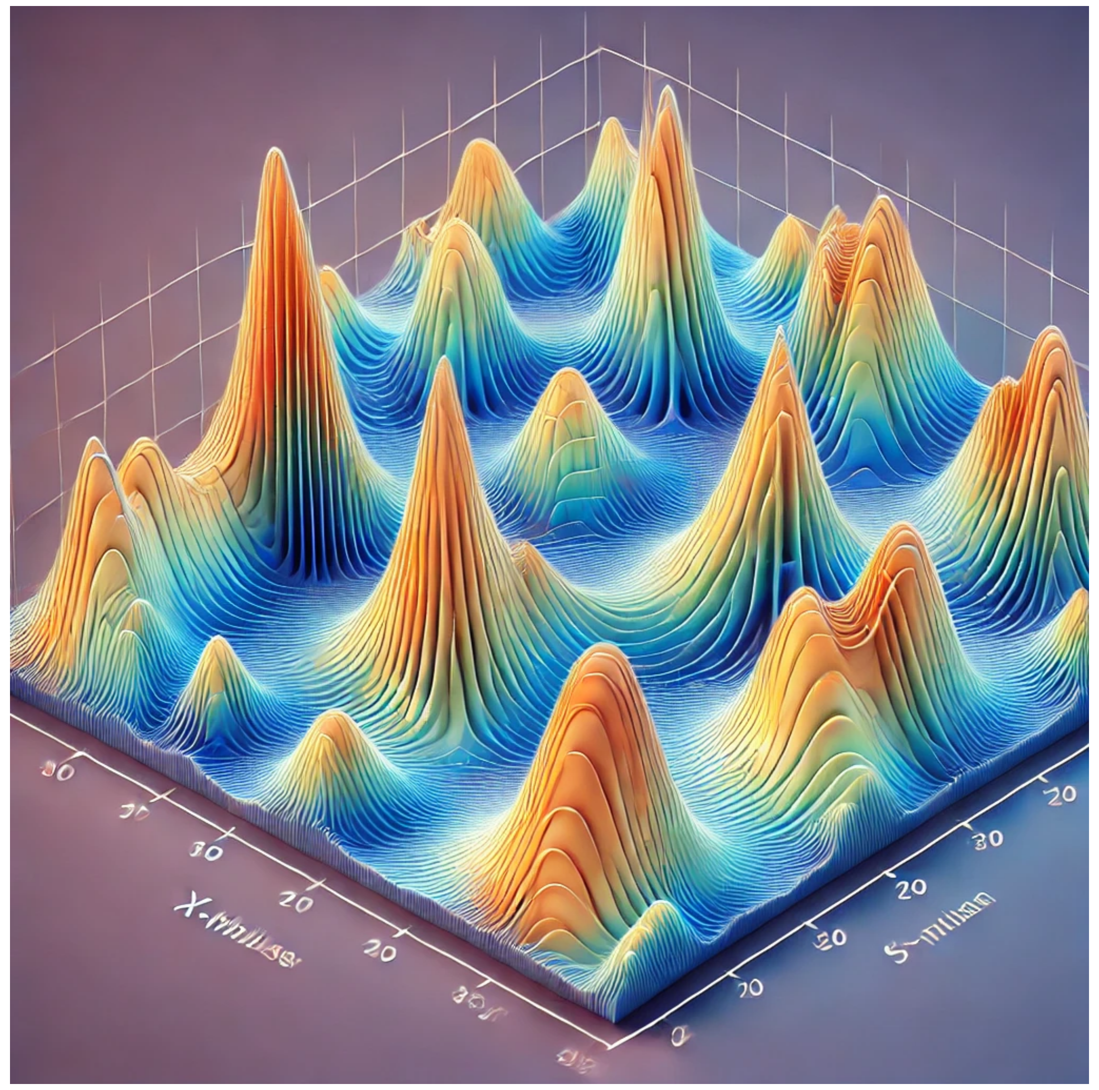

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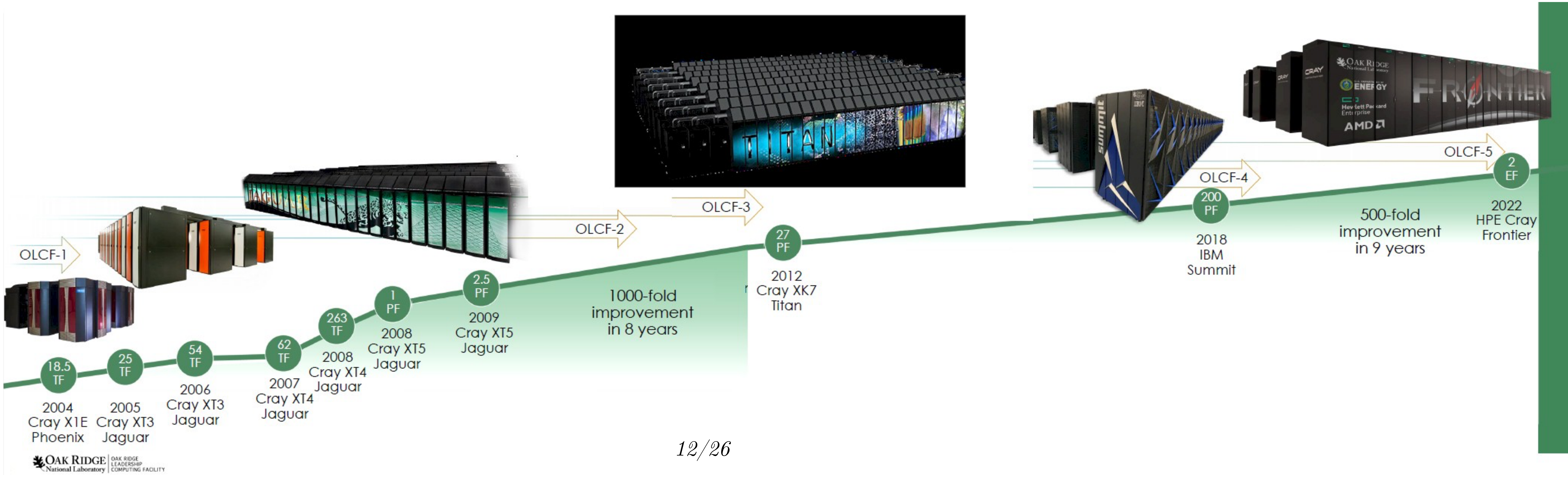
Can we find regions in the parameter space that reproduce seen data?

- computationally expensive likelihood → - emulators
- multimodal and high-D parameter space → - history matching
- *ab initio* errors difficult to quantify → - model comparisons (needs more work)

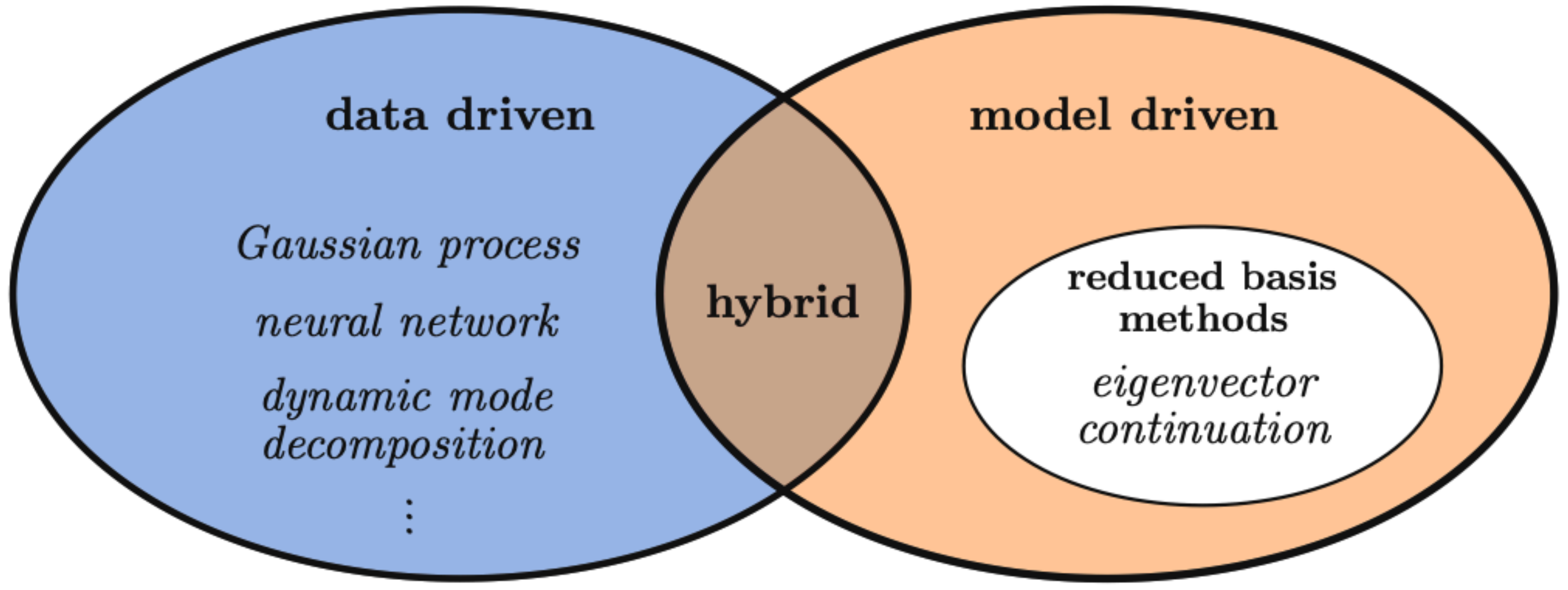
Computing nuclei: an HPC problem

Solving the Schrödinger equation for a large collection of strongly interacting nucleons typically requires substantial high-performance computing resources. Naively, the computational cost to solve the Schrödinger equation grows exponentially with nucleon number and basis size. Polynomially scaling methods exist but are still computationally expensive.



Emulators to the rescue

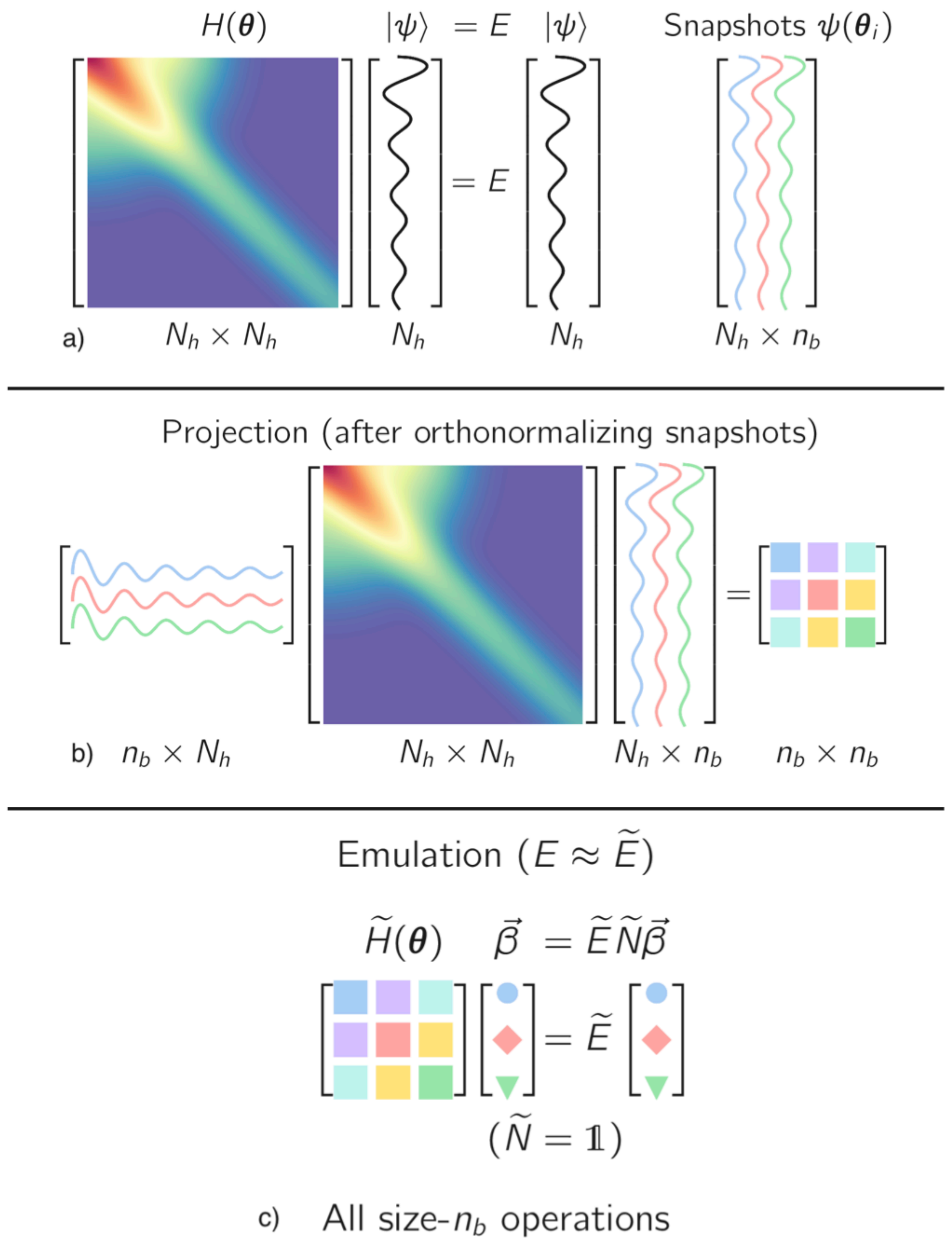
Eigenvector continuation (EC): a reduced-basis method (RBM) for fast and accurate emulation

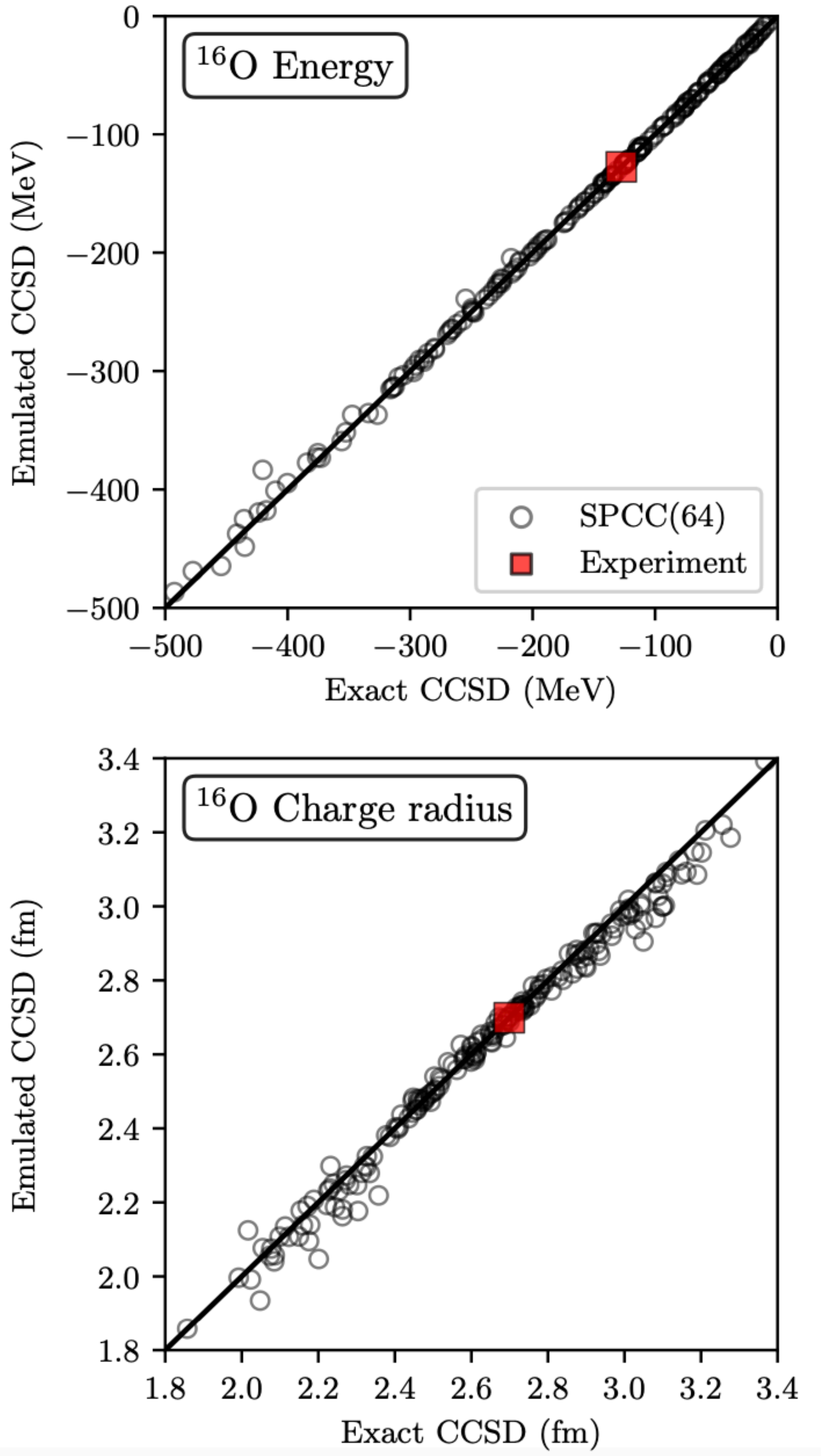


$$H(\alpha) = H_0 + \alpha H_1$$

continuous parameter

Eigenvector trajectories due to smooth changes of the Hamiltonian lie in a low dimensional manifold.





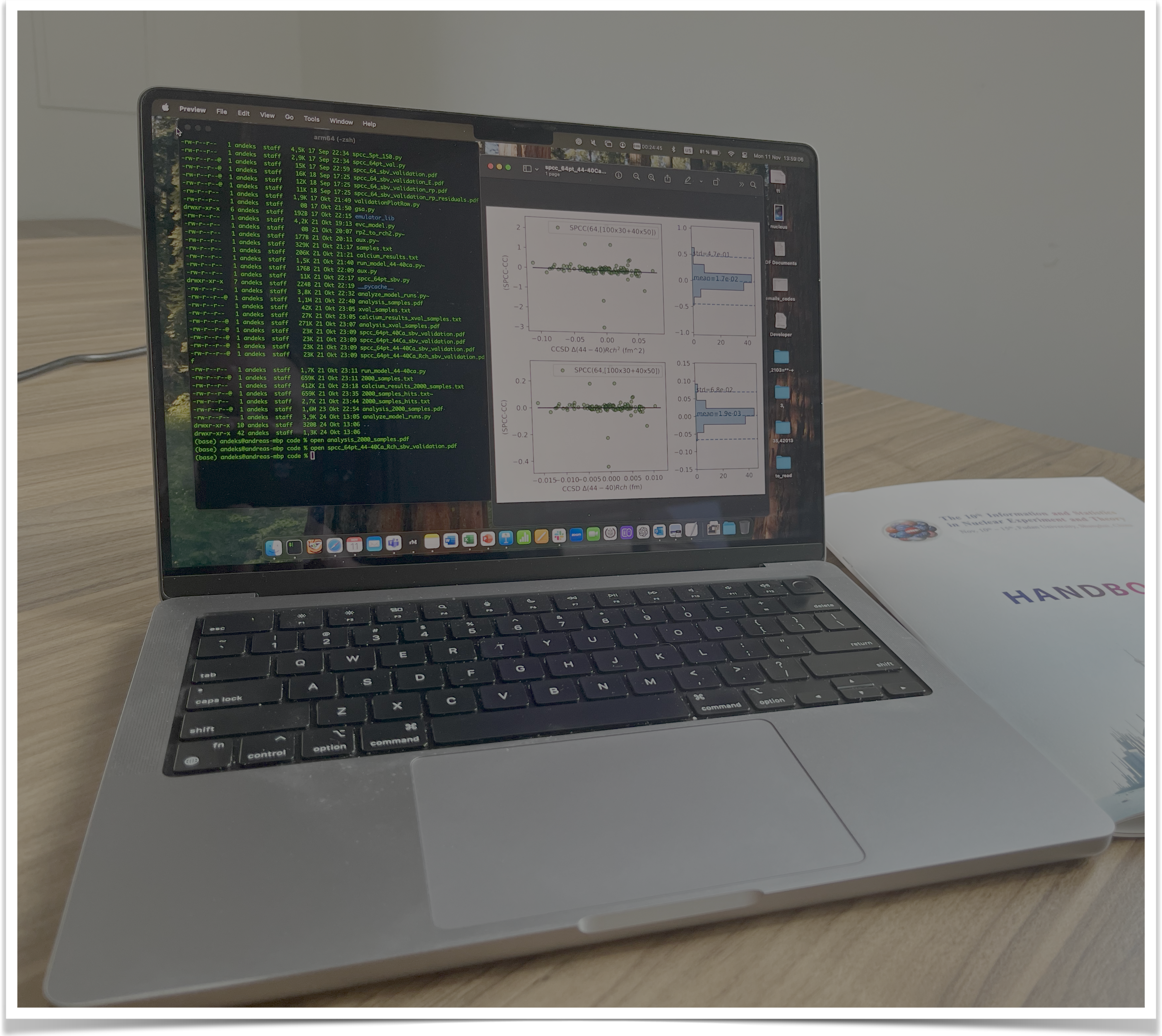
D. Frame, et al. Phys. Rev. Lett. (2018)
S. König, et al. Phys. Lett. B (2020)

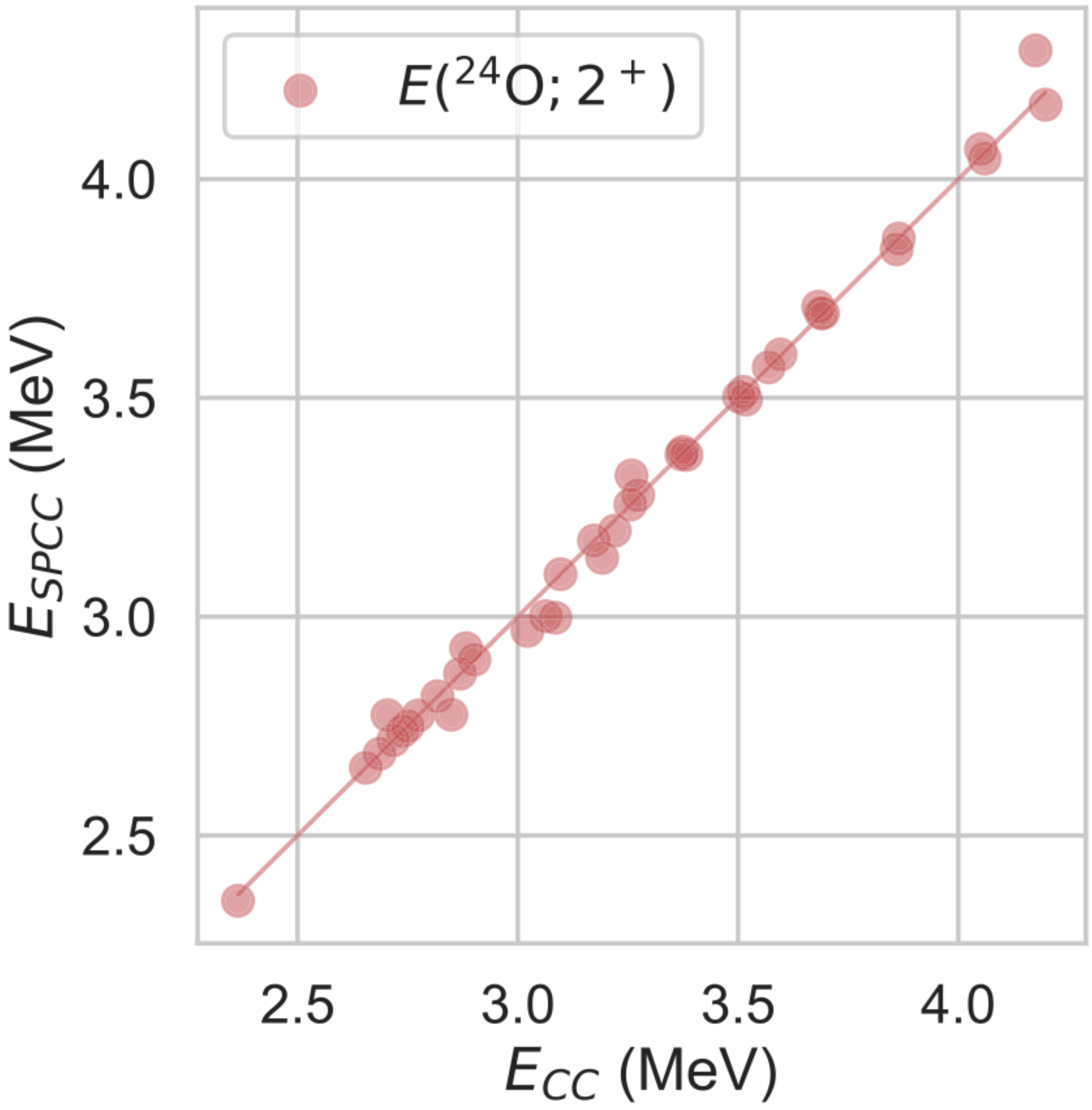
T. Duguet, et al, Rev. Mod. Phys (2024)

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

A computational statistics laboratory

- using fast and accurate emulators

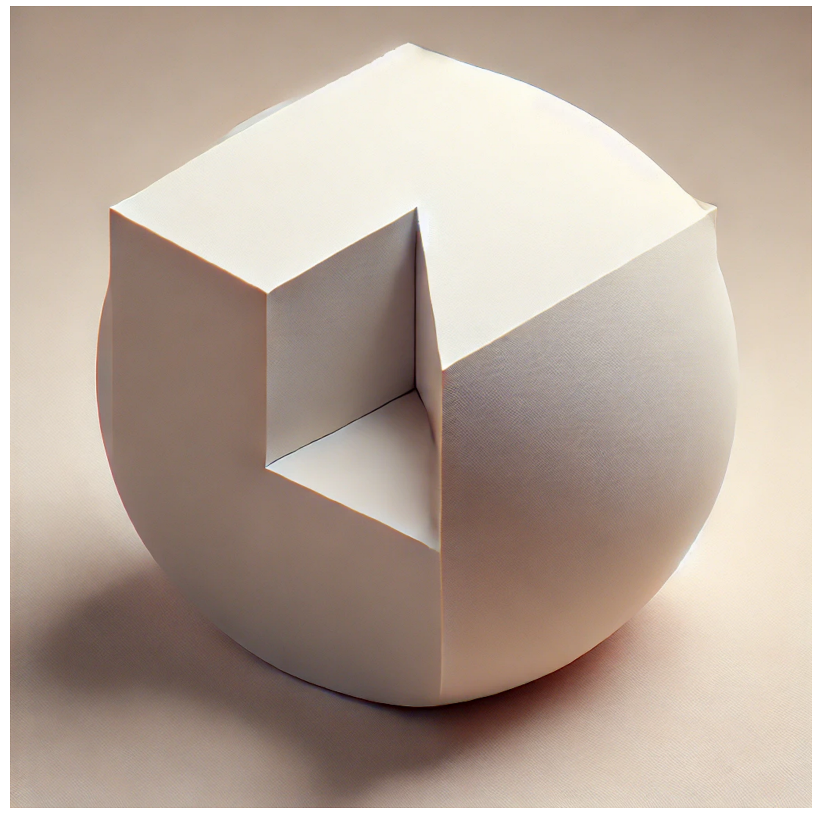


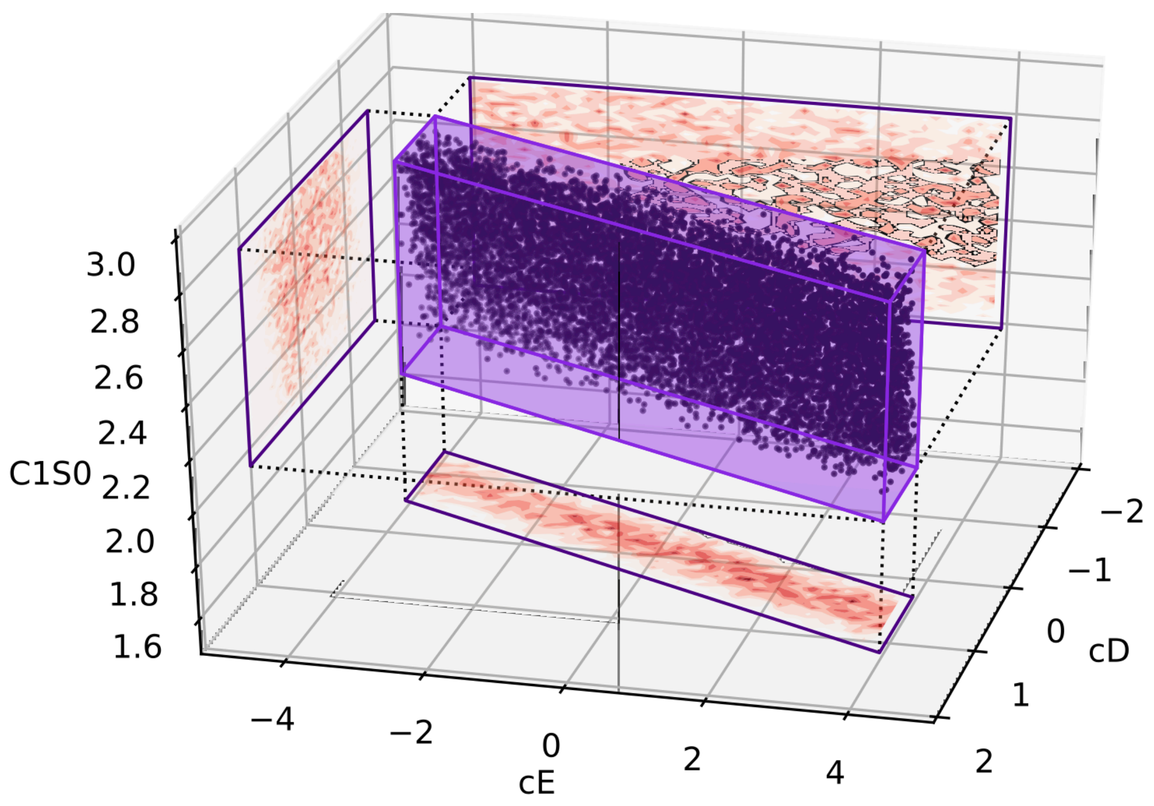


CCSDT-3

History matching as a first step towards ^{28}O

- excluding parts of parameter space that do not reproduce data





Easier to claim *implausibility* than to quantify posterior probability

$$\Theta(\vec{\alpha}) \text{ vs. } p(\vec{\alpha}\,|\,y, M, I) \text{ where } \Theta(\vec{\alpha}) = \begin{cases} 1 \text{ implausible} \\ 0 \text{ non} - \text{implausible} \end{cases}$$

Implausibility measure:

$$I^2(\vec{\alpha}) = \max_{y_{\text{exp}}^{(i)} \in y} \frac{|\mathbb{E}[y_{\text{th}}^{(i)}(\vec{\alpha})] - y_{\text{exp}}^{(i)}|^2}{\text{Var}[y_{\text{th}}^{(i)}(\vec{\alpha}) - y_{\text{exp}}^{(i)}]}$$

Iteratively rule out $\vec{\alpha}$ for $I(\vec{\alpha}) > 3$
(Pukelsheim)

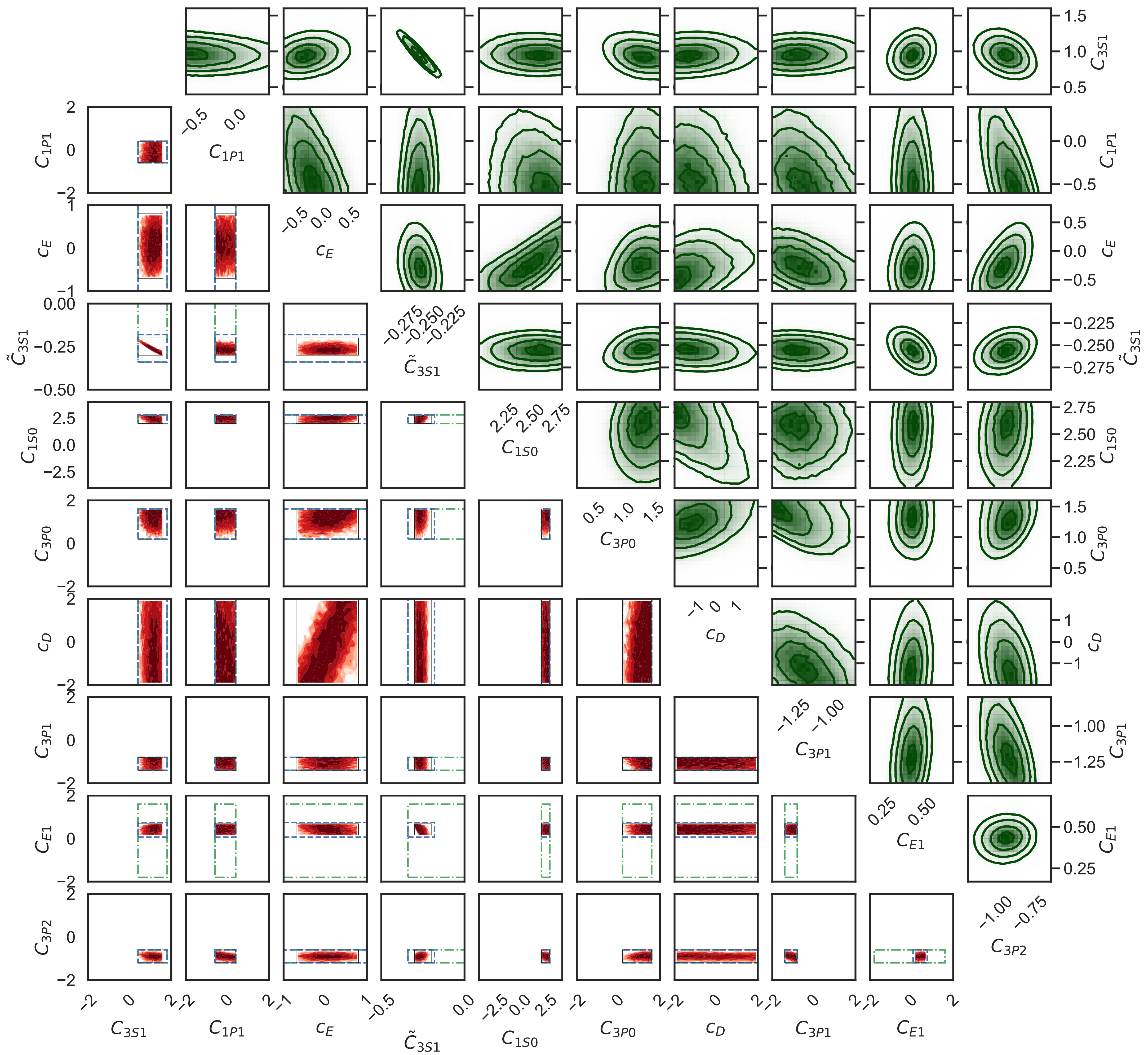
y	y_{exp}	ε_{exp}	$\varepsilon_{\text{model}}$	$\varepsilon_{\text{method}}$
$E(^2\text{H})$	−2.2298	0.0	0.05	0.0005
$r_p^2(^2\text{H})$	3.9030	0.0	0.02	0.0005
$Q(^2\text{H})$	0.27	0.01	0.003	0.0005
$E(^3\text{H})$	−8.4818	0.0	0.17	0.0005
$E(^4\text{He})$	−28.2956	0.0	0.55	0.0005
$r_p^2(^4\text{He})$	2.1176	0.0	0.045	0.0005
$E(^{16}\text{O})$	127.62	0.0	0.75	1.5
$r_p^2(^{16}\text{O})$	6.660	0.0	0.16	0.05
$\Delta E(^{22,16}\text{O})$	−34.41	0.0	0.4	0.5
$\Delta E(^{24,22}\text{O})$	−6.35	0.0	0.4	0.5
$E_{2+}(^{24}\text{O})$	4.79	0.0	0.5	0.25
$\Delta E(^{25,24}\text{O})$	0.77	0.02	0.4	0.25

Ian Vernon et al, Bayesian Analysis (2010)

Y. Kondo et al. Nature (2023)

Ab initio prediction of ^{28}O

Bayesian posterior pdf



history matching

- **History matching** identifies the parameter region where we expect the LEC posterior distribution to reside.
- **MCMC** + **emulators** to draw 10^8 samples of the LEC posterior at ΔNNLO with NN+3N interaction.

$$\mathrm{p}(\vec{\alpha}|A = 2-24)$$

- We assume uniform prior + uncorrelated normal likelihood. Effects of heavier-tail (Student's t) correlations ($\rho \approx 0.6$) not great.
- Very informative to update the parameter posterior with $\Delta E(^{25}\mathrm{O},{}^{24}\mathrm{O})$. Subsequently draw 121 parameter samples that we employ in our prediction of oxygen-27/28.

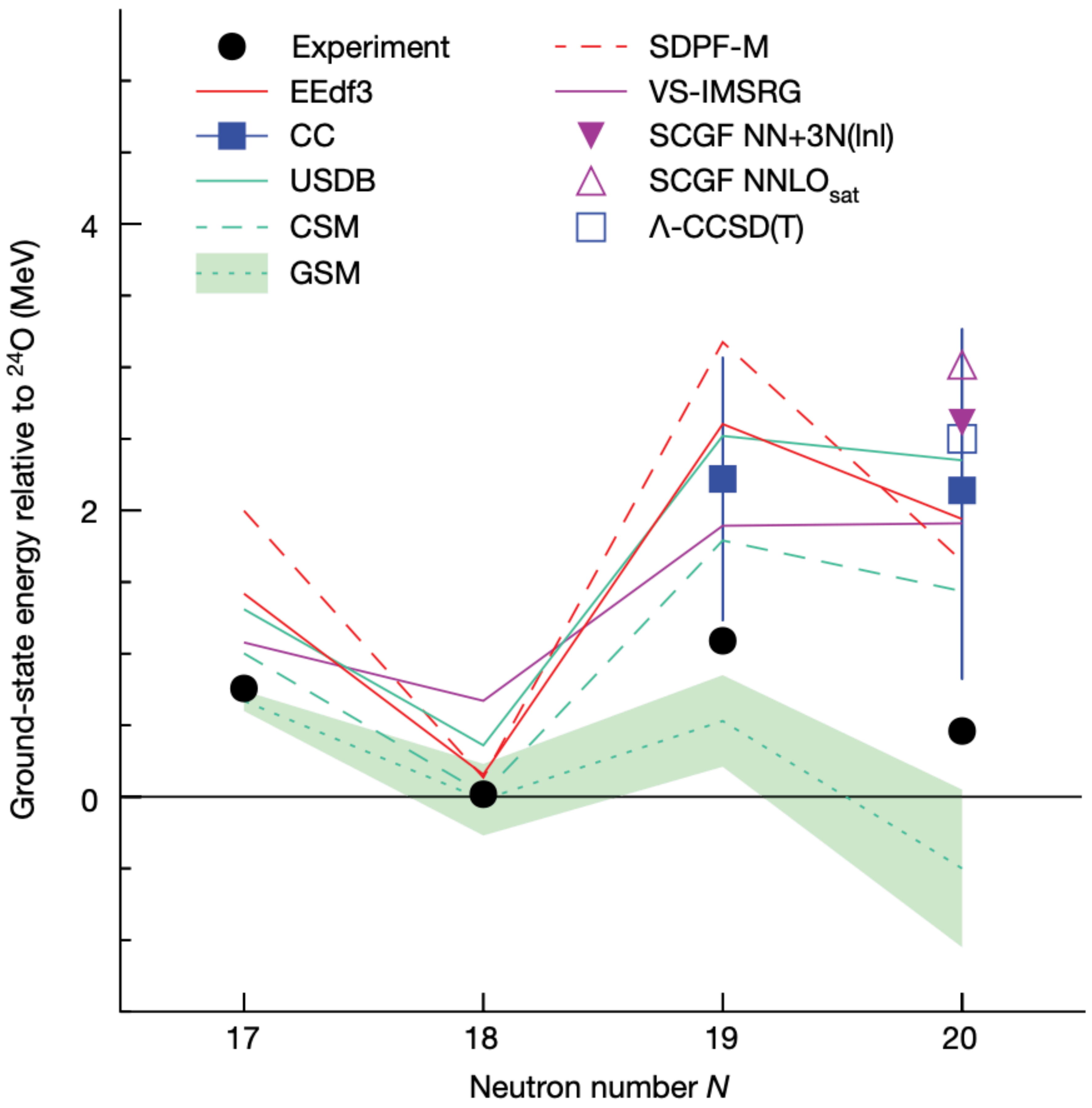
$$\vec{\alpha} \sim \mathrm{p}(\vec{\alpha}|A = 2-25)$$

Y. Kondo et al. Nature (2023)

PPD for complex nuclei

^{28}O separation energies

- We claim with 98% certainty that ^{28}O is unbound with respect to ^{24}O:
- The experimental data point (red star) is away from the posterior maximum. This suggests that only a few finely-tuned chiral interactions are able to reproduce low-energy and exotic oxygen structure Y. Kondo et al. Nature (2023)

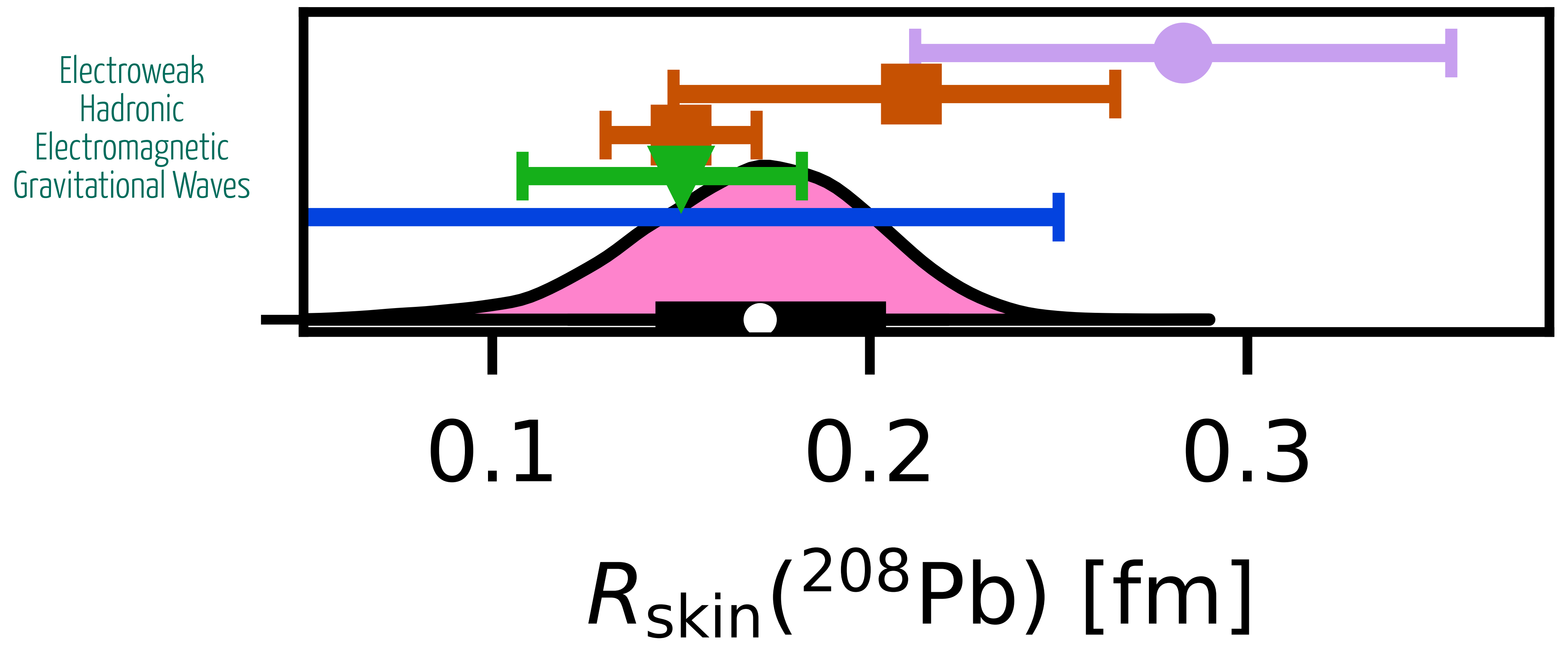


^{208}Pb neutron skin-thickness

n.b. similarly curated history matching data

- We predict a small skin thickness 0.14-0.20 fm in mild (1.5σ) tension with electroweak (PREX) measurement.

B. Hu et al Nature Physics (2022)



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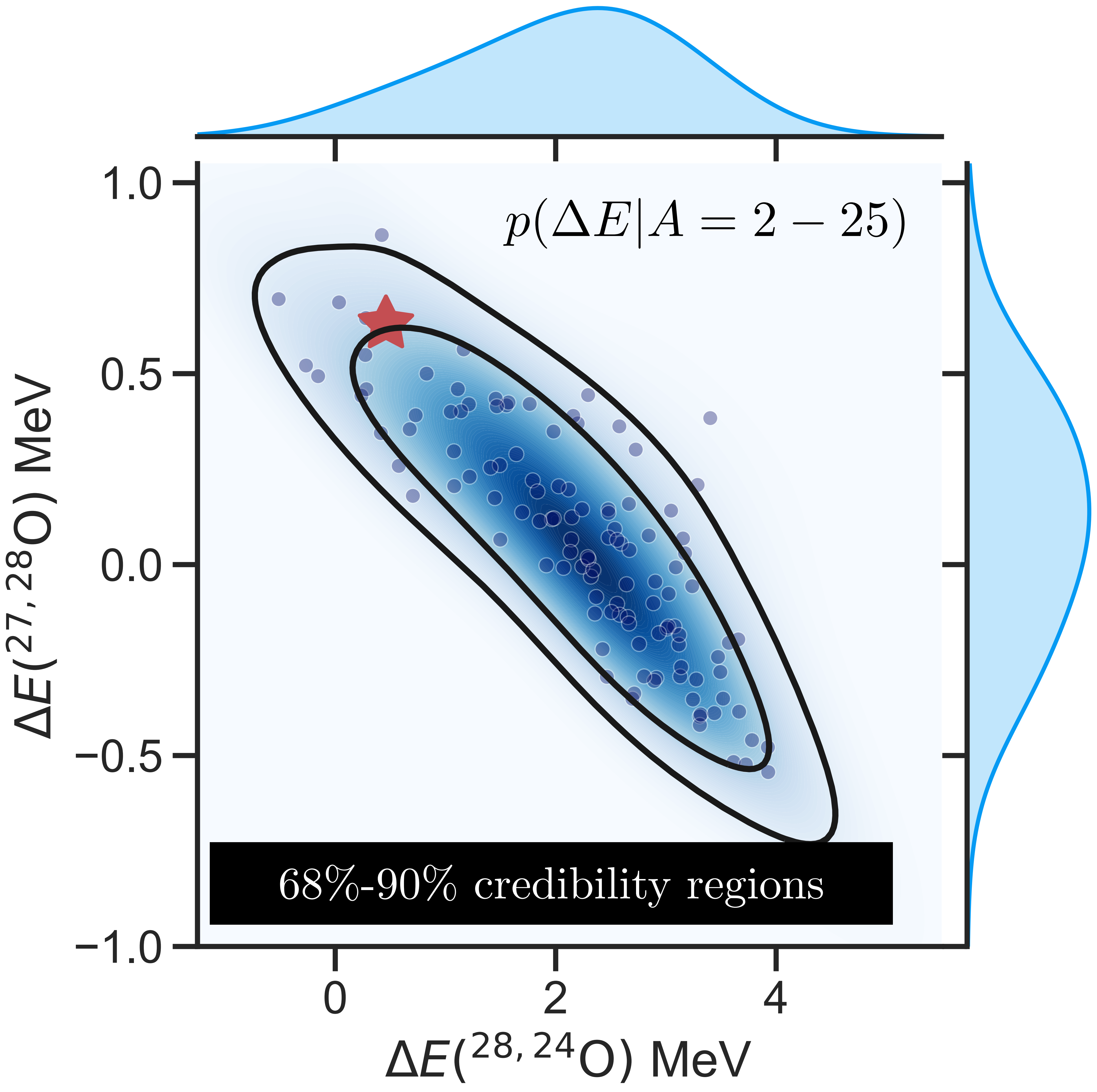

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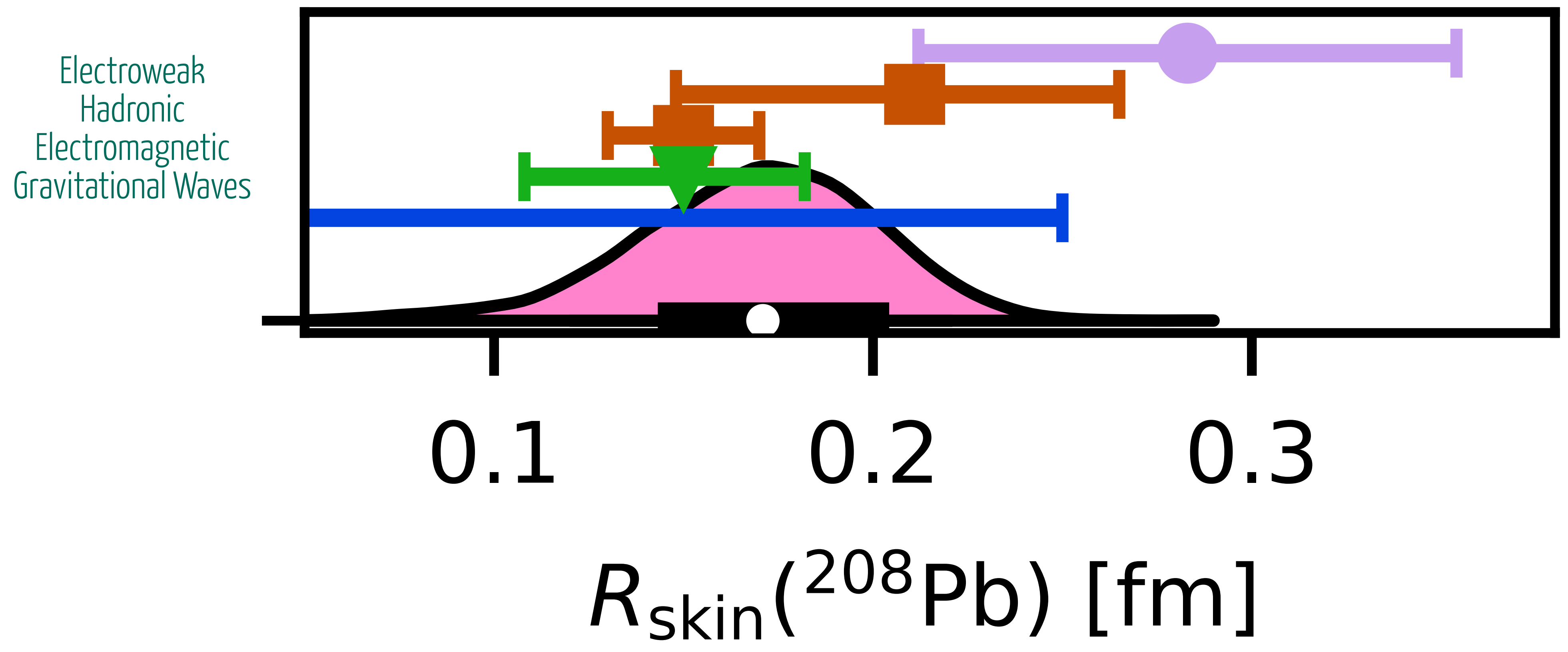
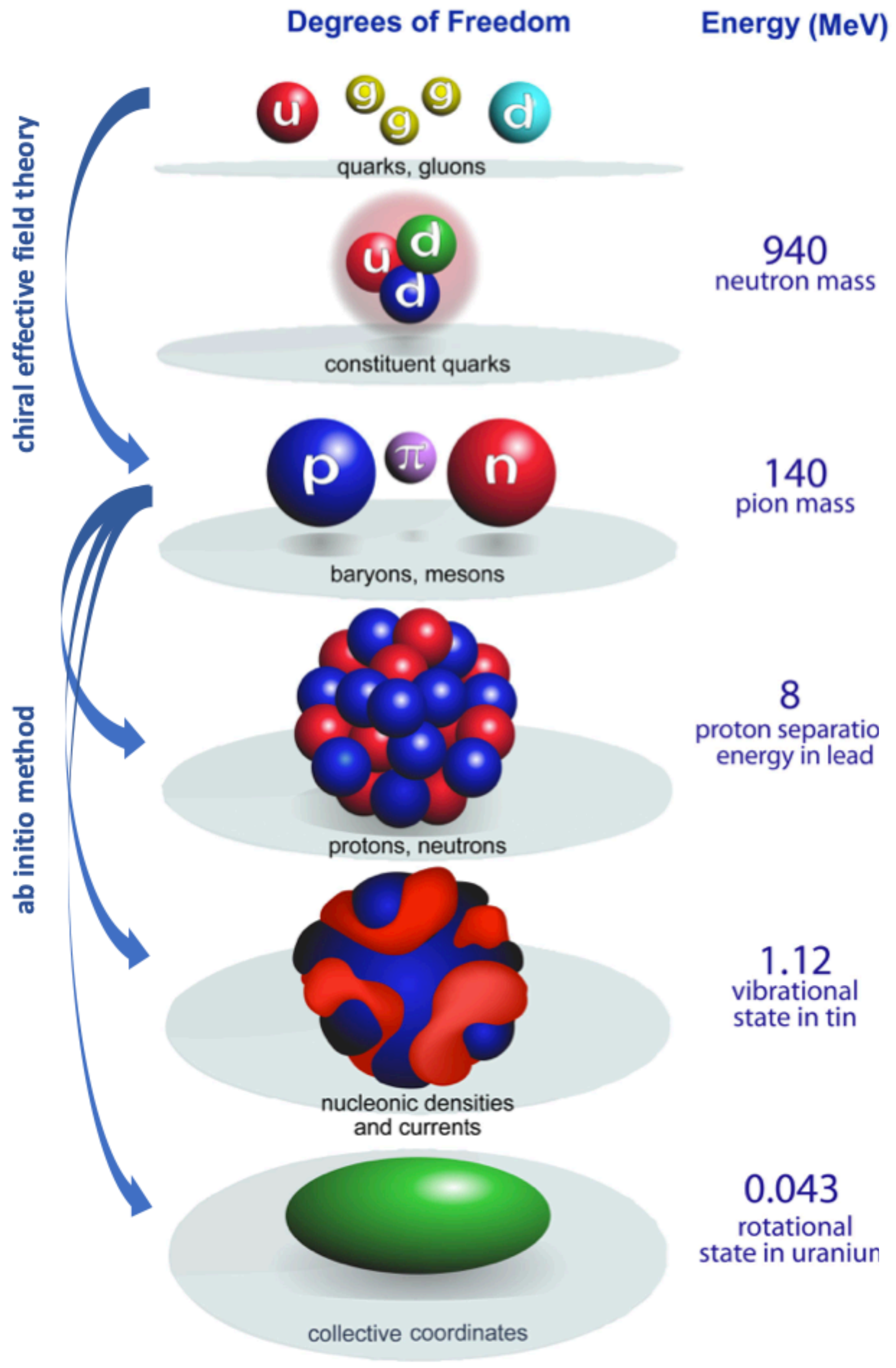
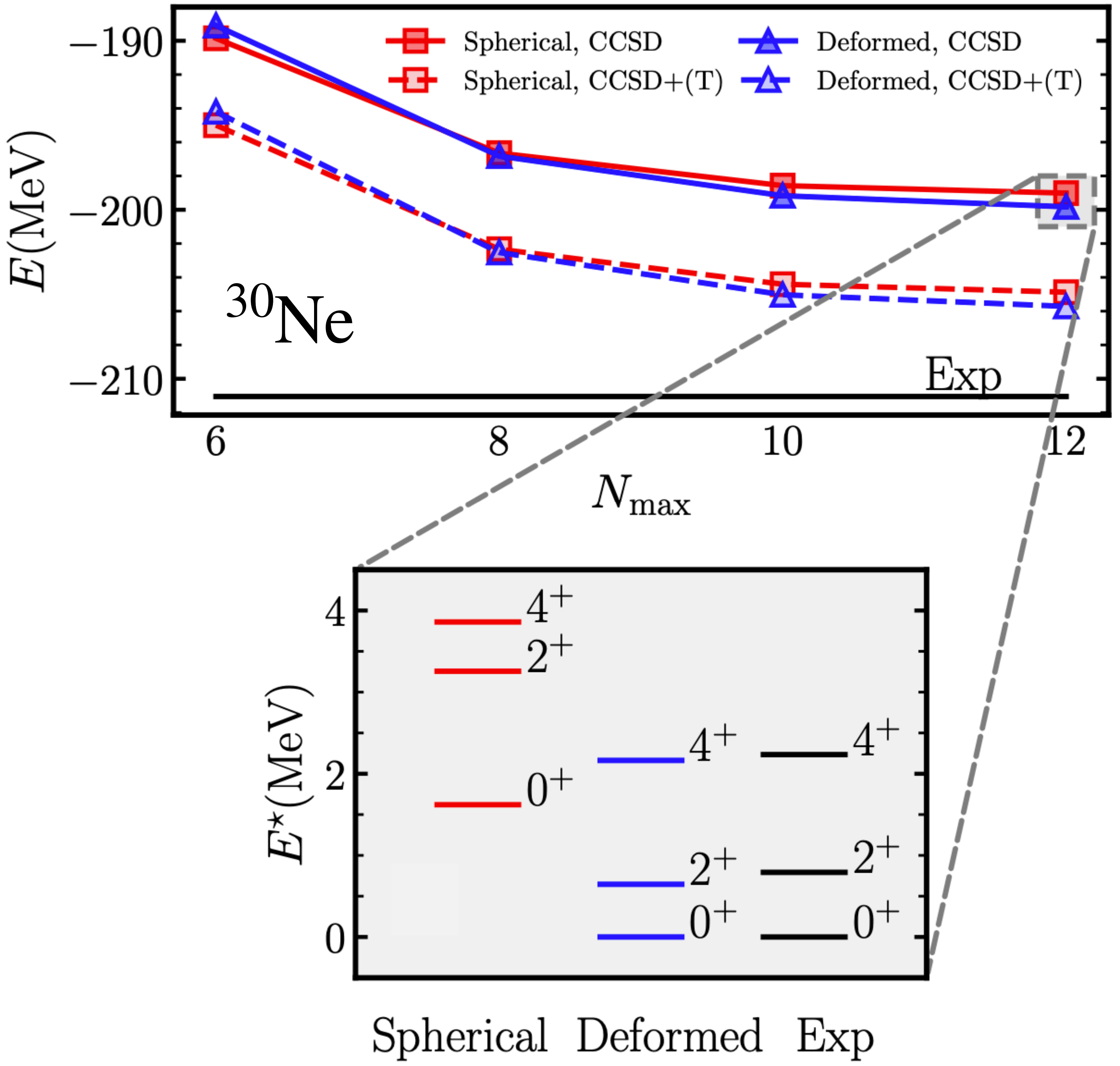


Multiscale physics of atomic nuclei from *ab initio*

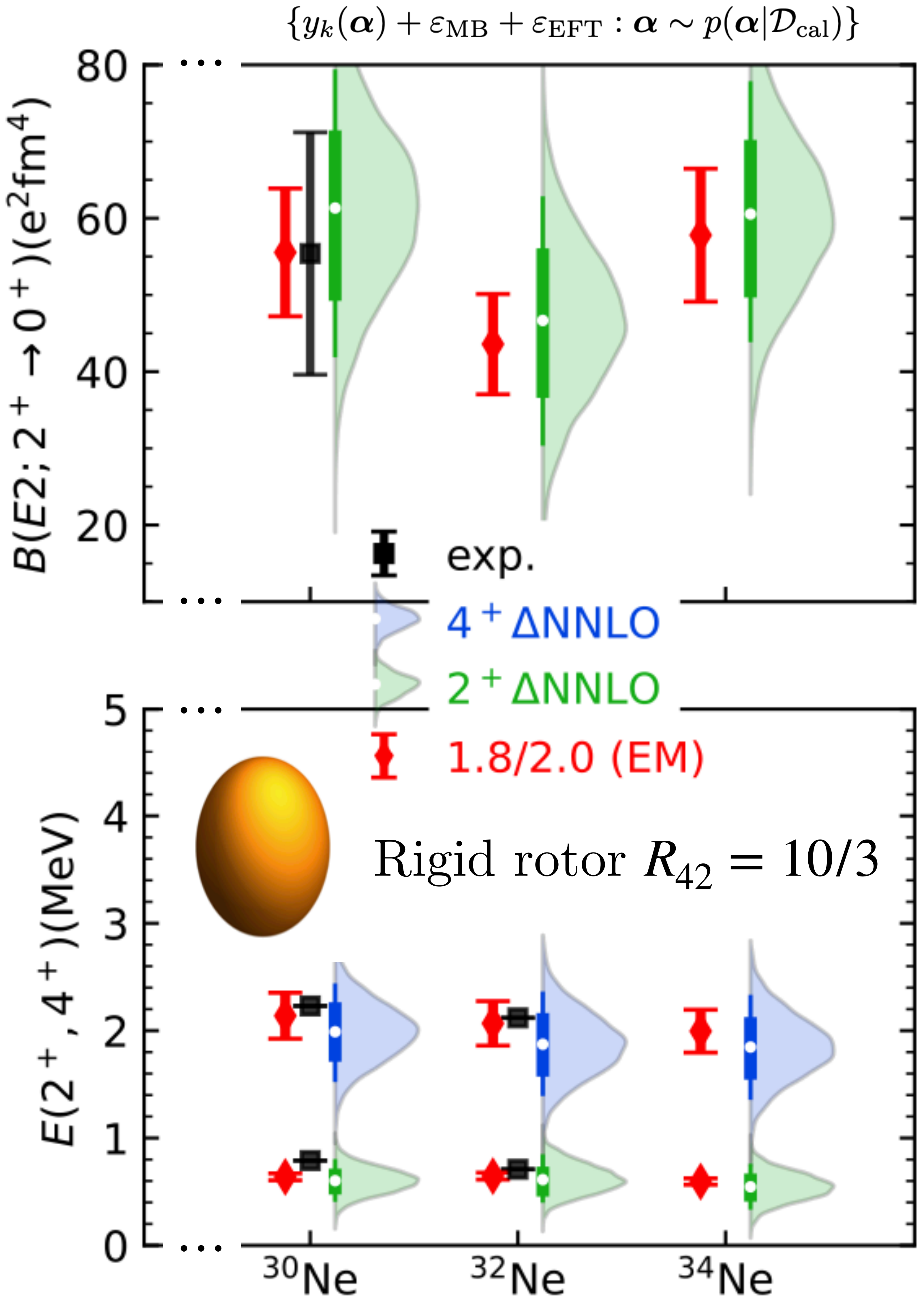


Adapted from NSAC LRP (2007)

PPDs sampled starting from LEC values obtained in the 28-O History Matching.



Z. H. Sun, et al. arXiv (2024)



Global sensitivity analysis

- what is responsible for the variance in the output?

A sensitivity analysis addresses the question *'How much does each model parameter contribute to the uncertainty in the prediction?'*

Variance-based methods for GSA decompose the variance of a certain model output in terms of each input and their combinations.

Global methods deal with the uncertainties of the outputs due to input variations over the whole domain.

Bottleneck: Converging the MC sampling of the variance integrals require approximately 10^6 samples

A. Saltelli et al. Global sensitivity analysis: the primer, John Wiley & Sons

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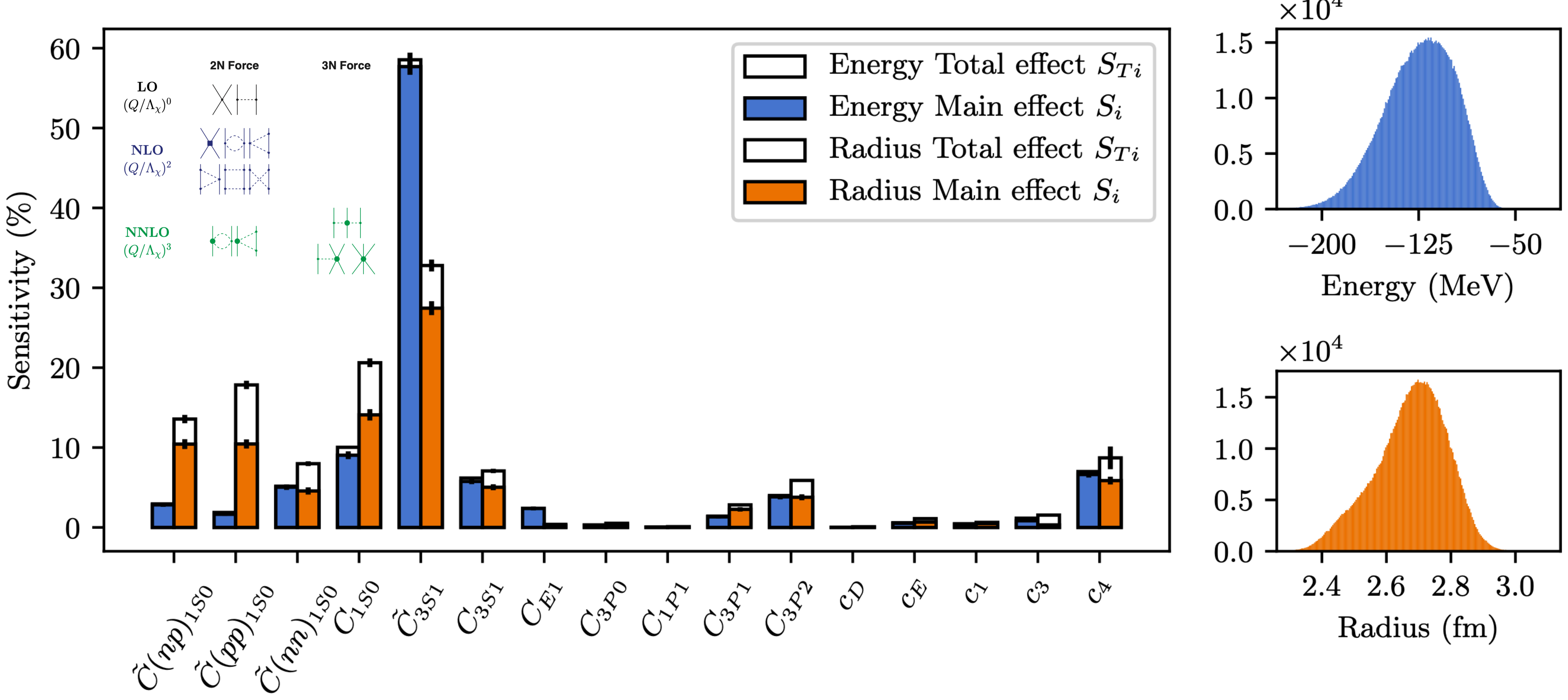
Challenge: relaxing the iid assumption

A. Saltelli et al. Global sensitivity analysis: the primer, John Wiley & Sons

Global sensitivity analysis of an atomic nucleus (^{16}O)

- Radii higher-order sensitivity to low-energy constants



Ekström and Hagen Phys Rev Lett (2019)

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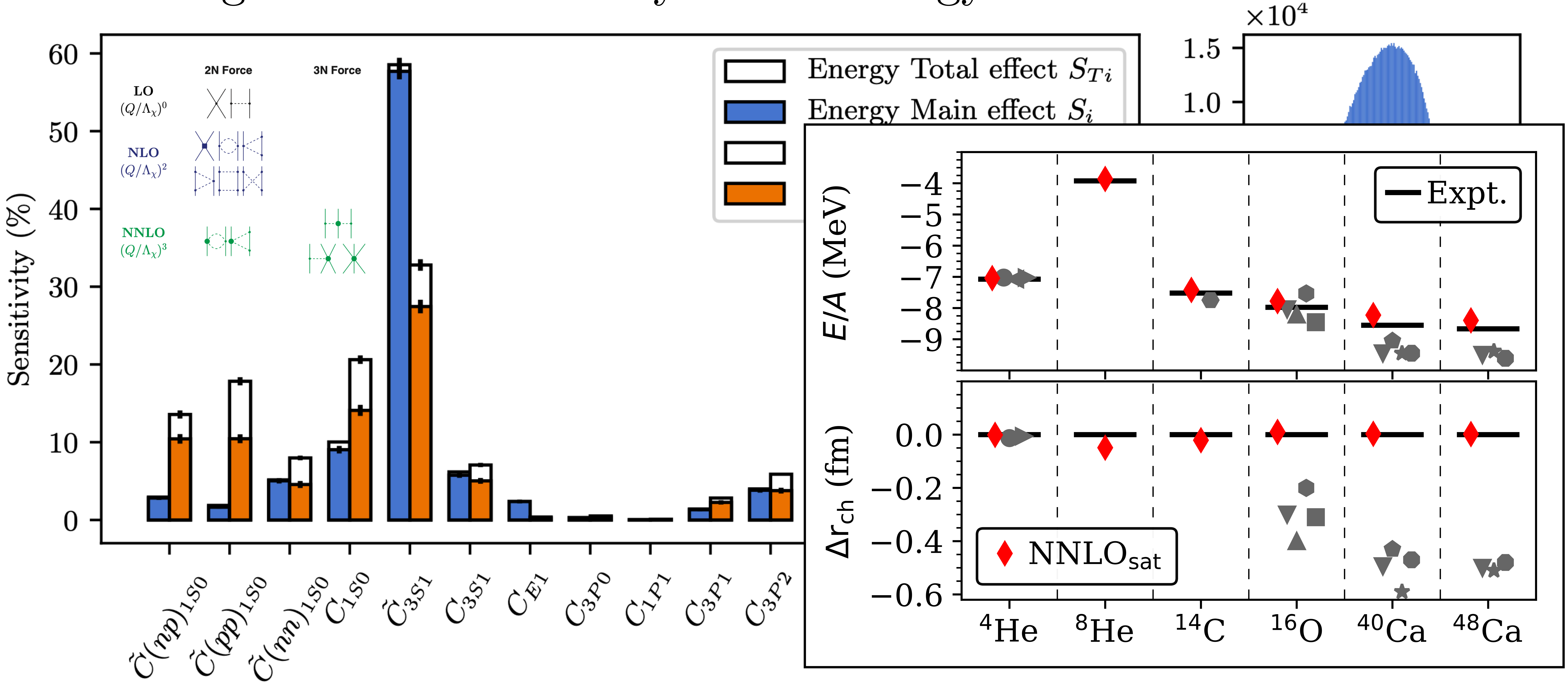
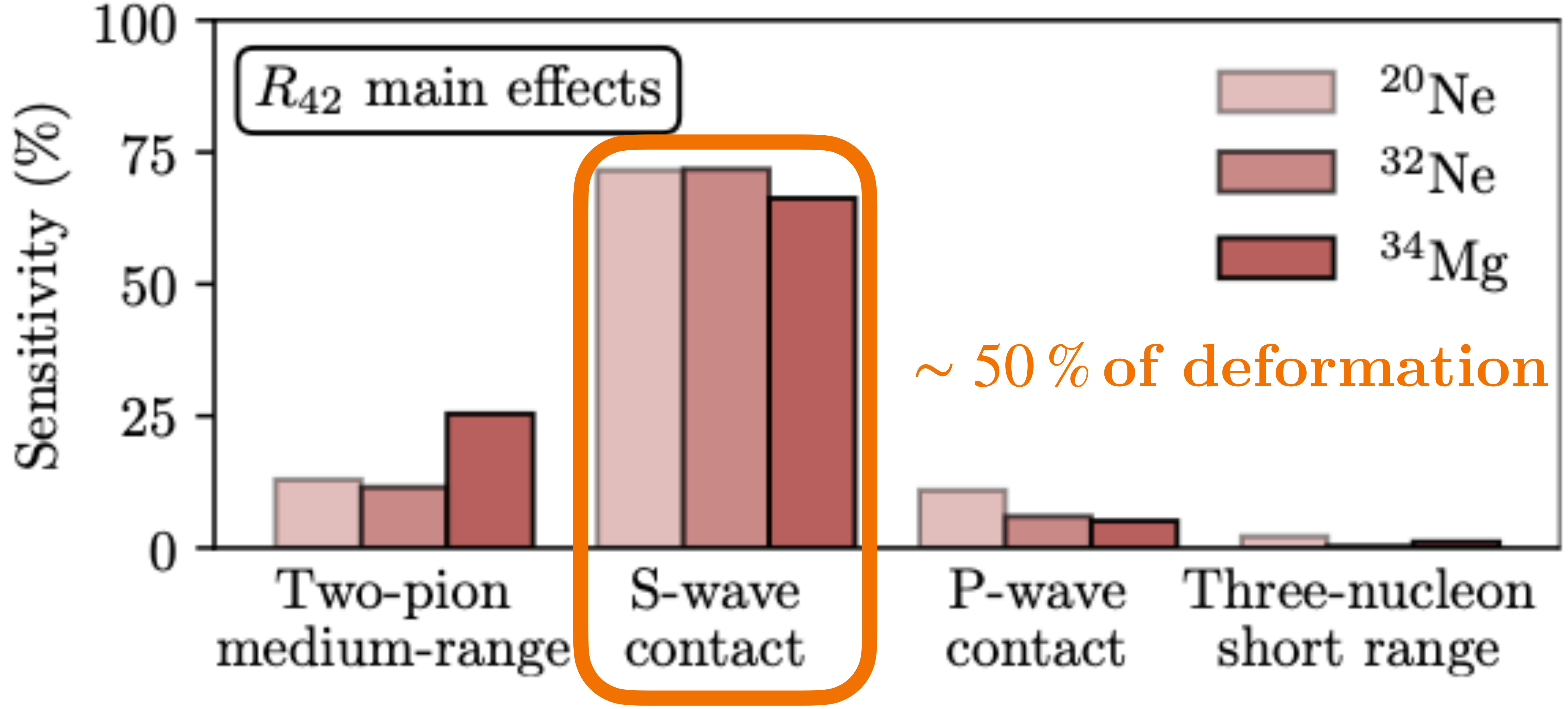


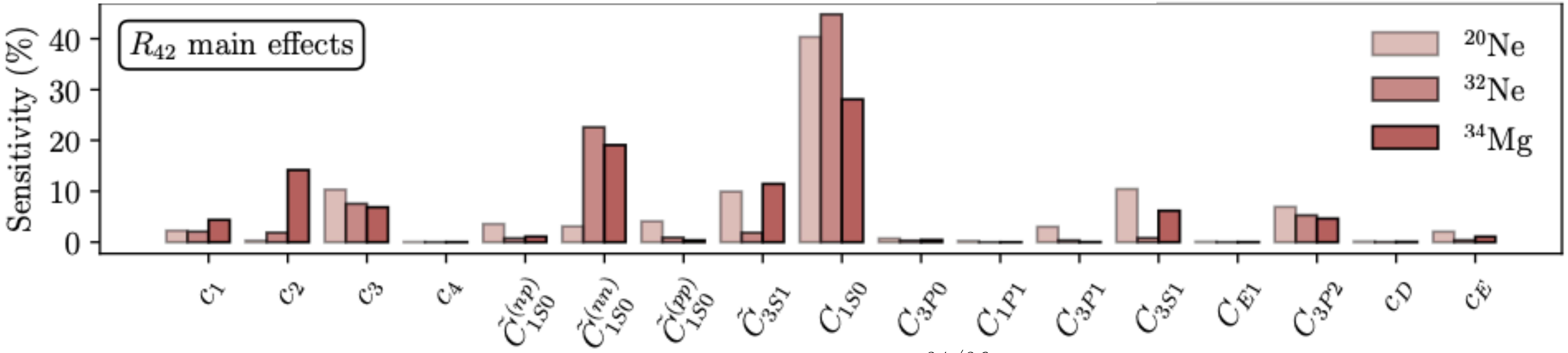
Ekström and Hagen Phys Rev Lett (2019)

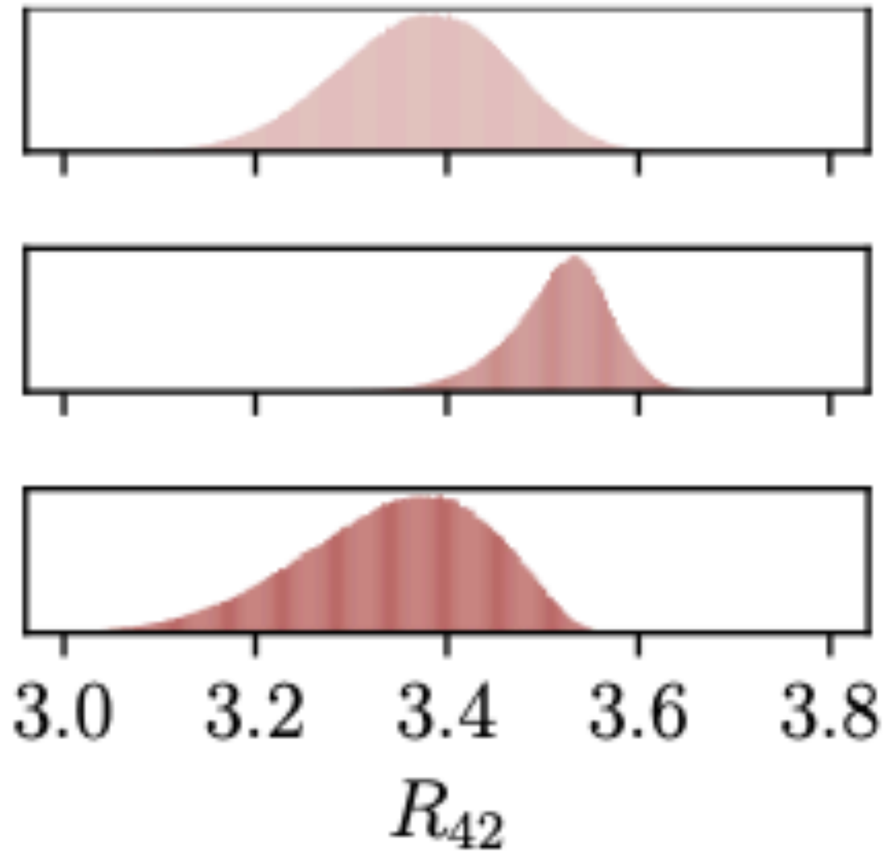
Linking deformation and chiral nuclear forces



$$S_i = \frac{\mathrm{Var}_i(\mathbb{E}_{X-i}[Y|X_i])}{\mathrm{Var}(Y)} \in [0,1]$$ 10^6 Monte Carlo samples

- Adding short-range repulsion appears to increase deformation, probably via reduced pairing.
- Increasing medium-range 2π-exchange increases deformation, presumably by adding attraction in higher partial waves





Z. H. Sun, et al. arXiv (2024)

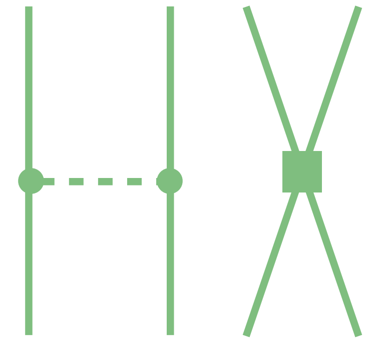
RG-invariant χEFT: proposal by Long & Yang

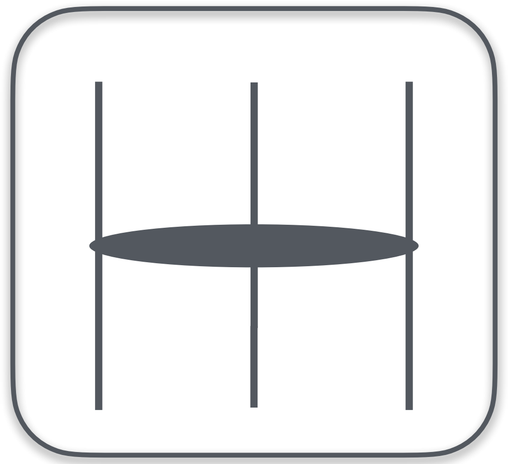
amplitude expanded in (Q/Λ_χ)

non-perturbative one-pion-exchange

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

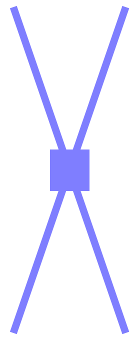
All other partial waves

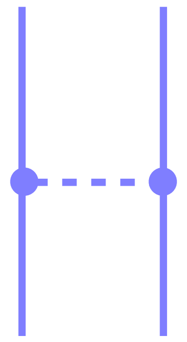
LO g_A  $C_{^1S_0}, C_{^3S_1}, D_{^3P_0}, D_{^3P_2}$



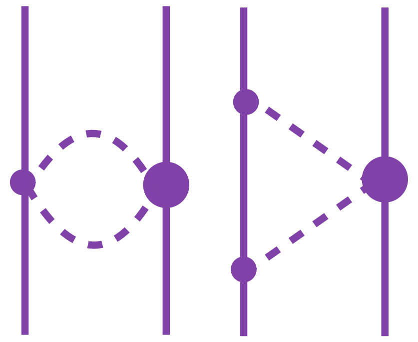
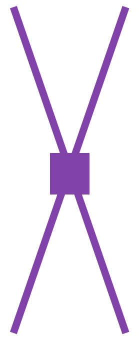
promote?

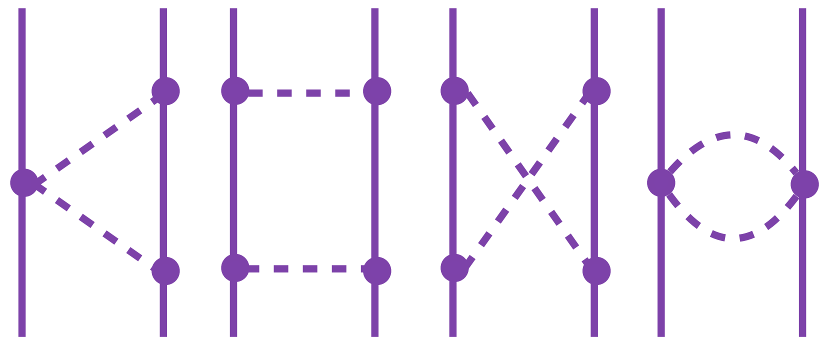
perturbative contritutions

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  $c_{1,3,4}$  $F_{^1S_0}$



Several other RG-invariant PCs exist: Kolck, Kaplan, Savage, Wise, Long, Valderrama, Griesshammer, Yang, Birse, Arriola, Phillips, ...

RG-invariant χEFT: proposal by Long & Yang

non-perturbative one-pion-exchange

Challenge: analyze RG-invariance for $A \gtrsim 4$ systems

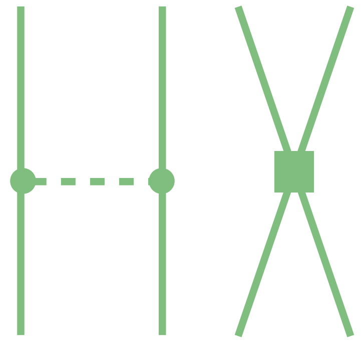
$^3S_0, ^3S_1 - ^3D_1, ^3P_{0,1}, ^3P_2 - ^3F_2, ^1P_1$

All other partial waves

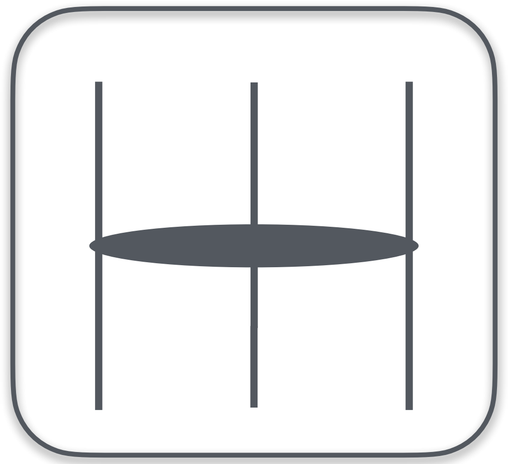
amplitude expanded in (Q/Λ_χ)

perturbative contritutions

LO g_A

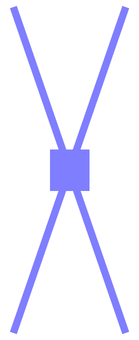


$C_{^1S_0}, C_{^3S_1}, D_{^3P_0}, D_{^3P_2}$



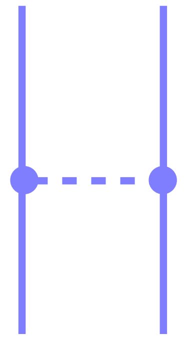
promote?

NLO



$D_{^1S_0}$

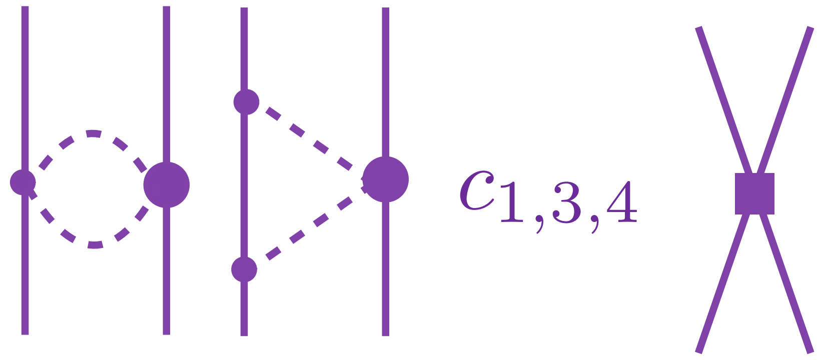
g_A



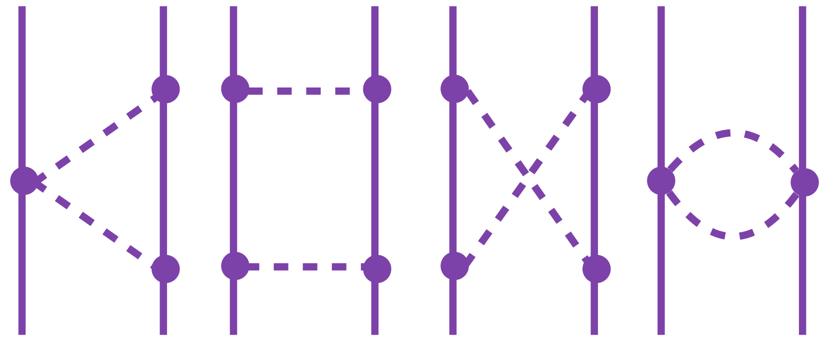
N²LO

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

N³LO



$c_{1,3,4}$ $F_{^1S_0}$



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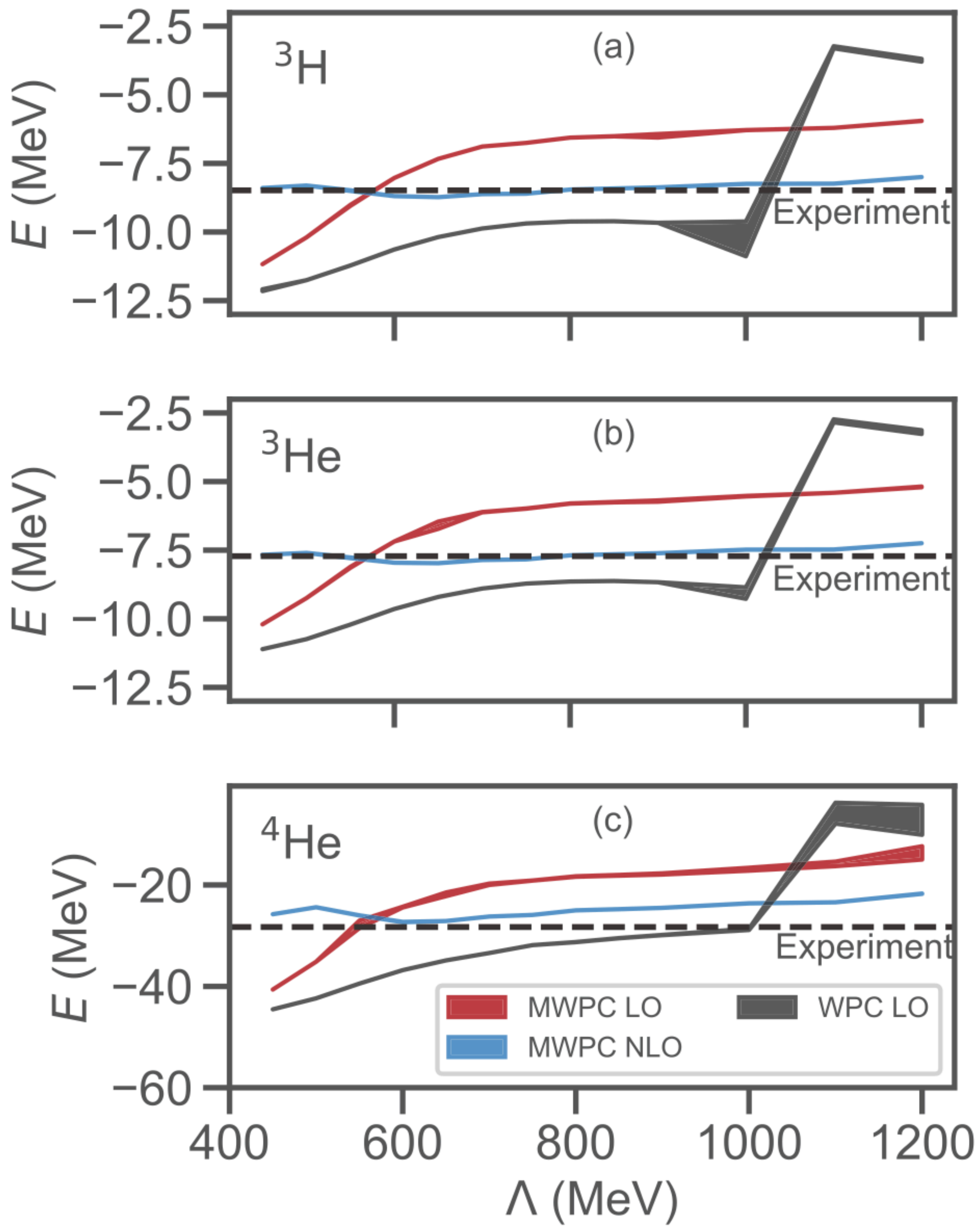
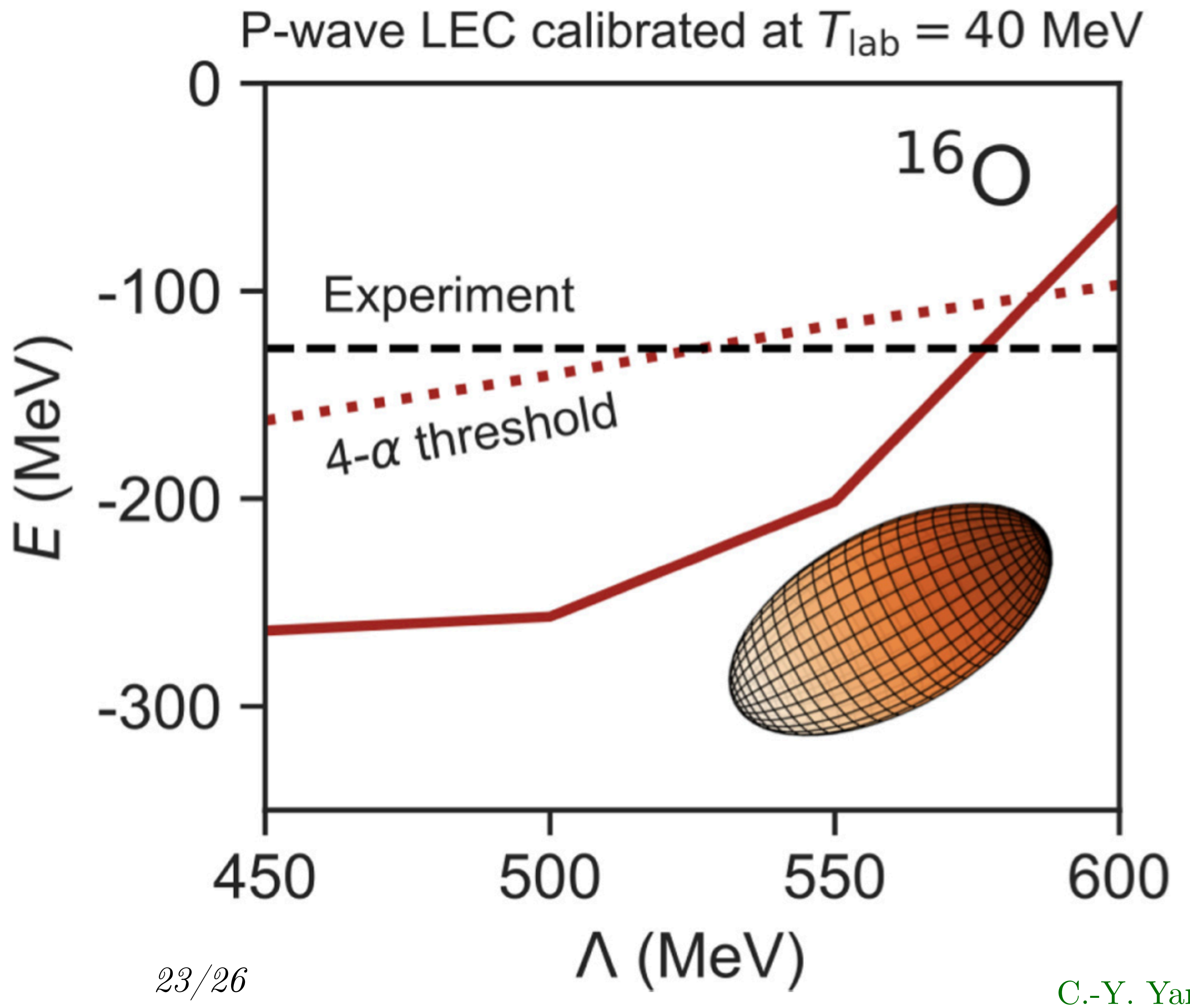
Problems at leading order in χEFT

Atomic nuclei with A>4 unstable



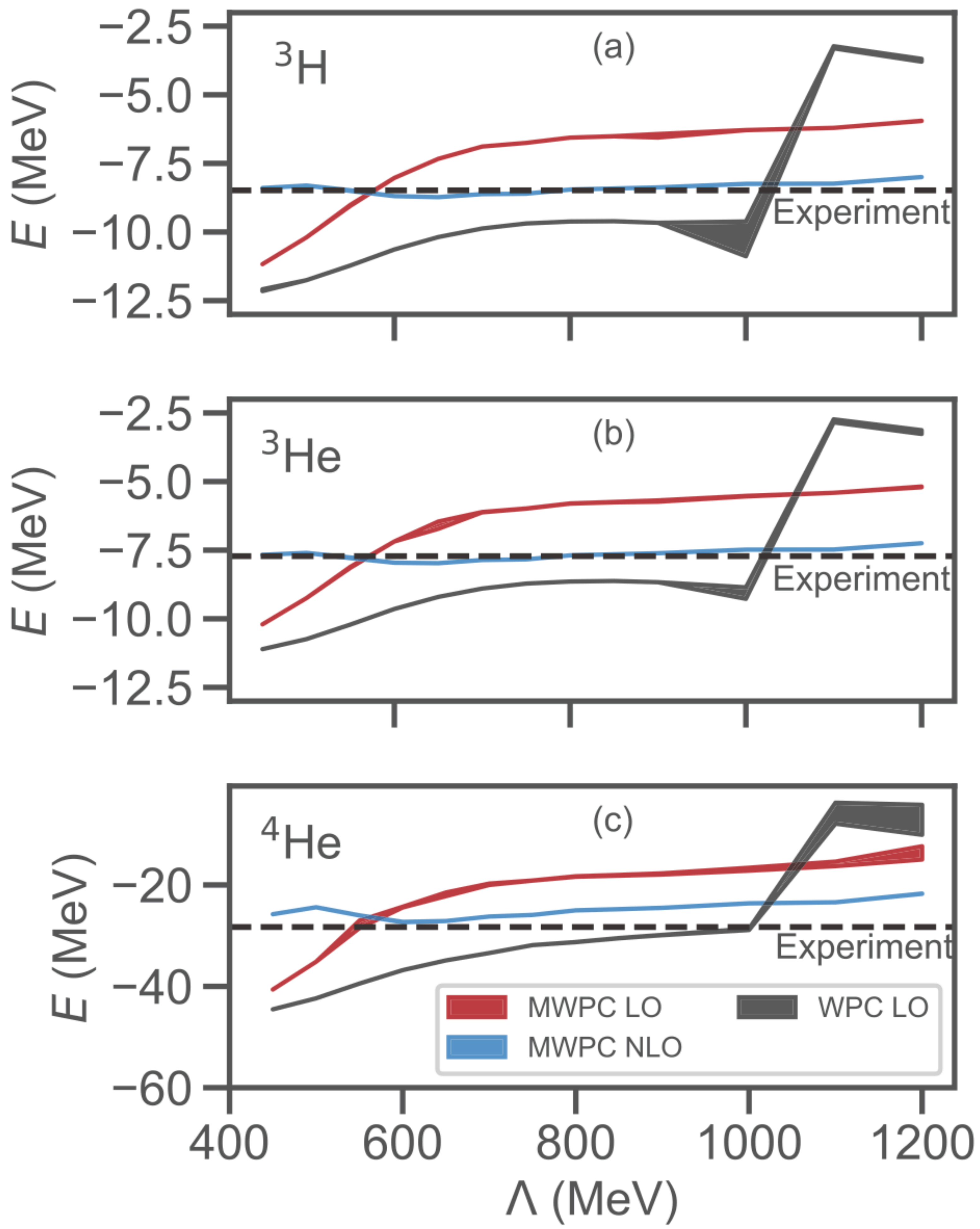


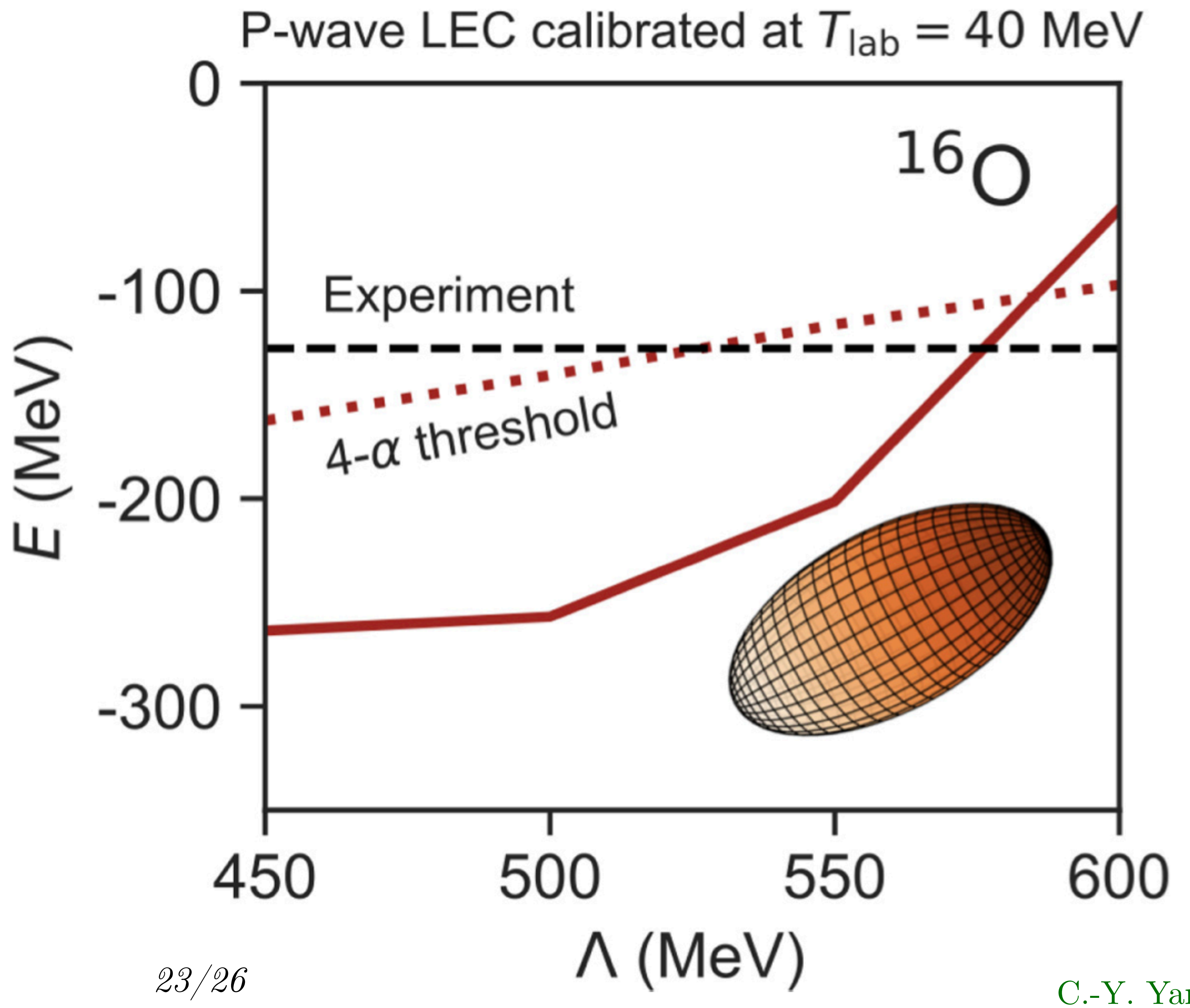
C.-Y. Yang, et al. Phys. Rev. C (2021)

Problems at leading order in χEFT

Atomic nuclei with A>4 unstable

Challenge: possible fine tuning effects? flawed power counting?





C.-Y. Yang, et al. Phys. Rev. C (2021)

A possible solution: promote many-body forces

A combinatorial argument

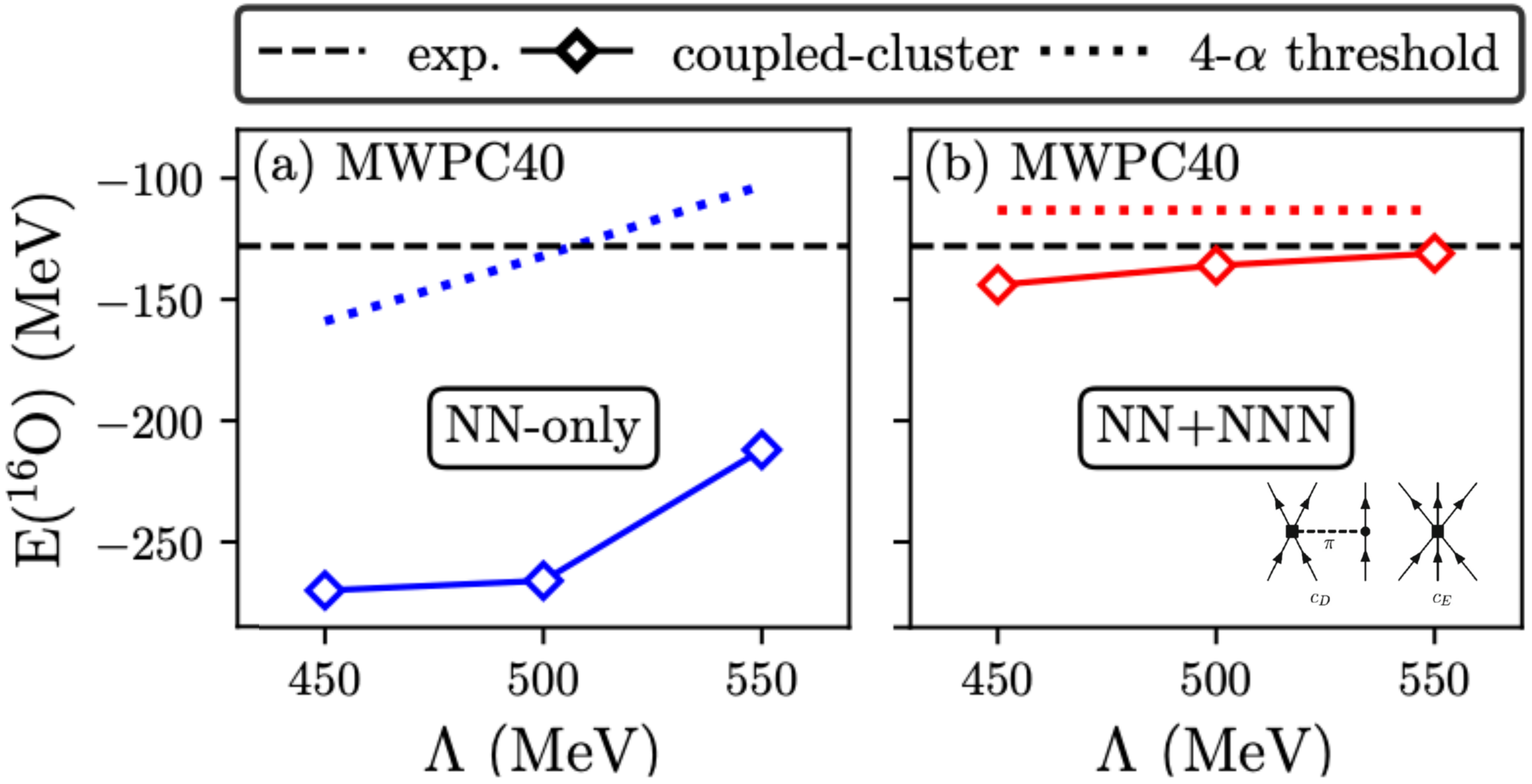


Table 1 Binding energy per nucleon (B_A/A) obtained with NN-only and NN+NNN interactions at LO. Here MWPC40 and Λ=450 MeV is adopted

B_A/A	^{3}H	^{4}He	^{16}O	^{40}Ca
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C.-J. Yang, et al. The European Physical Journal A (2023)

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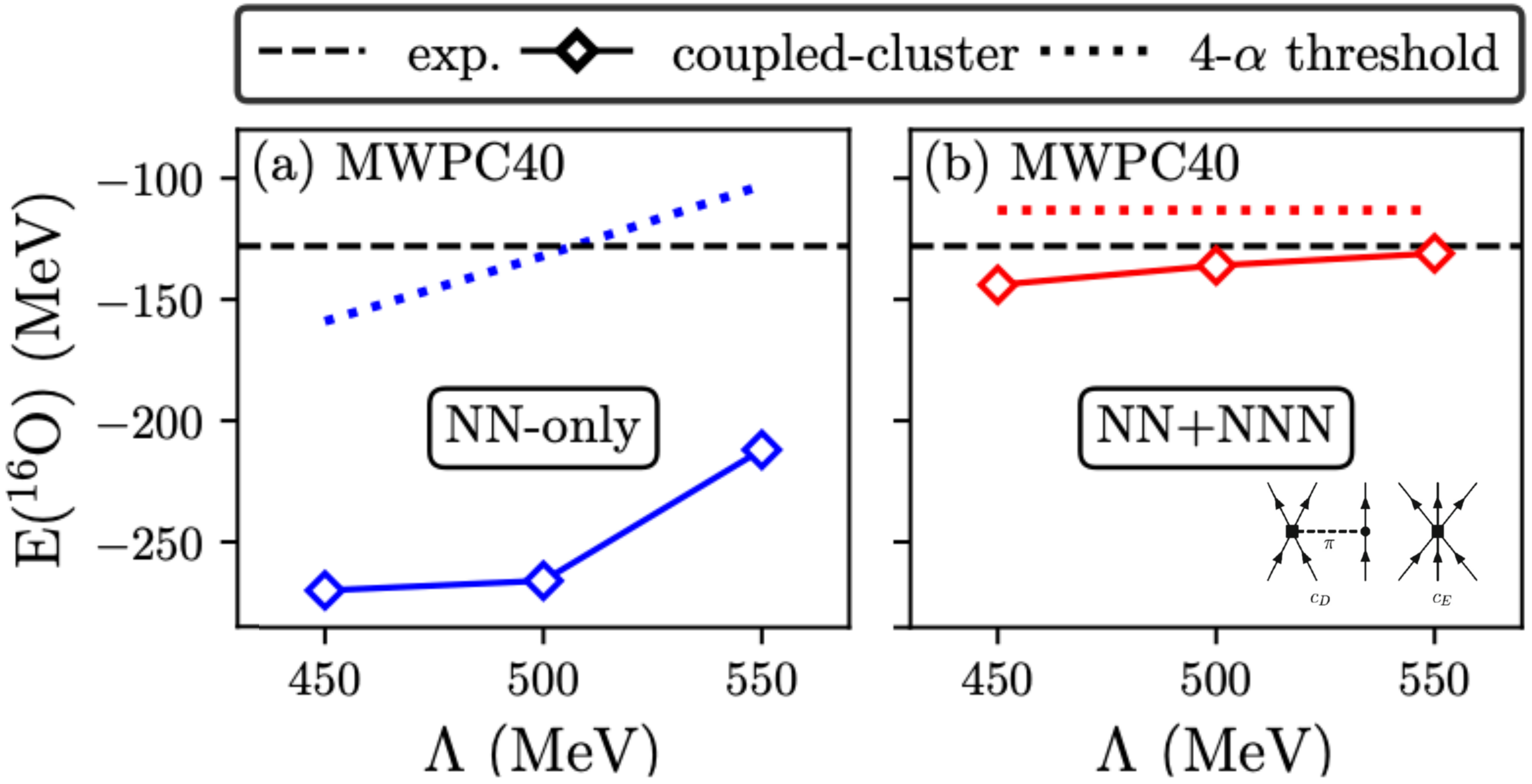

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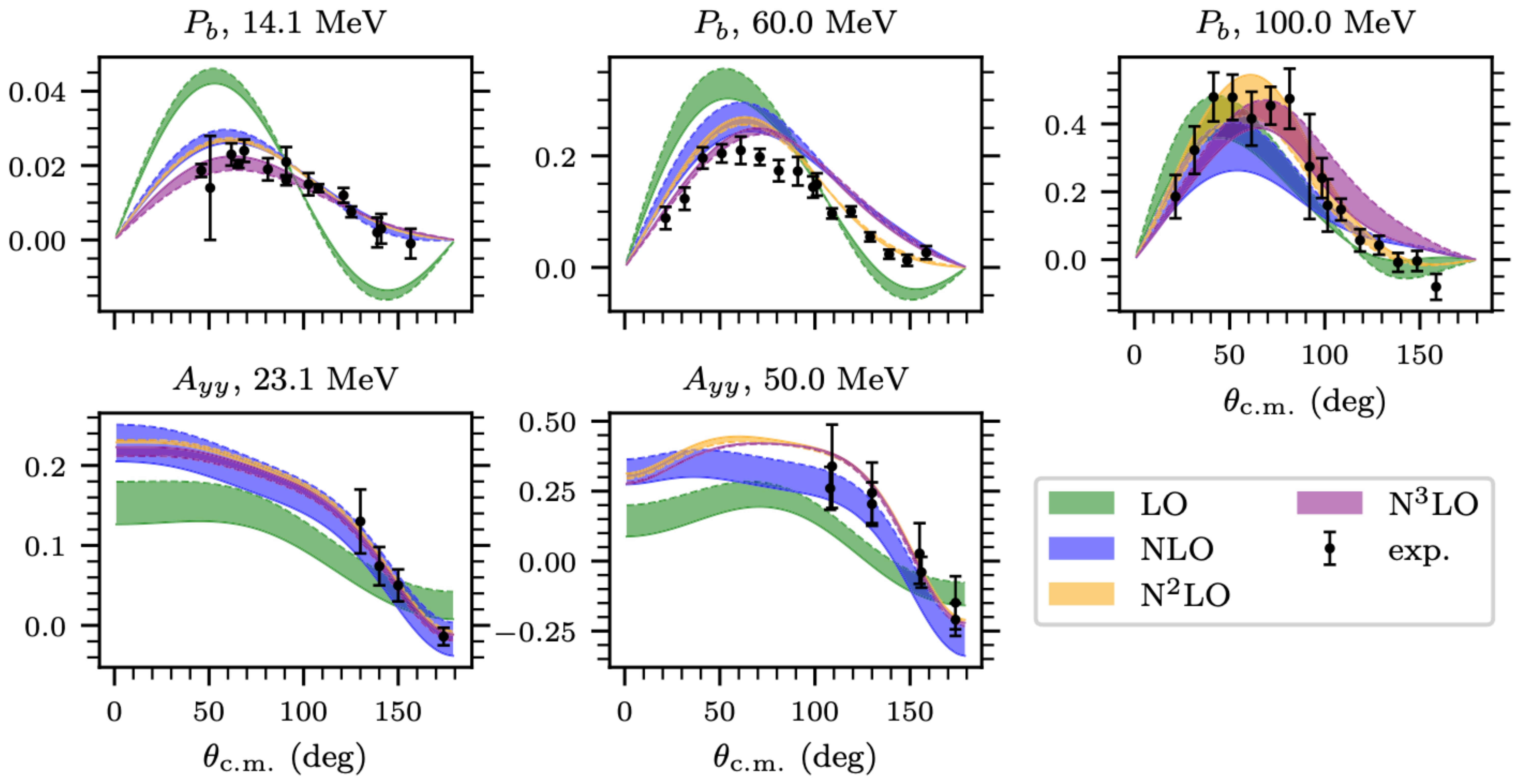
Challenge: explore enhanced importance of 3/4-body forces for increasing mass number and quantify uncertainties

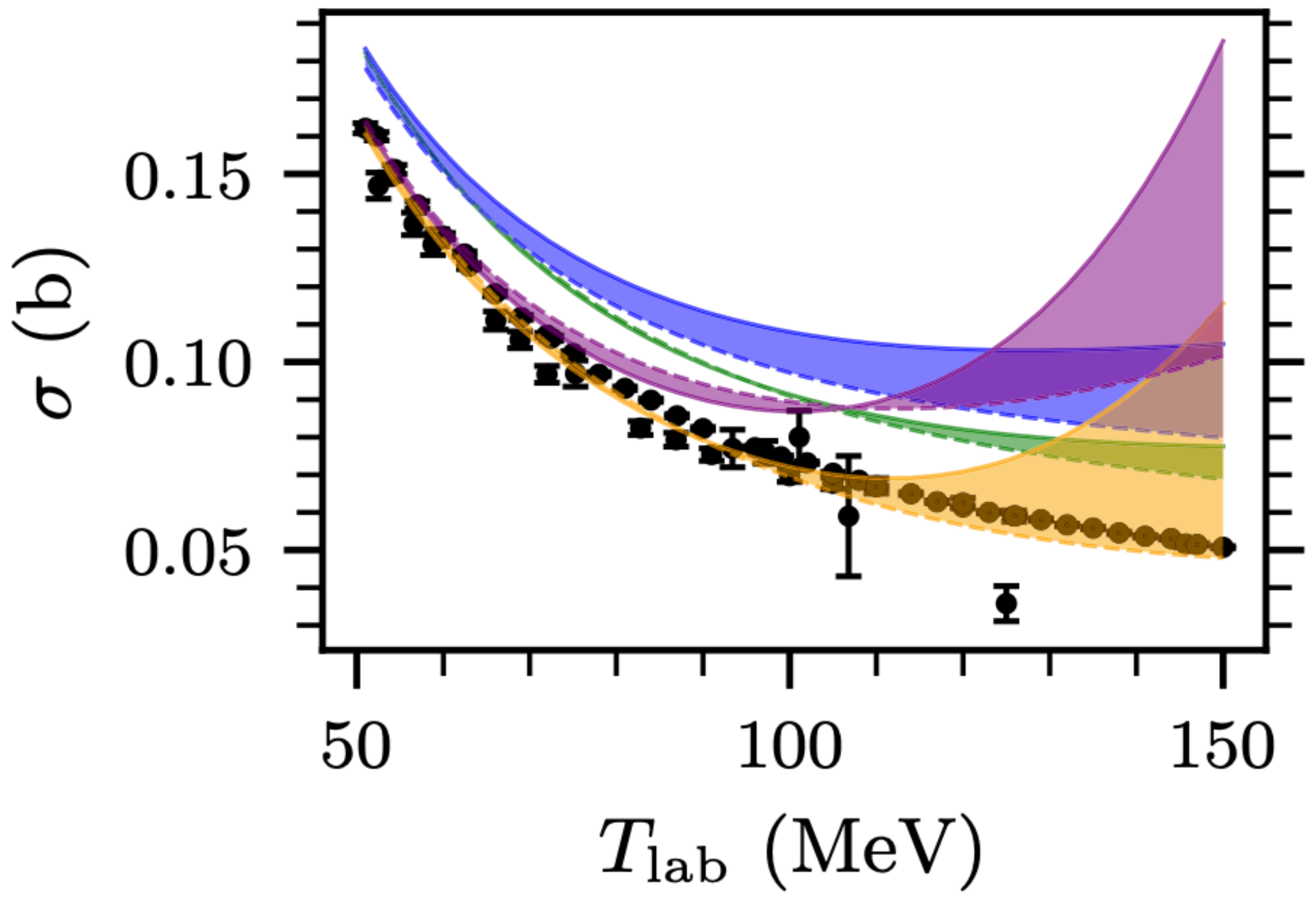
C.-J. Yang, et al. The European Physical Journal A (2023)

A possible solution: mitigate overfitting

Preparing for Bayesian inference and A>4 predictions beyond NLO MWPC

Bands indicate $\Lambda = 500 - 2500\,\mathrm{MeV}$





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

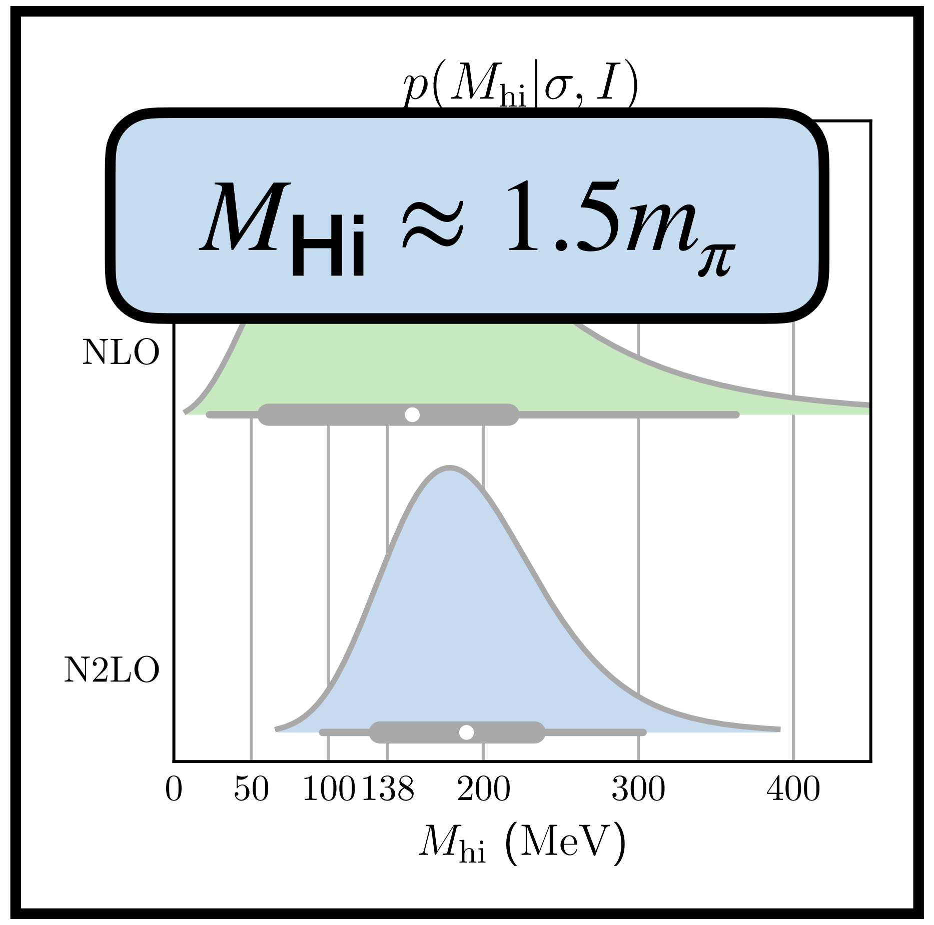
$p(\Lambda_b | y, I)$?

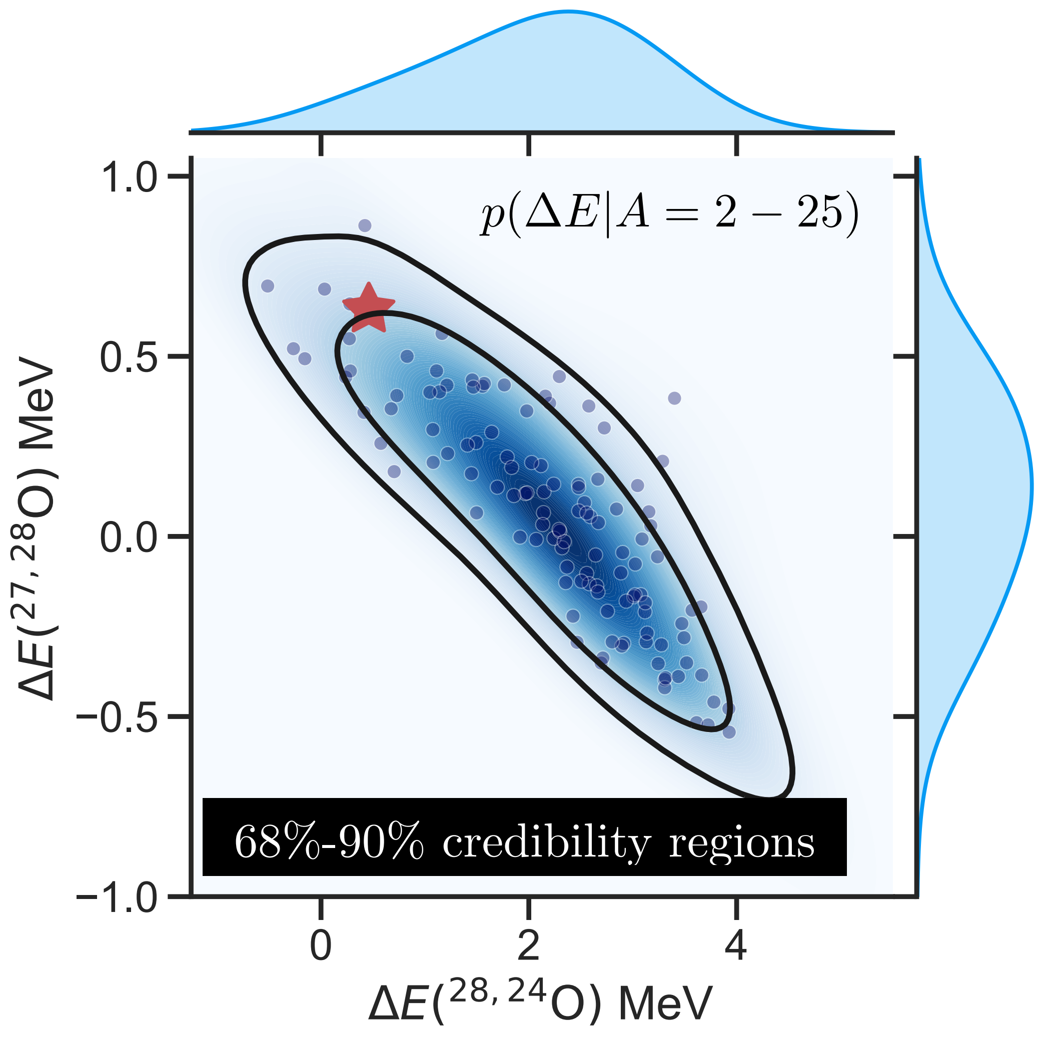
O. Thim, et al, Phys. Rev. C (2024)

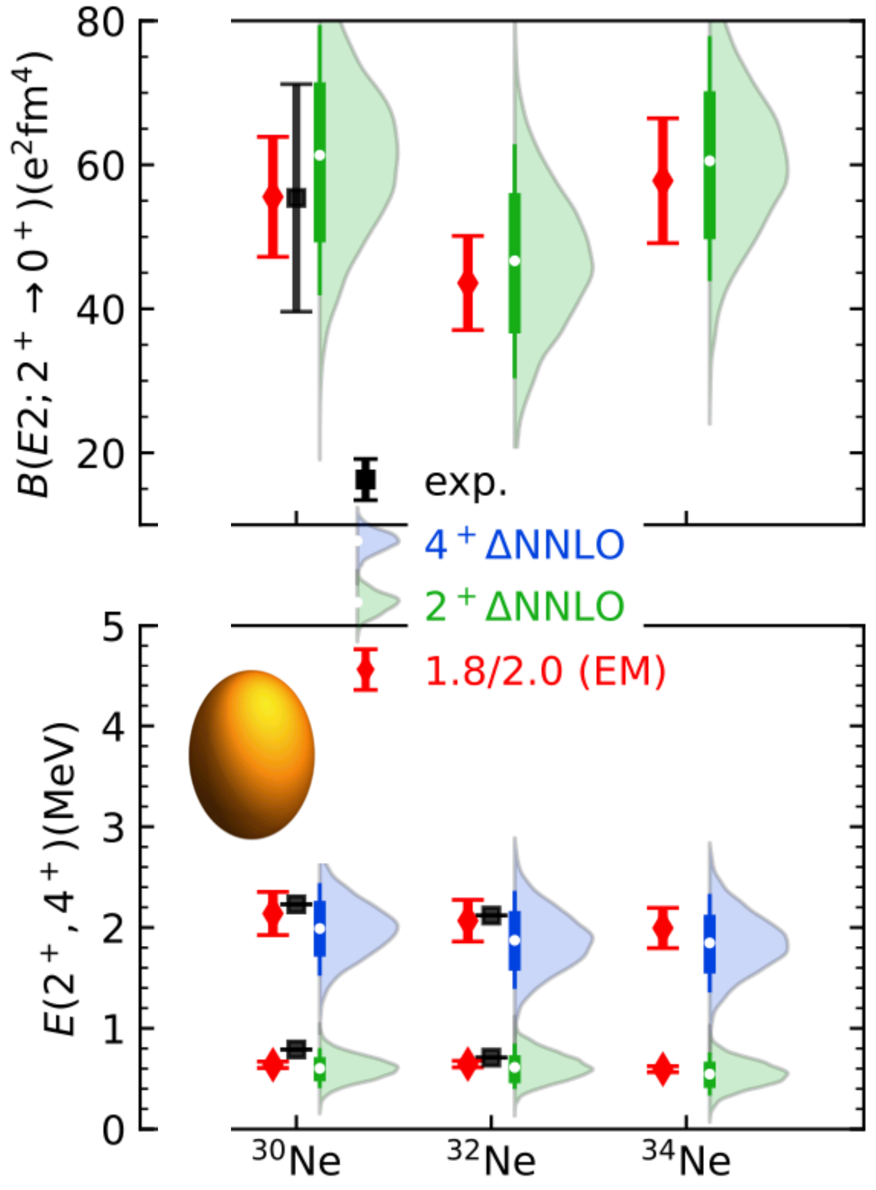
Summary

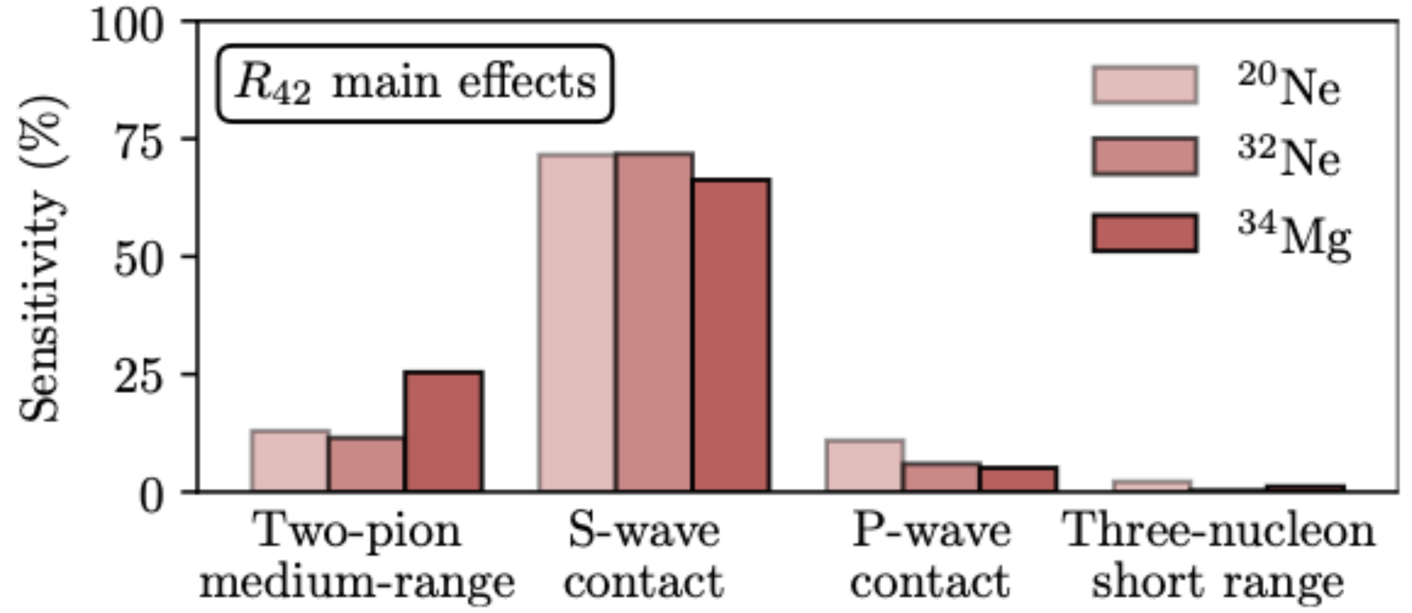
Nuclear *ab initio:* a *systematically improvable* approach for quantitatively describing nuclei using the finest resolution scale possible while maximizing its predictive capabilities.

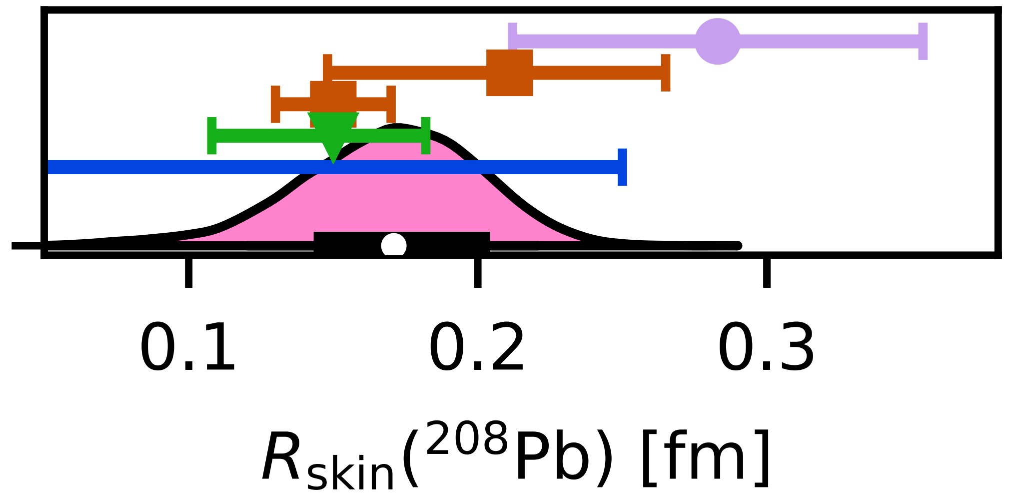
We are quantifying posterior predictive distributions and sensitivities of nuclear observables











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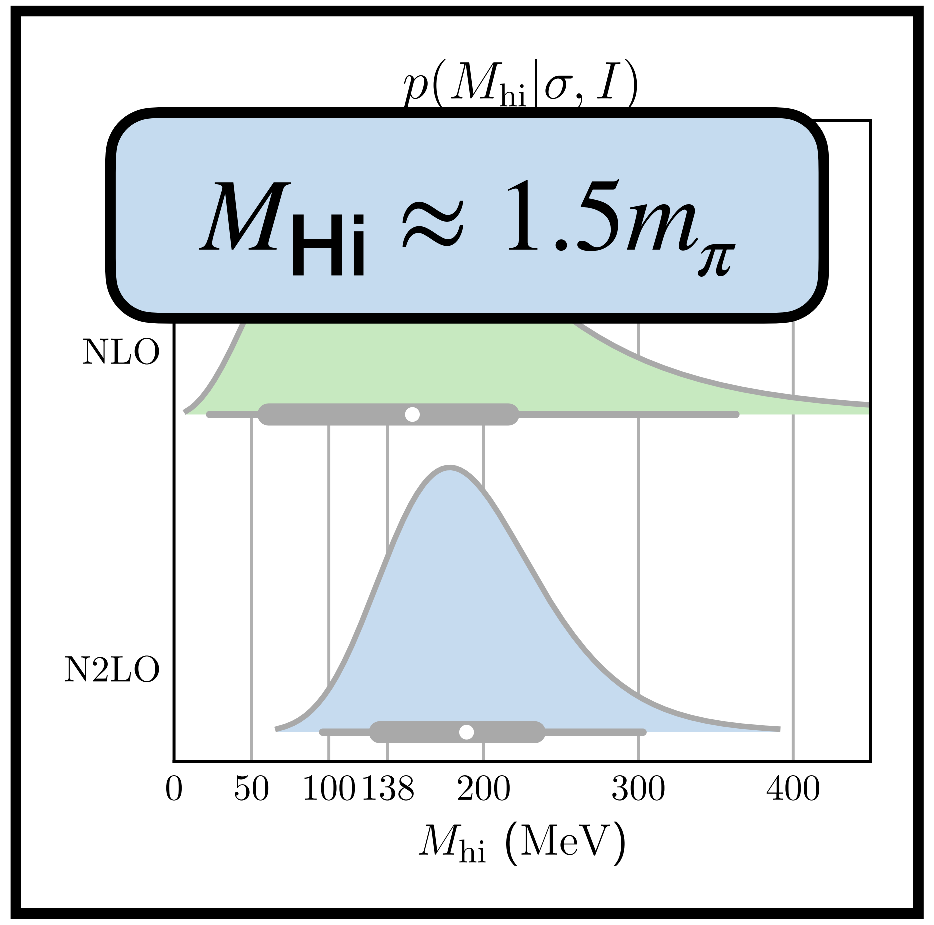

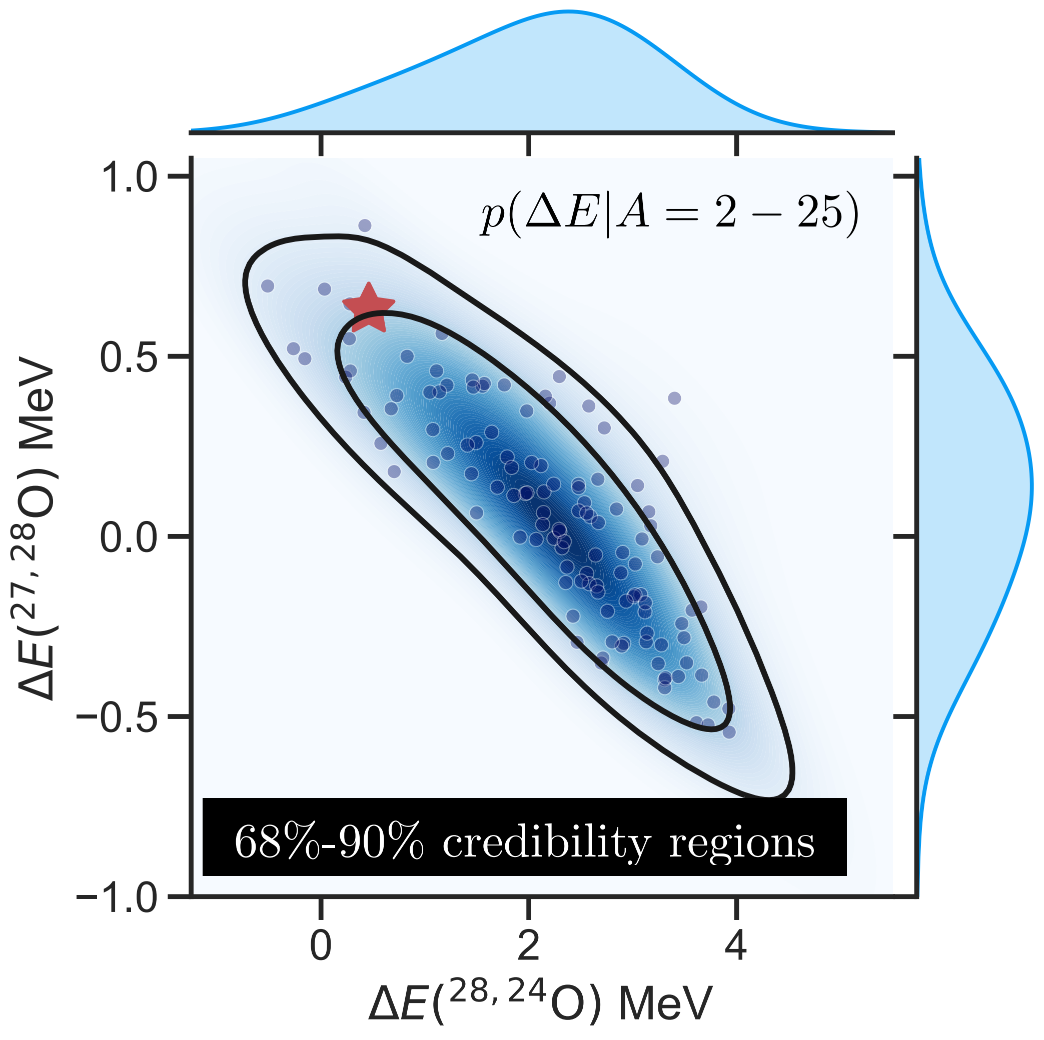

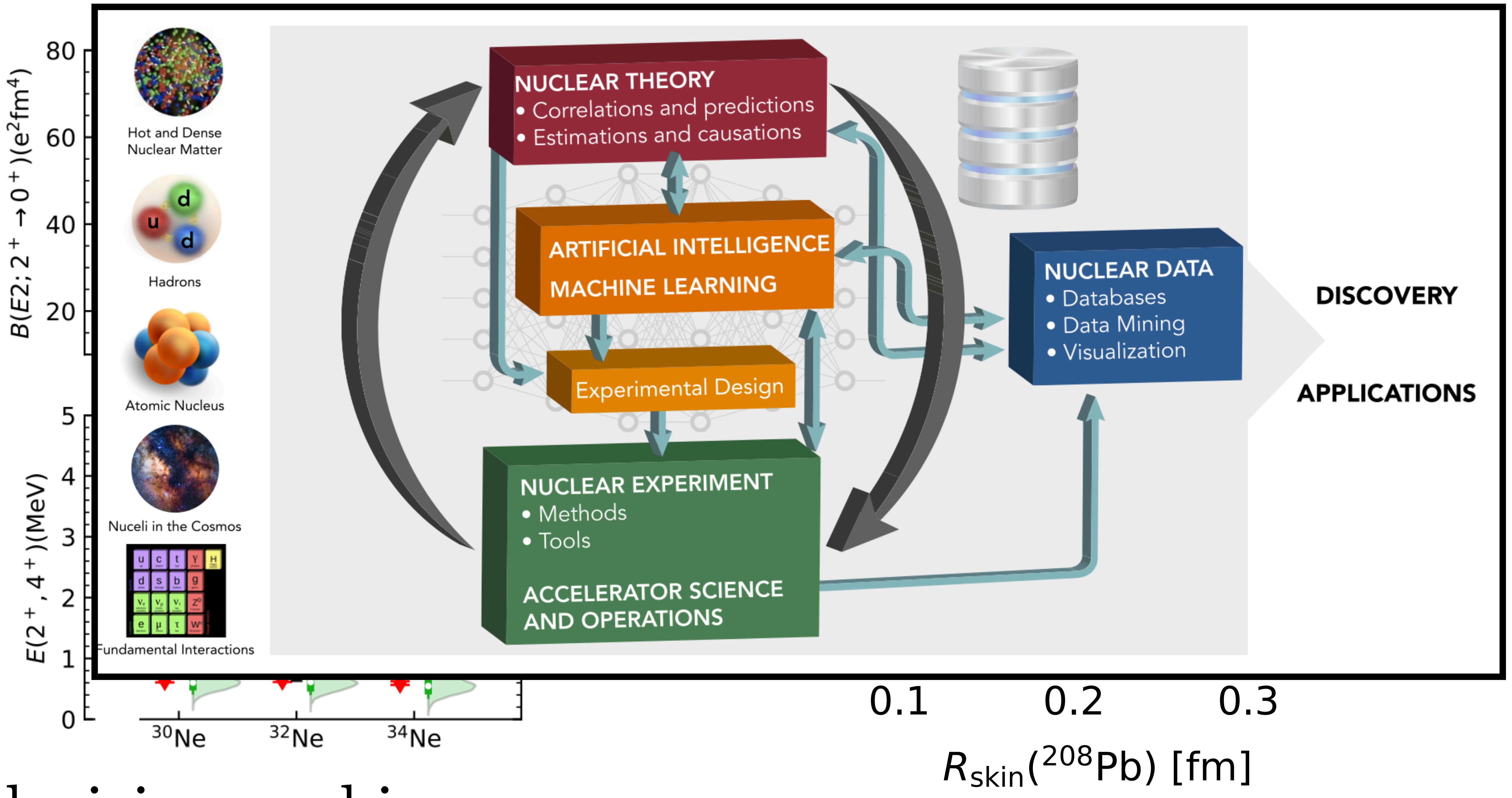

Next, we should try to utilize them in our decision making process

Thank you for your attention!