

Uncertainty quantification of $0\nu\beta\beta$ NMEs

INT26-2a

Antoine Belley

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Acknowledgement



- Ronald Fernando Garcia Ruiz
- **Jose Miguel Muños Arias**



- **Taiki Shickele**



- **Alex Todd**



- Jason Holt



- Ragnar Stroberg



- Heiko Hergert



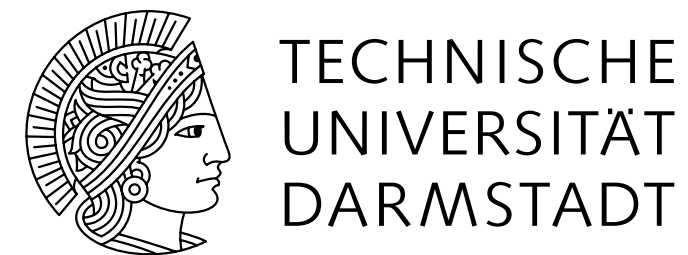
- Jiangming Yao



- **Jack Pitcher**



- Takayuki Miyagi



- Lotta Jokiniemi

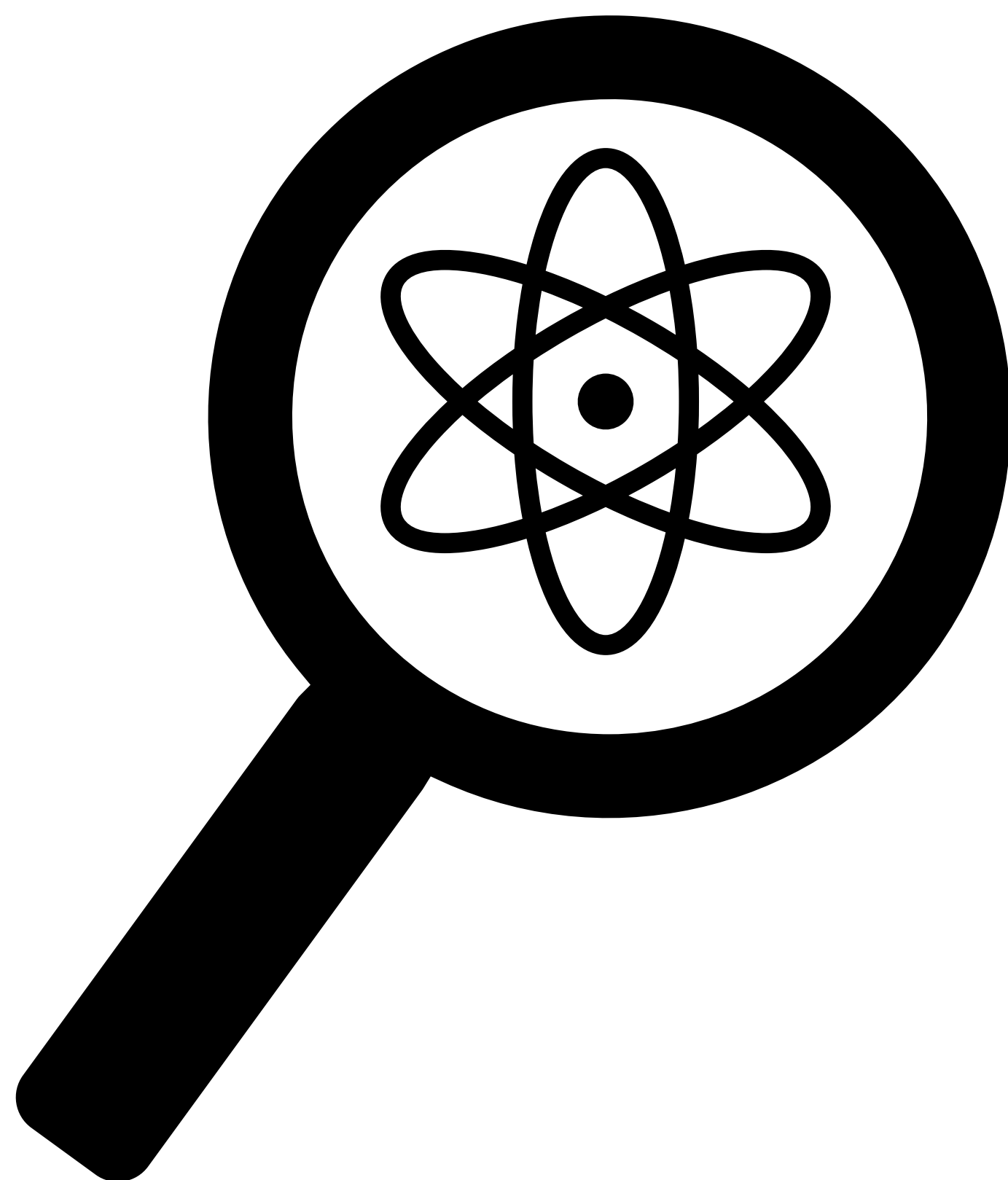


- Bingcheng He



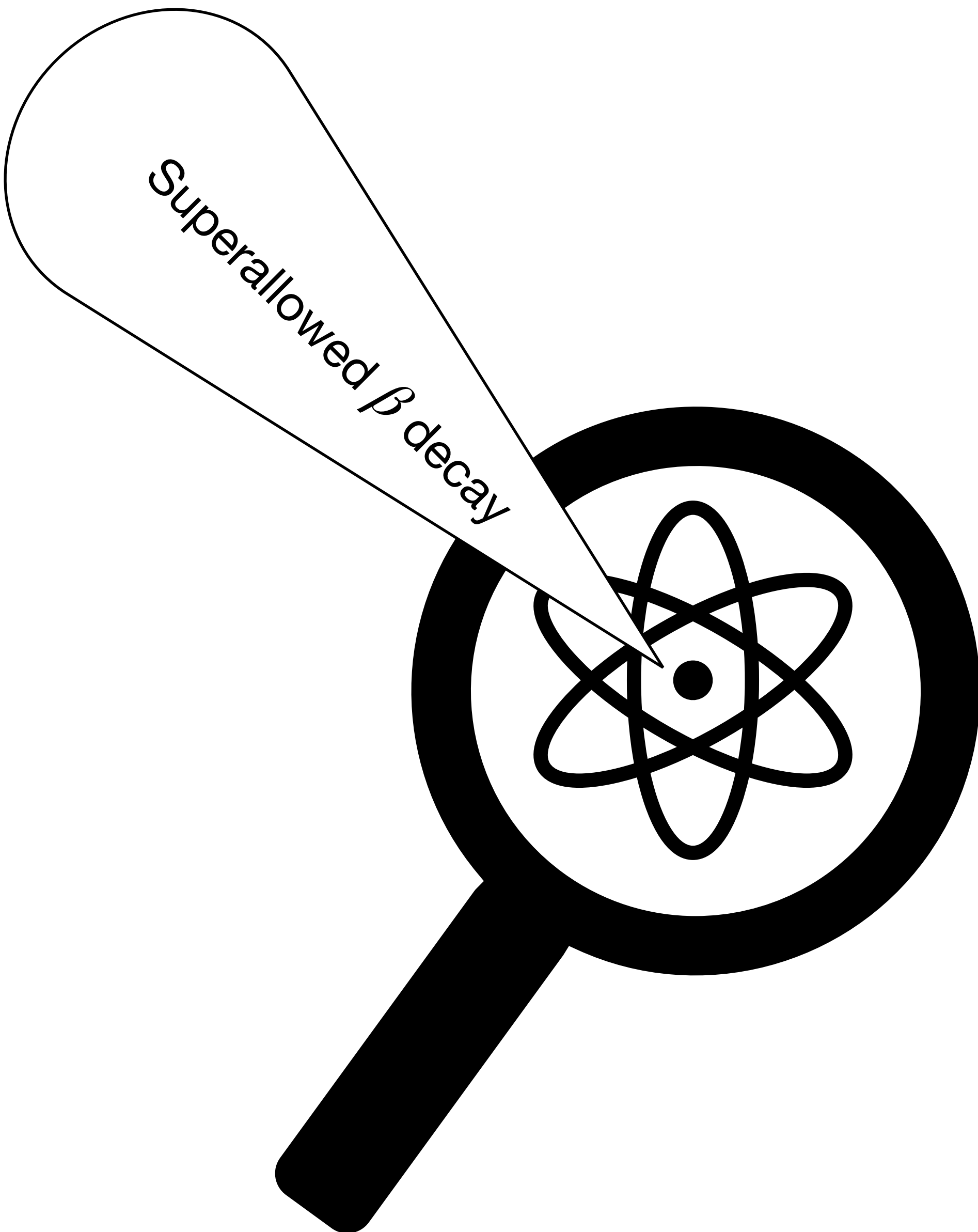


Atomic Nucleus as a Probe



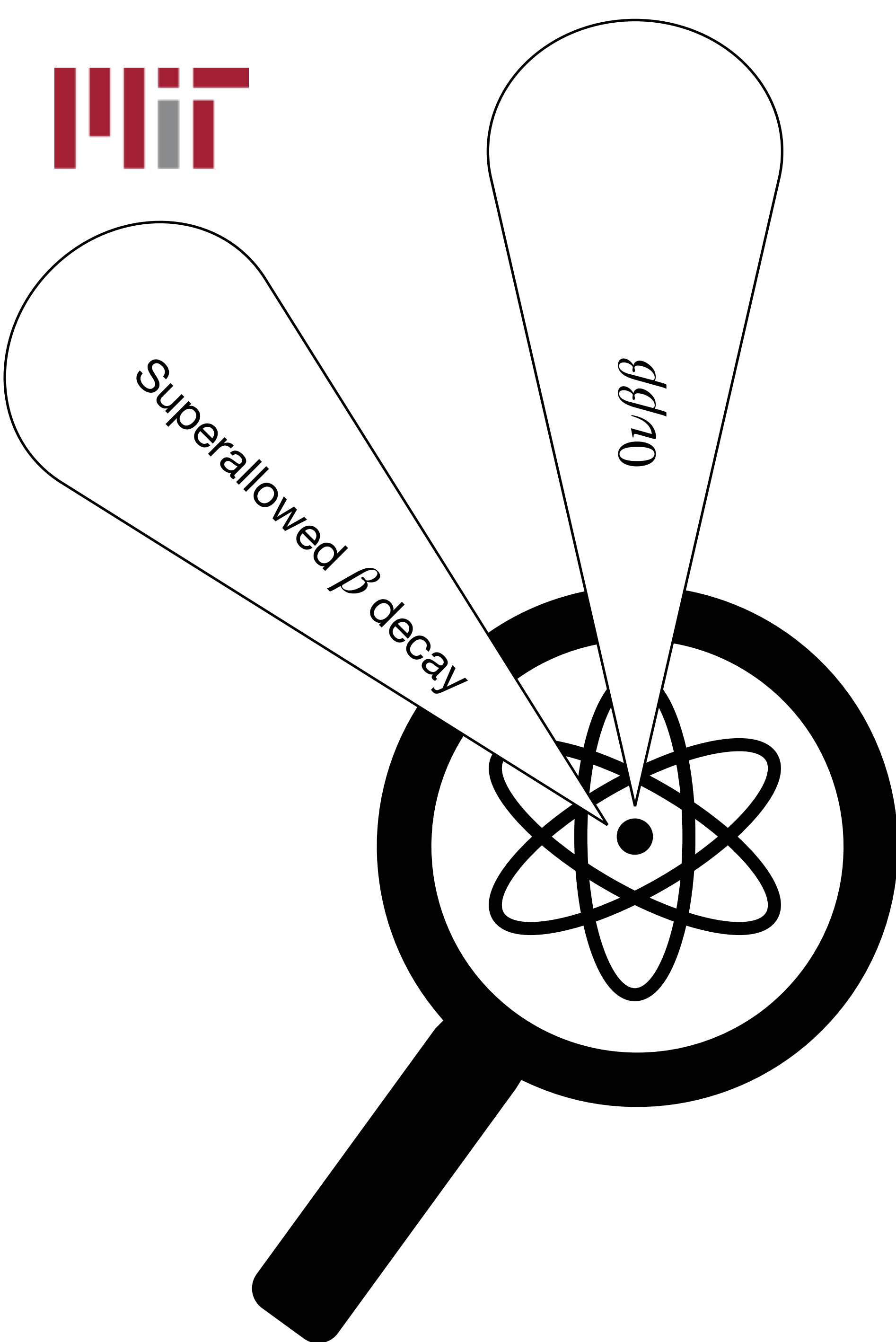


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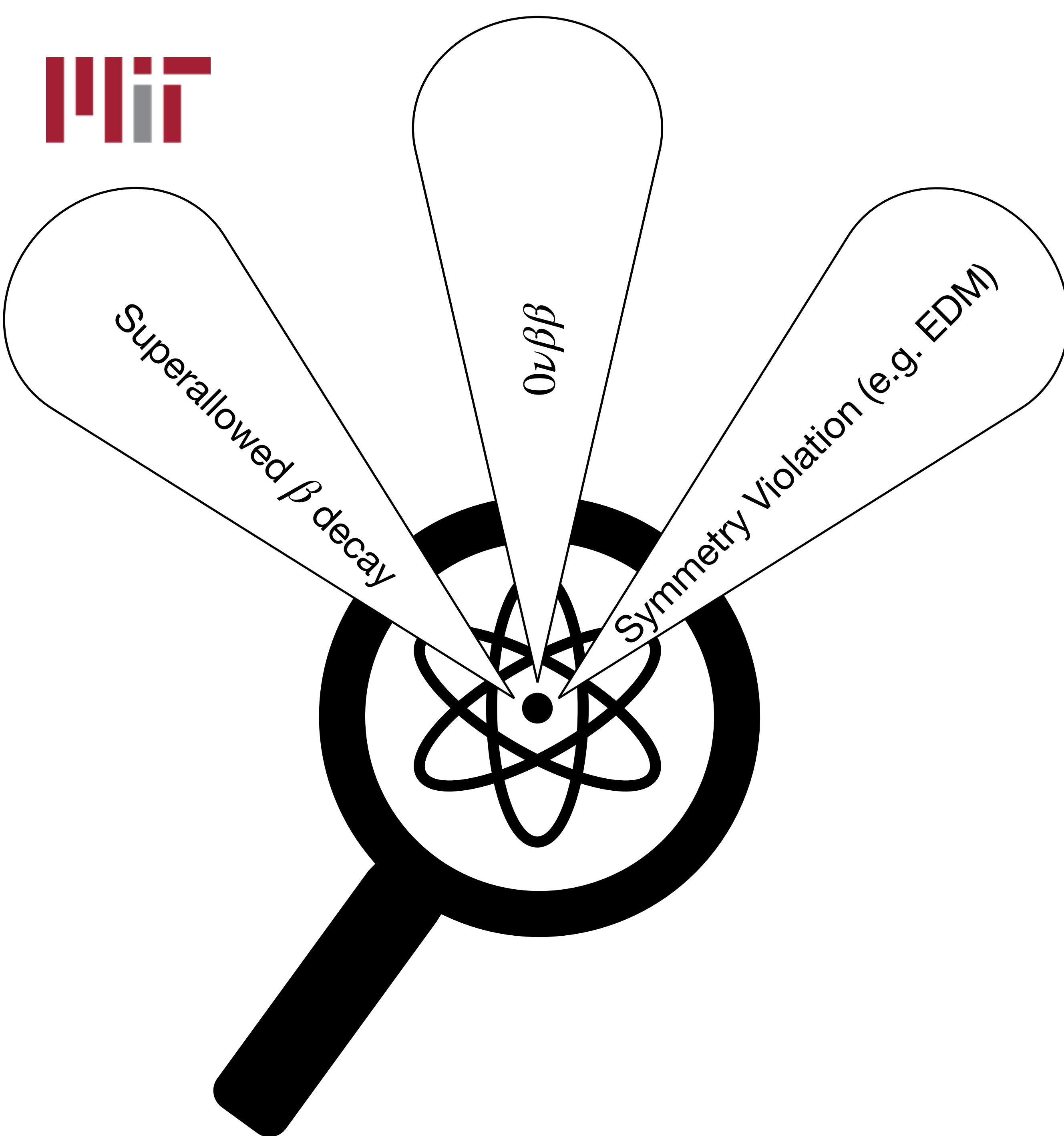


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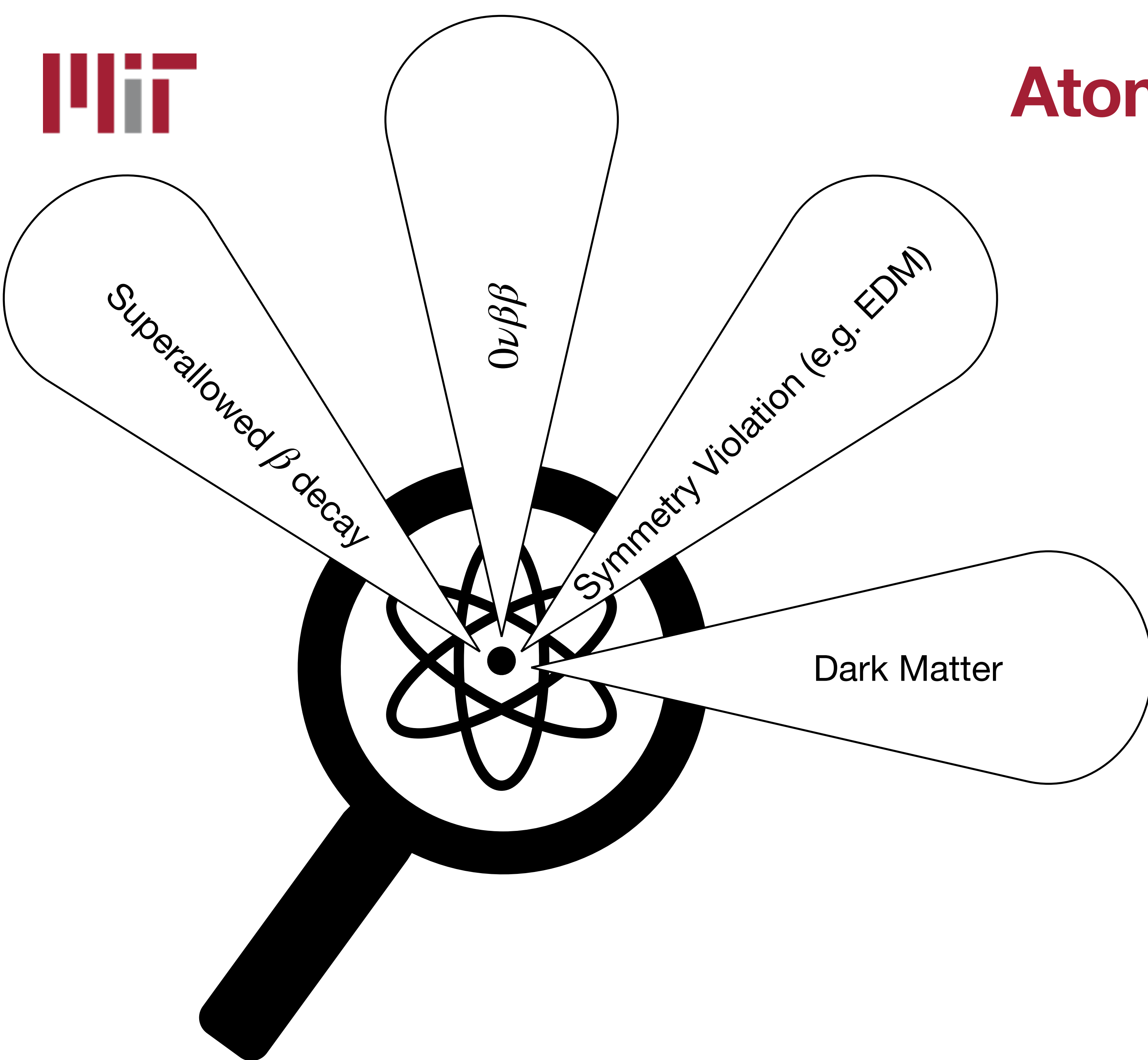


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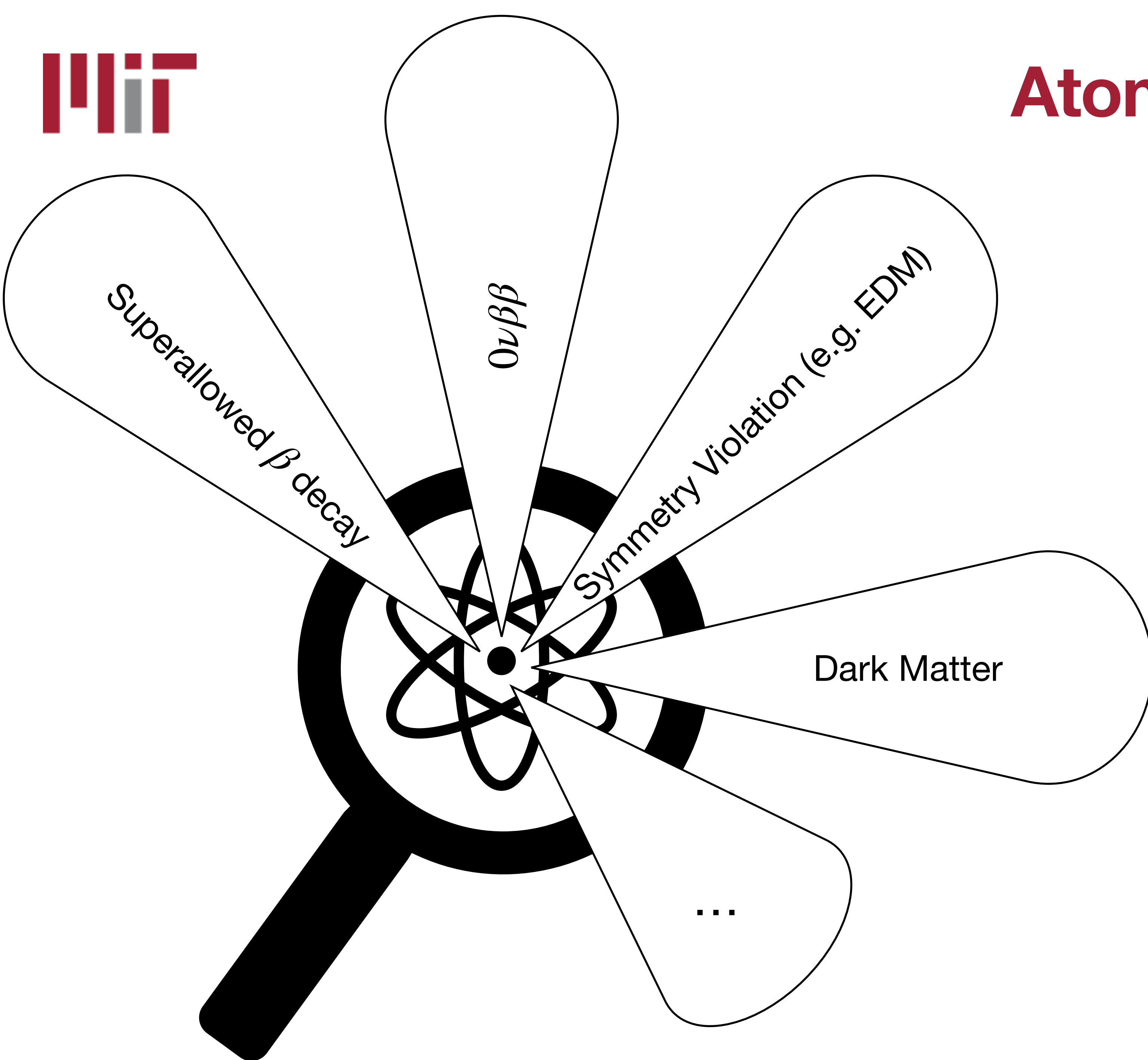


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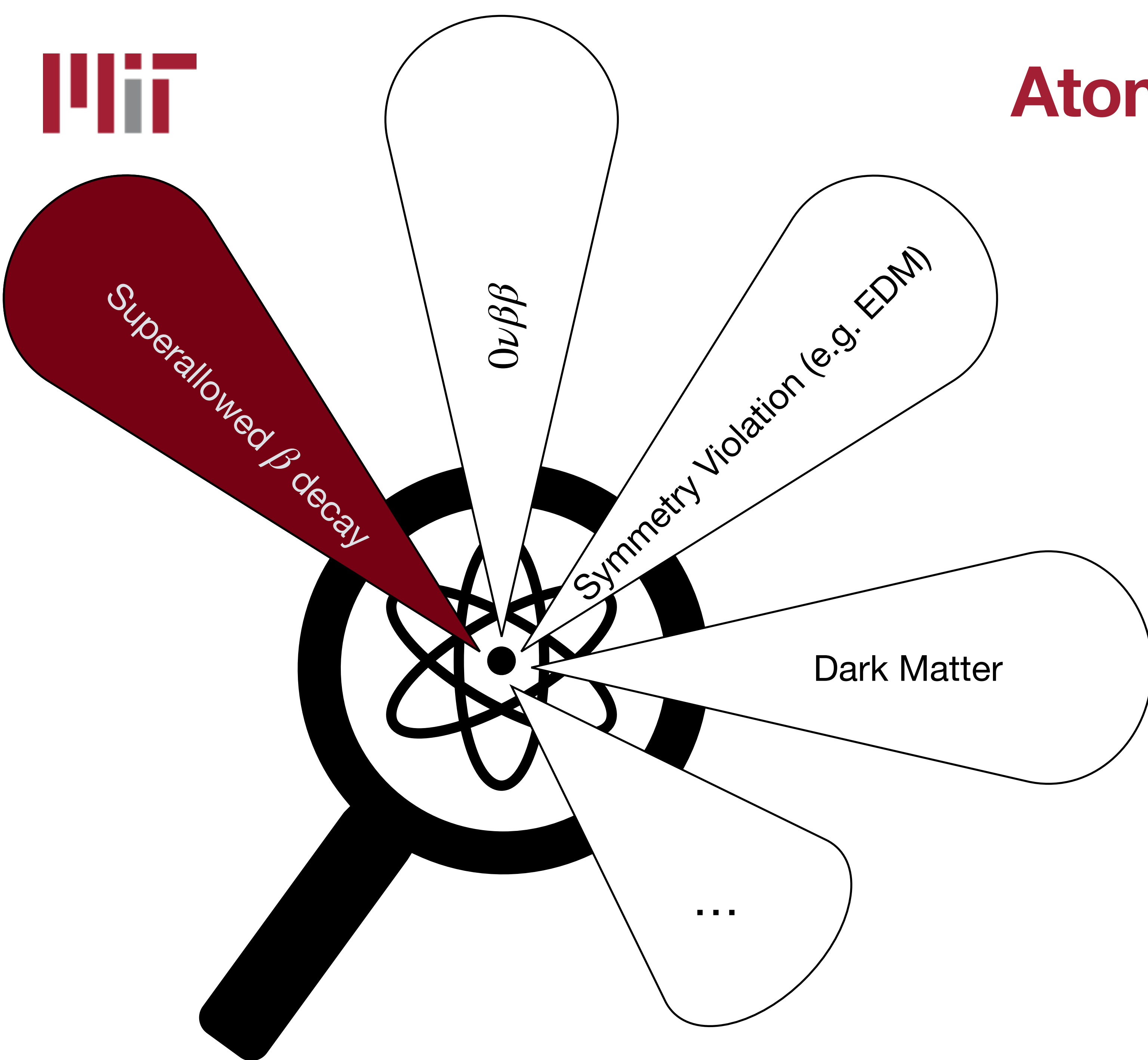


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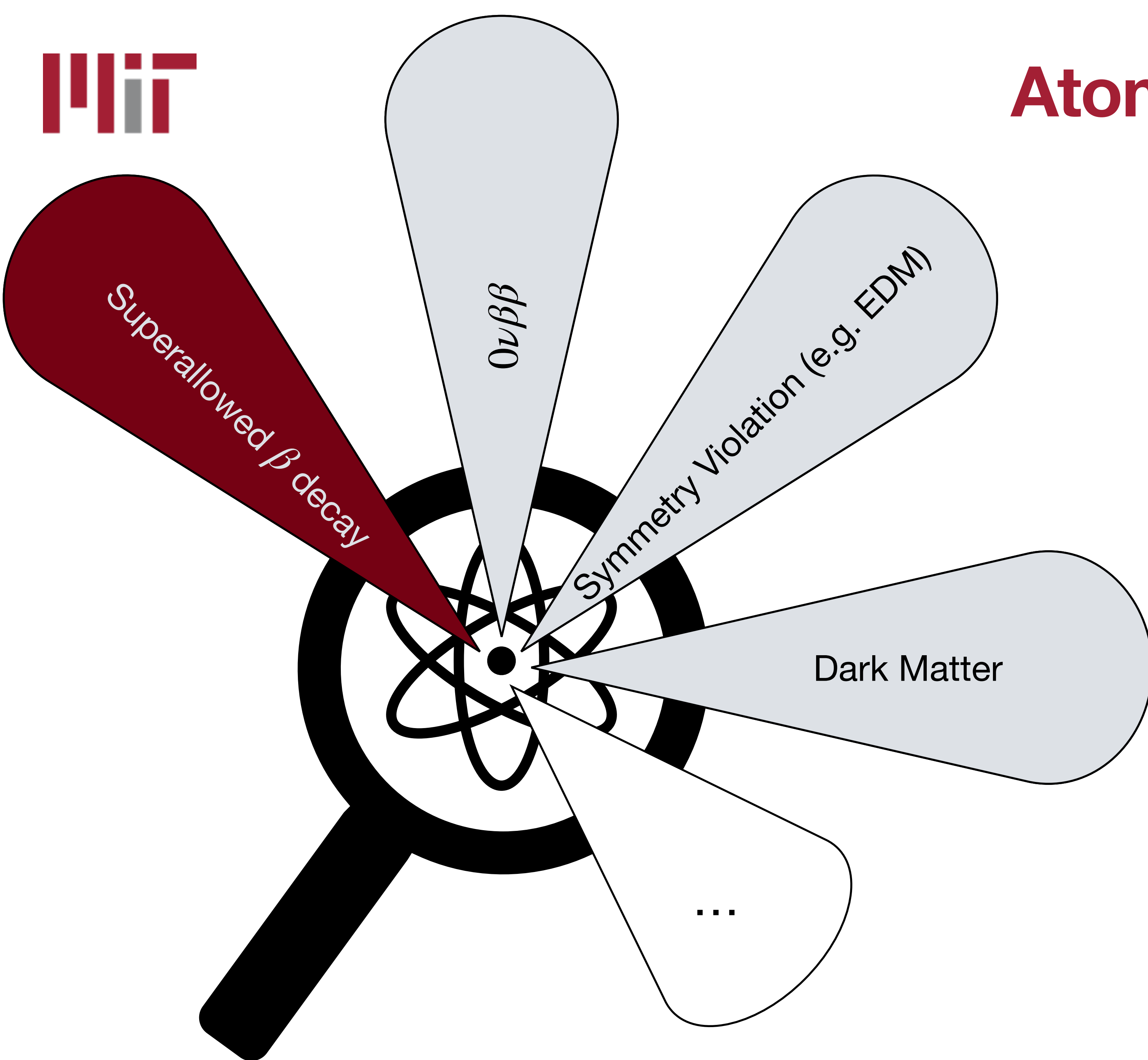


Atomic Nucleus as a Probe



1. Looking at deviation from Standard Model prediction.

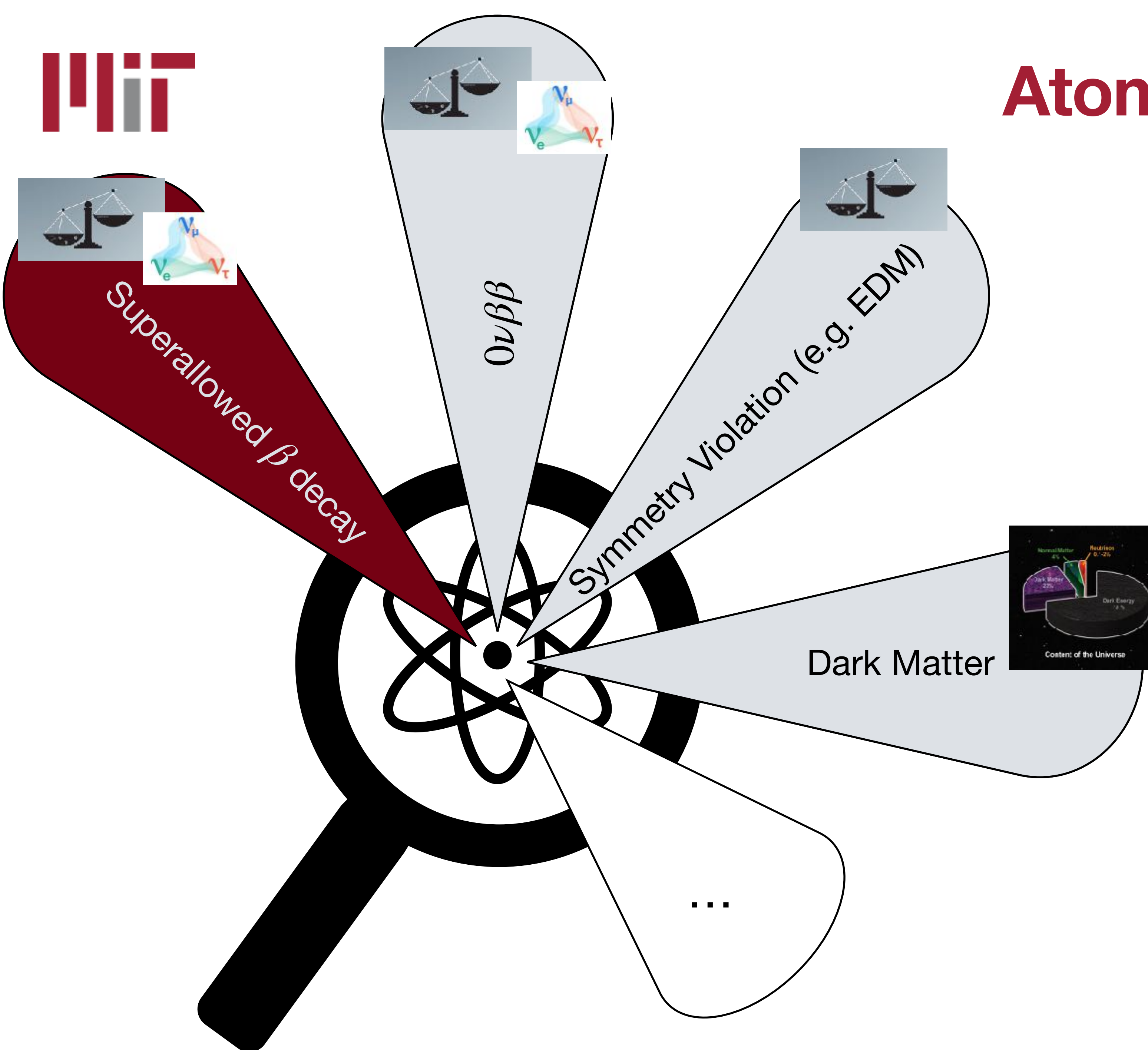
Atomic Nucleus as a Probe



1. Looking at deviation from Standard Model prediction.

2. Search for phenomena not predicted by the Standard Model.

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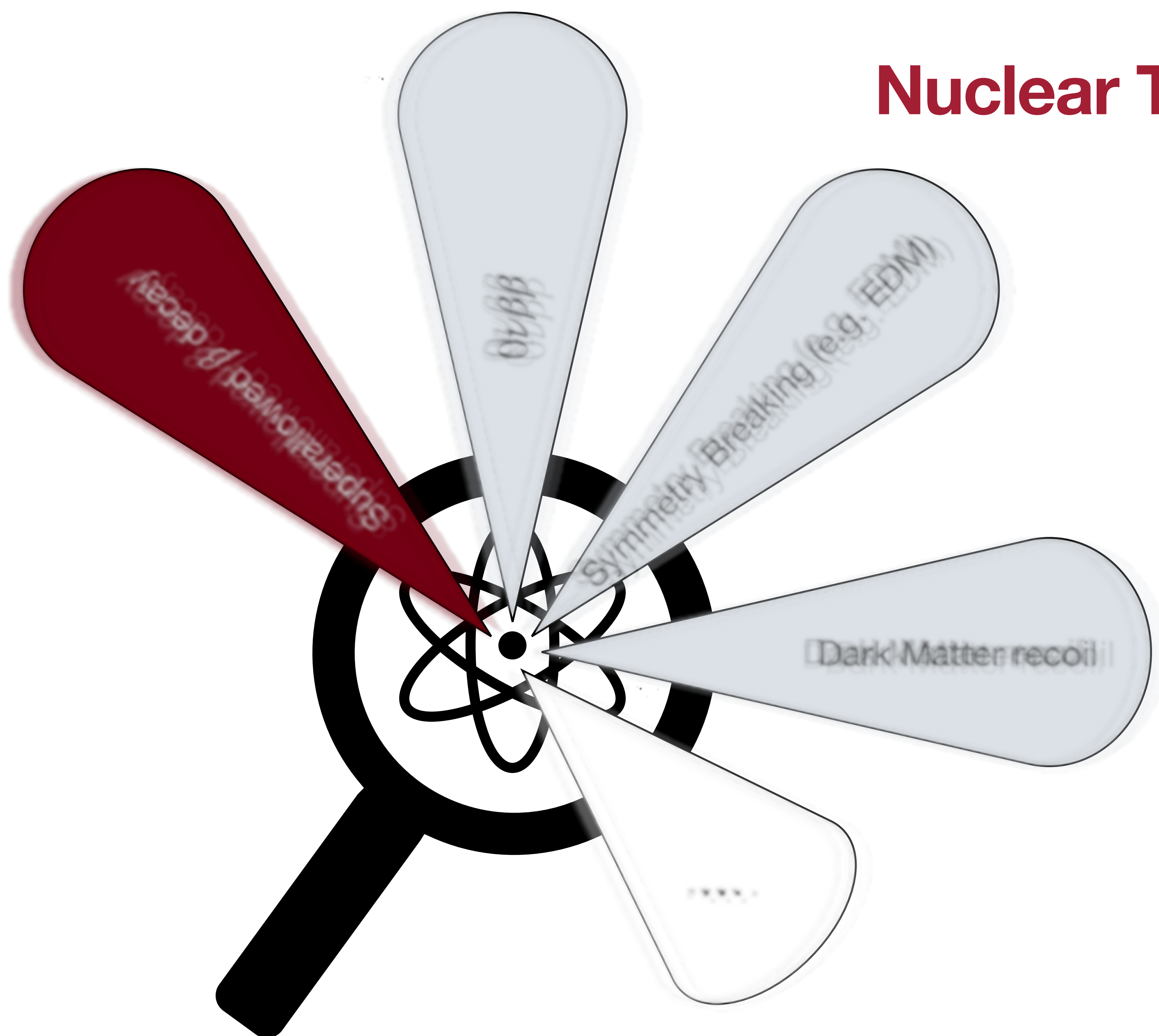
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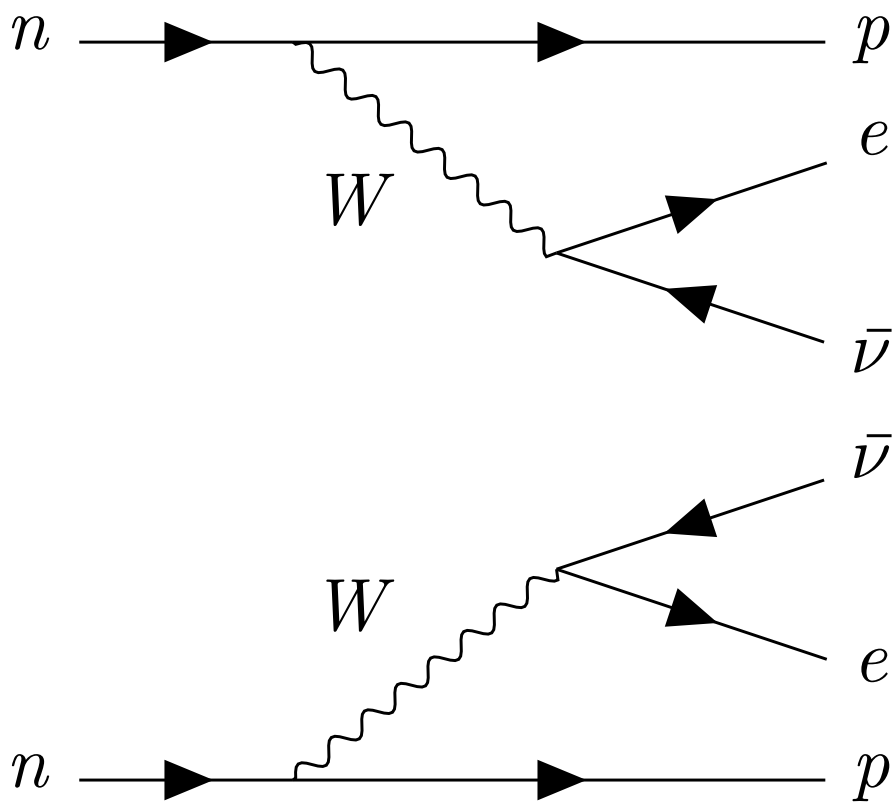
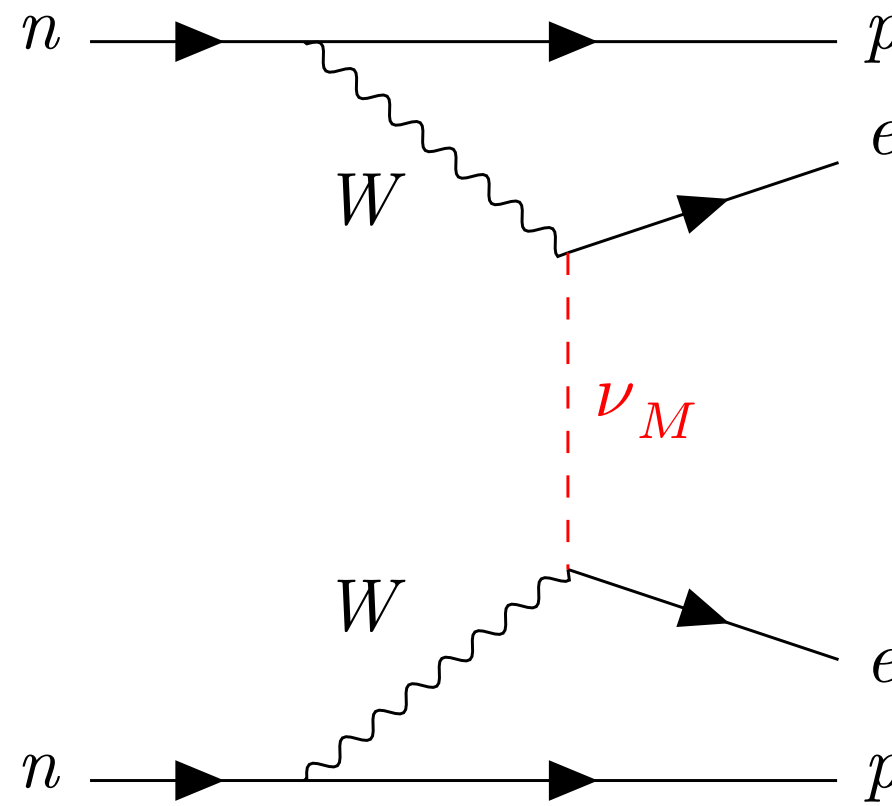


The Need for Nuclear Theory

In all cases, nuclear theory inputs are required in order to interpret experimental results:

- **Superaligned β decay:** Corrections from Standard Model δ_{NS} and δ_C .
- **$0\nu\beta\beta$:** Nuclear matrix elements $M^{0\nu}$.
- **Electric Dipole Moment:** The nuclear Schiff Moment.
- **Dark Matter Scattering:** WIMP Scattering structure factor S_A .
- ...

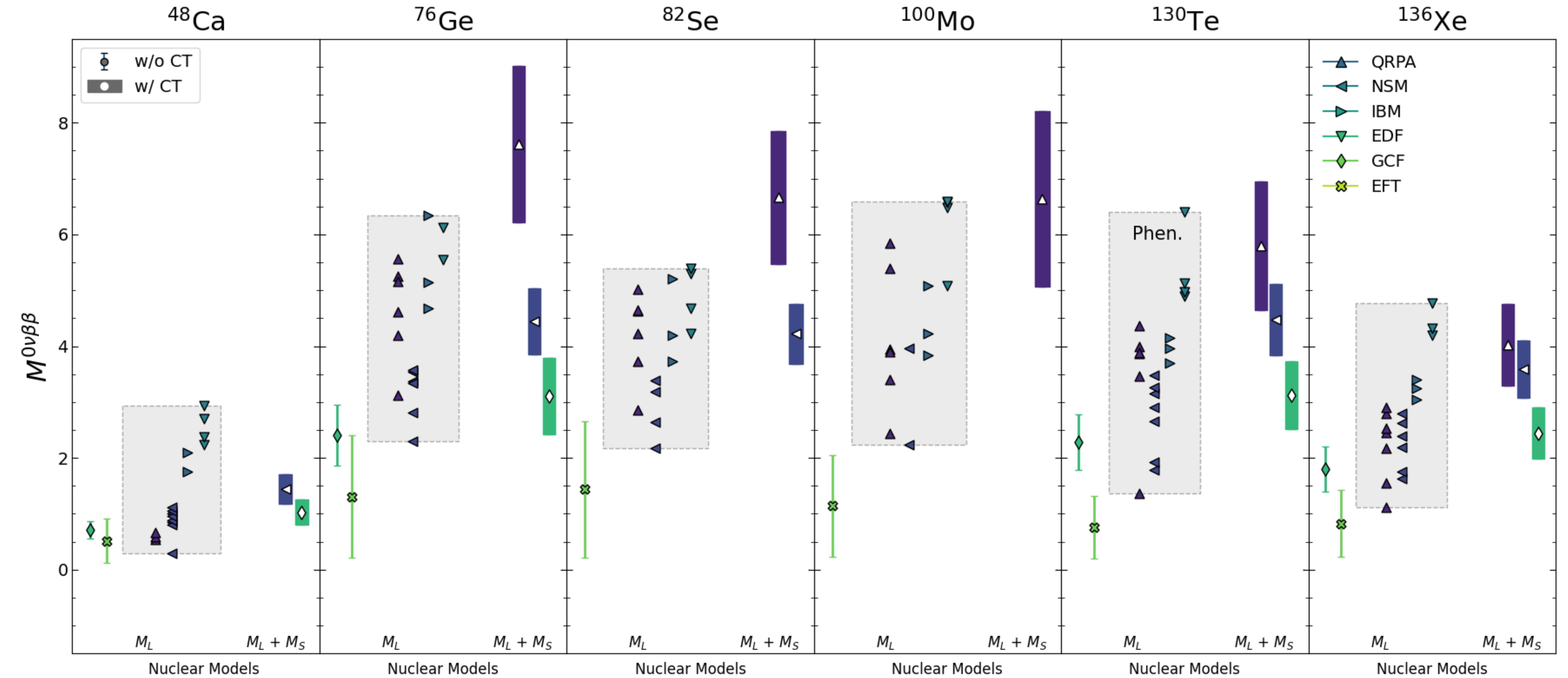


Decay	$2\nu\beta\beta$	$0\nu\beta\beta$
Diagram		
Half-life Formula	$[T_{1/2}^{2\nu}]^{-1} = g_A^4 G^{2\nu} M^{2\nu} ^2$	$[T_{1/2}^{0\nu}]^{-1} = g_A^4 G^{0\nu} M^{0\nu} ^2 \left(\frac{\langle m_{\beta\beta} \rangle}{m_e} \right)^2$
NME Formula	$M^{2\nu} \approx M_{GT}^{2\nu}$	$M^{0\nu} = M_{GT}^{0\nu} - \left(\frac{g_V}{g_A} \right)^2 M_F^{0\nu} + M_T^{0\nu} - 2g_{\nu\nu} M_{CT}^{0\nu}$

*NME : Nuclear matrix elements

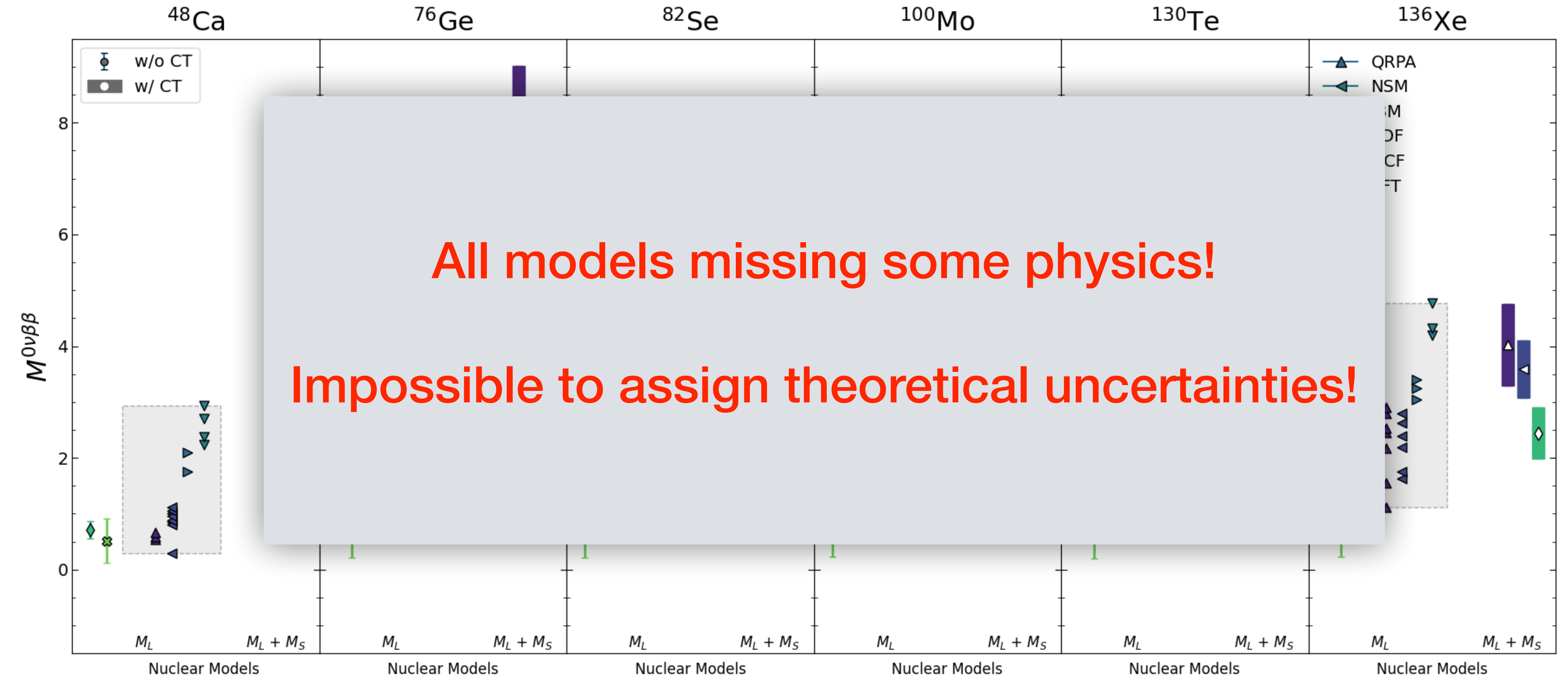


Status of $0\nu\beta\beta$ -decay Matrix Elements



Values from Engel and Menéndez, Rep. Prog. Phys. **80** 046301 (2017); Yao, Sci. Bull. 10.1016 (2020); Brase et al, Phys. Rev. C **106**, 034309 (2021)

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Nuclear Theory Challenges

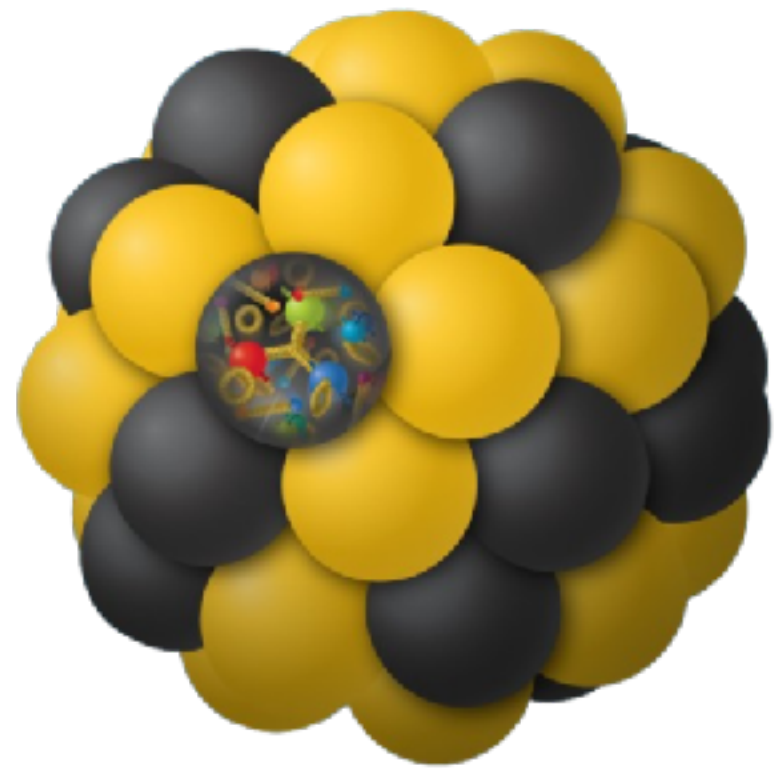
Understanding nuclear structure from microscopic physics



Nuclear Theory Challenges

Understanding nuclear structure from microscopic physics

Nuclear Interactions



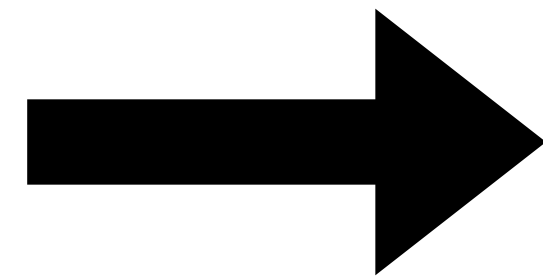
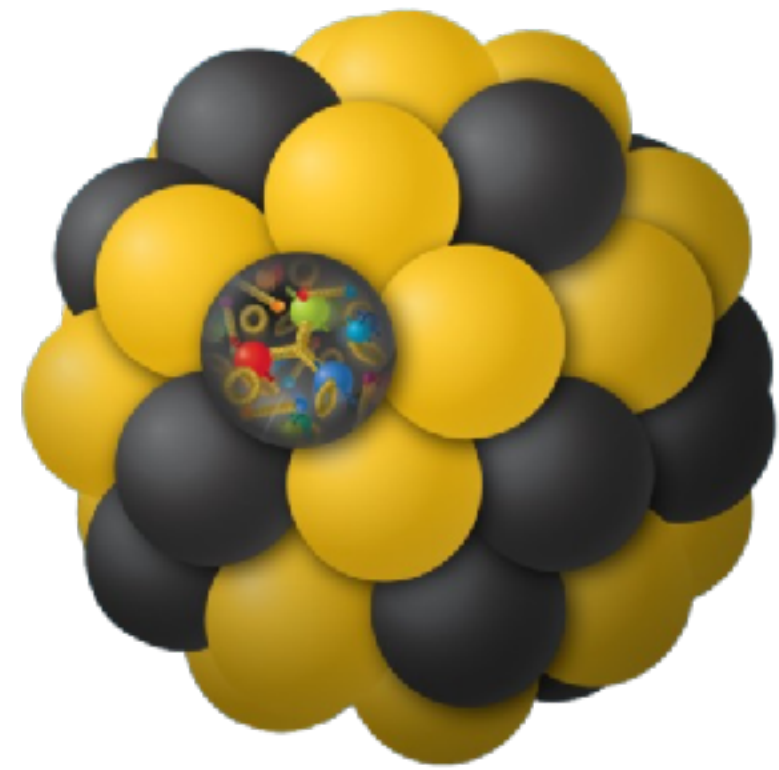


Nuclear Theory Challenges

Understanding nuclear structure from microscopic physics

Nuclear Interactions

Wave functions



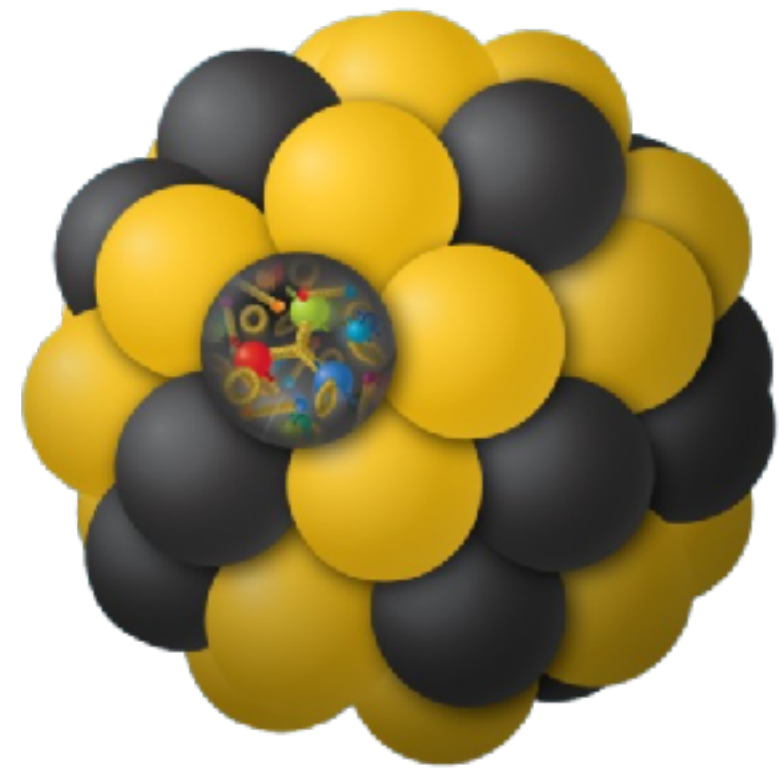
$$H|\Psi\rangle = E|\Psi\rangle$$



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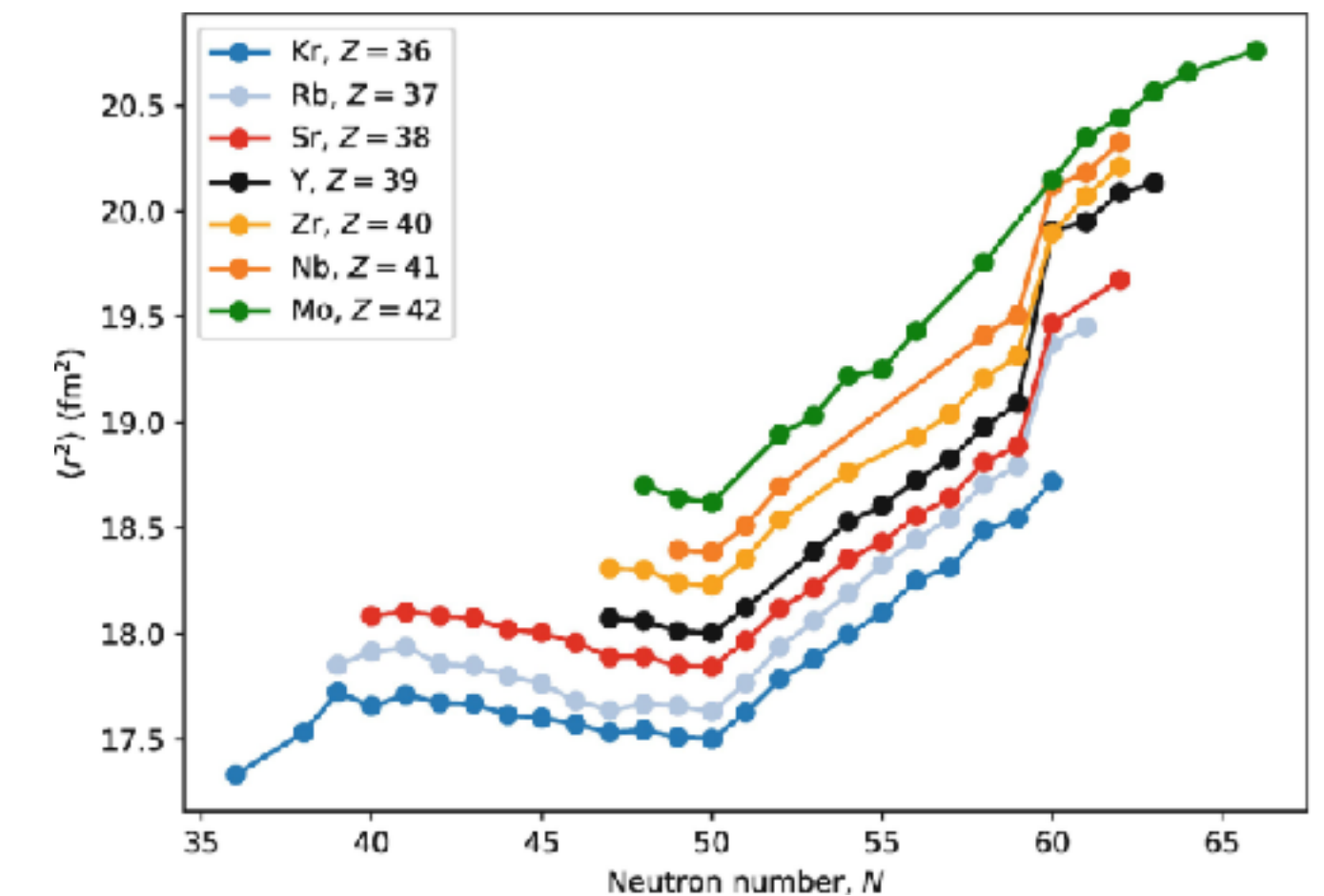
Nuclear Interactions



Wave functions

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Observables



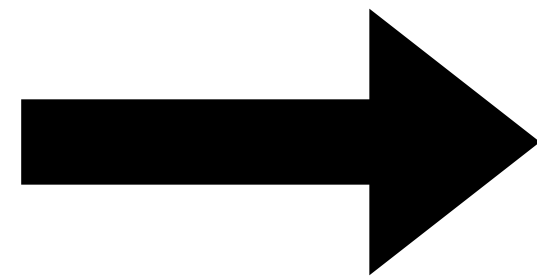
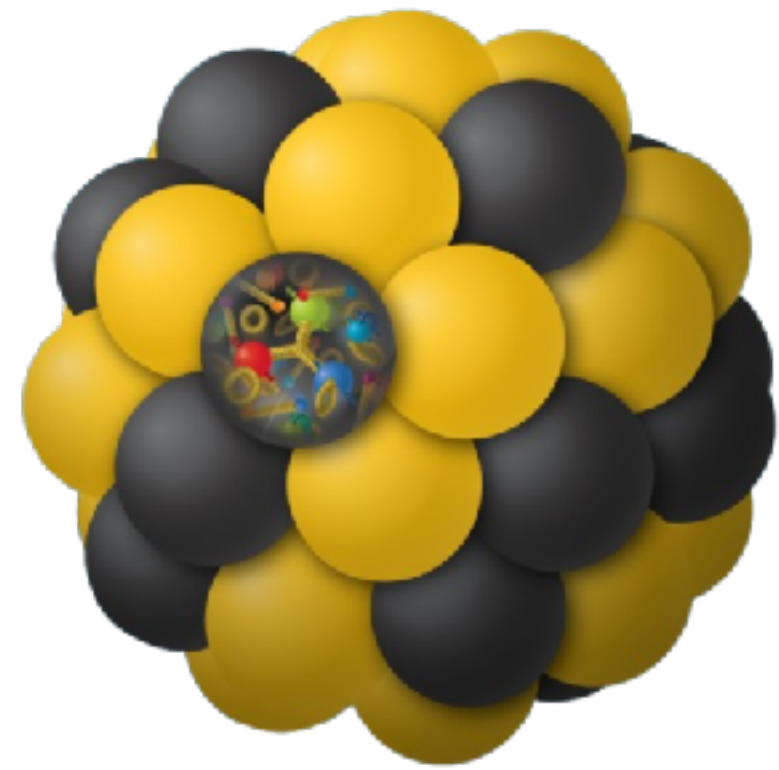
Figures courtesy of J. Muñoz



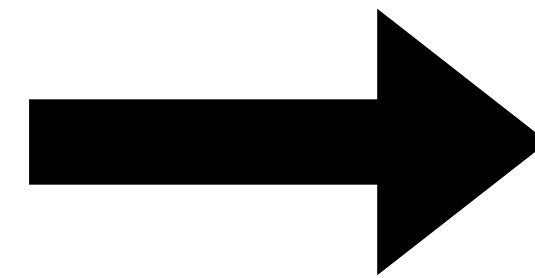
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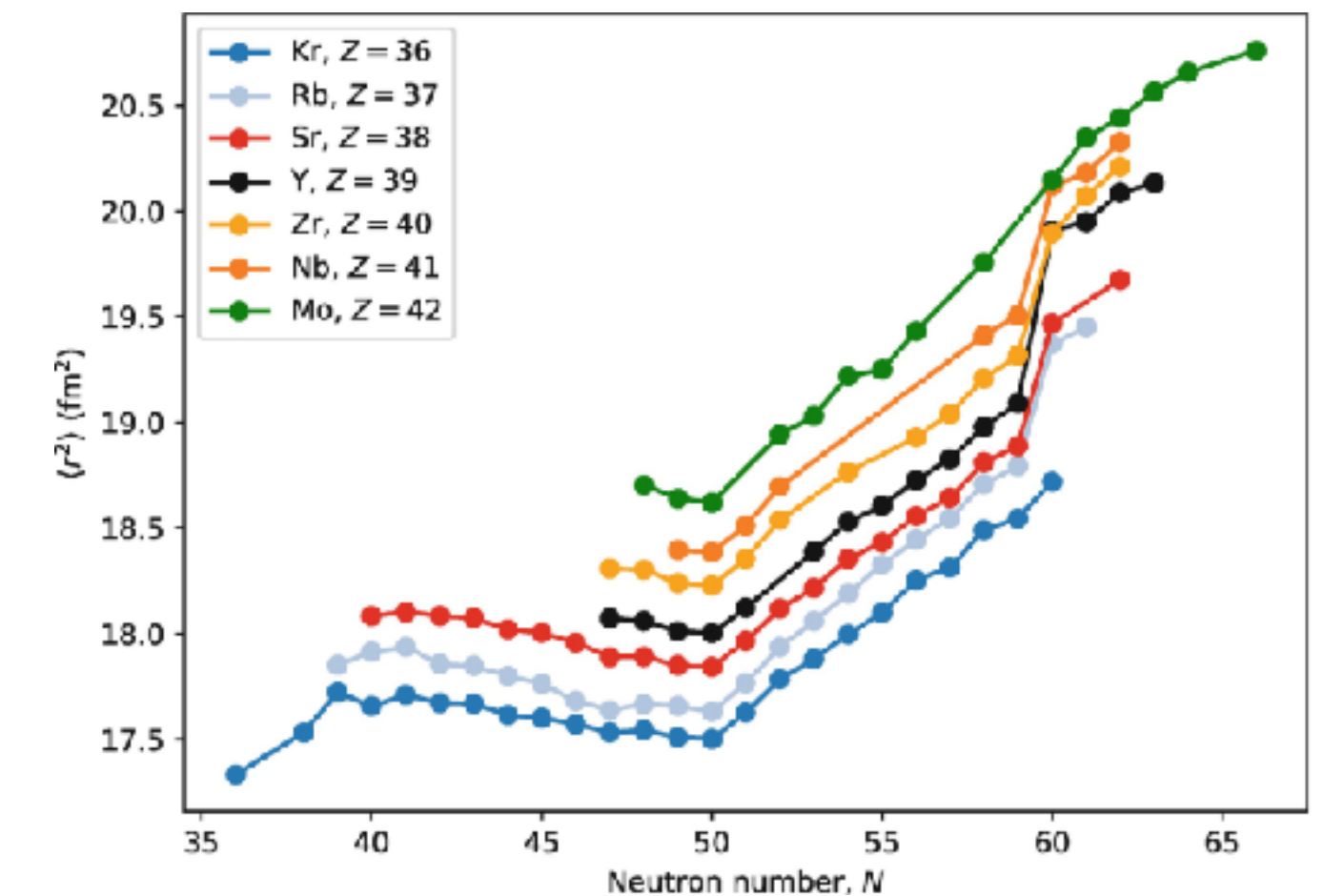
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List of Challenges



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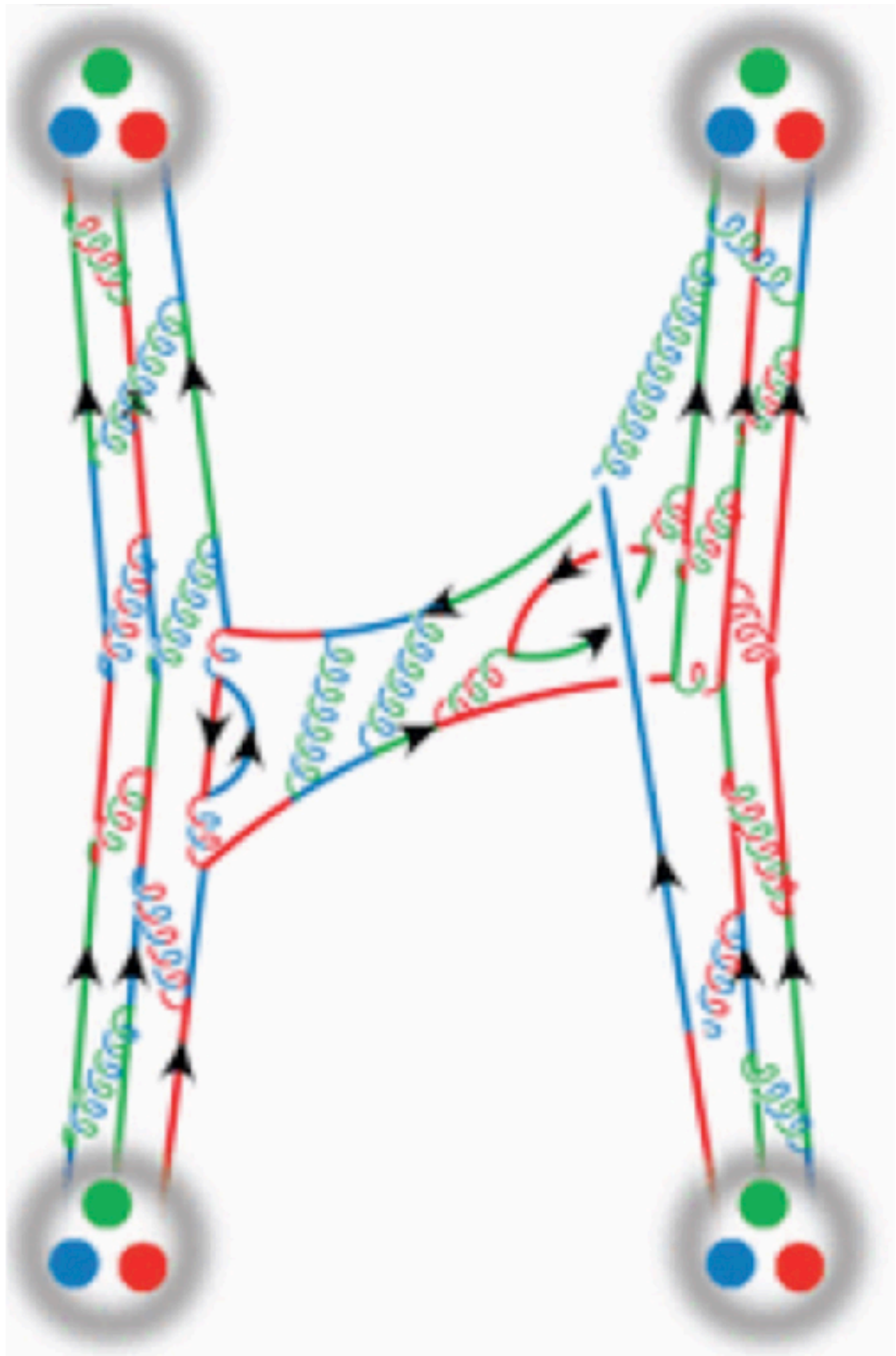
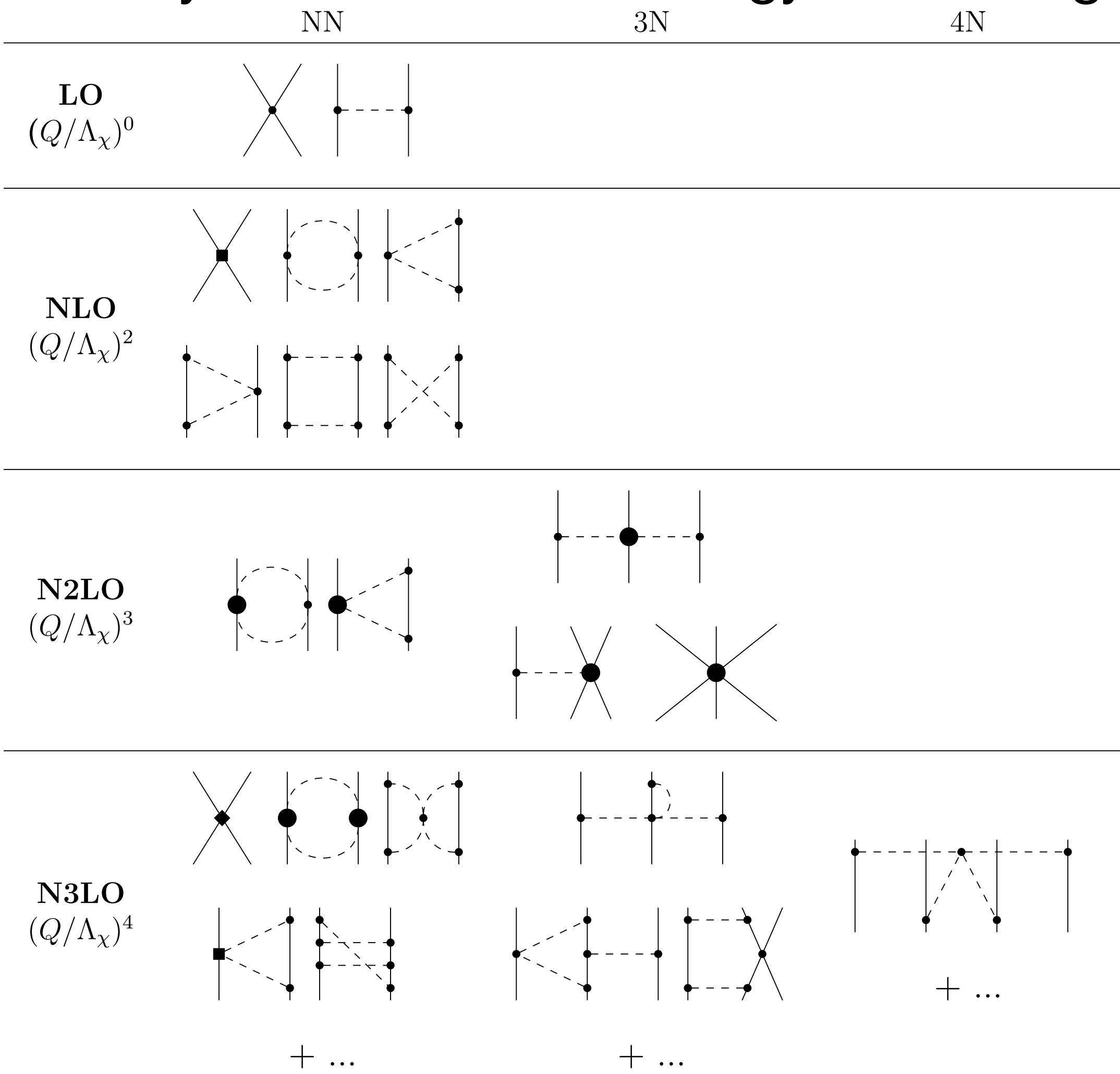
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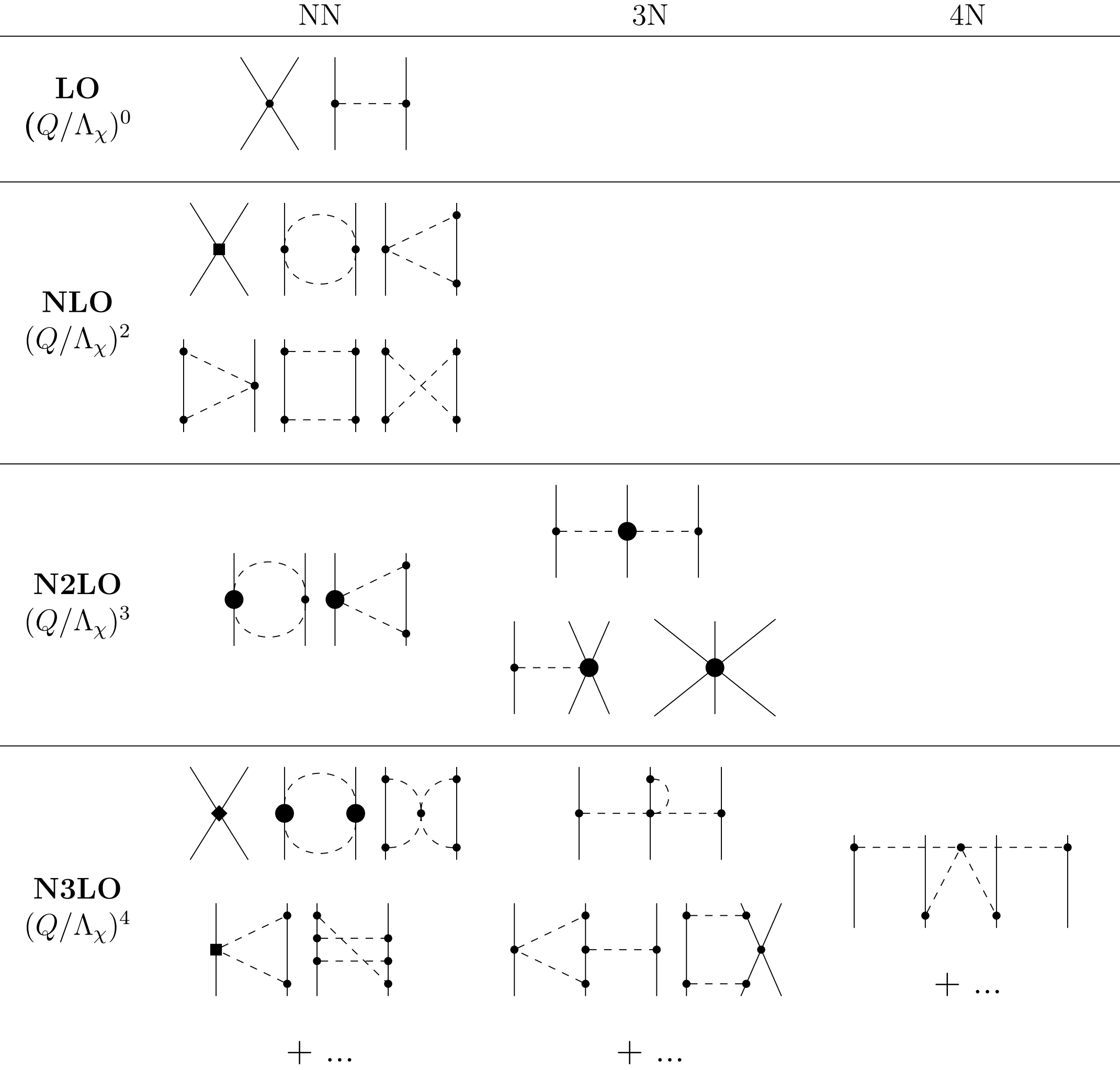
Expansion order by order of the nuclear forces

Reproduces symmetries of low-energy QCD using nucleons as fields and pions as force carriers.



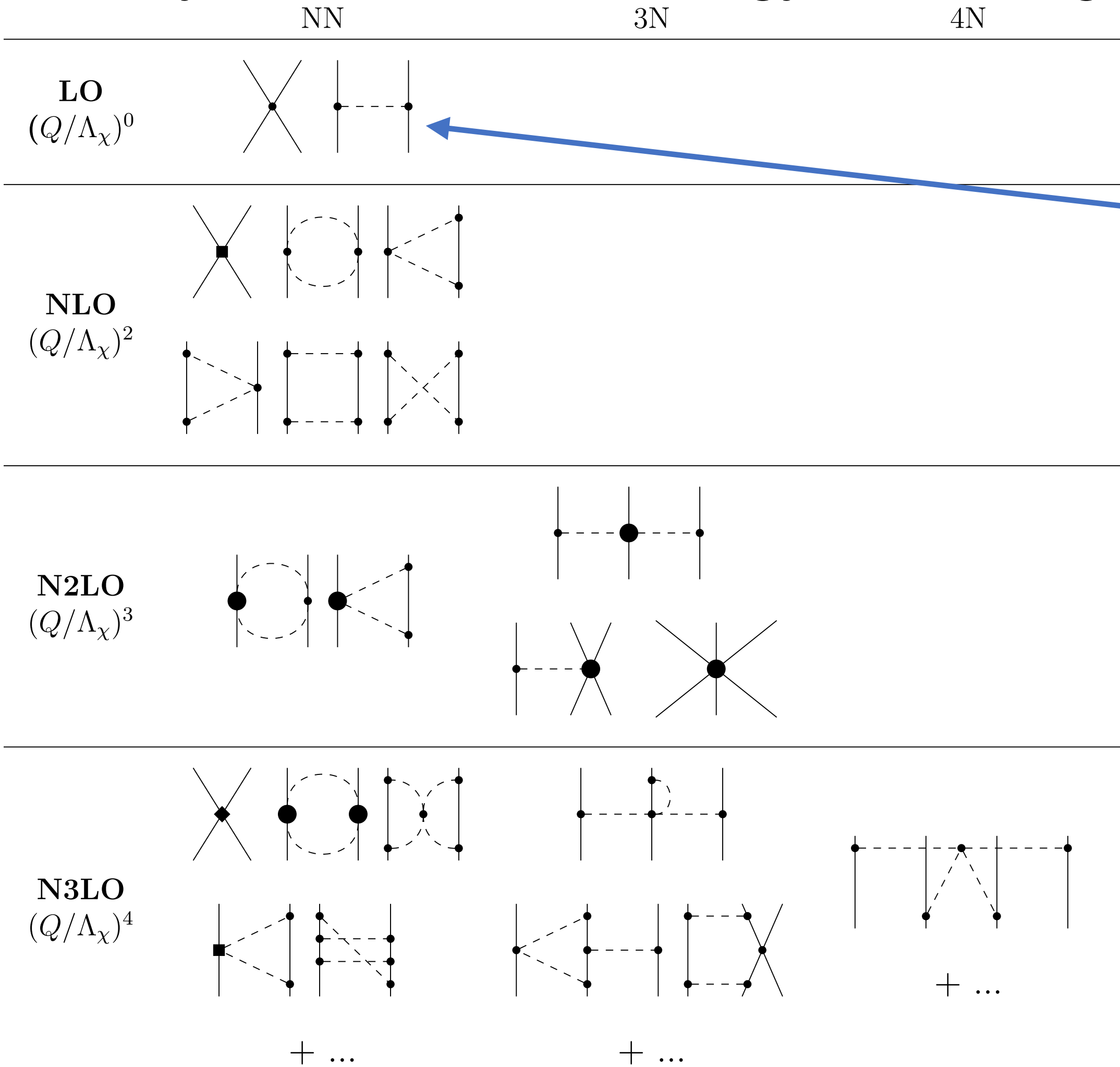
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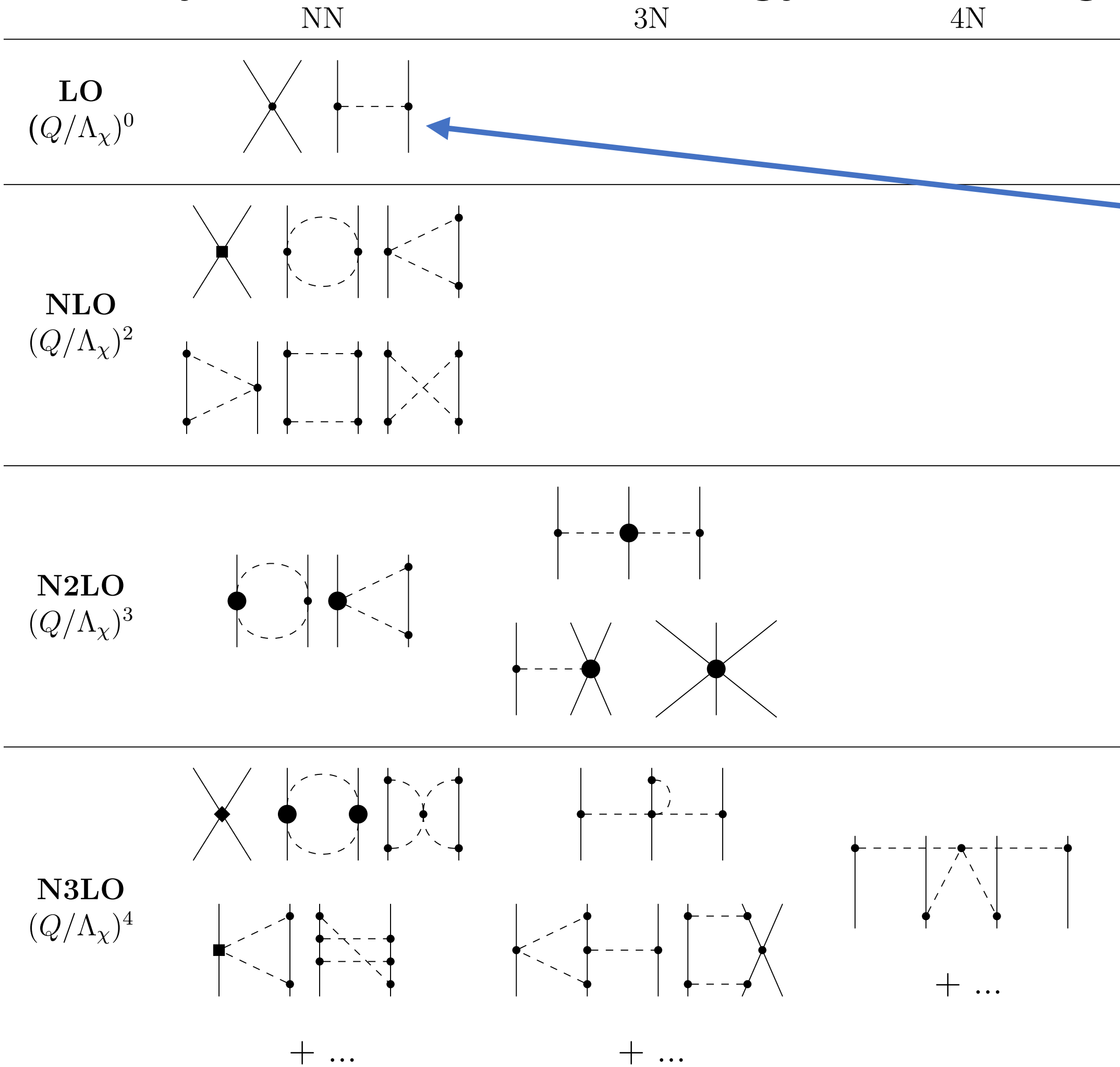


The different low energy coupling constants (LECs) are fitted to few-nucleon data.

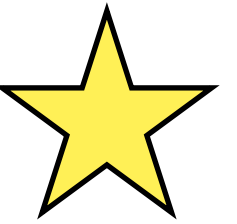


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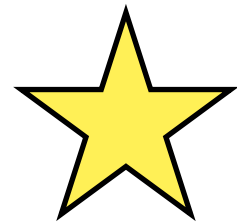
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Need to truncate at some order.

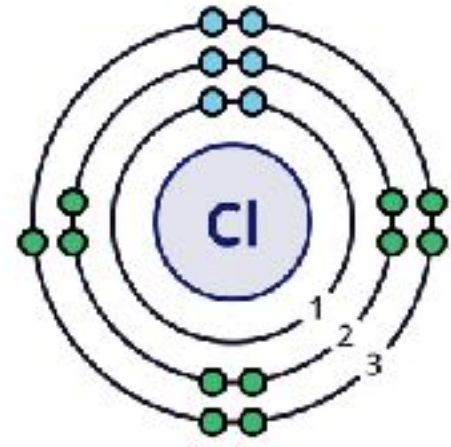


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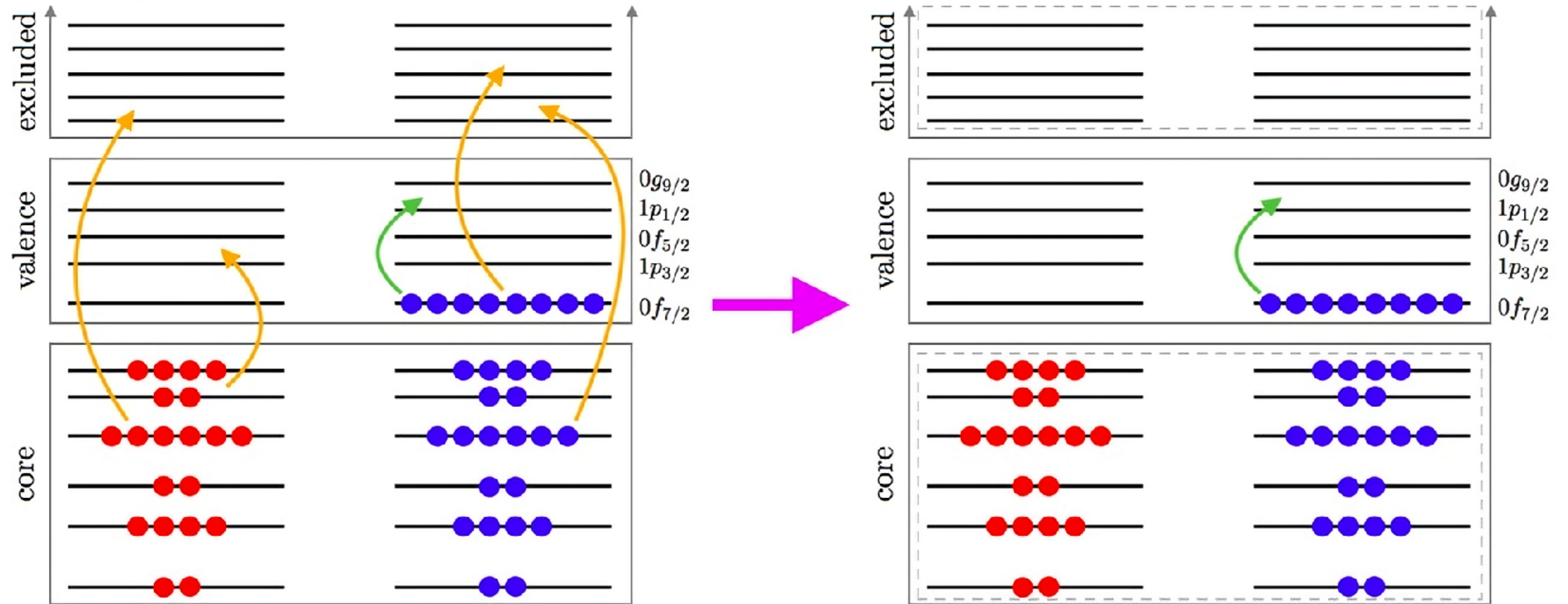
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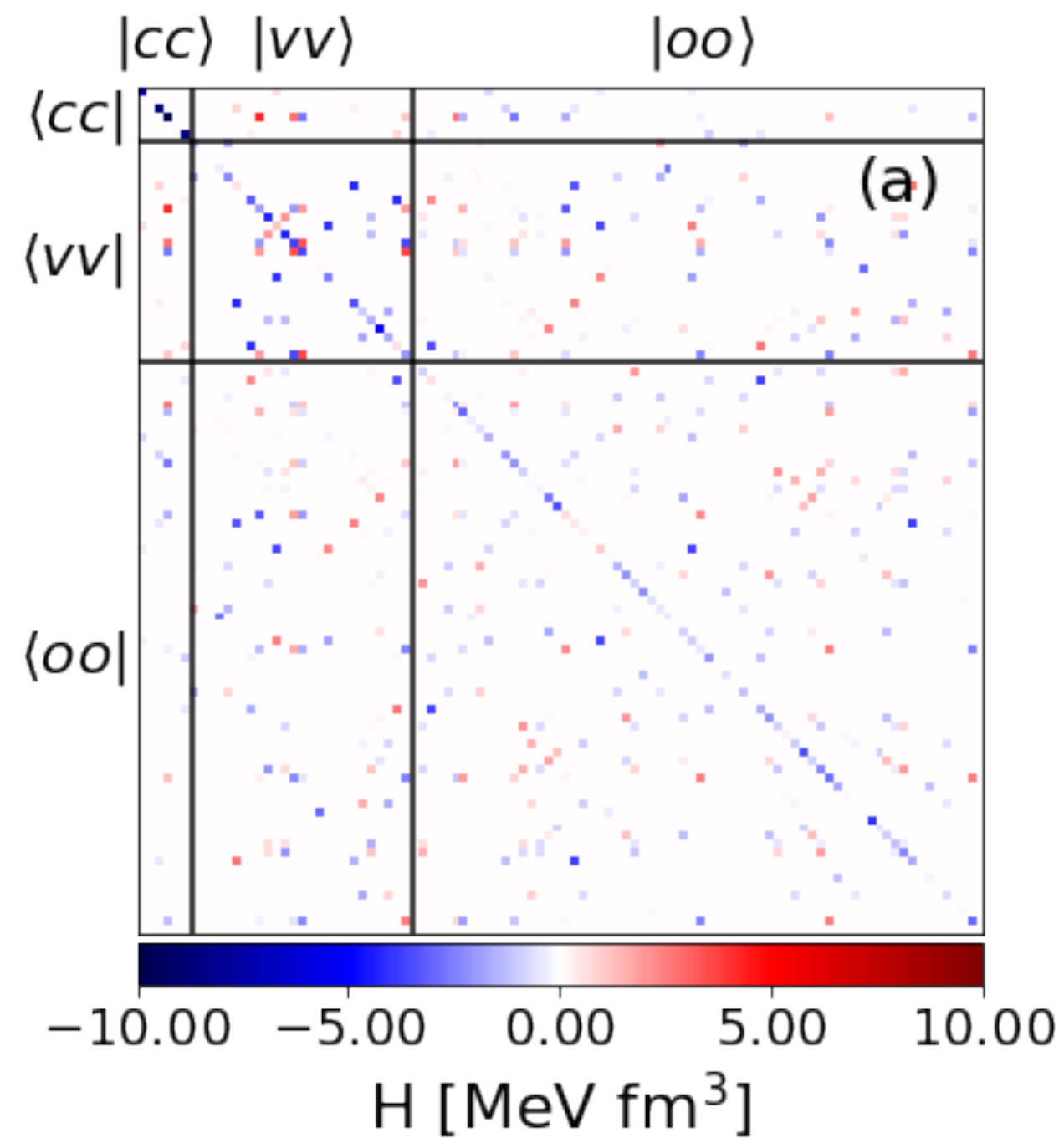


Valence Space In Medium Similarity Renormalization Group



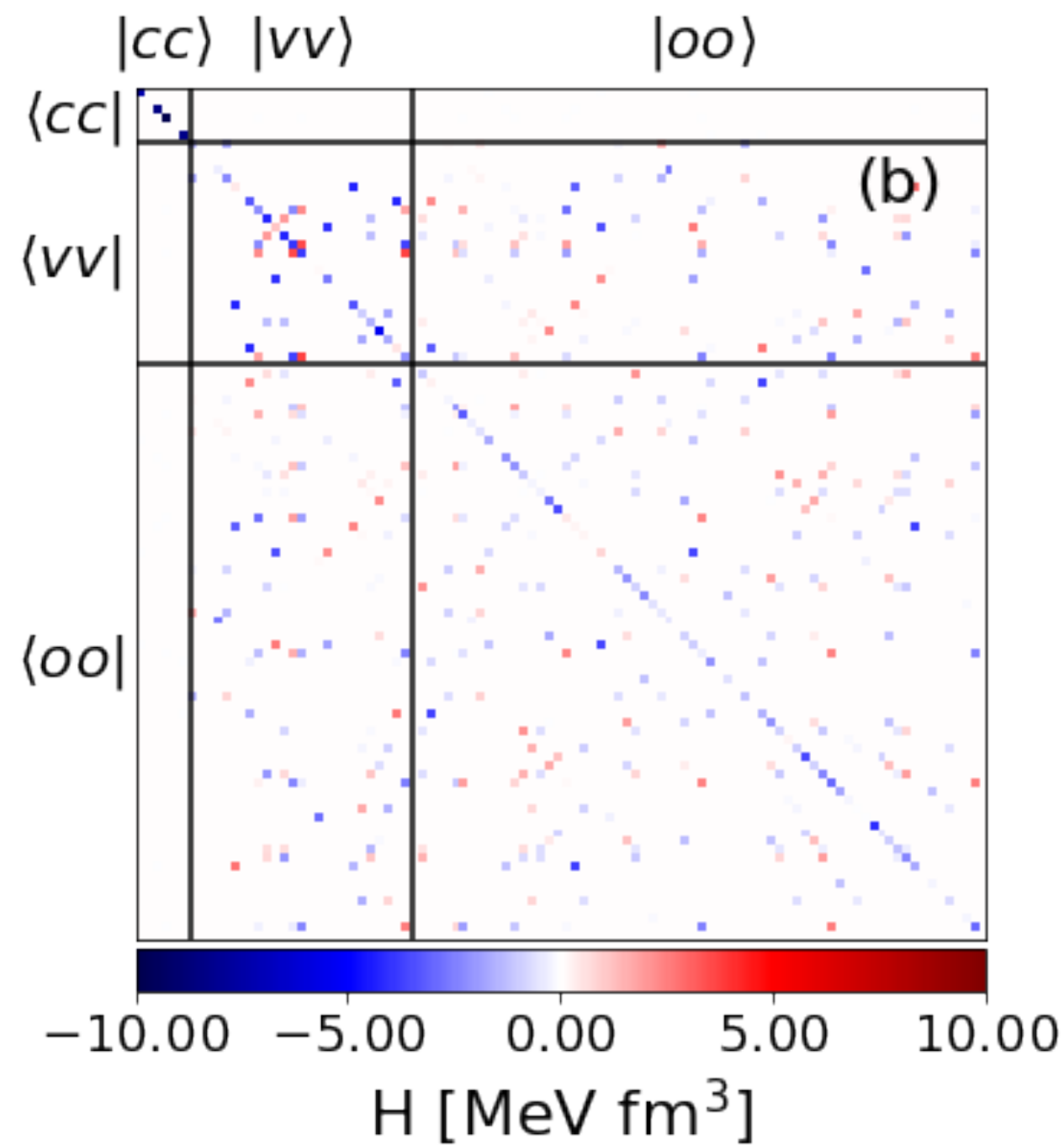
Charlie Payne, Master's Thesis, UBC (2018)

Valence-Space In Medium Similarity Renormalization Group



Bare Hamiltonian

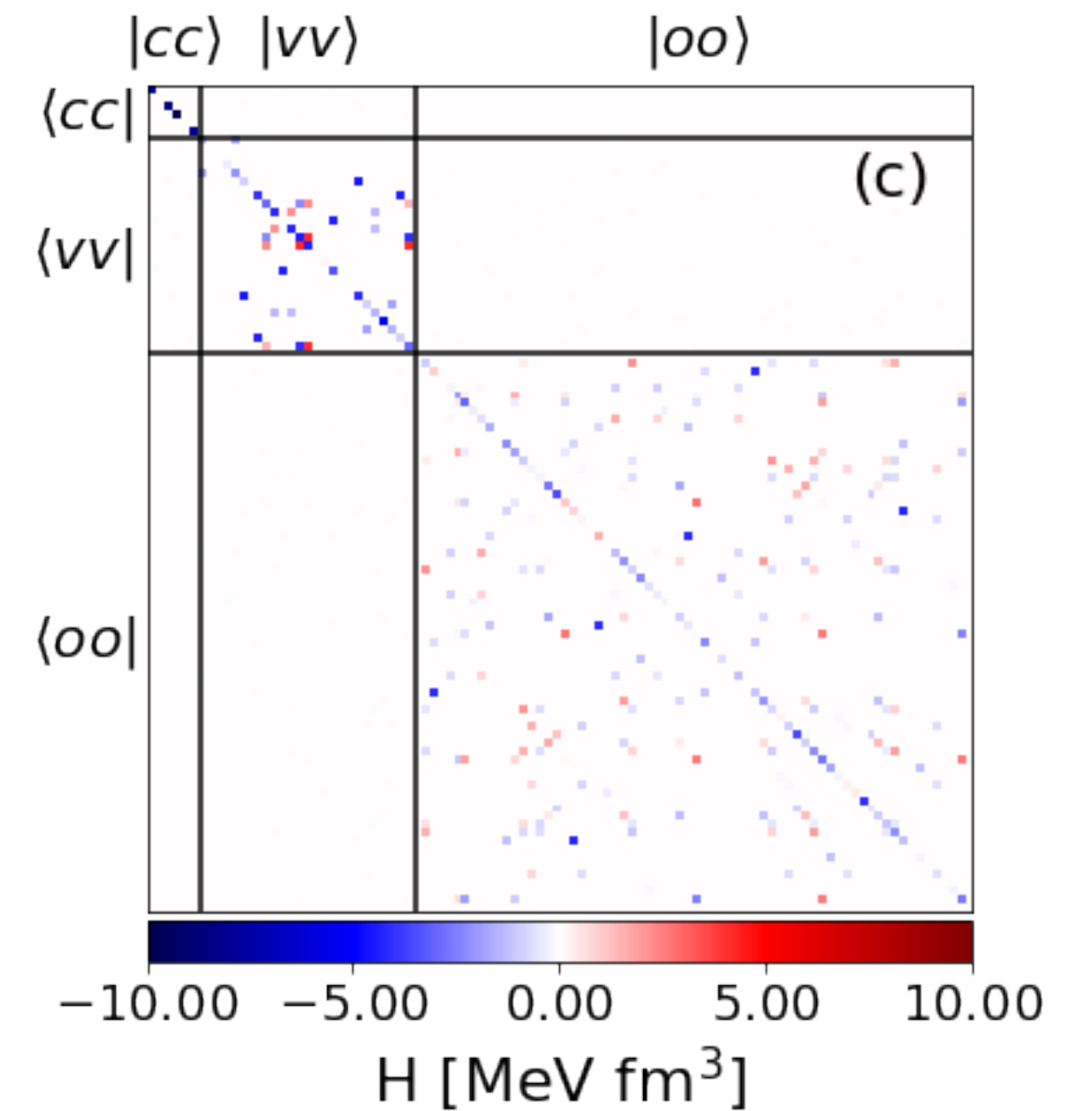
$$\hat{H}(0)$$



Core is decoupled

$$\hat{H}(s) = e^{\Omega_c(s)} \hat{H}(0) e^{-\Omega_c(s)}$$

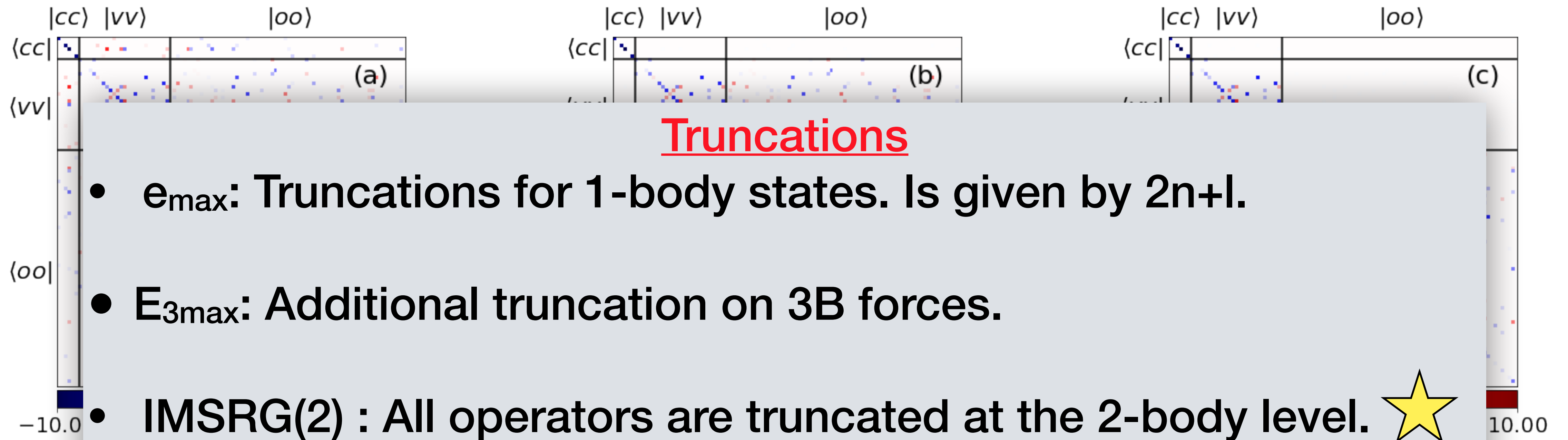
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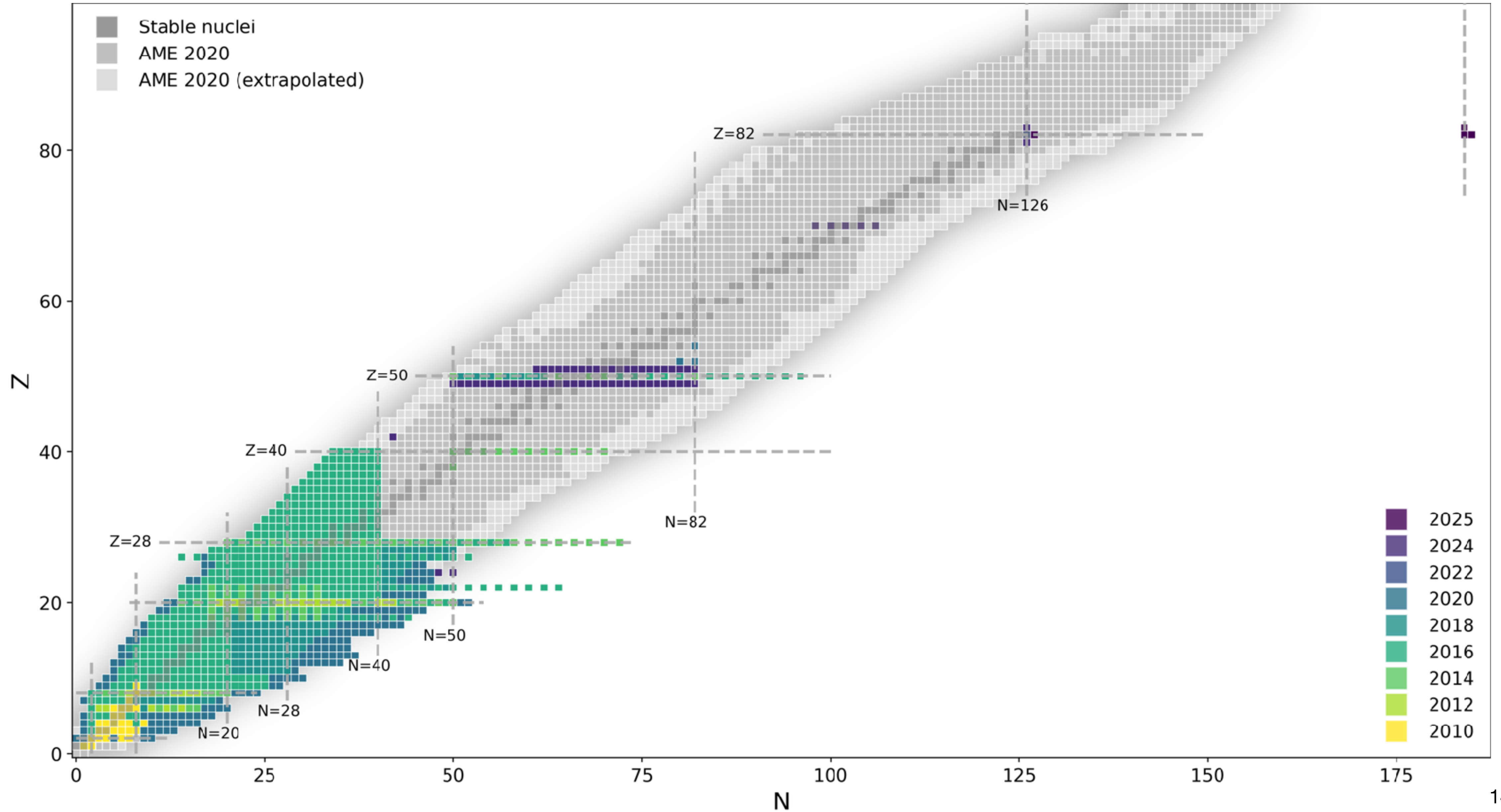
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Ab initio Revolution



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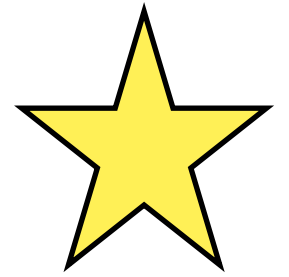
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EFT Corrections to the Operator

Complete approach based on EFT allows to find corrections to operators:

$$[T_{1/2}^{0\nu}]^{-1} = g_A^4 G^{0\nu} | M_{LR}^{0\nu} + M_{SR}^{0\nu} + M_{\text{usoft}}^{0\nu} + M_{\text{loops}}^{0\nu} |^2 \left(\frac{m_{\beta\beta}}{m_e} \right)^2$$



V. Cirigliano et al., Phys. Rev. C 97, 065501 (2018), Phys. Rev. Lett. 120, 202001 (2018), Phys. Rev. C 100, 055504 (2019)

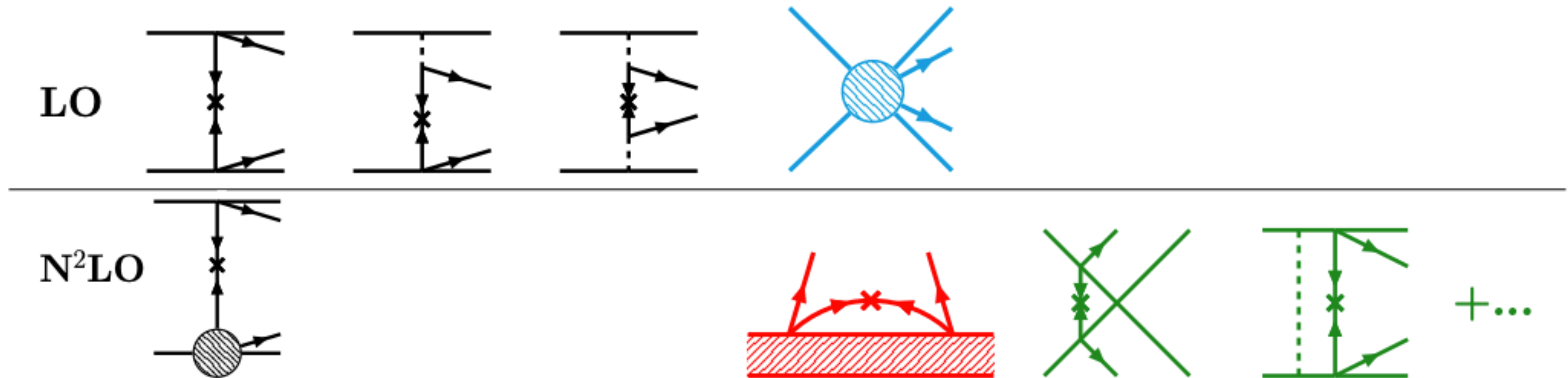
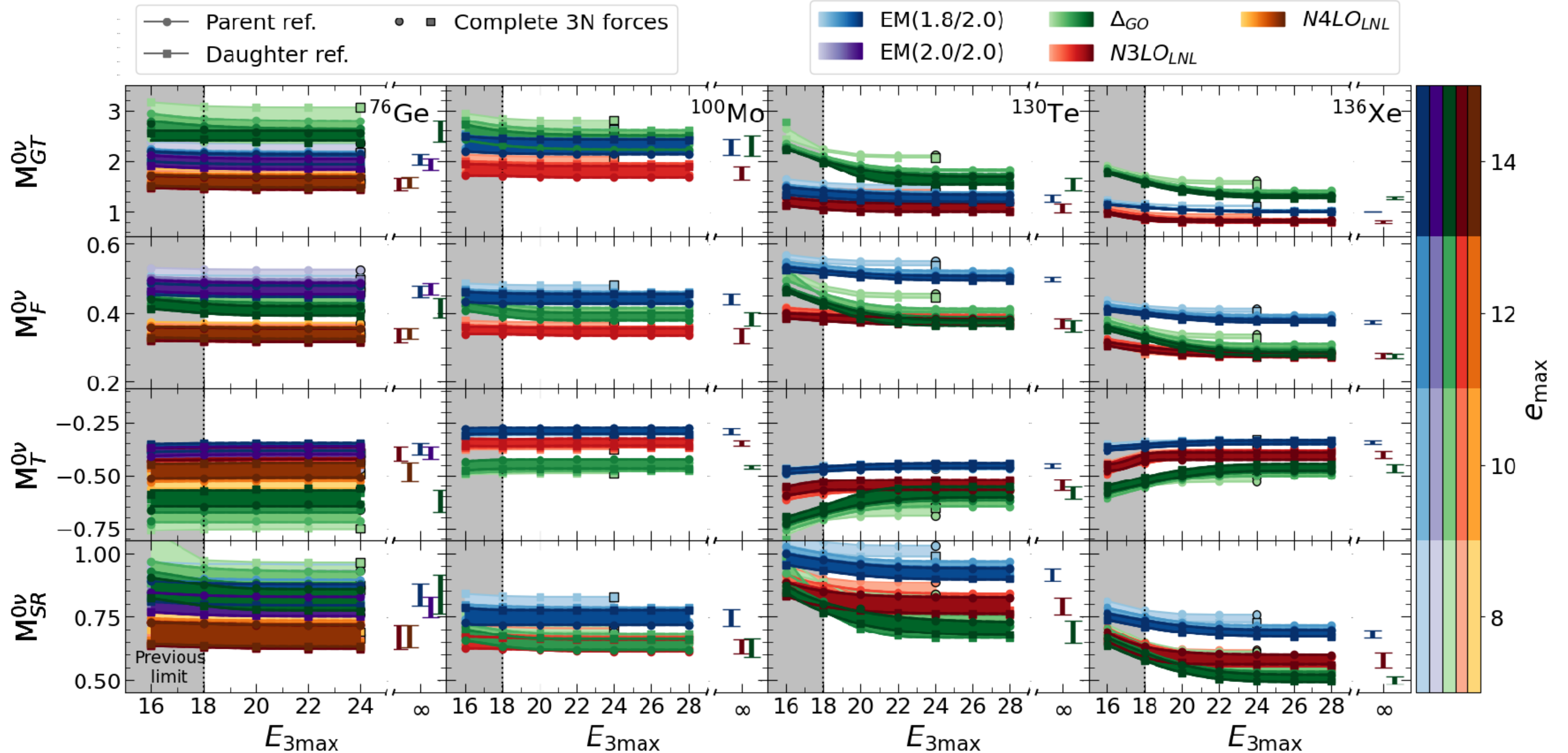
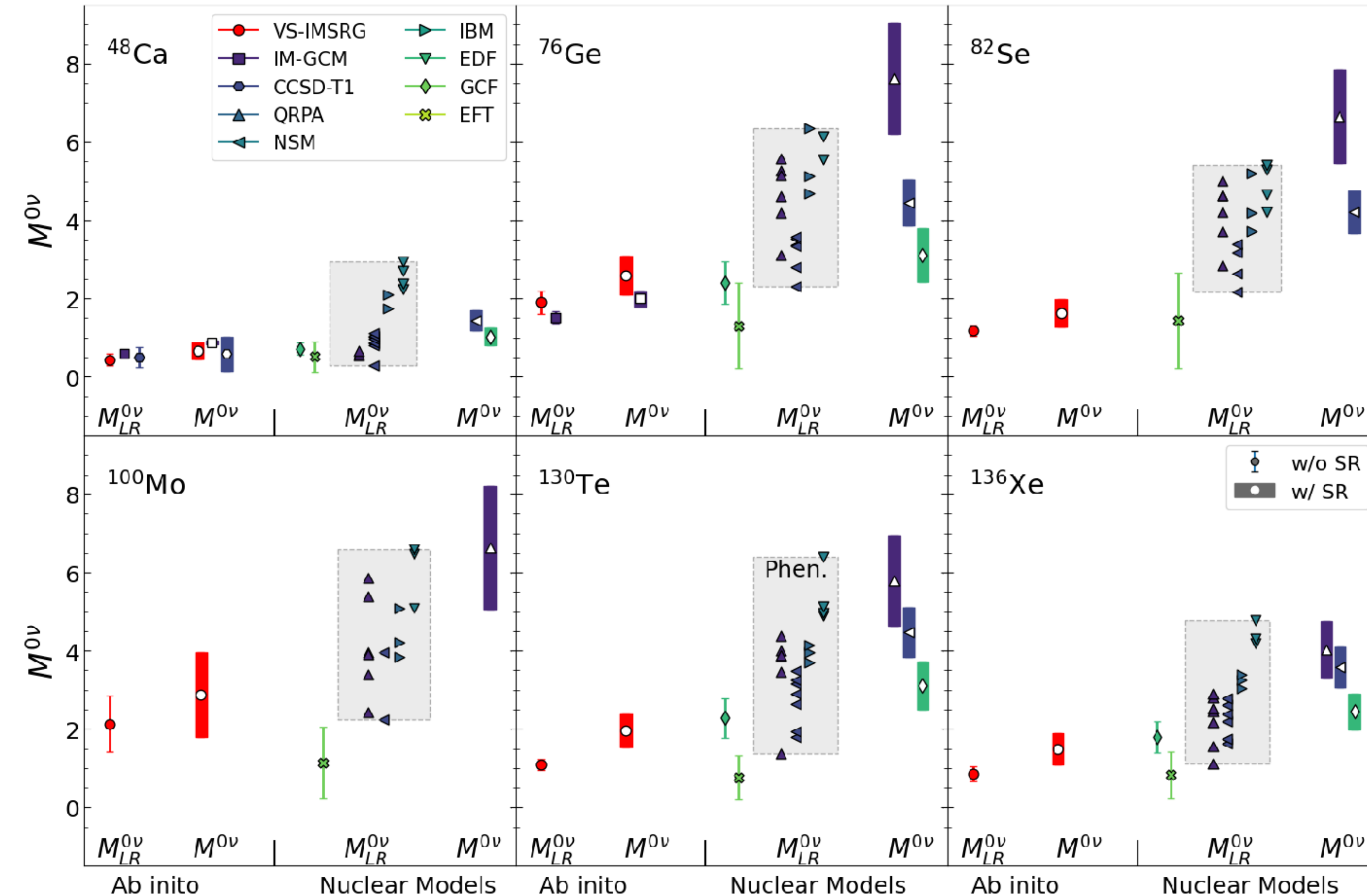


Figure courtesy of L. Jokiniemi



Results in Heavy Nuclei

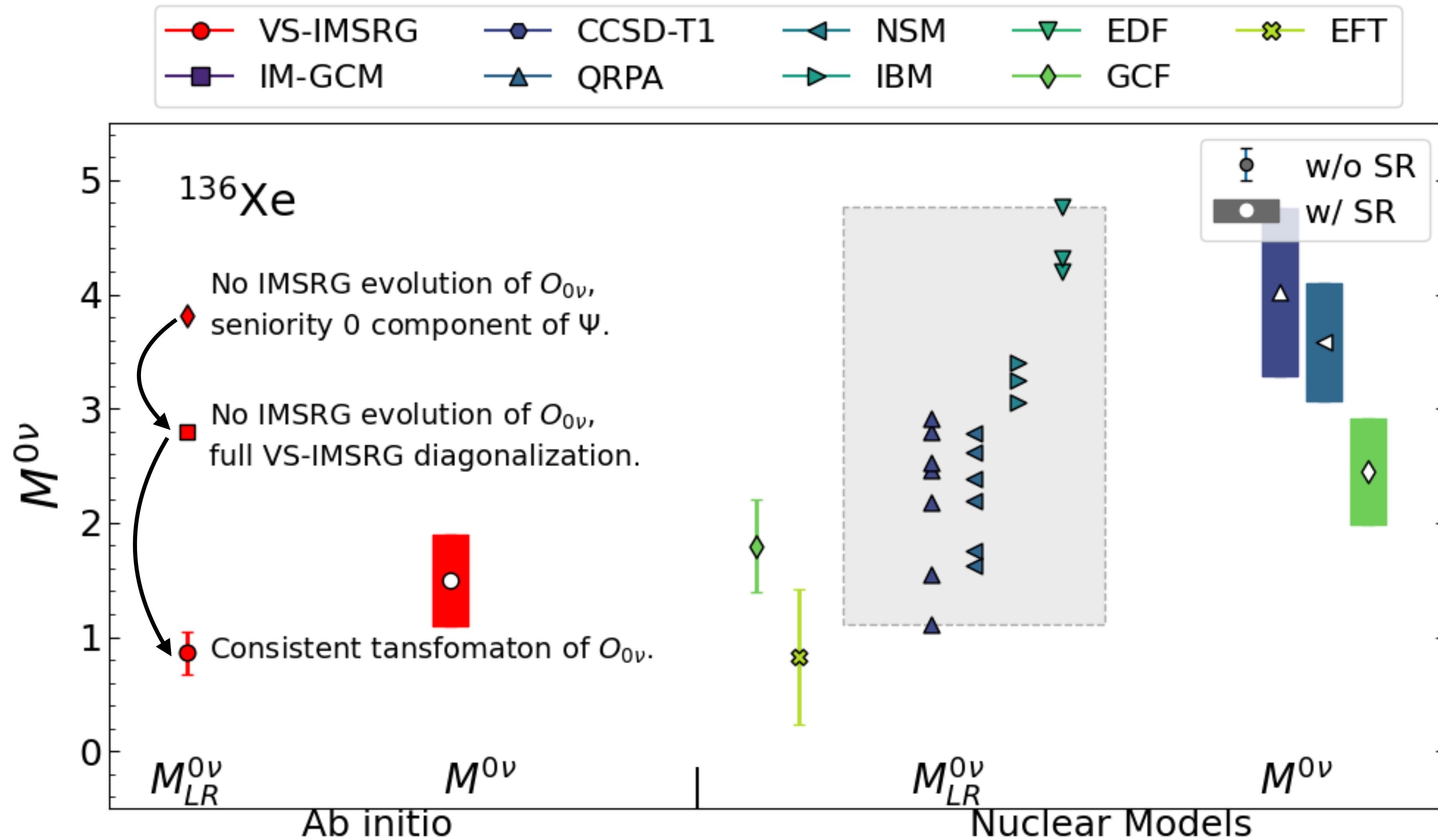




Values from:

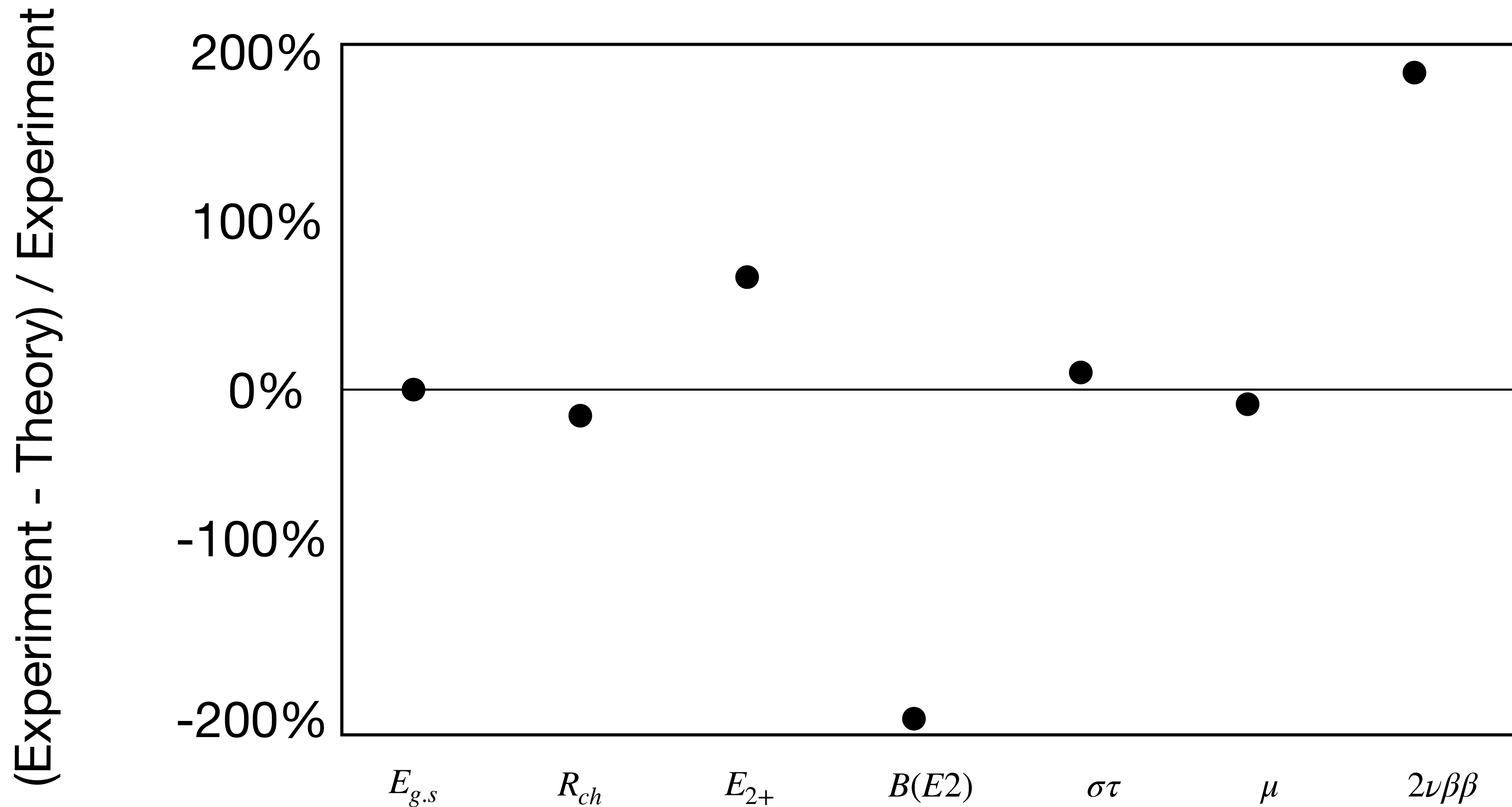
- Agostini et al., Rev. Mod. Phys. 95, 025002 (2023);
- Yao, Sci. Bull. 10.1016 (2020);
- **Belley** et al., Phys. Rev. Lett. 126, 042502 (2020);
- Brase et al., Phys. Rev. C 106, 034309 (2021);
- Weiss et al., Phys. Rev. C 106, 064401 (2022);
- **Belley** et al., arXiv:2307.15156 (2023);
- **Belley** et al., Phys. Rev. Lett. 132, 182502 (2024).

Comparison with Previous Results





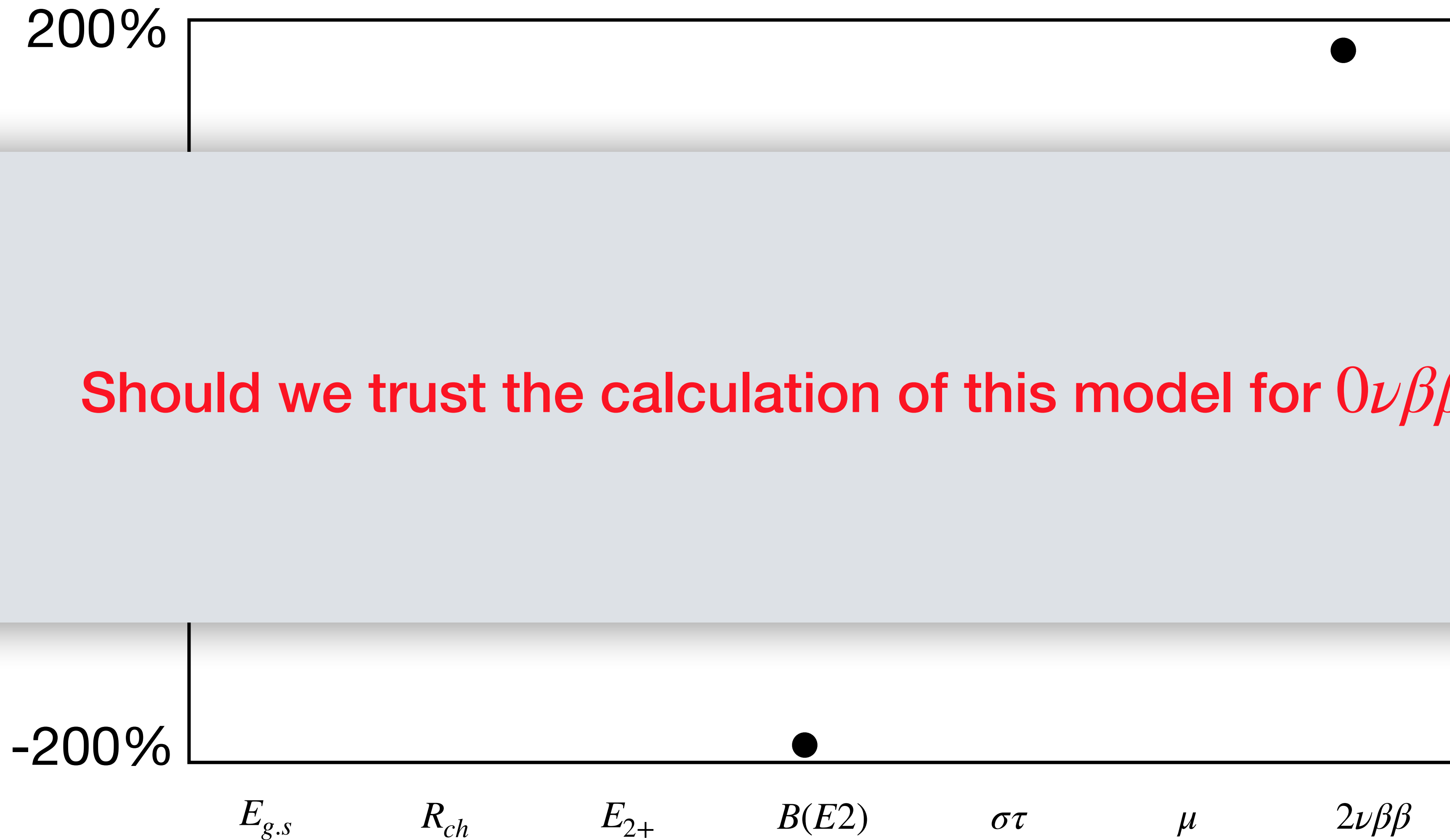
Using other observables





Using other observables

(Experiment - Theory) / Experiment





List of Challenges



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- Deriving an expression for the nuclear potential (χ -EFT)
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 - Uncertainty Quantification

Uncertainty quantification



Propagating the LECs Error

Recall that the nuclear potential depends on a set of LECs α :

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that are fitted to NN and few-nucleon data, i.e. each LEC has an uncertainty $\delta\alpha$ associated with it.



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Bayesian Statistics!



Bayesian Approach

We read $\textit{prob}(A | B)$ as
probability of A given B

$$\textit{prob}(\alpha | y, I) \propto \textit{prob}(y | \alpha, I) \times \textit{prob}(\alpha | I)$$



Bayesian Approach

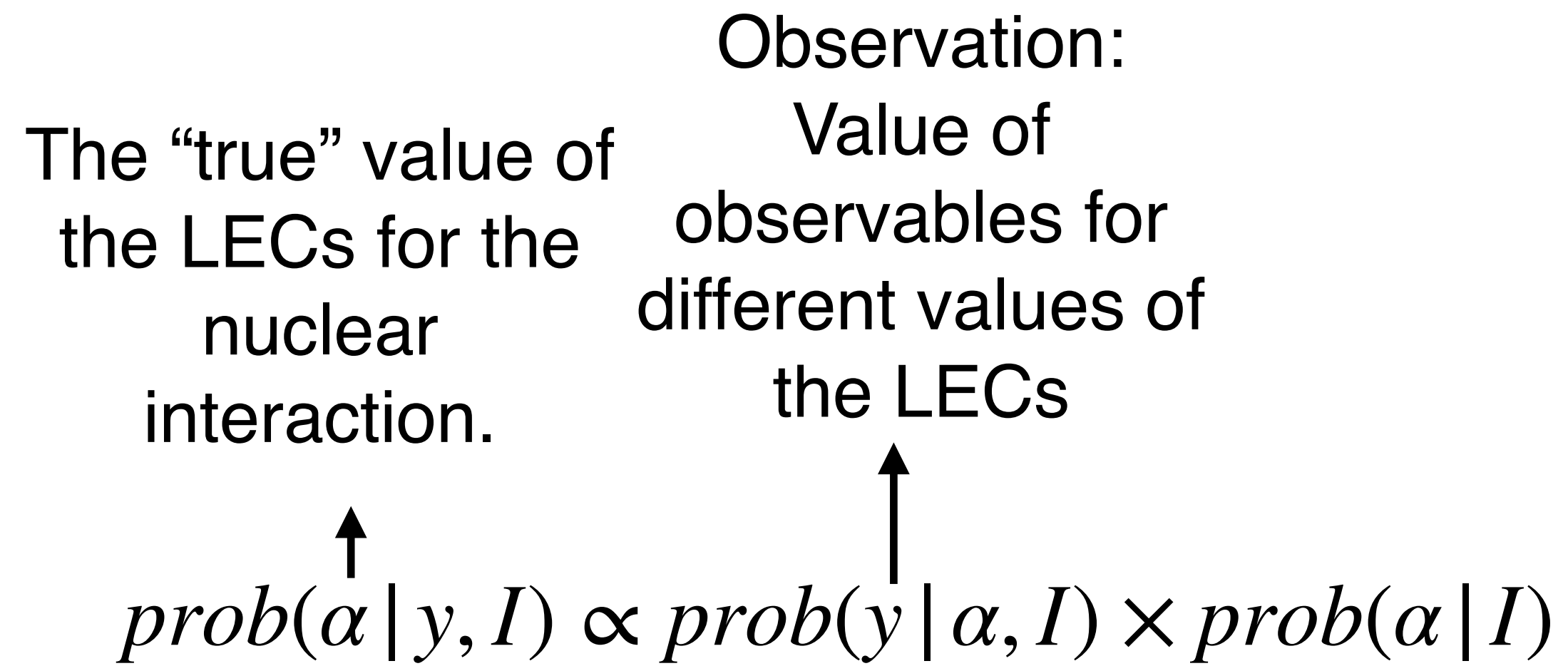
The “true” value of
the LECs for the
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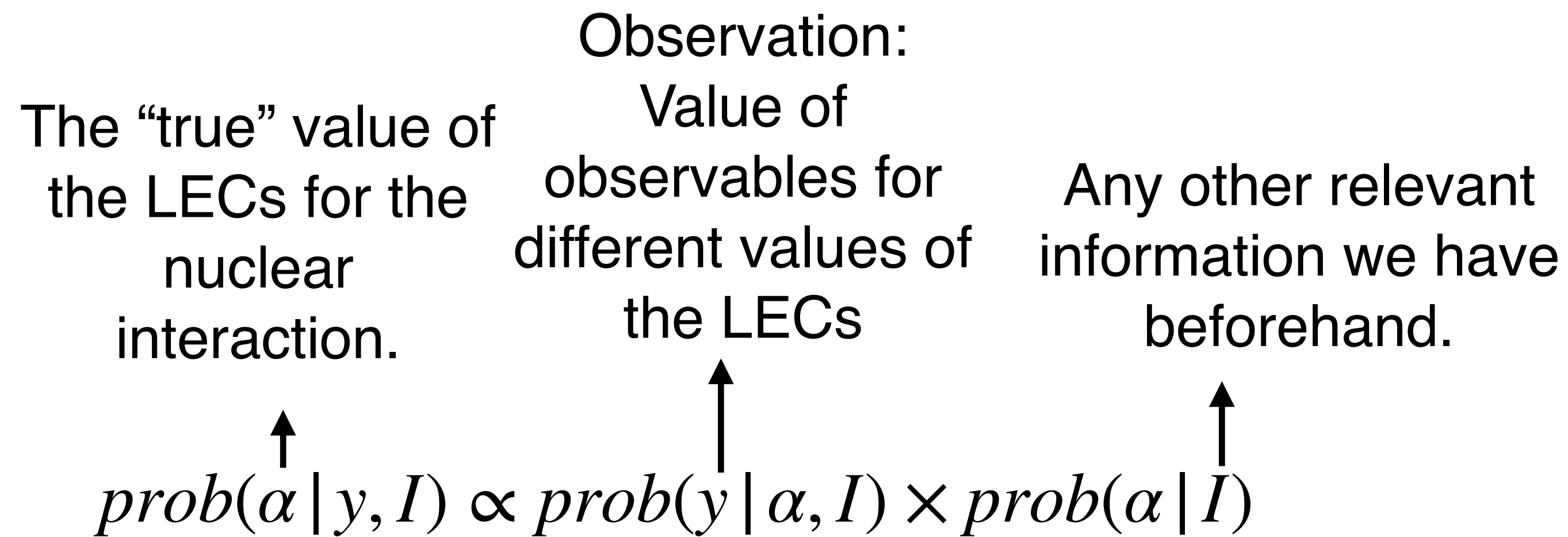
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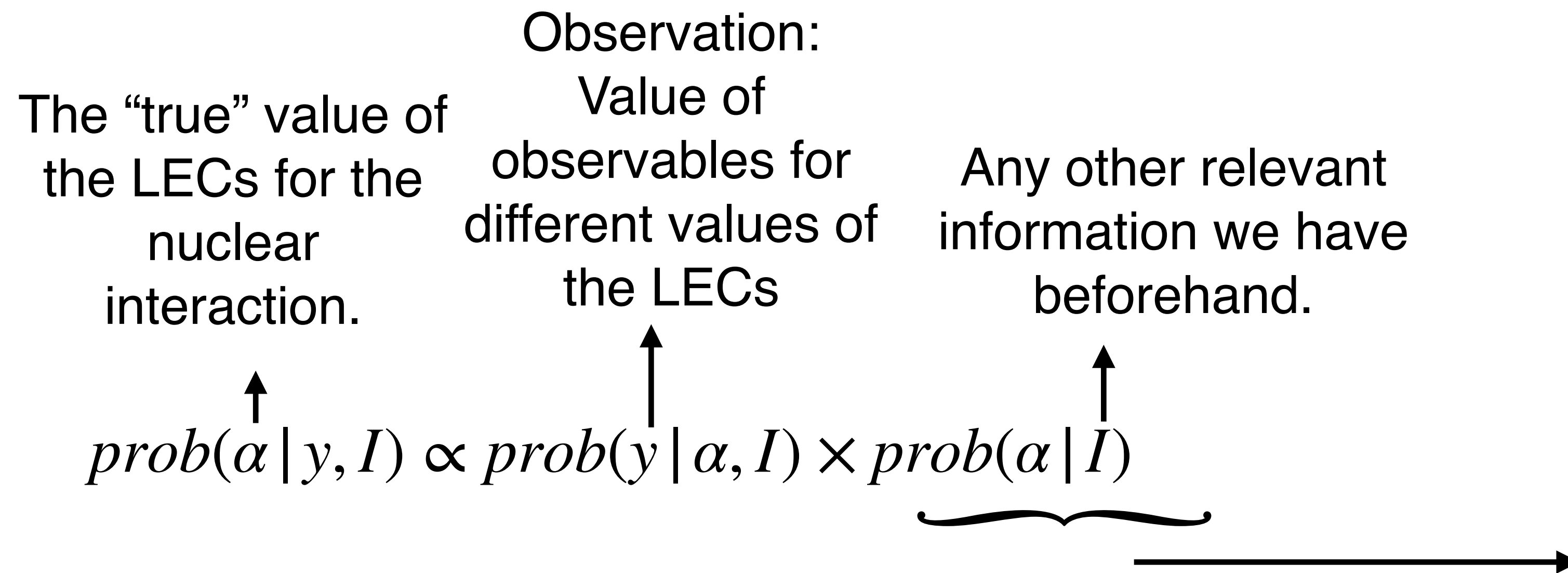
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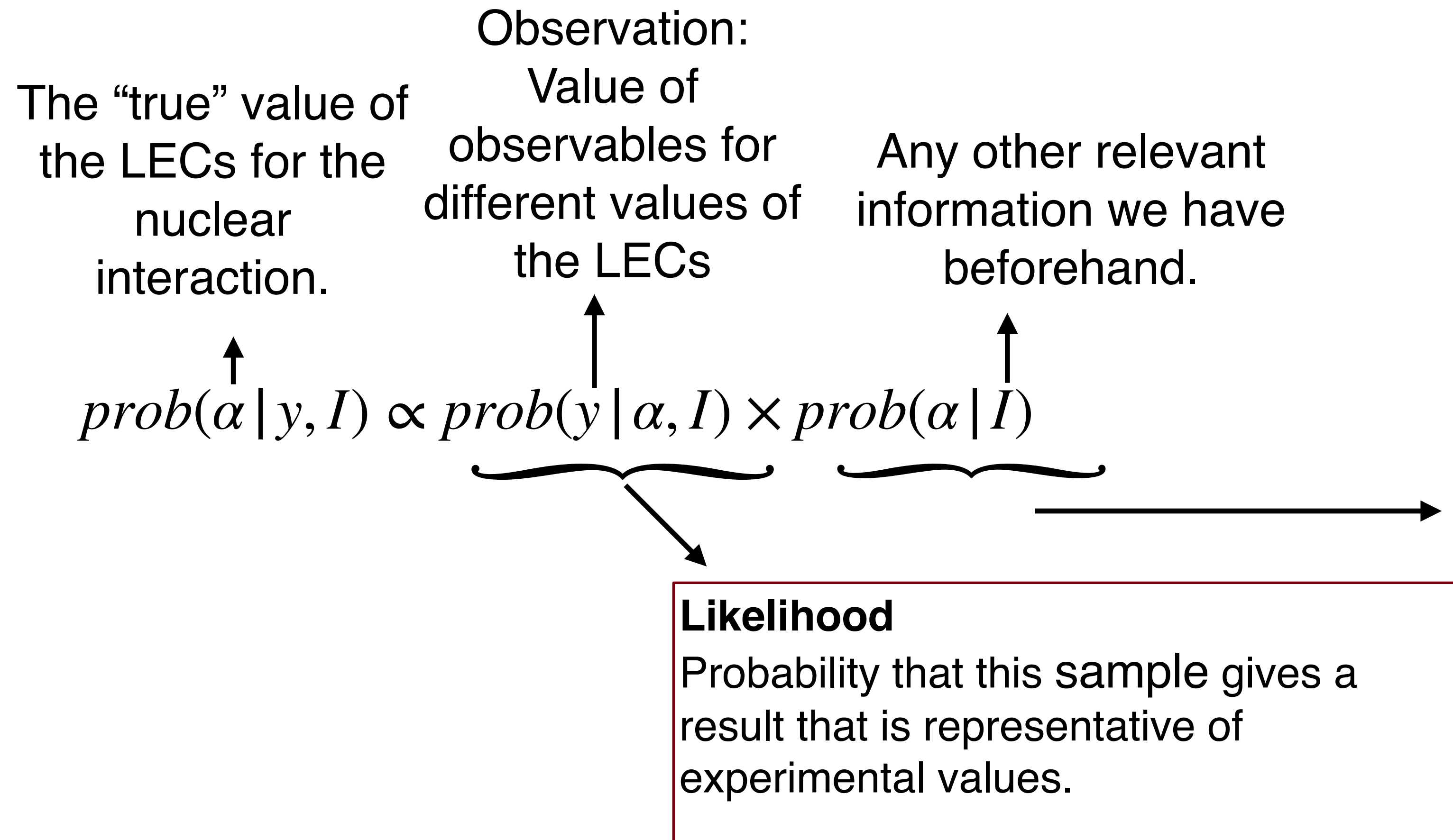
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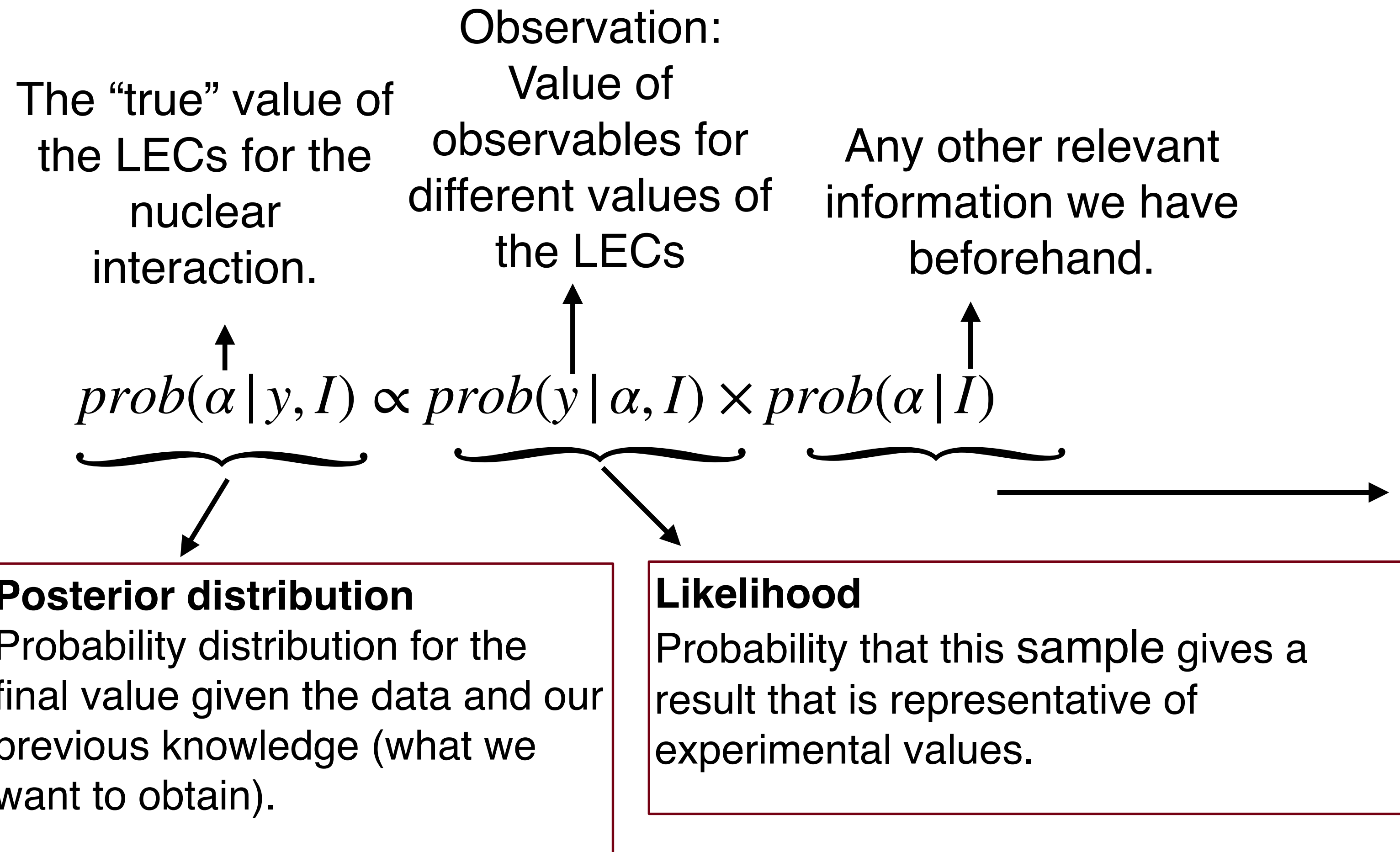


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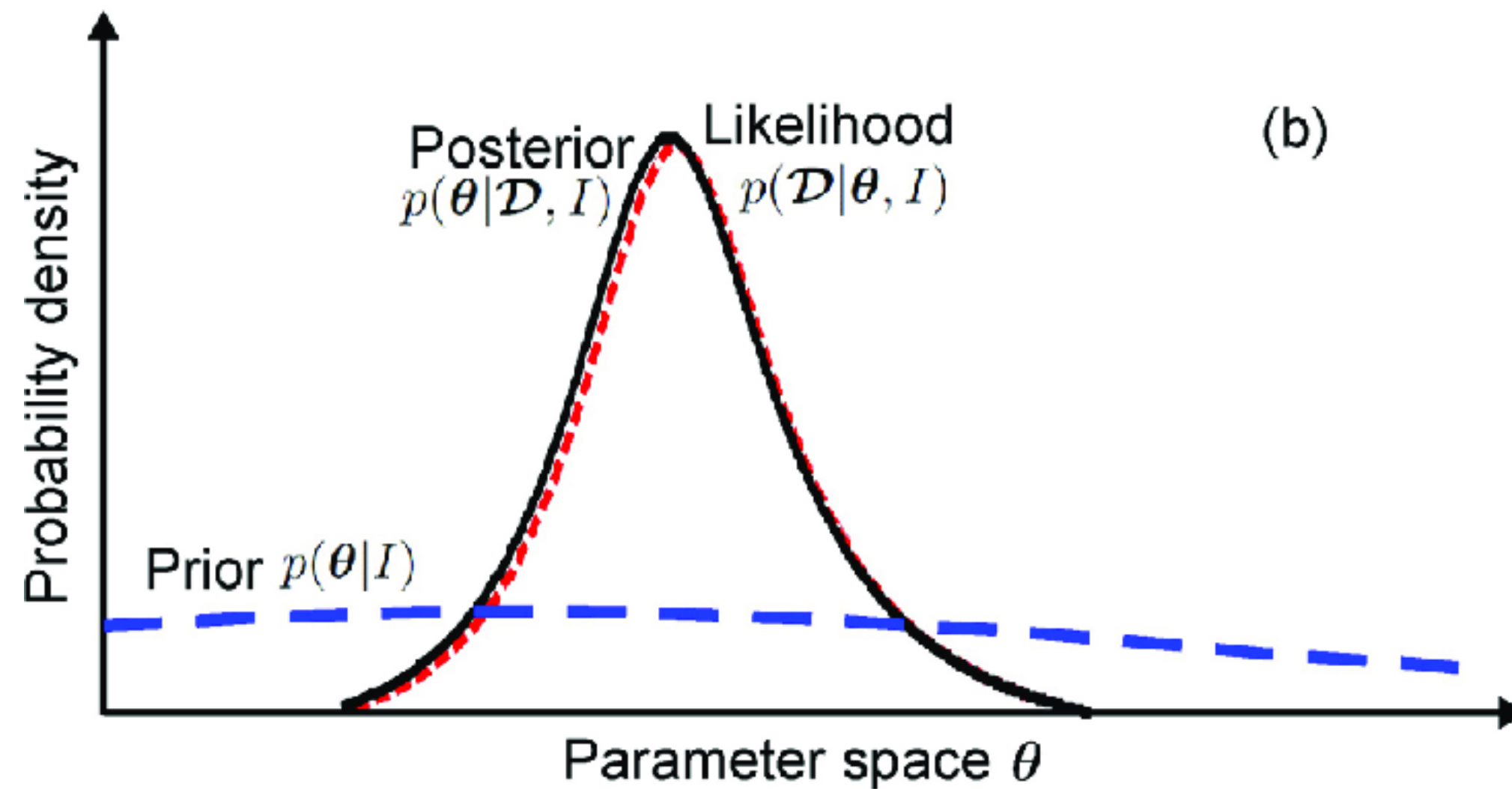
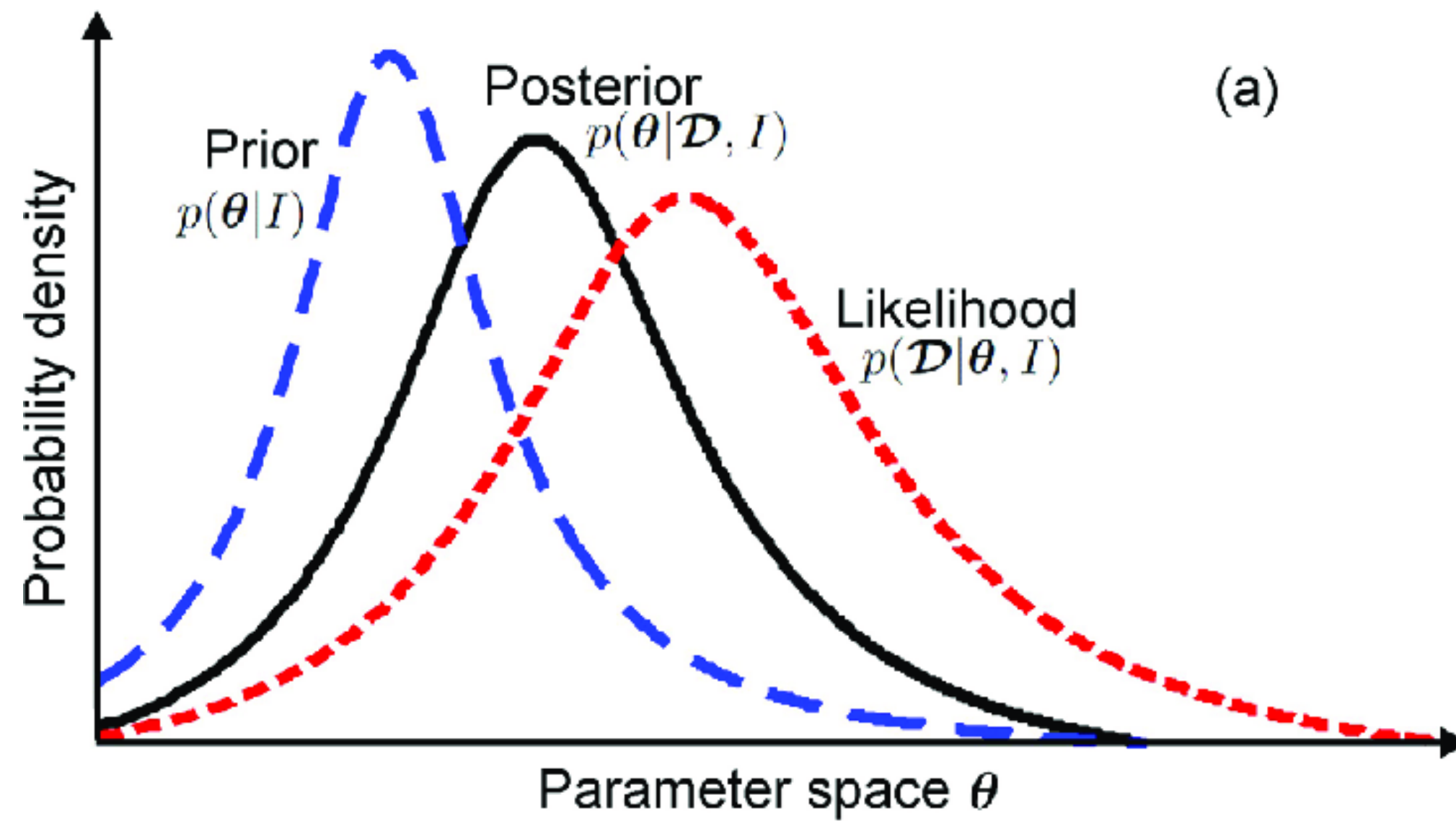


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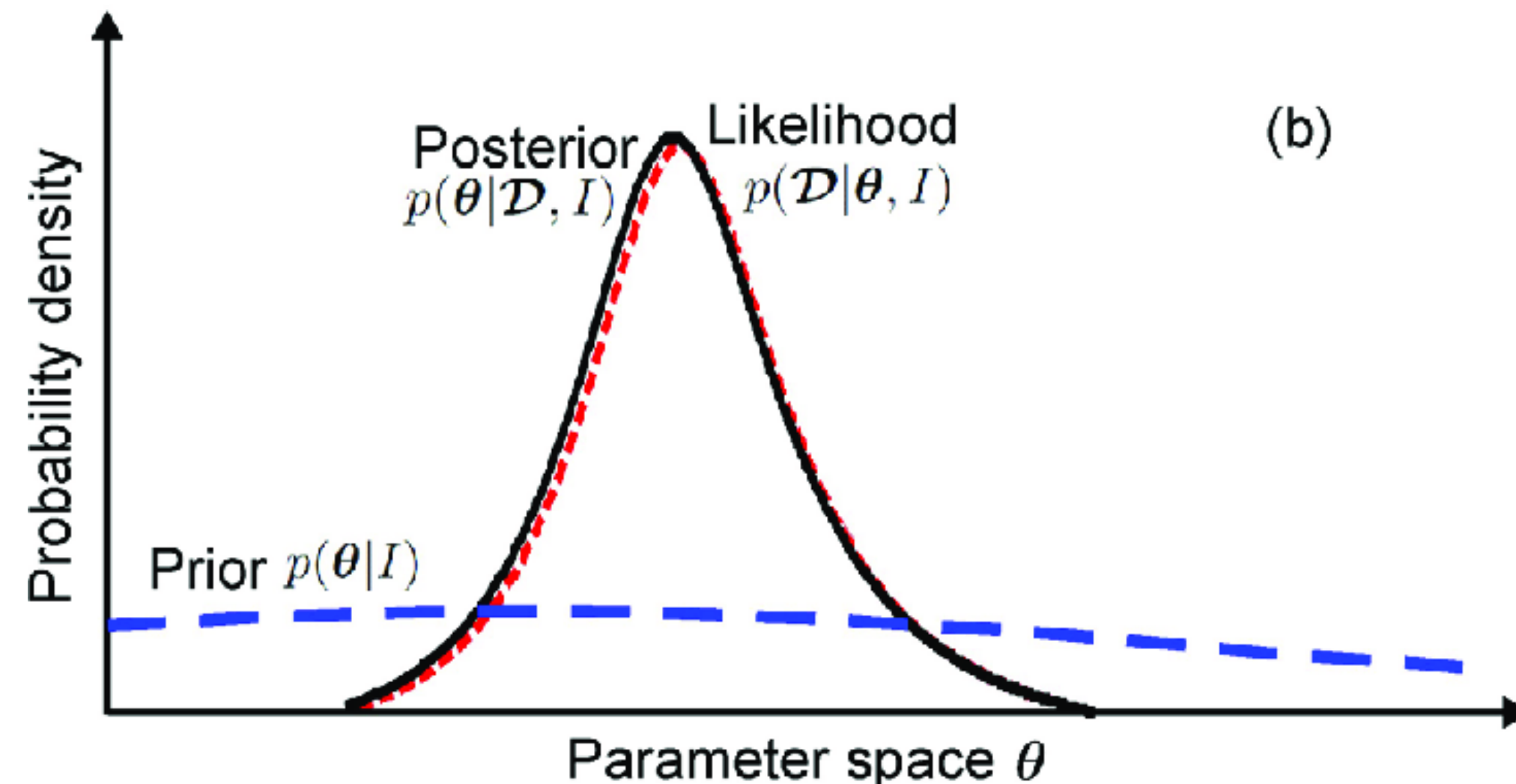
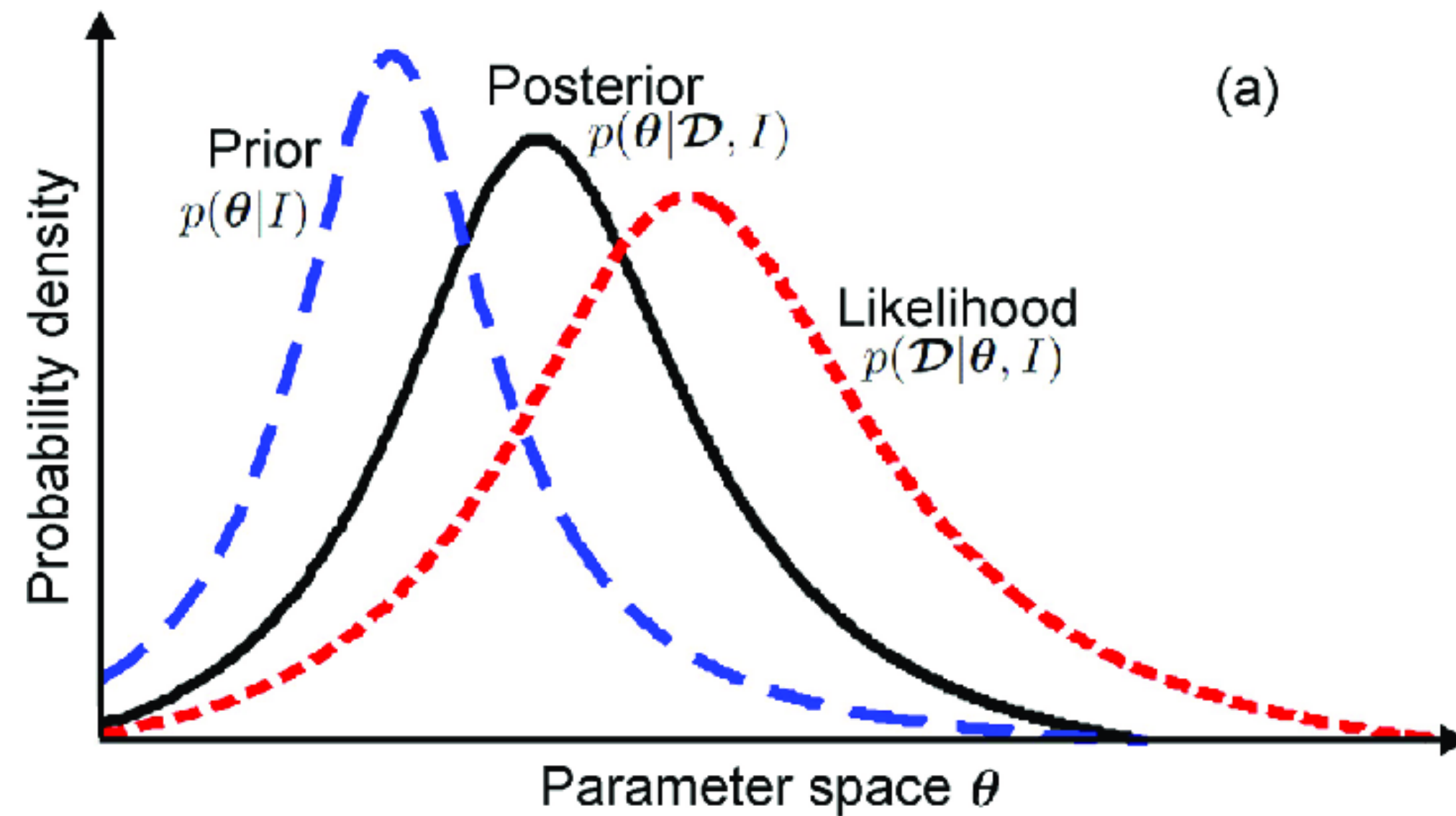


Procedure for UQ in the Bayesian Approach





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The catch

Need many samples.

Due to the large cost of many-body methods, for 1 isotope:

- Take ~1 year to compute all samples on HPC cluster.
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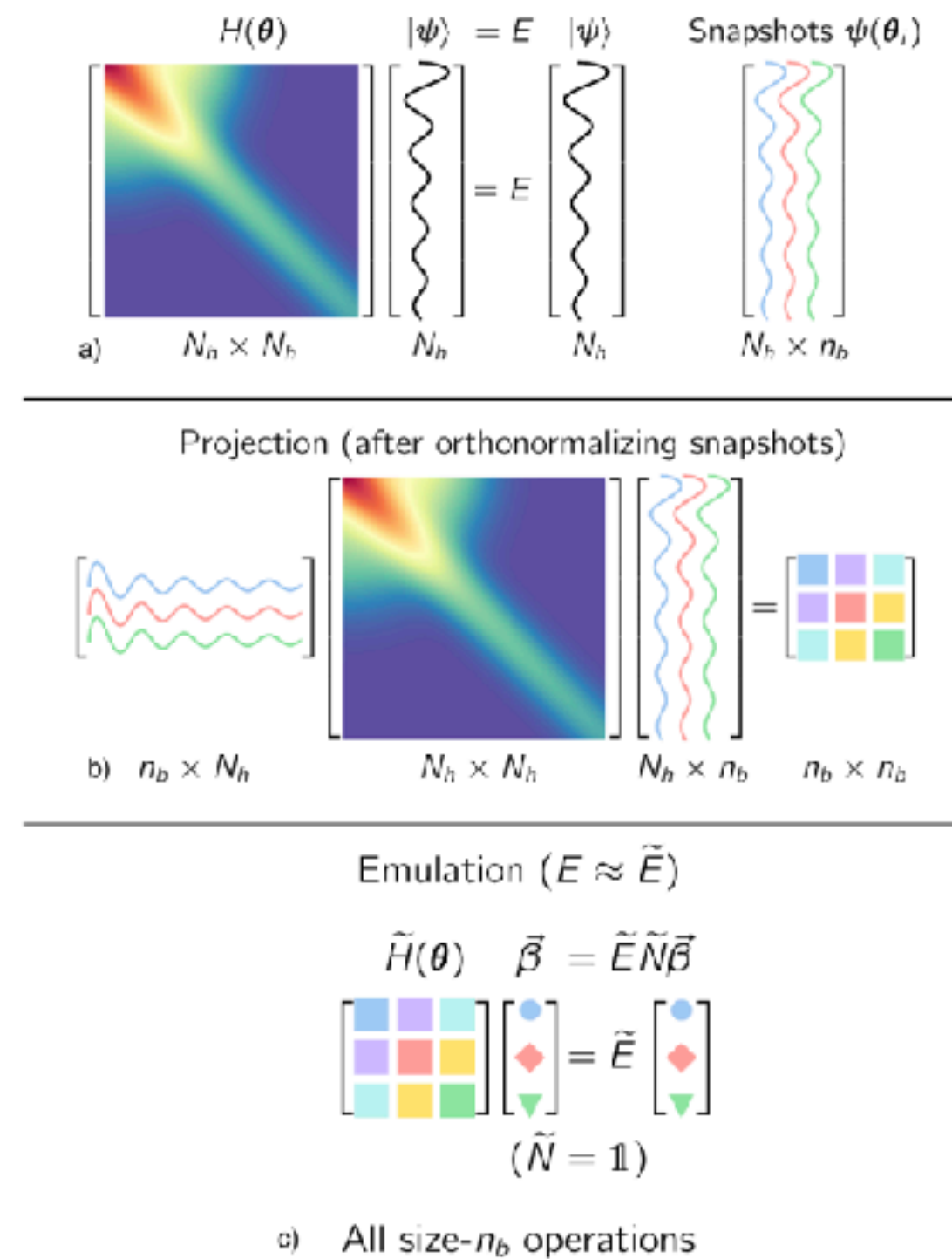


Emulators for Many-Body Methods

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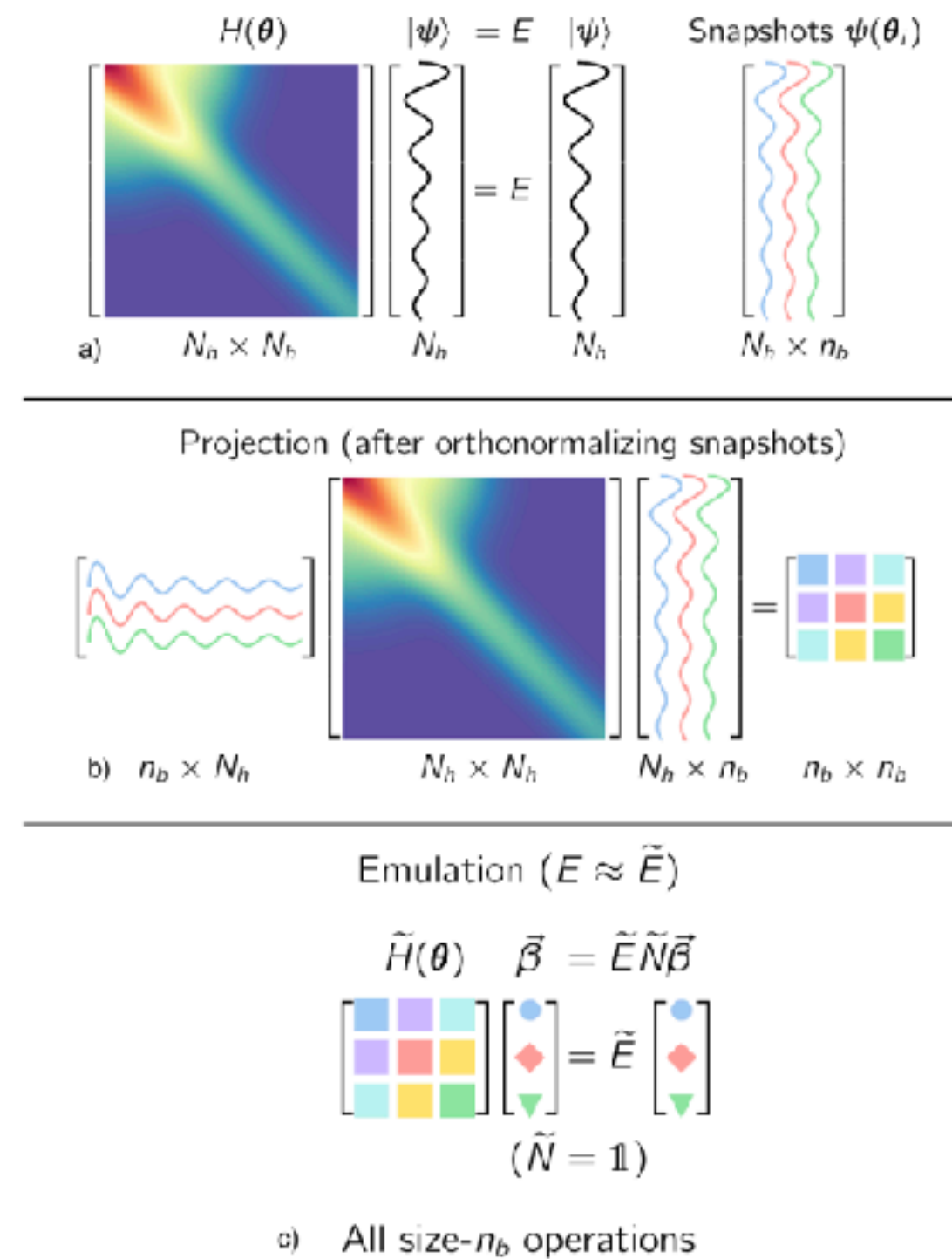
1. Physics driven



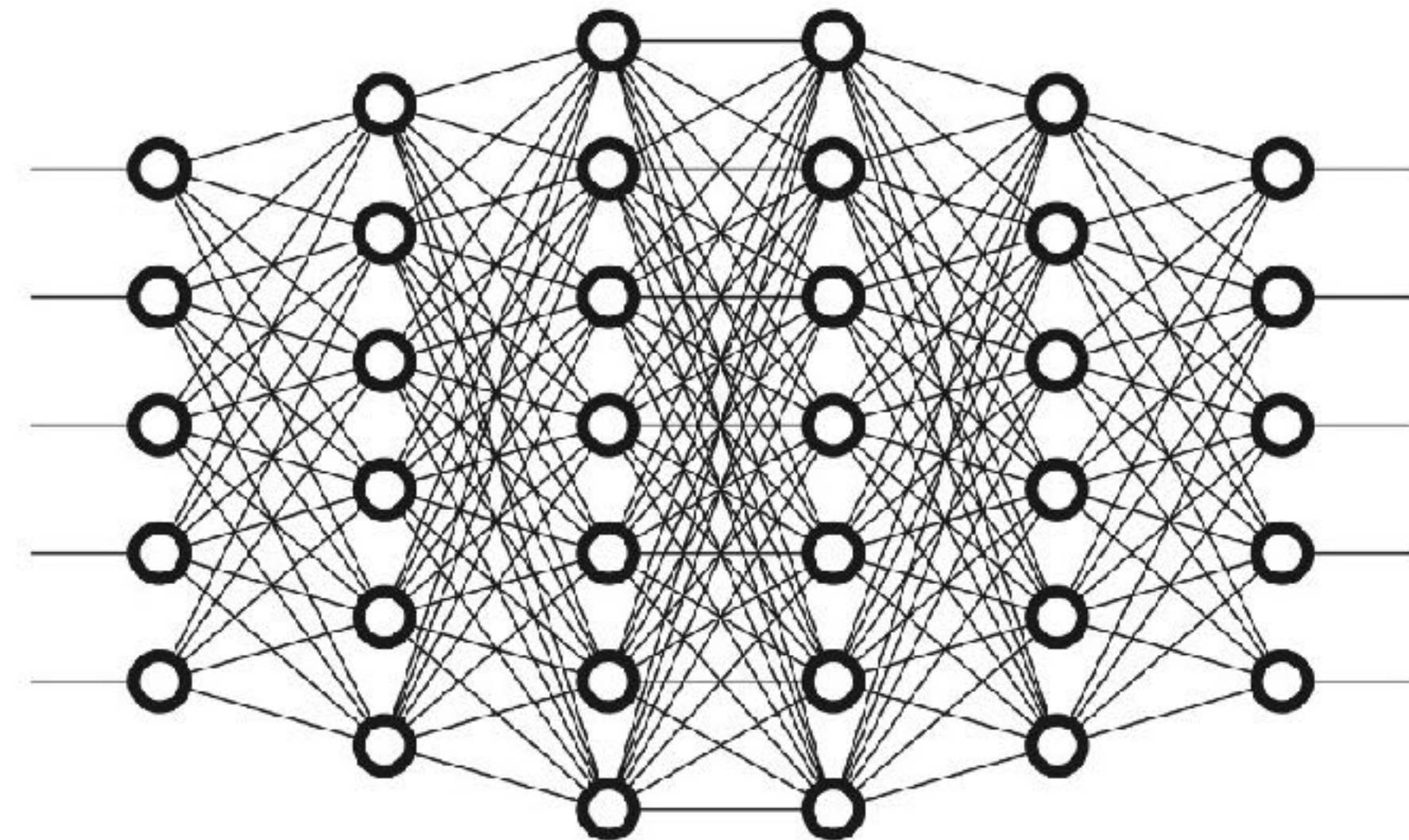
Emulators for Many-Body Methods

There are two ways to build an emulator for nuclear physics:

1. Physics driven



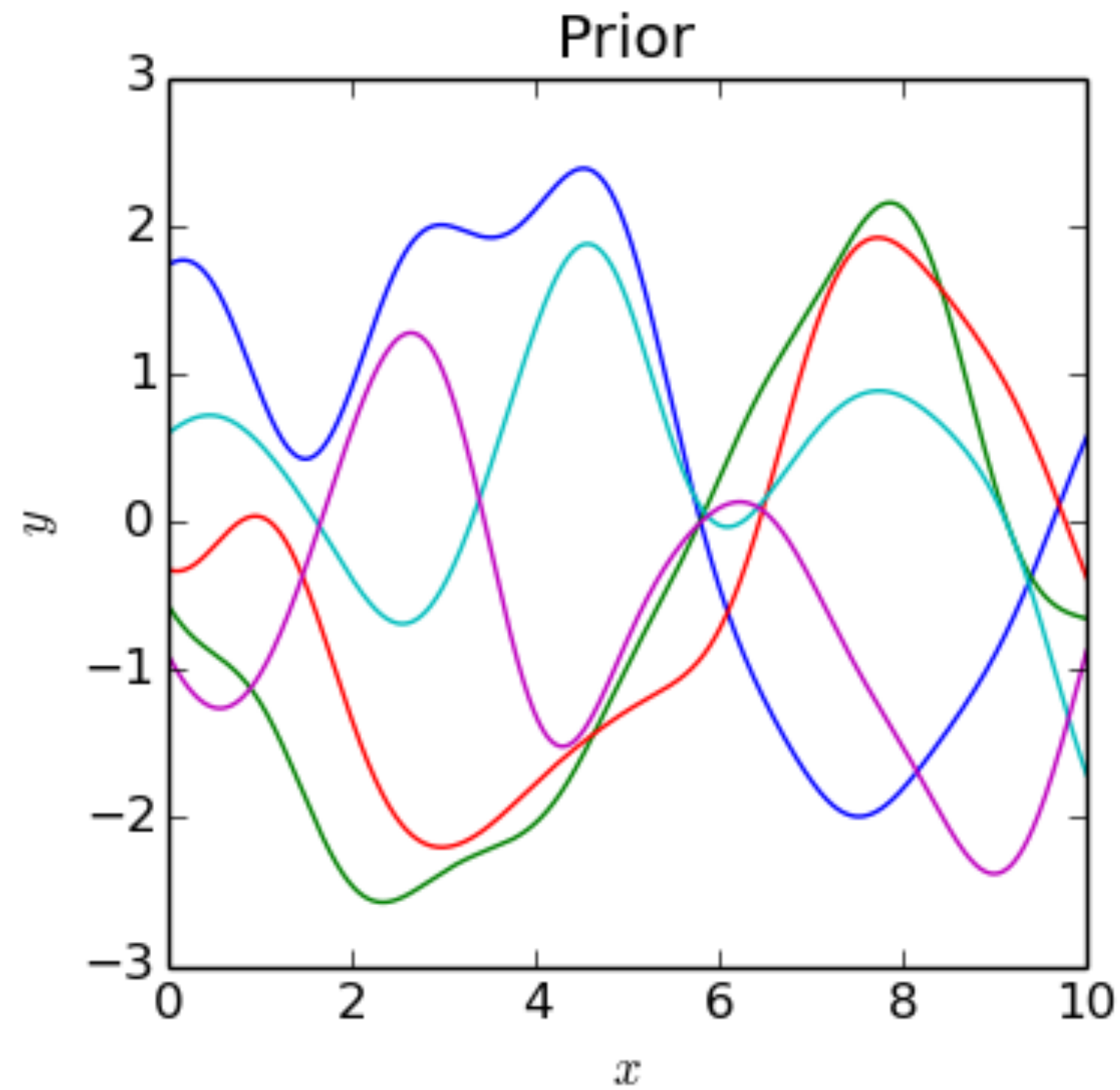
2. Data driven





Using Gaussian Process as an Emulator

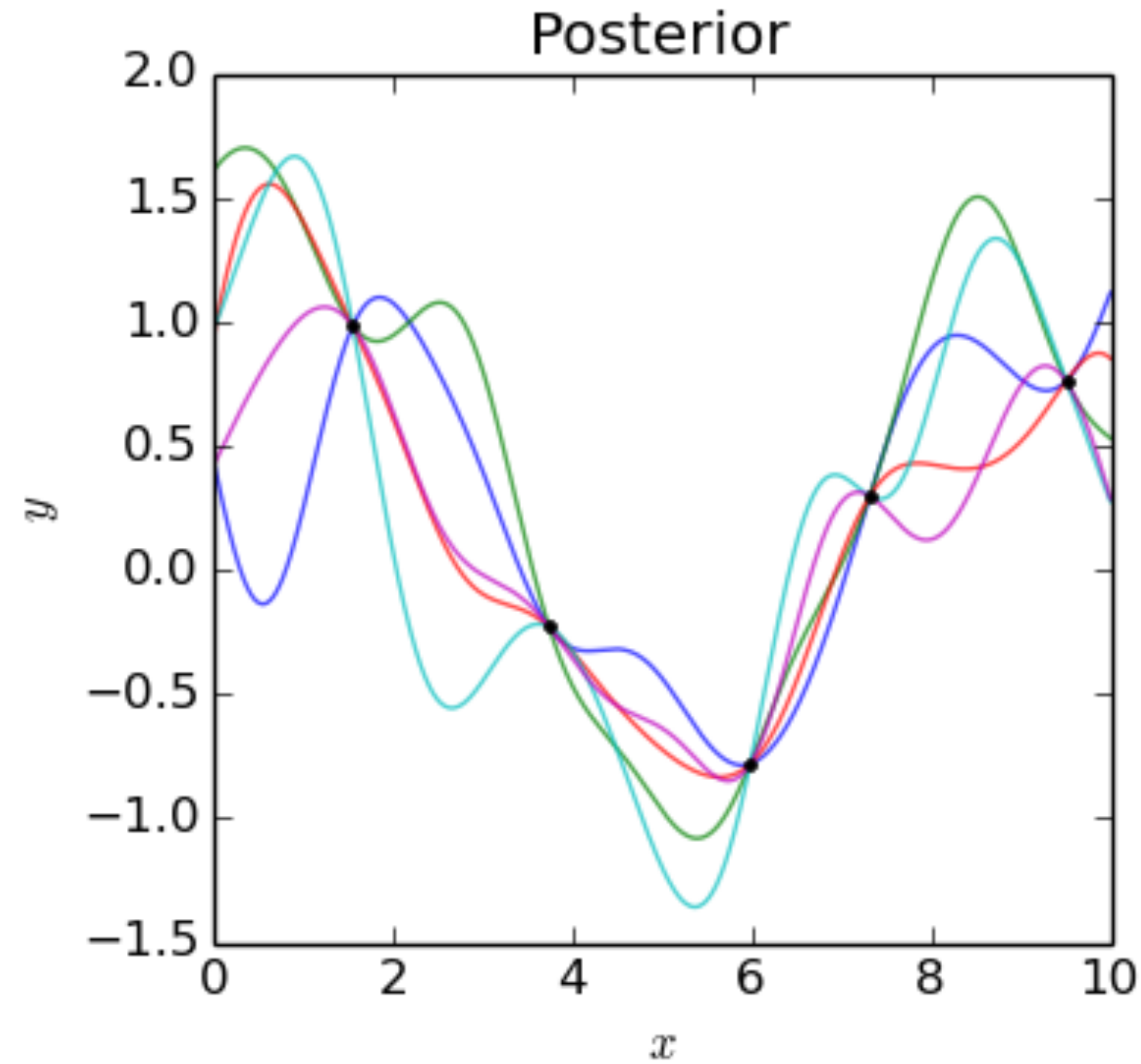
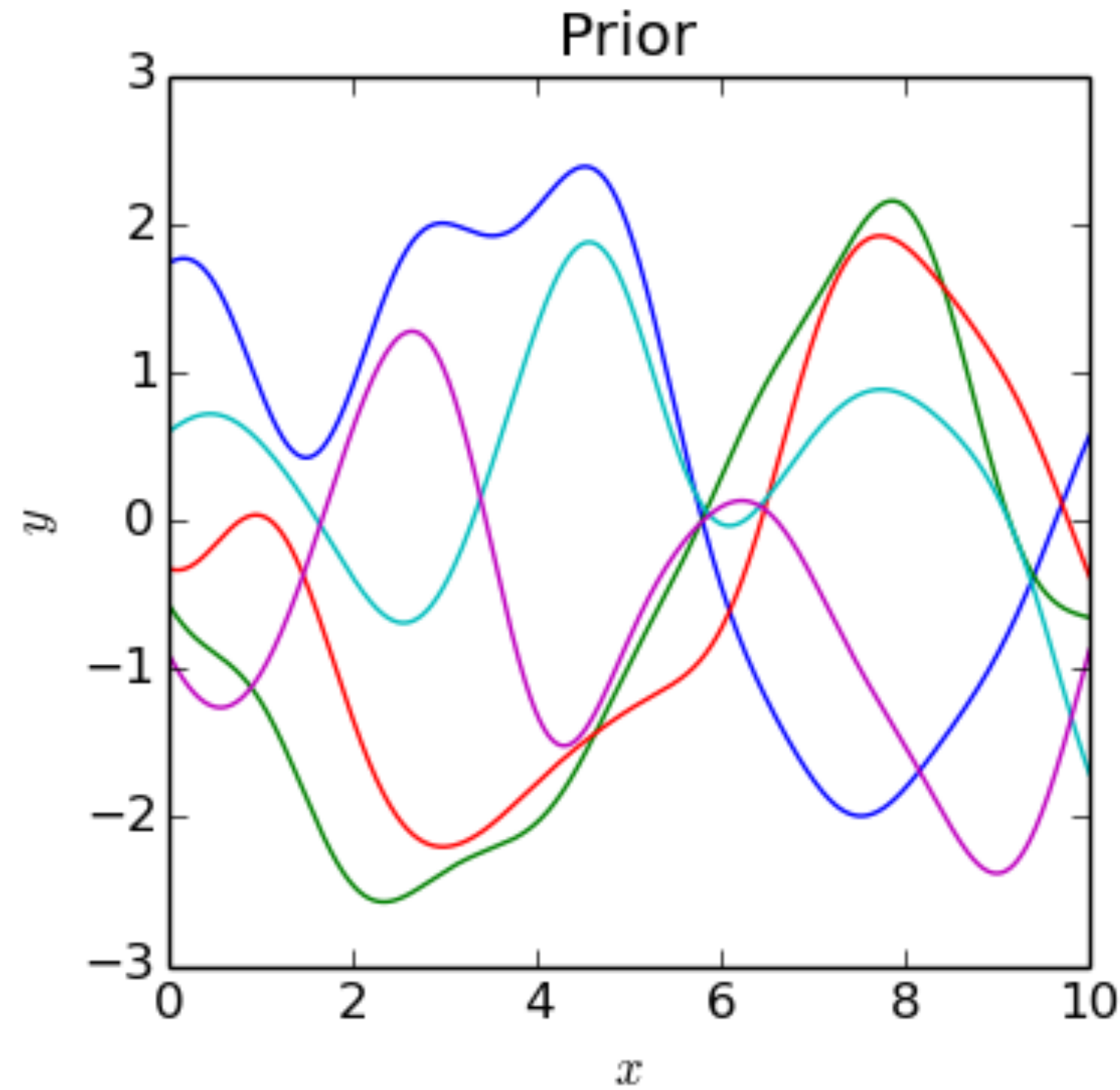
Cdipaolo - <https://commons.wikimedia.org/w/index.php?curid=47589433>
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$$f(\mathbf{x}) = \mathcal{N}(\mu, K(\mathbf{x}, \mathbf{x}))$$

Using Gaussian Process as an Emulator

Cdipaolo - <https://commons.wikimedia.org/w/index.php?curid=47589433>
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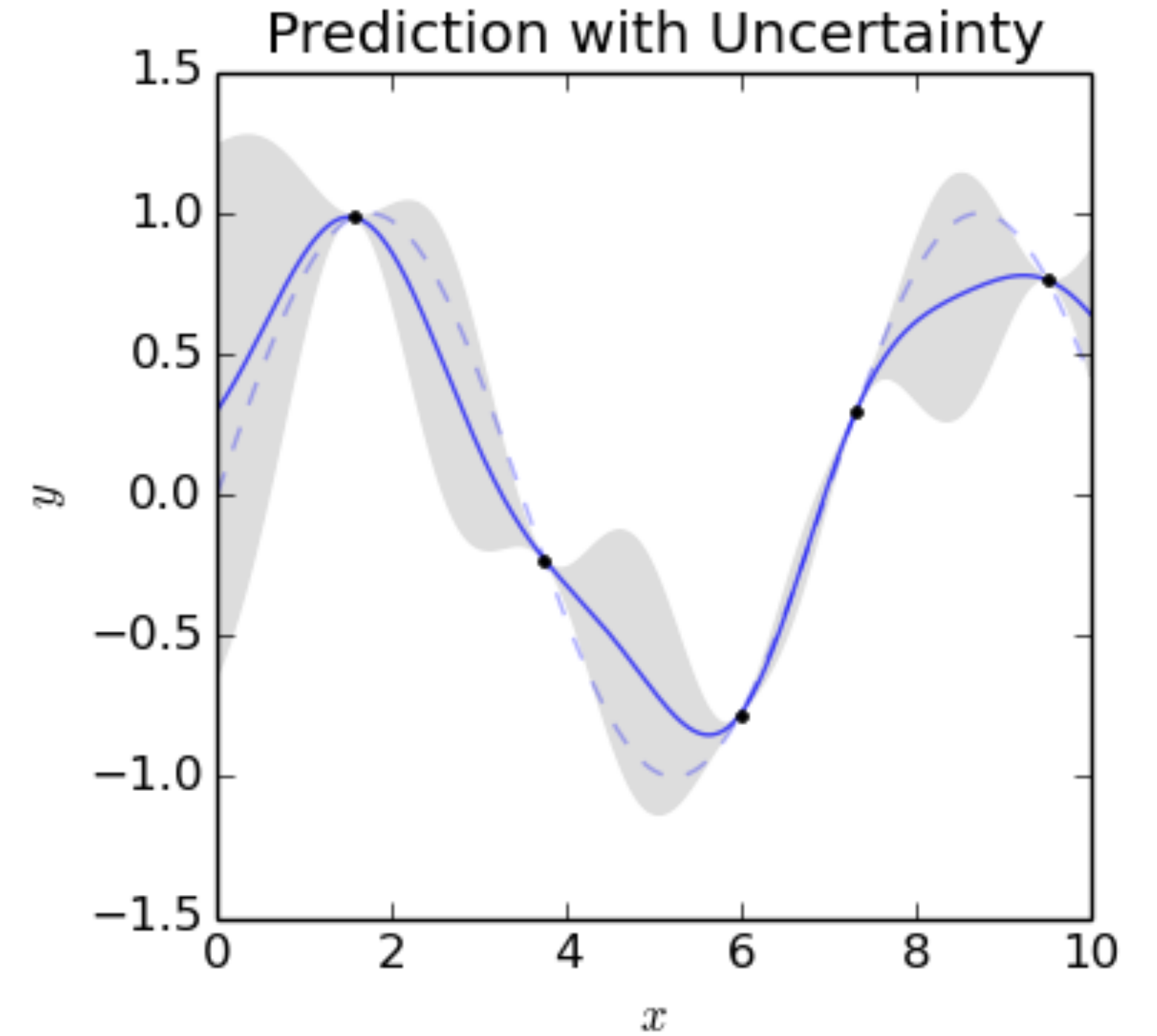
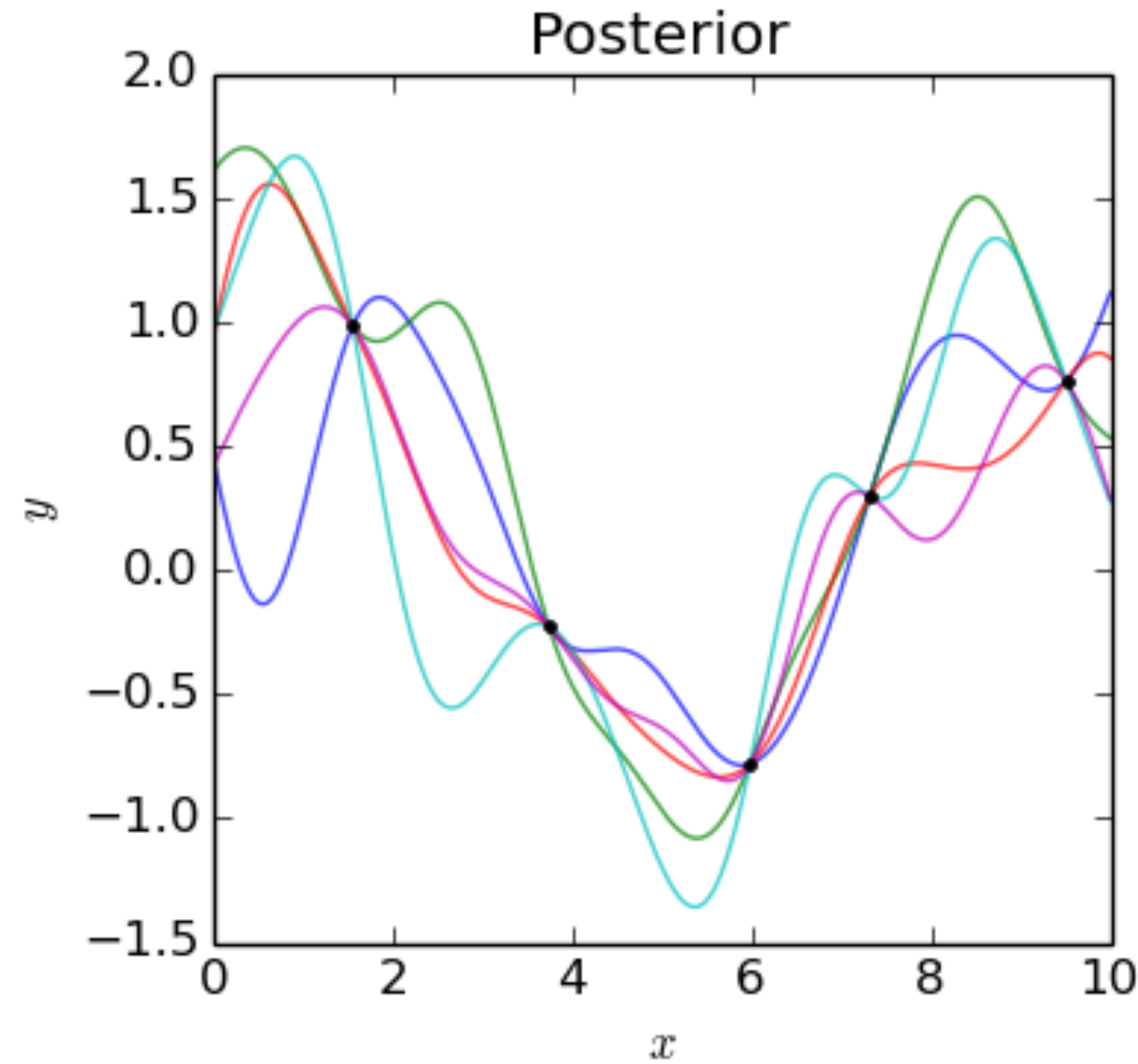
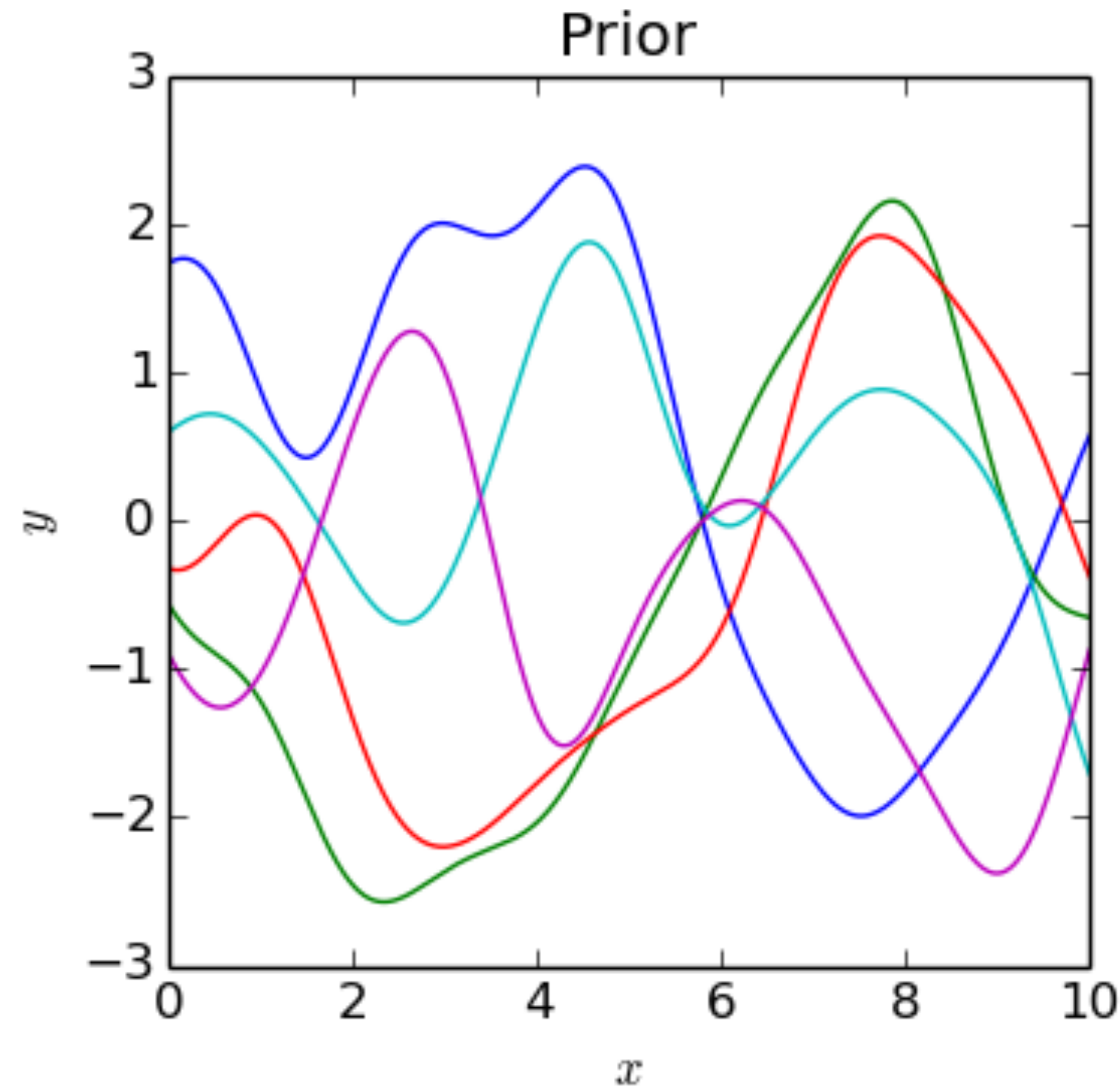


$$f(\mathbf{x}) = \mathcal{N}(\mu, K(\mathbf{x}, \mathbf{x}))$$

$$P_{Y^*|Y} \sim \mathcal{N}(\Sigma_{X^*X}\Sigma_{XX}^{-1}Y, \Sigma_{X^*X^*} - \Sigma_{X^*X}\Sigma_{XX}^{-1}\Sigma_{XX^*})$$

Using Gaussian Process as an Emulator

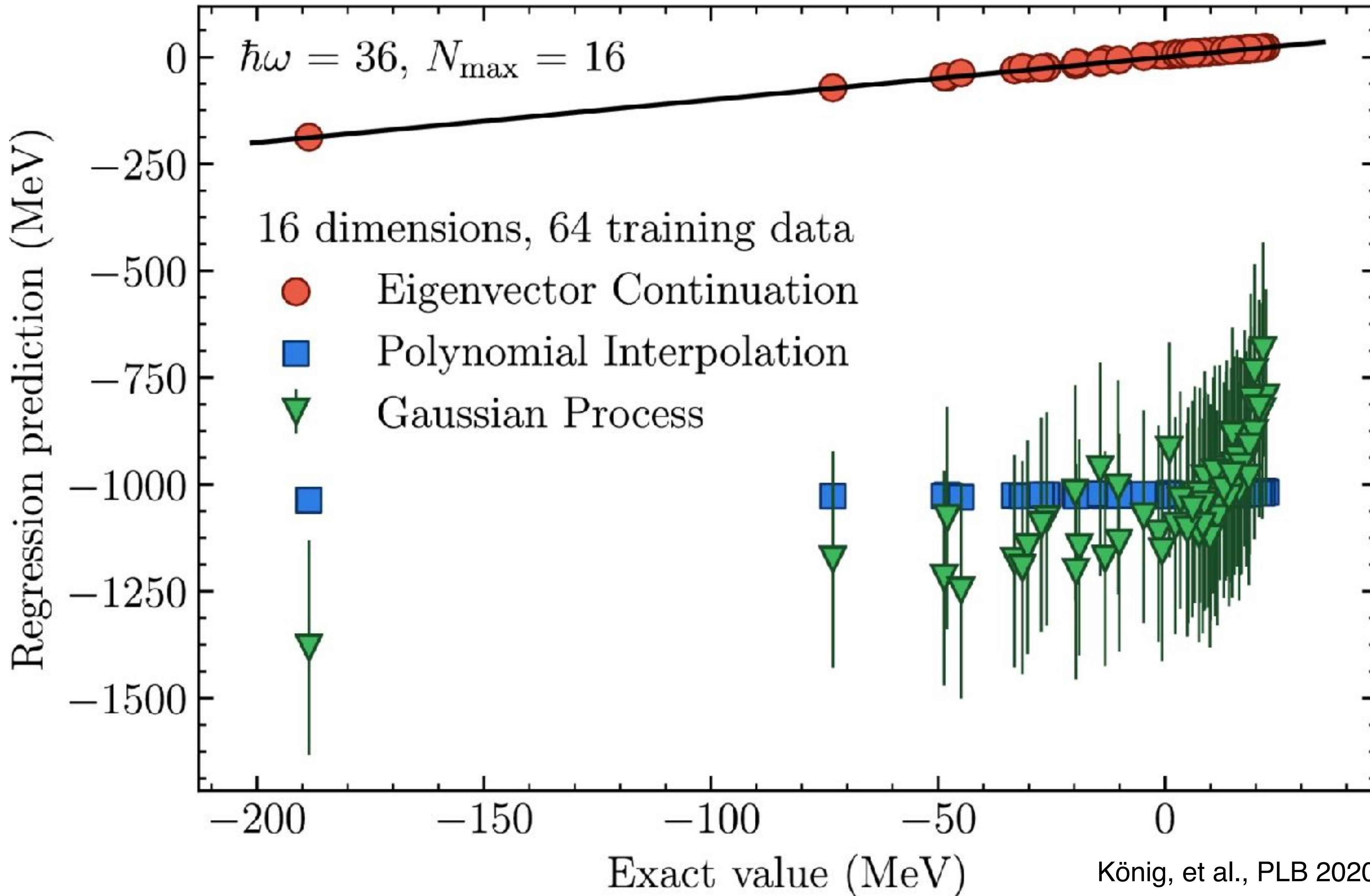
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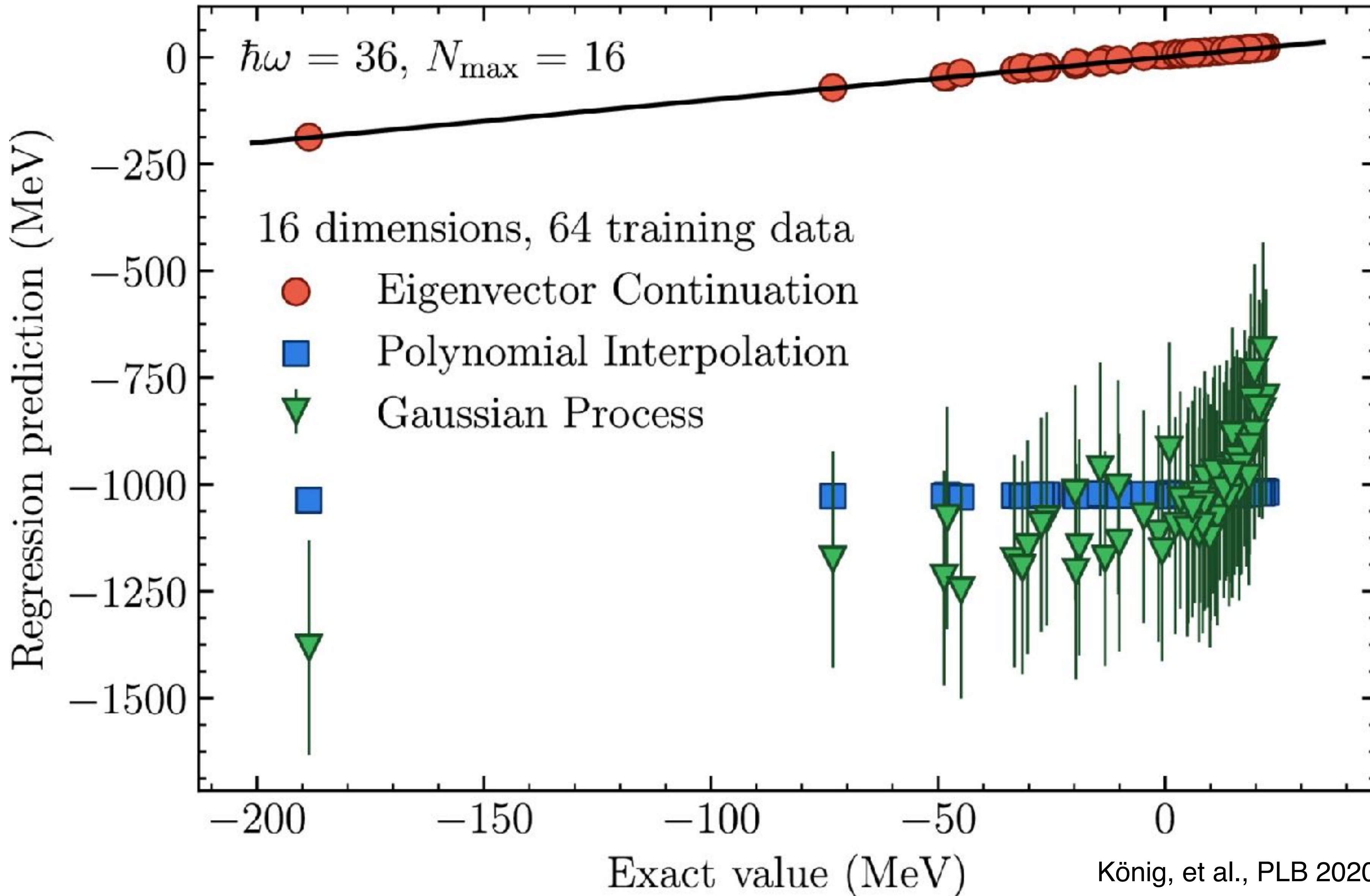
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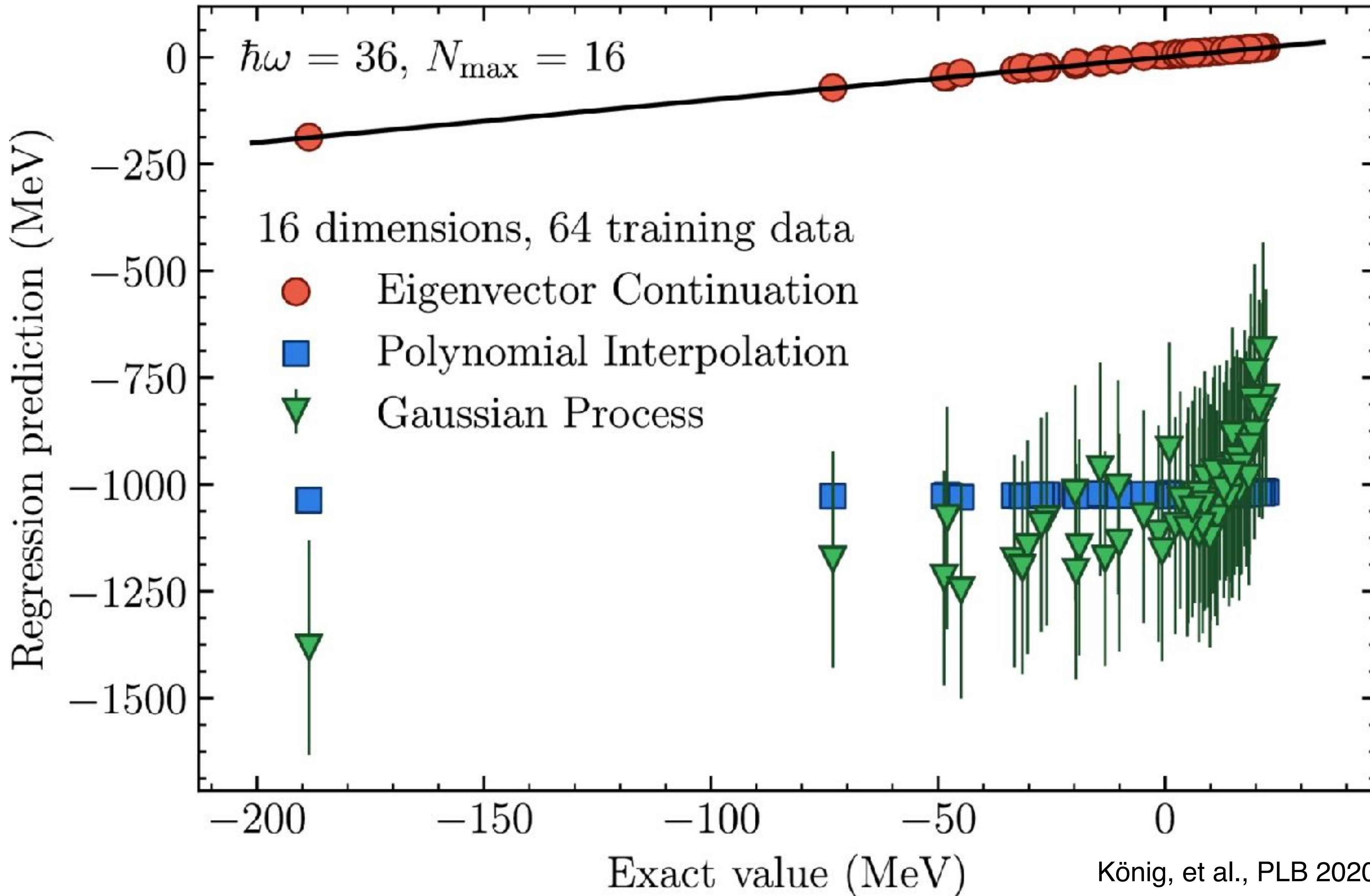
Using Gaussian Process as an Emulator



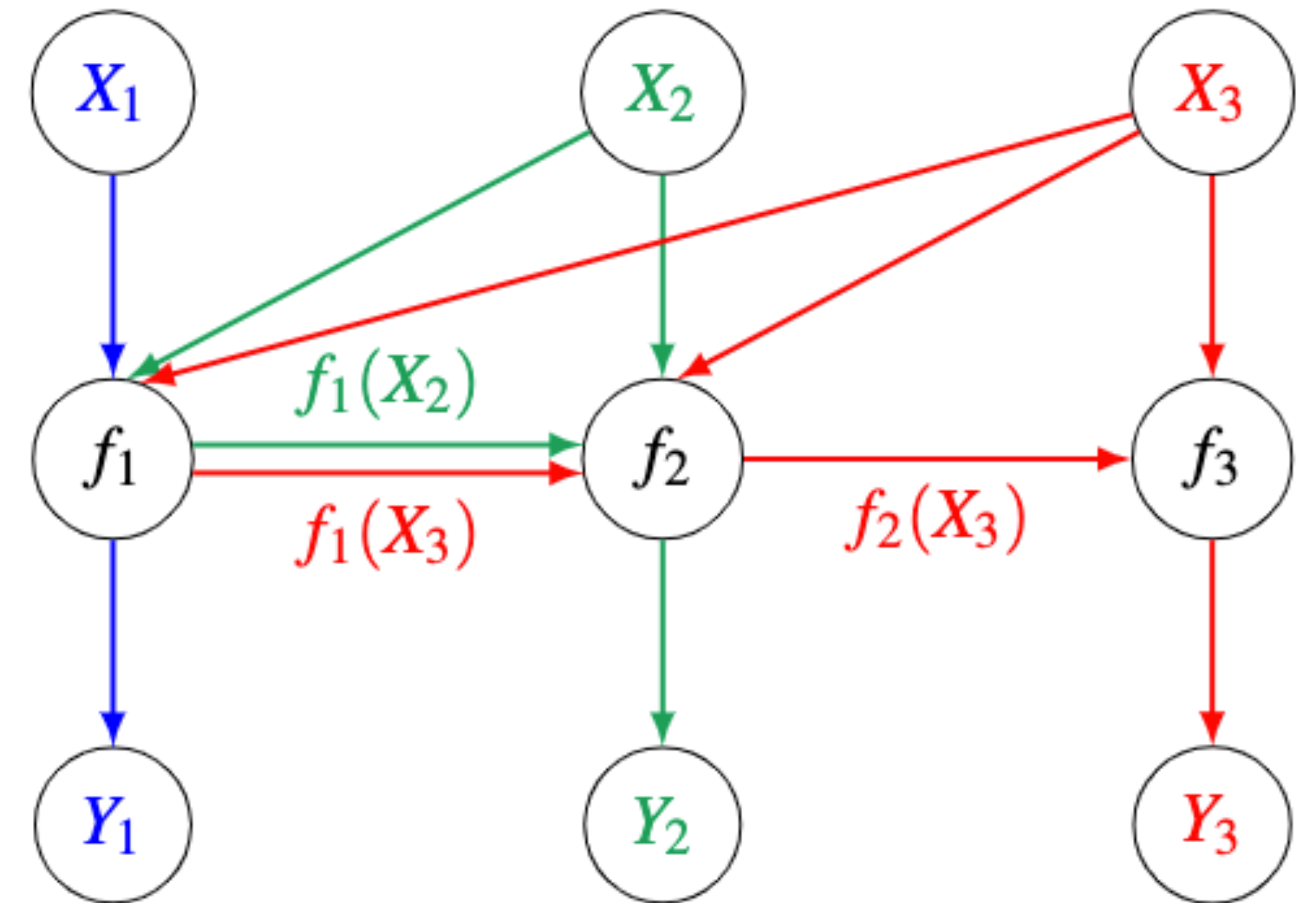
Using Gaussian Process as an Emulator



Using Gaussian Process as an Emulator



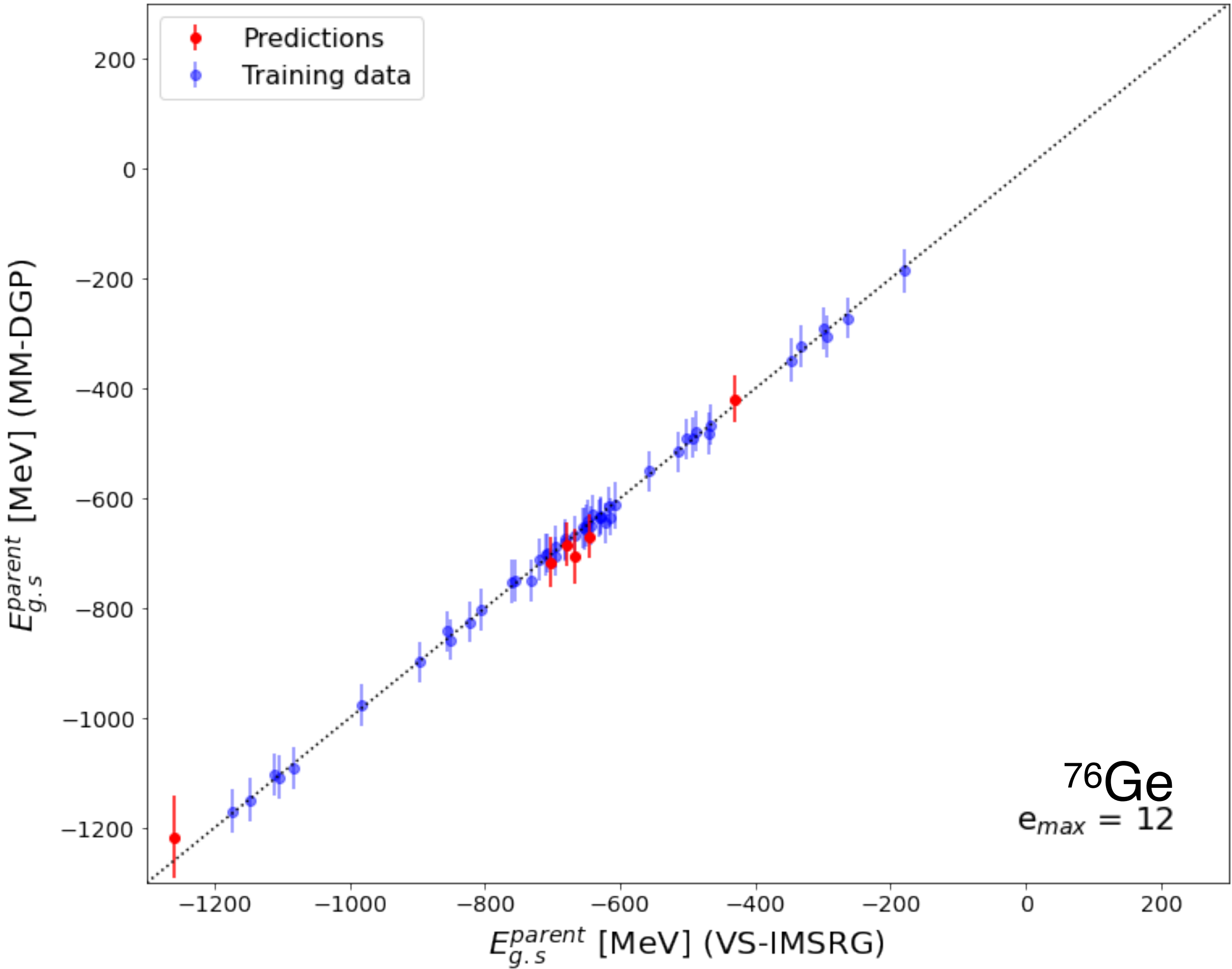
- **Deep Gaussian Processes [1]:** Stack multiple GPs in a neural network-like architecture for improved hierarchical learning.
- **Multi-Fidelity Modelling:** Model low-to-high fidelity differences by passing outputs from one fidelity as inputs to the next.
- **MM-DGP Extension:** Adapted to handle multiple outputs across fidelity levels, creating the **Multi-output Multi-fidelity Deep Gaussian Process (MM-DGP)**.



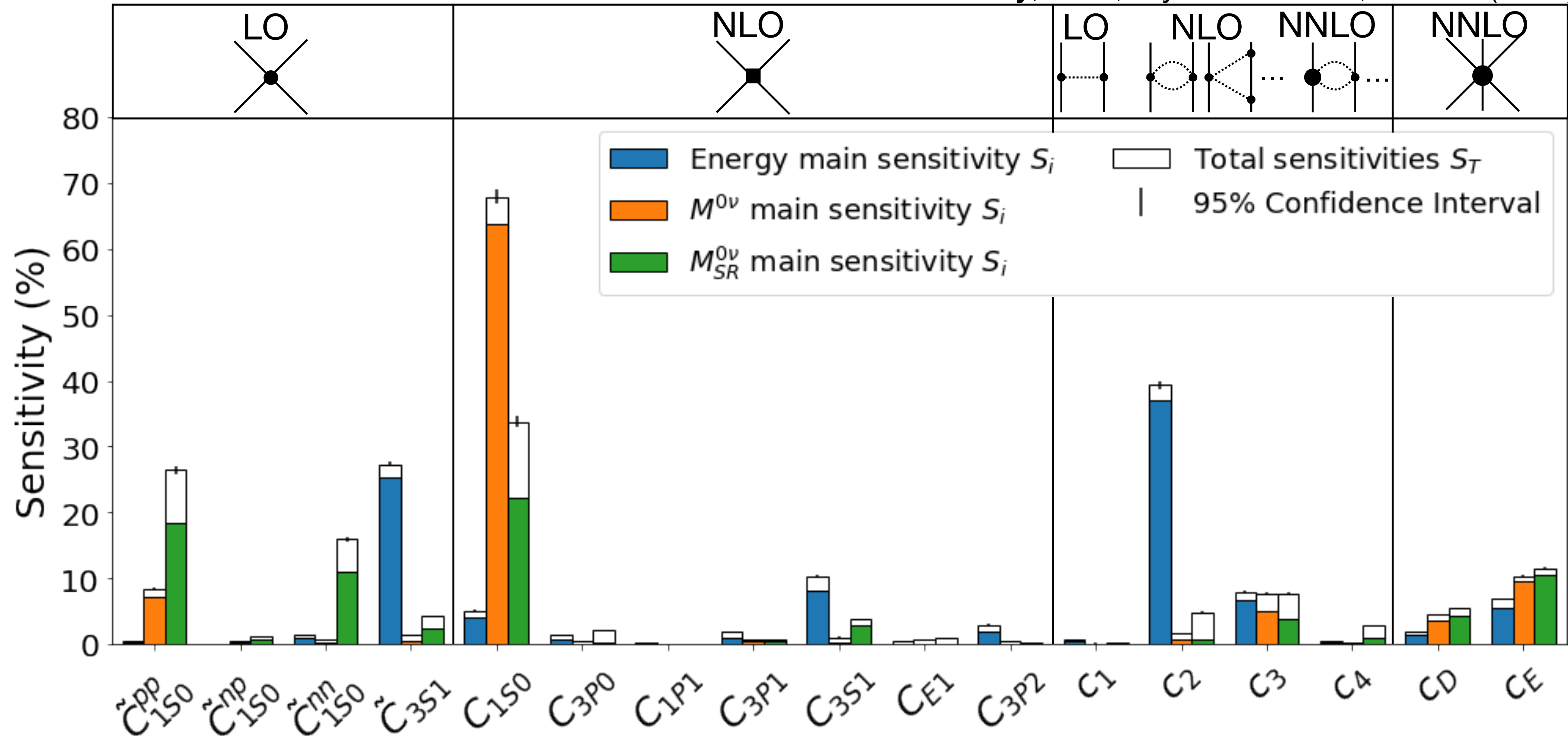


The MM-DGP Algorithm: Energies

$e_{\max}$	# of training points
4	250
6	100
8	90
10	50
12	50

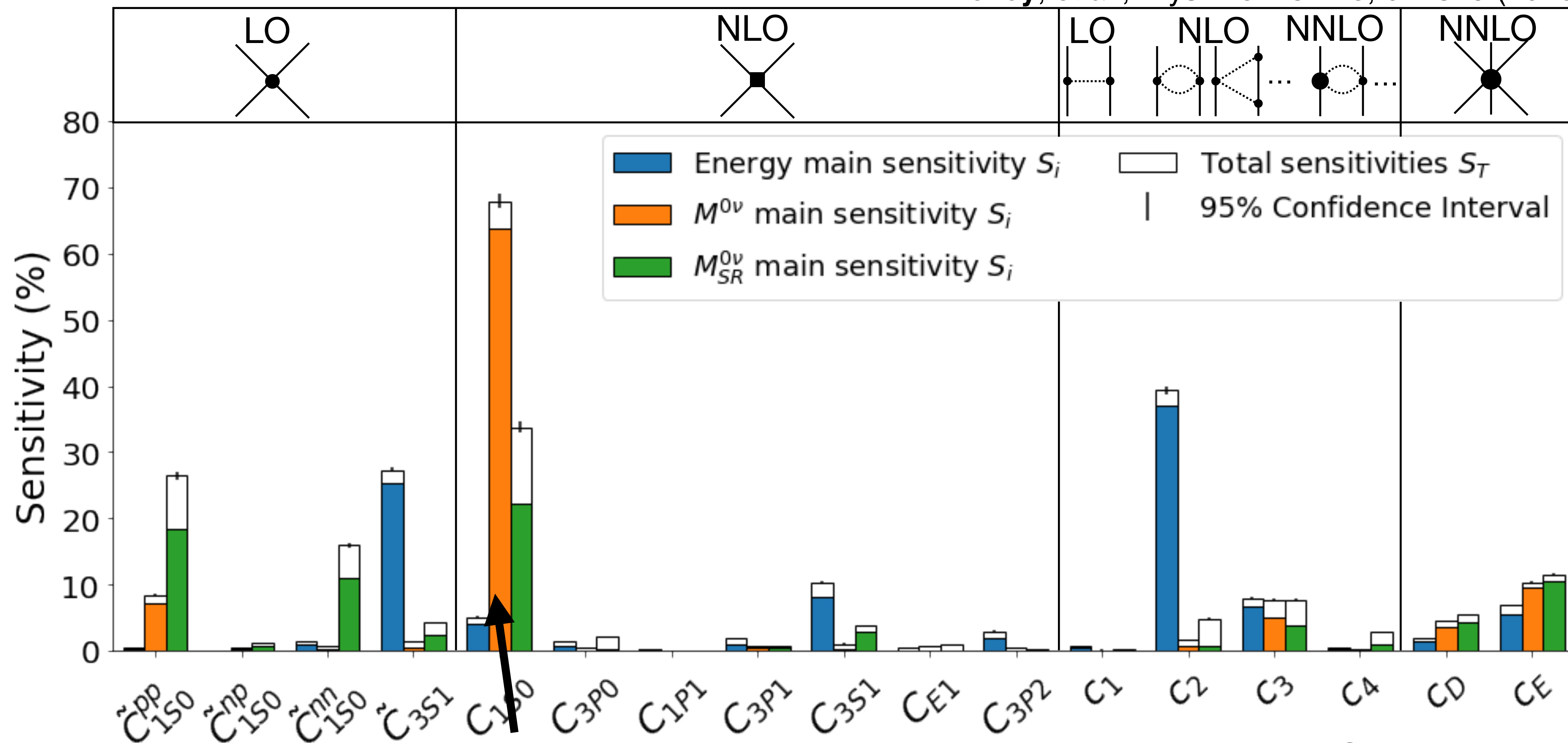


Belley, et al., Phys. Rev. C **113**, 014319 (2026)



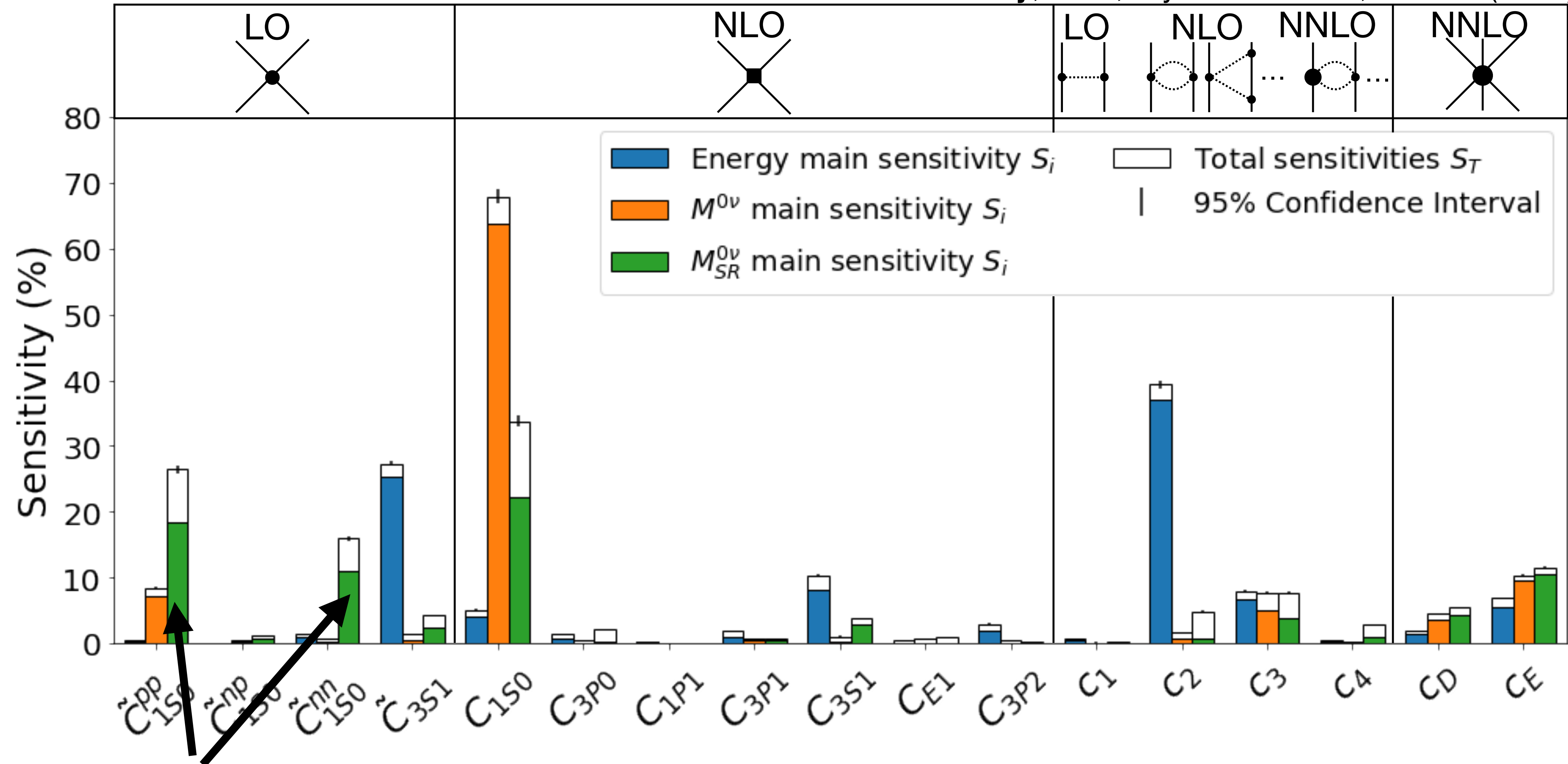
Low-energy constants, i.e. parameters of the nuclear force

Belley, et al., Phys. Rev. C **113**, 014319 (2026)



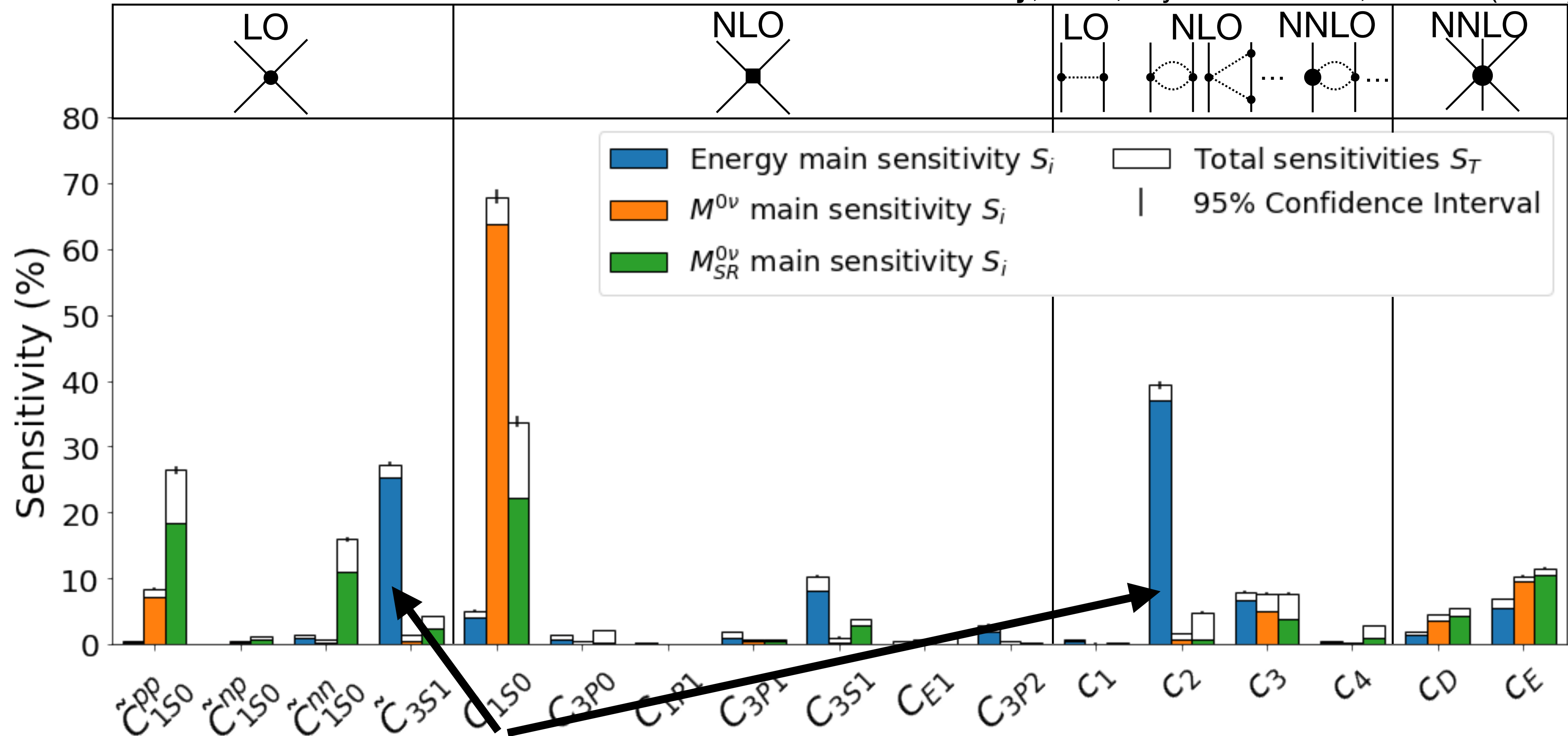
The total matrix element mostly depends on one LEC!

Belley, et al., Phys. Rev. C **113**, 014319 (2026)



The short-range matrix element however sees other contributions from LECs associated to the short-range nuclear interaction.

Belley, et al., Phys. Rev. C **113**, 014319 (2026)



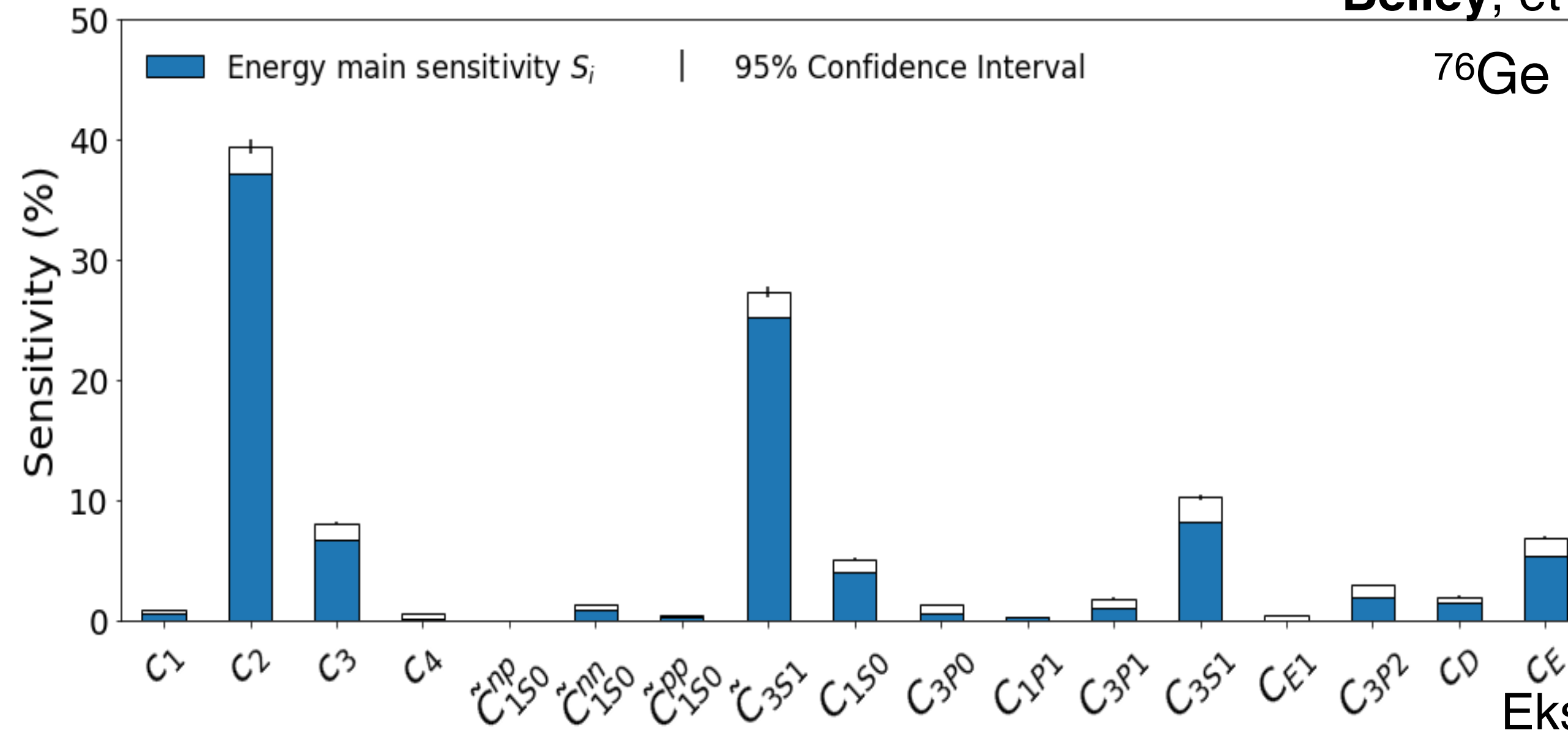
Results for energies are consistent with results of physics-based emulators of the coupled cluster method.



The MM-DGP Algorithm: GSA

Belley, et al., Phys. Rev. C **113**, 014319 (2026)

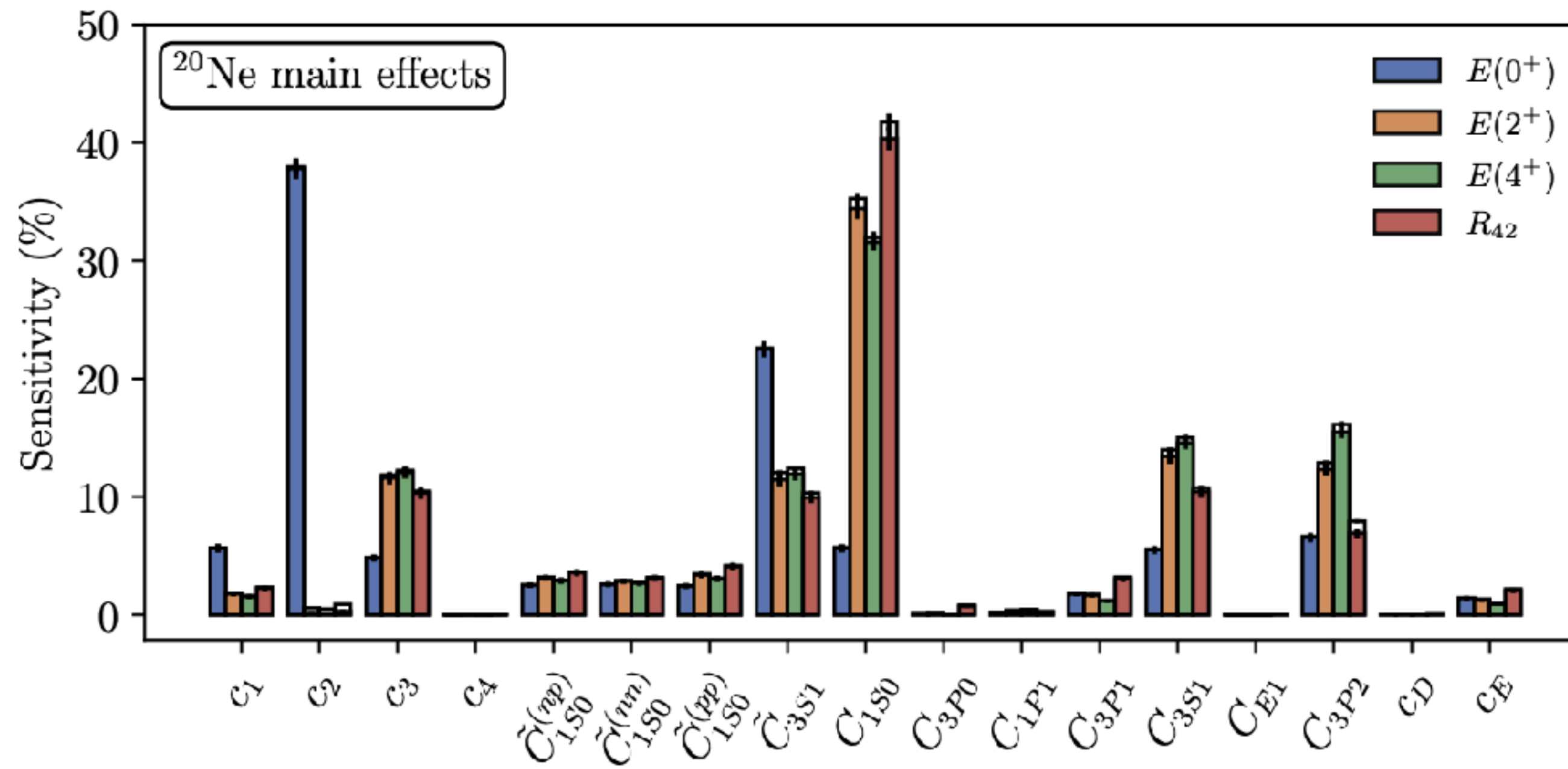
Data driven
MM-DGP



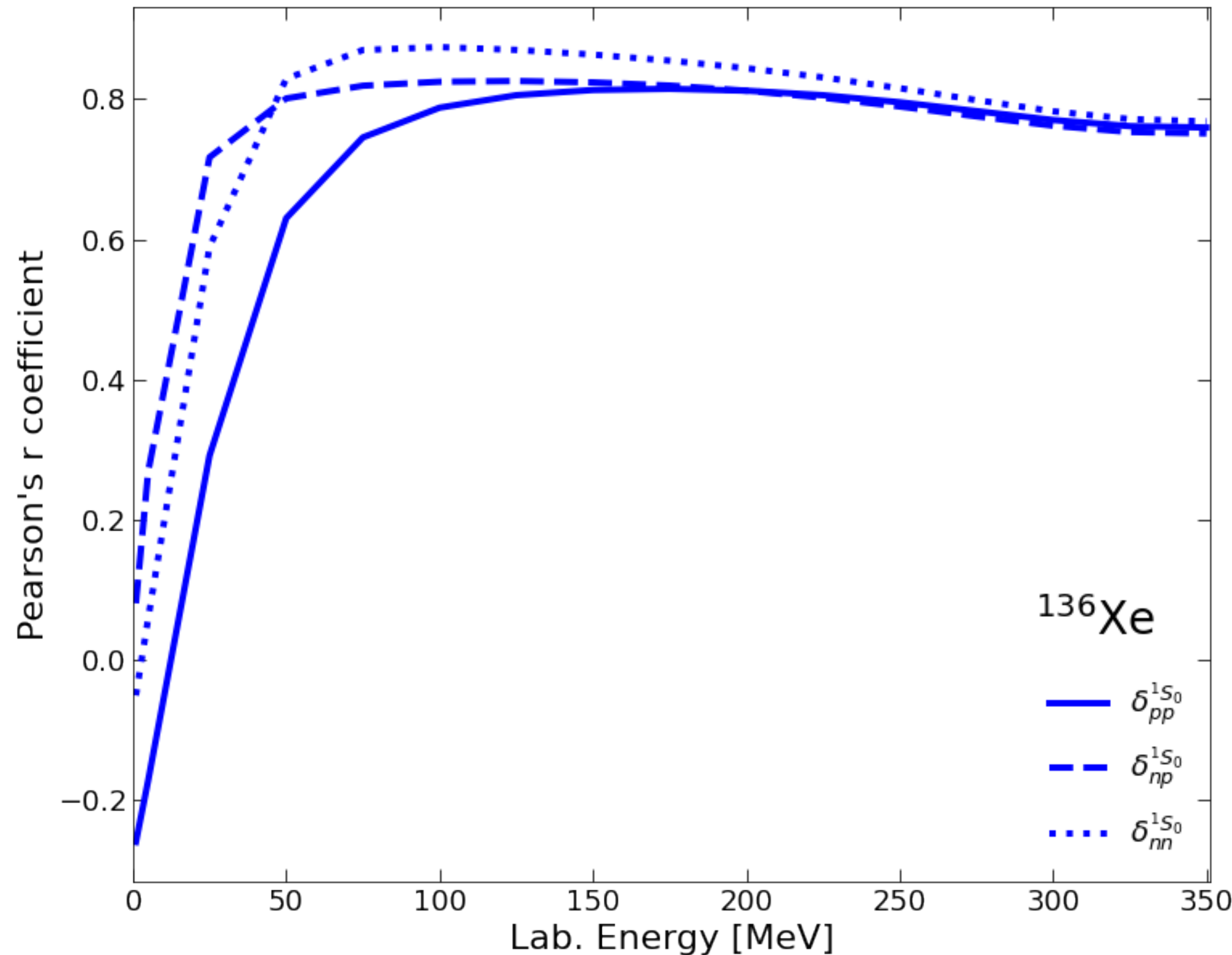
Ekström, et al., arXiv:2305.06955 (2023)

VS

Physics
Driven



Correlation with Phase-Shift



Strong correlation for energies > 50 MeV

$\Rightarrow$

The size of matrix elements is mostly constrained by the interaction between the two nucleons that undergo the decay, given they are close enough from each other.



Getting Posterior Distributions



Getting Posterior Distributions

Prior: 8188 “non-implausible” samples (Phys. Rev. C 109, 064314)



Getting Posterior Distributions

Prior: 8188 “non-implausible” samples (Phys. Rev. C 109, 064314)

“Solve” many-body with emulator for all samples



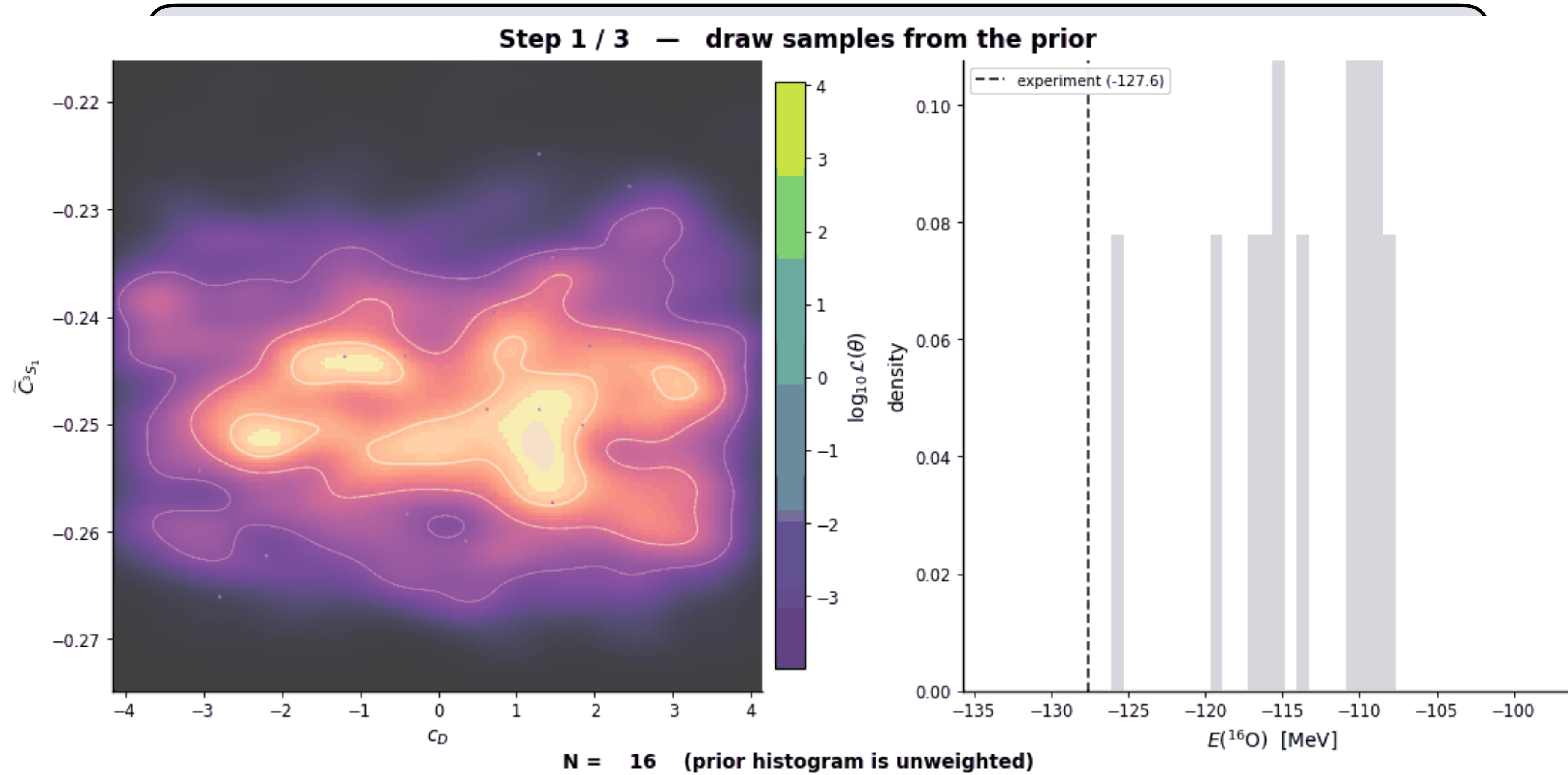
Getting Posterior Distributions

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Weight the samples by a likelihood for some calibration observables
(correlation with target observable)

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$$y = y_{LECs} + \epsilon_{emulator} + \epsilon_{EFT} + \epsilon_{many-body} + \epsilon_{operator}$$

where y_{LECs} is sampled from the weighted interactions

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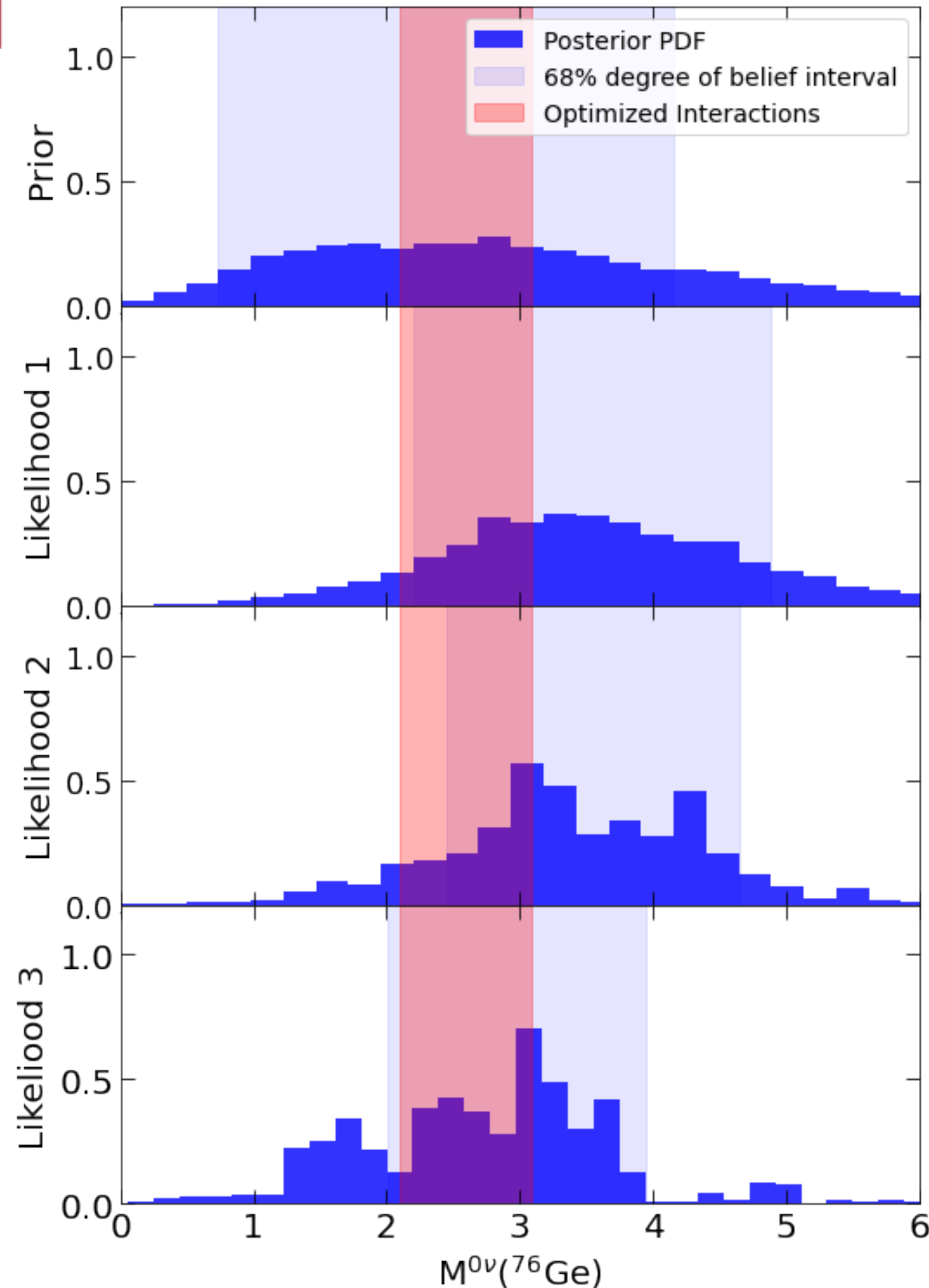
where y_{LECs} is sampled from the weighted interactions

The different sources of errors ϵ are assumed to be normally distributed and independent

ϵ 's do not necessarily correlate between isotopes and observables!!!



Choosing a Likelihood



Likelihood 1: Only contains 1S_0 neutron-proton phase shifts at 50 MeV.

Likelihood 2: Contains 1S_0 neutron-proton phase shifts at 50 MeV and observables for A=2-4.

Likelihood 3: Contains 1S_0 neutron-proton phase shifts at 50 MeV and observables for A=2-4,16.

$$L \propto \exp\left(-1/2 \sum_n \frac{(O_n^{exp.} - O_n^{th.})^2}{\sigma_n^2}\right)$$

Include both theoretical and experimental errors

A2-4: E(^2H), R_p(^2H), Q(^2H), E(^3H), E(^4He), R_p(^4He)

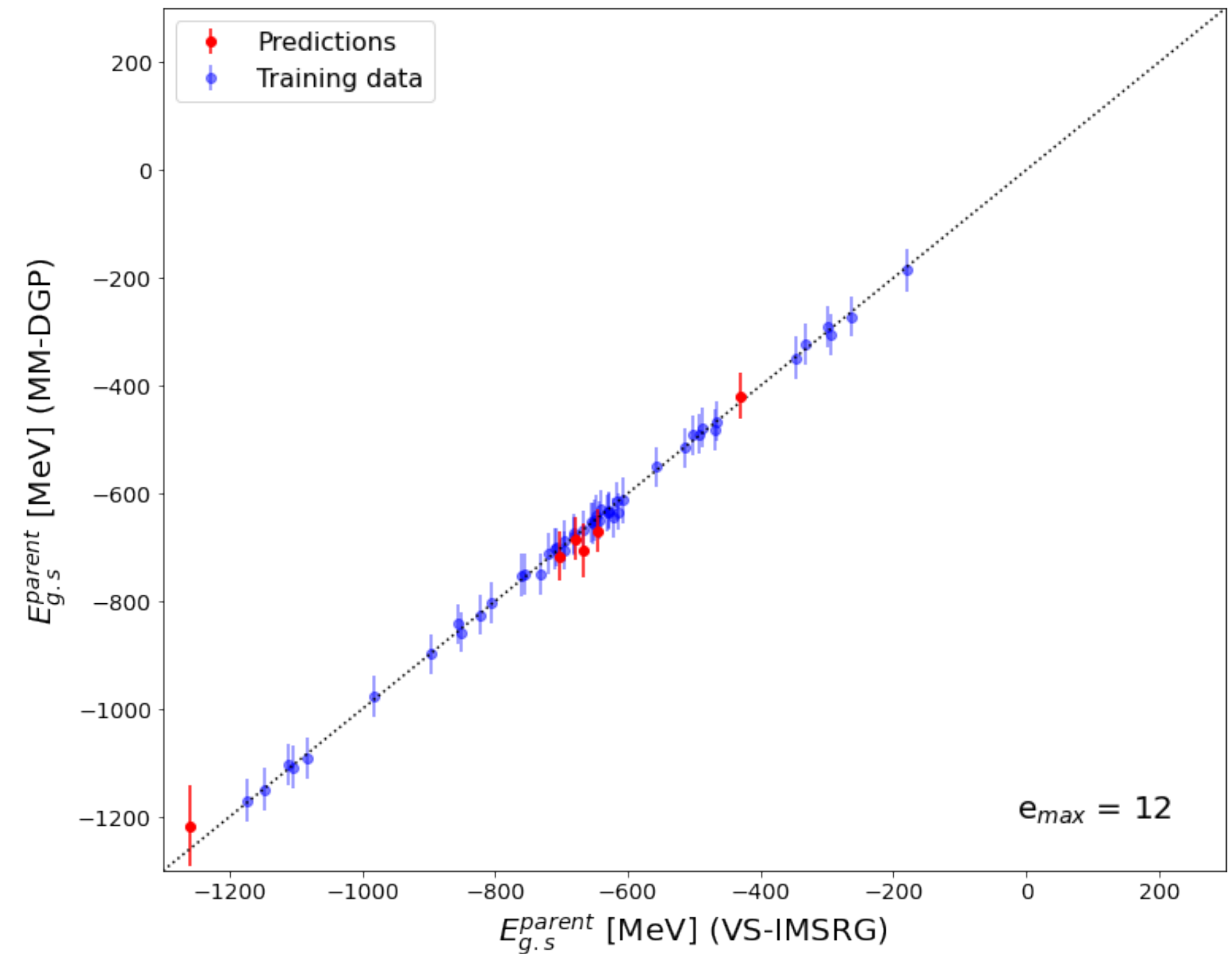
A16: E(^{16}O), R_p(^{16}O)



Emulator Error

$$y = y_{MM-DGP} + \epsilon_{emulator} + \epsilon_{EFT} + \epsilon_{many-body} + \epsilon_{operator}$$

This error is given directly by the Gaussian Process and depends on the LECs (i.e. each predicted point has its own error).





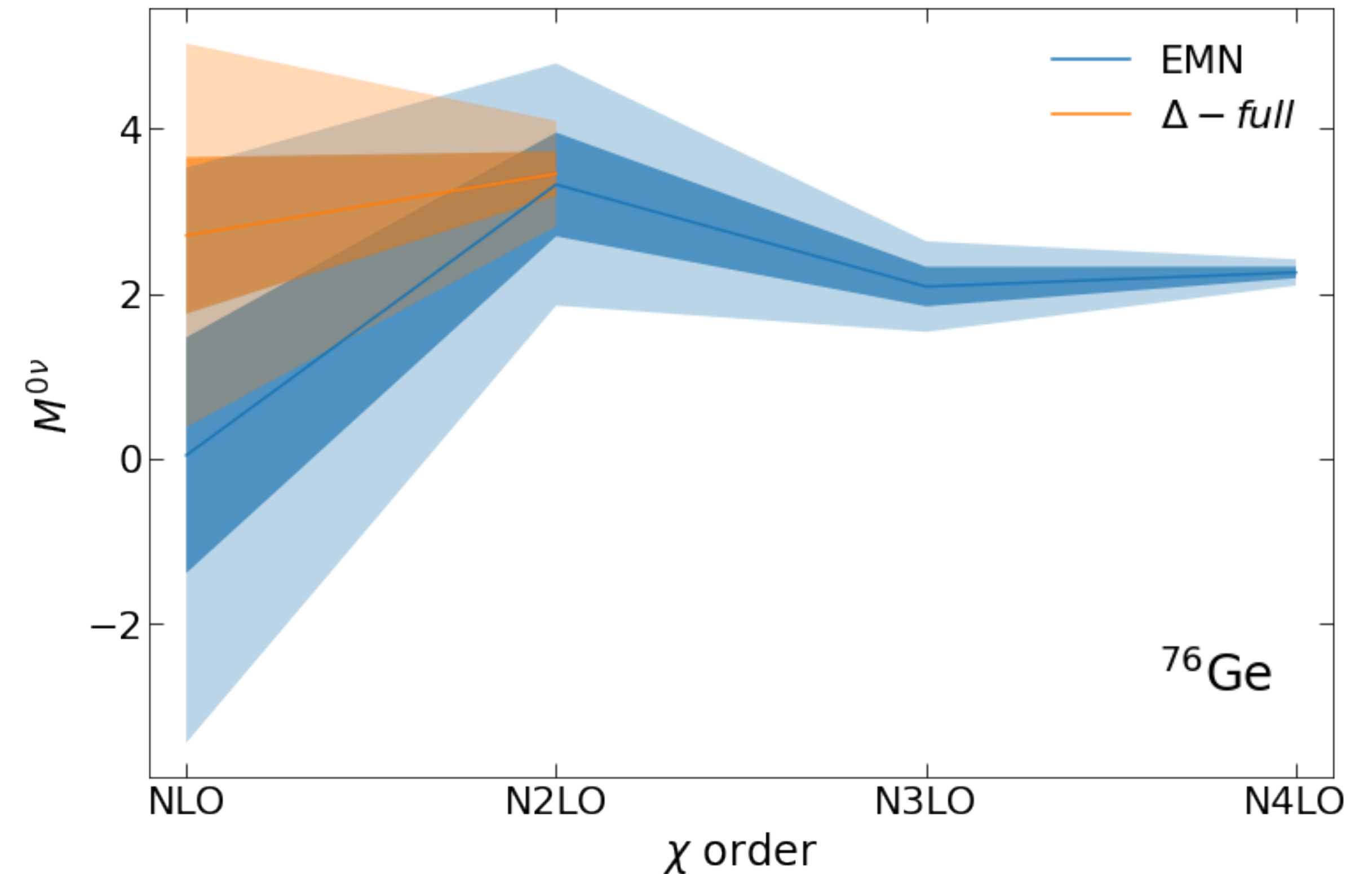
EFT Truncation Error

$$y = y_{MM-DGP} + \epsilon_{emulator} + \epsilon_{EFT} + \epsilon_{many-body} + \epsilon_{operator}$$

Error due to the truncation of the nuclear interactions (the samples are truncated at N2LO, including delta excitations).

Use EMN interaction at NLO, N2LO, N3LO and N4LO.

Using expansion from BUQEYE collaboration, we get $\epsilon_{EFT} = 0.3$.





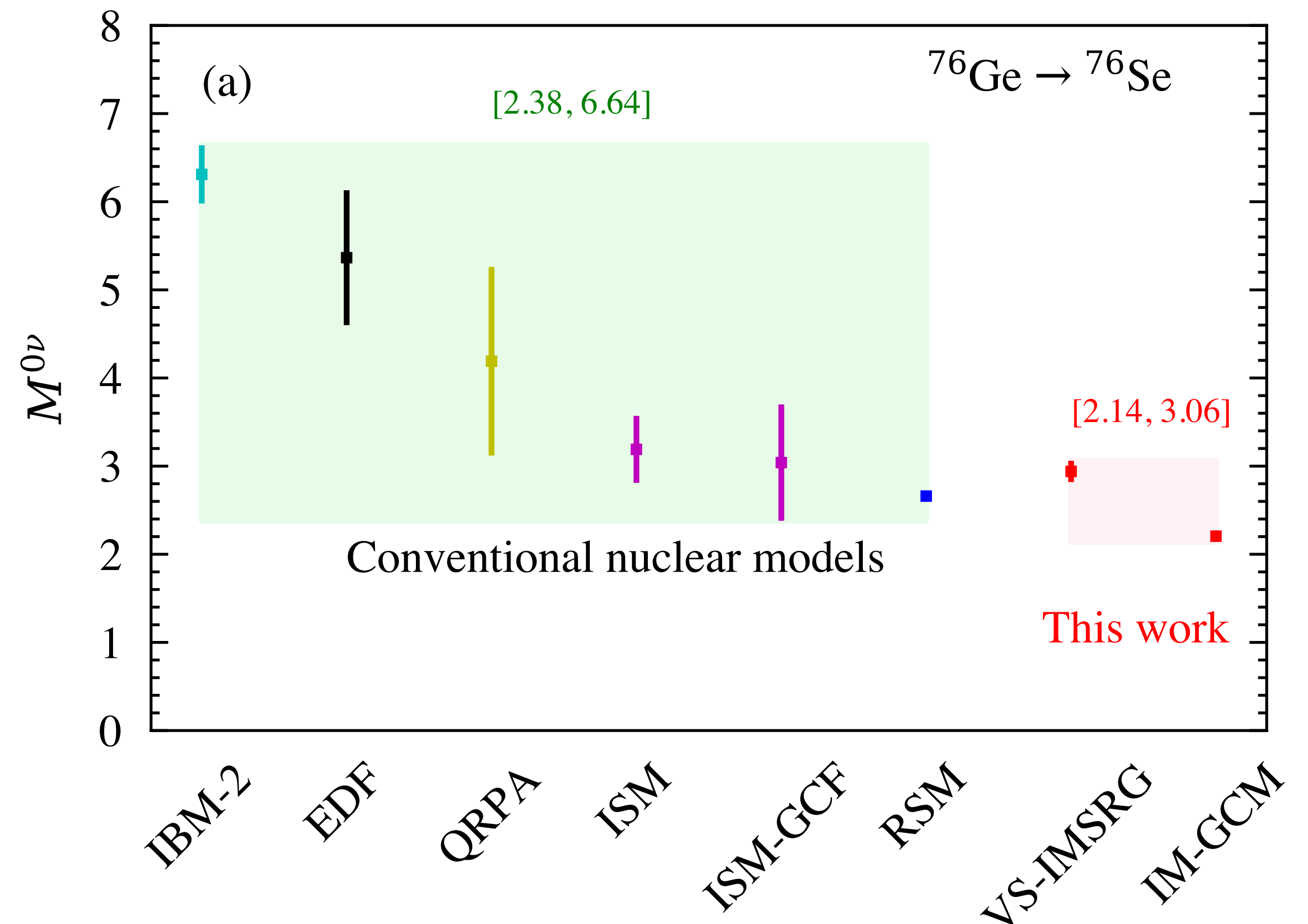
Many-Body Truncation Error

$$y = y_{MM-DGP} + \epsilon_{emulator} + \epsilon_{EFT} + \epsilon_{many-body} + \epsilon_{operator}$$

Error due to the truncation of the many-body method. This is studied by comparing the results of the IM-GCM and VS-IMSRG using the magic interaction.

This error is surprisingly large as we find $\epsilon_{many-body} = 0.88$.

By far the weakest point of the analysis!!!

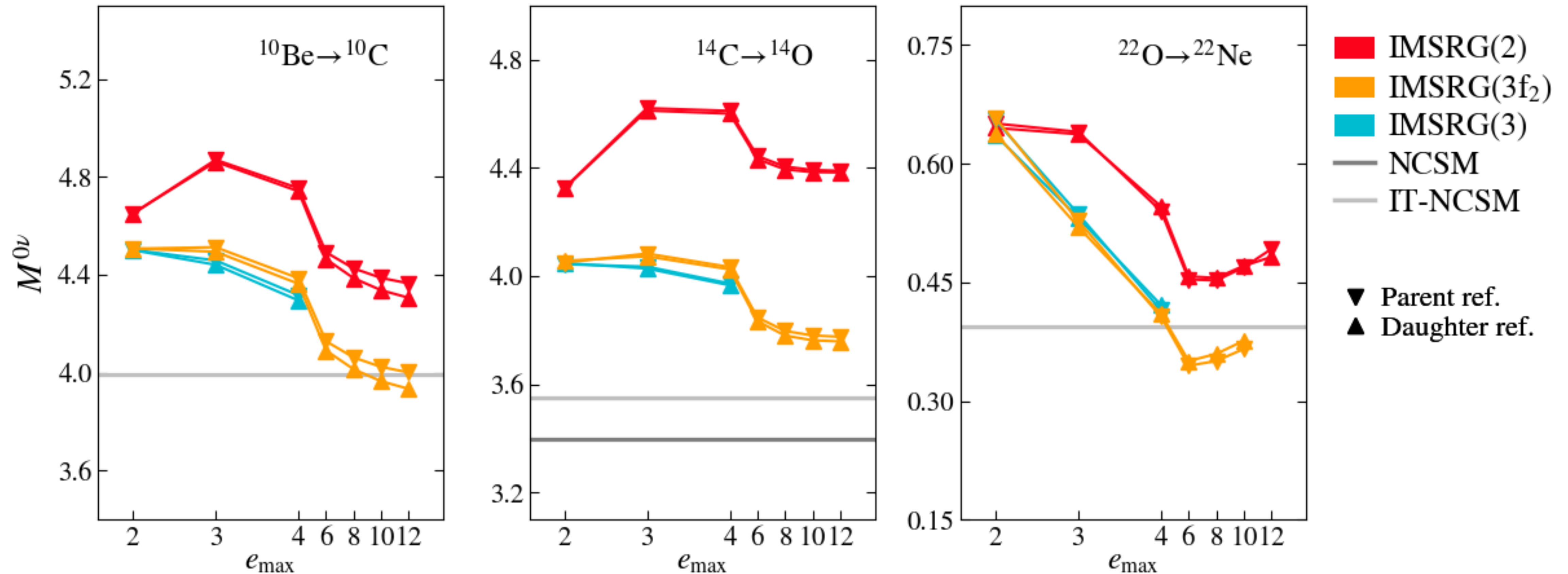




Alex Todd

Many-Body Truncation Error

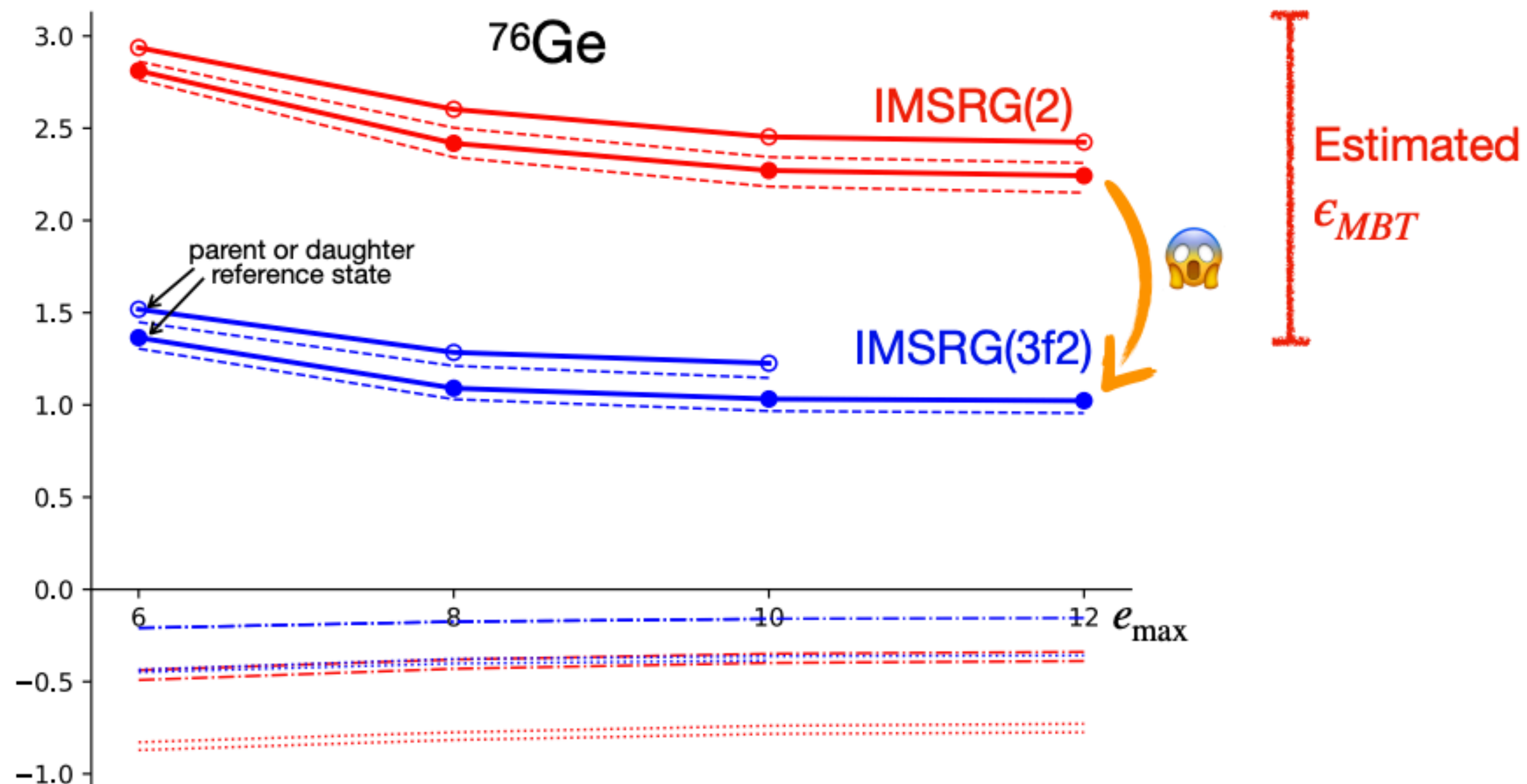
Preliminary results of IMSRG(3f2) show expected improvements.



Many-Body Truncation Error

$$y = y_{MM-DGP} + \epsilon_{emulator} + \epsilon_{EFT} + \epsilon_{many-body} + \epsilon_{operator}$$

Effect from IMSRG(3f2) is larger than the error we originally estimated...





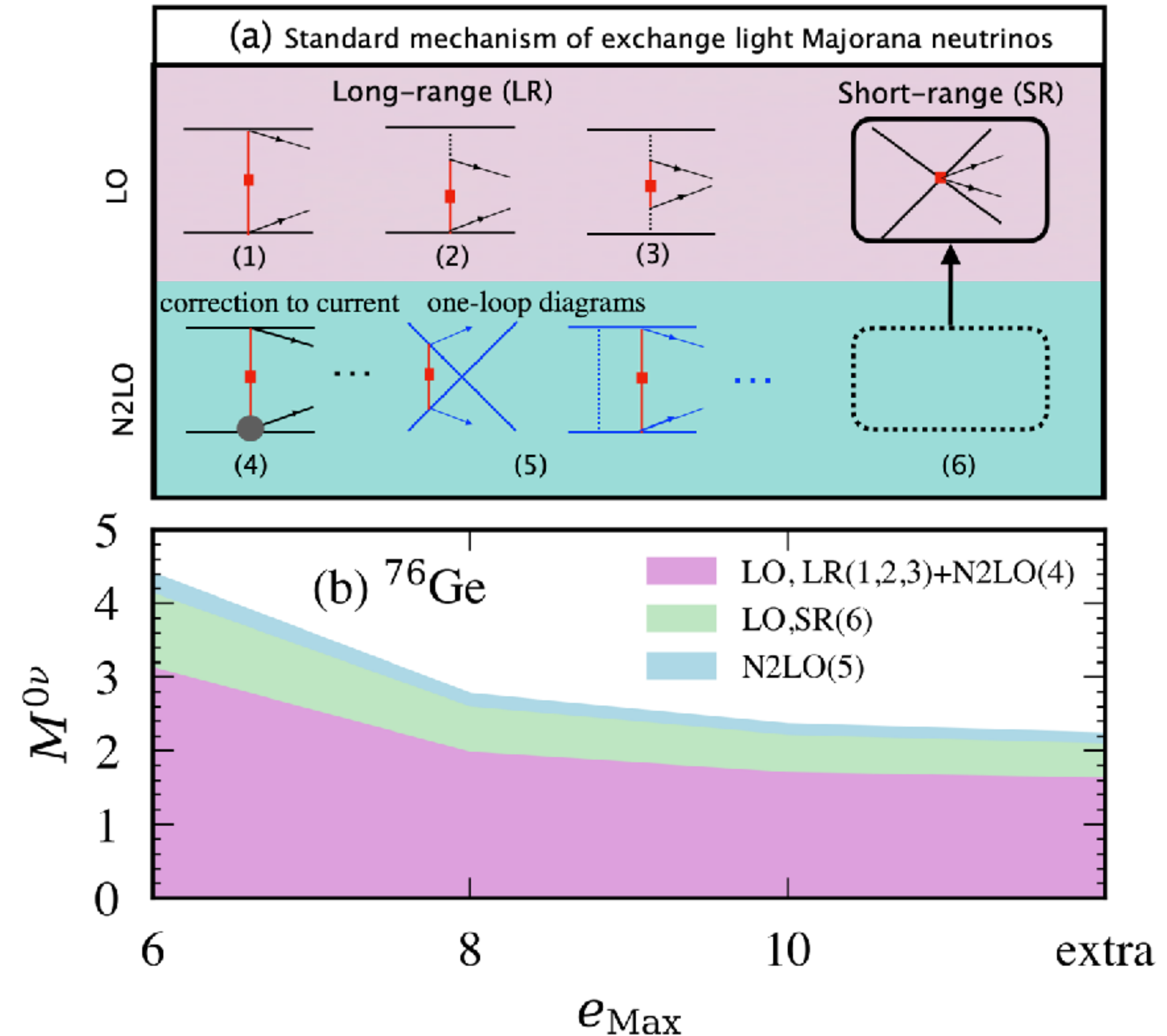
Operator Error

$$y = y_{MM-DGP} + \epsilon_{emulator} + \epsilon_{EFT} + \epsilon_{many-body} + \epsilon_{operator}$$

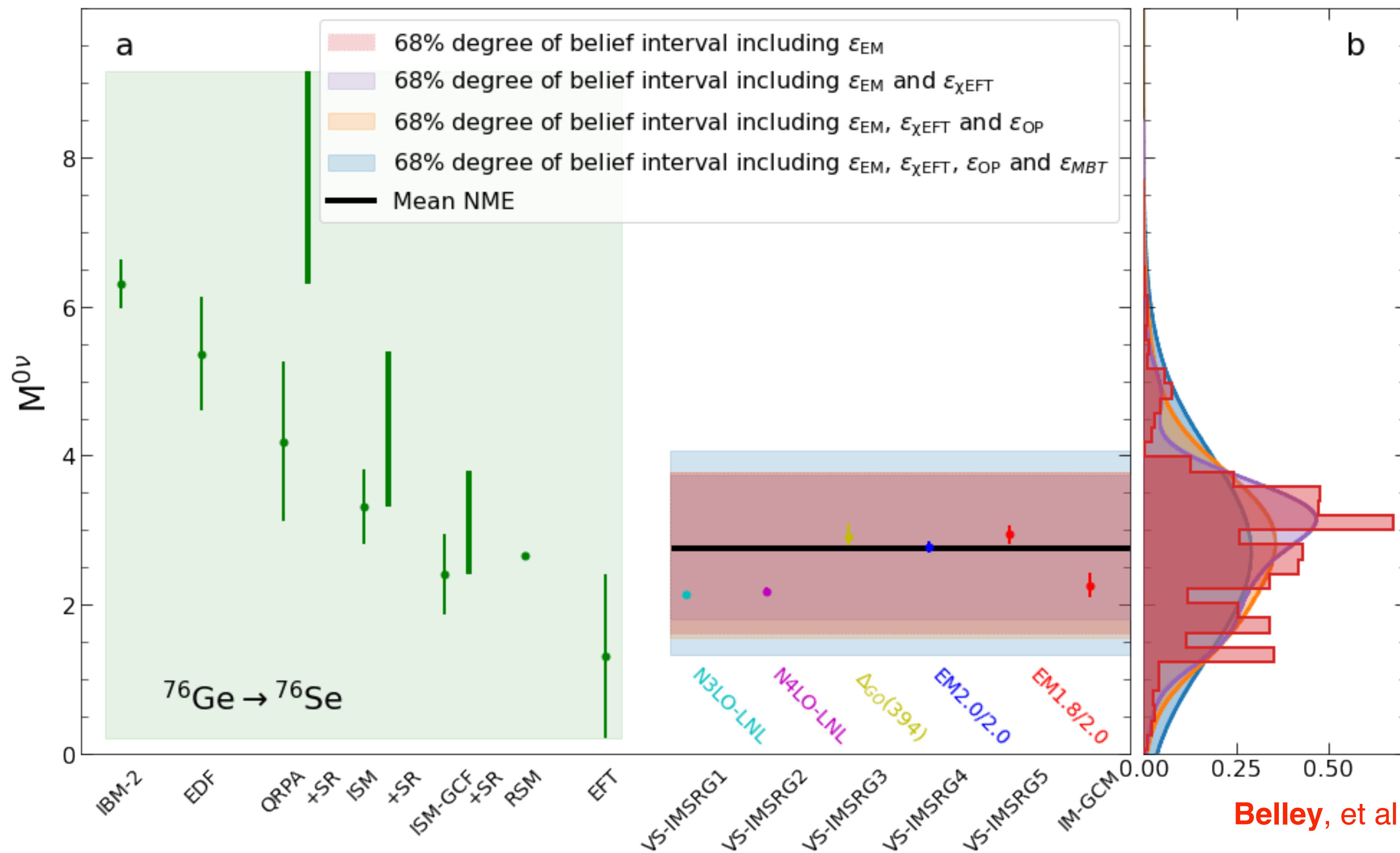
Error due to the truncation of the operator in chiral expansion + closure energy correction + value of the contact LEC.

Adding N2LO operators has very small contribution (< 0.2). Biggest contribution comes from determination of contact term.

Total error amounts to $\epsilon_{operator} = 0.47$.



Combining All Sources of Uncertainty

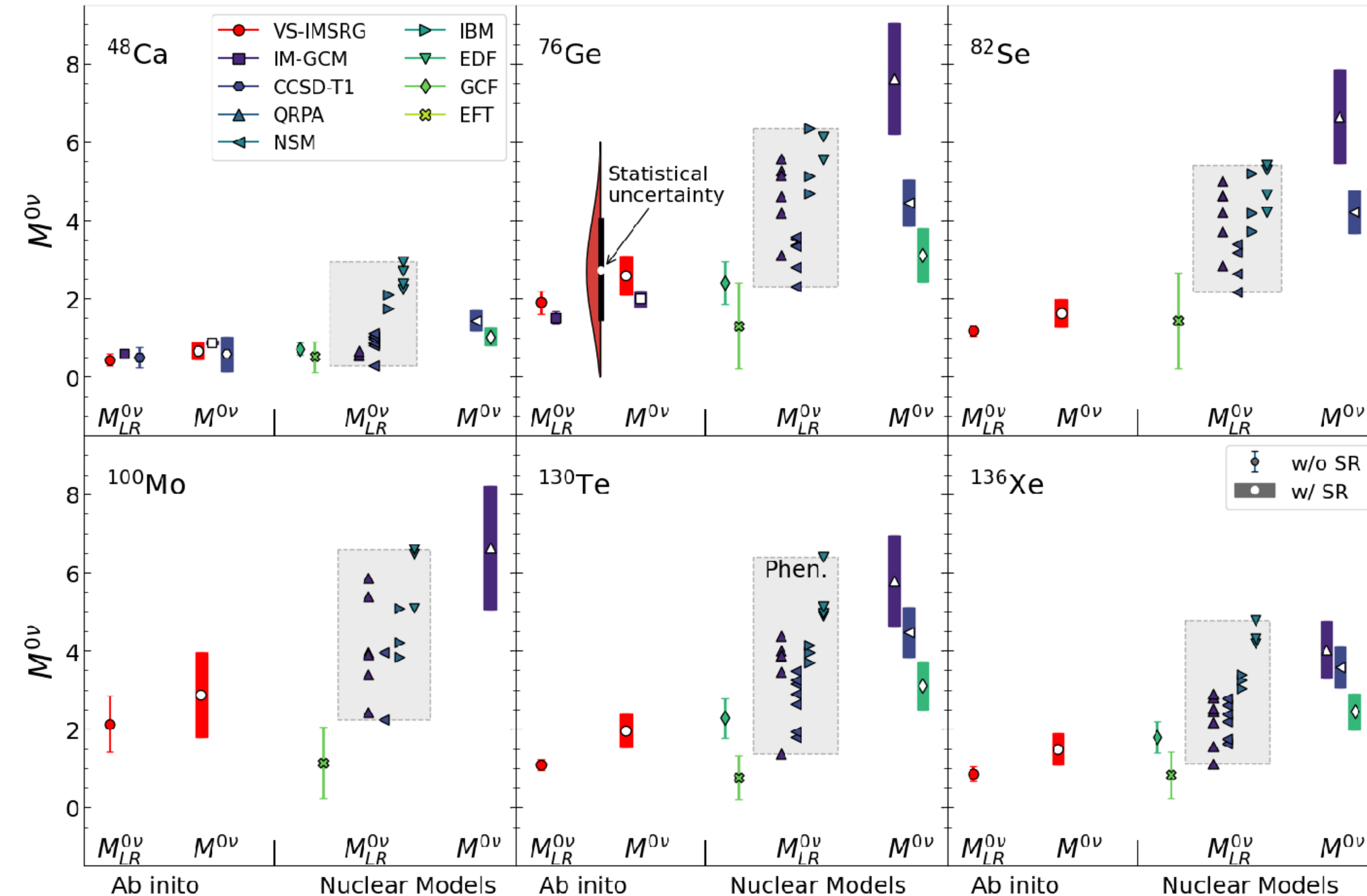


$$M^{0\nu\beta\beta} = 2.60^{+1.28}_{-1.36}$$

Belley, et al., Phys. Rev. Lett. 132, 182502



The Current Picture



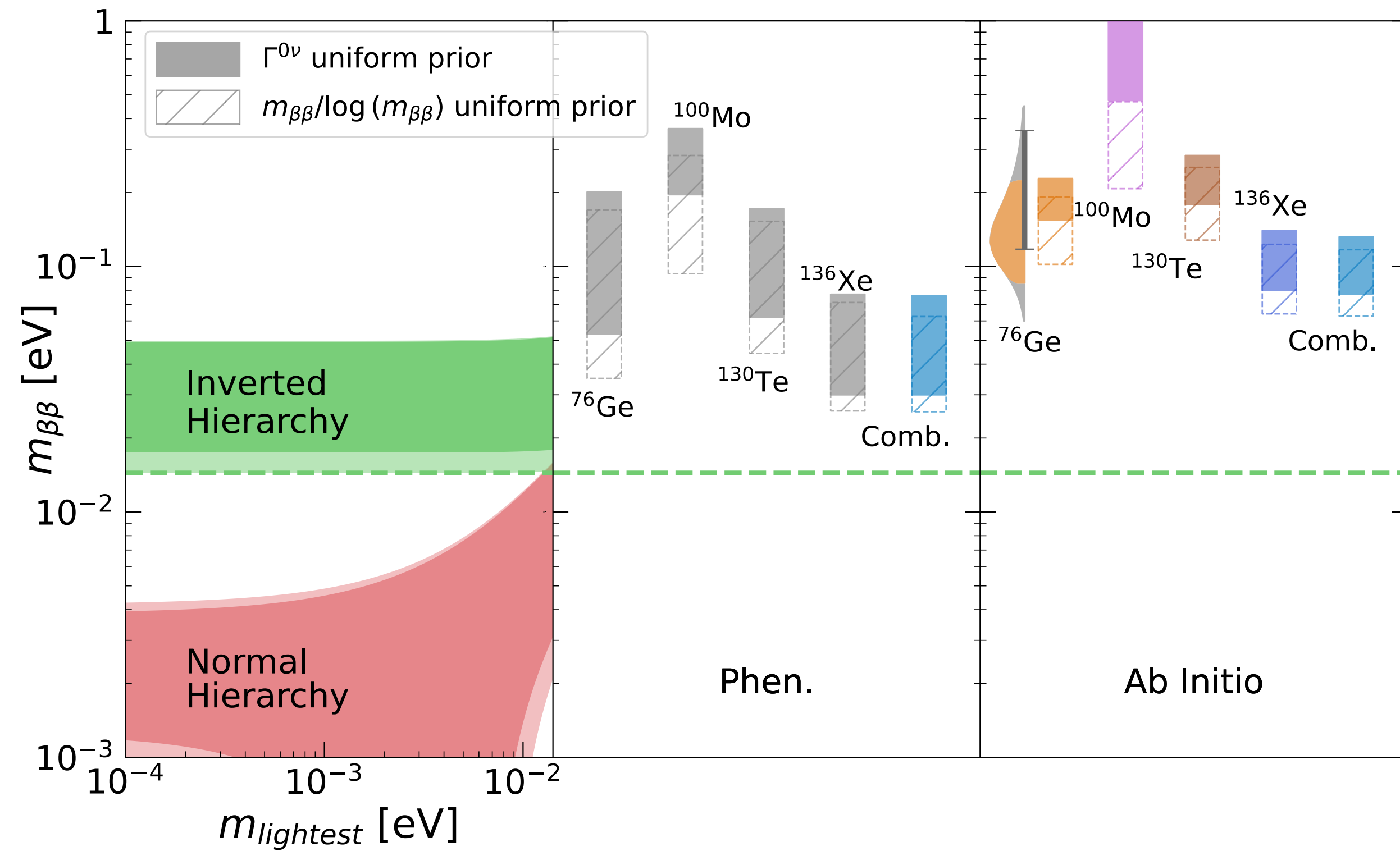
Values from:

- Agostini et al., Rev. Mod. Phys. 95, 025002 (2023);
- Yao, Sci. Bull. 10.1016 (2020);
- **Belley** et al., Phys. Rev. Lett. 126, 042502 (2020);
- Brase et al., Phys. Rev. C 106, 034309 (2021);
- Weiss et al., Phys. Rev. C 106, 064401 (2022);
- **Belley** et al., arXiv:2307.15156 (2023);
- **Belley** et al., Phys. Rev. Lett. 132, 182502 (2024).



Taiki Shickele

Combining Limits of Different Isotopes

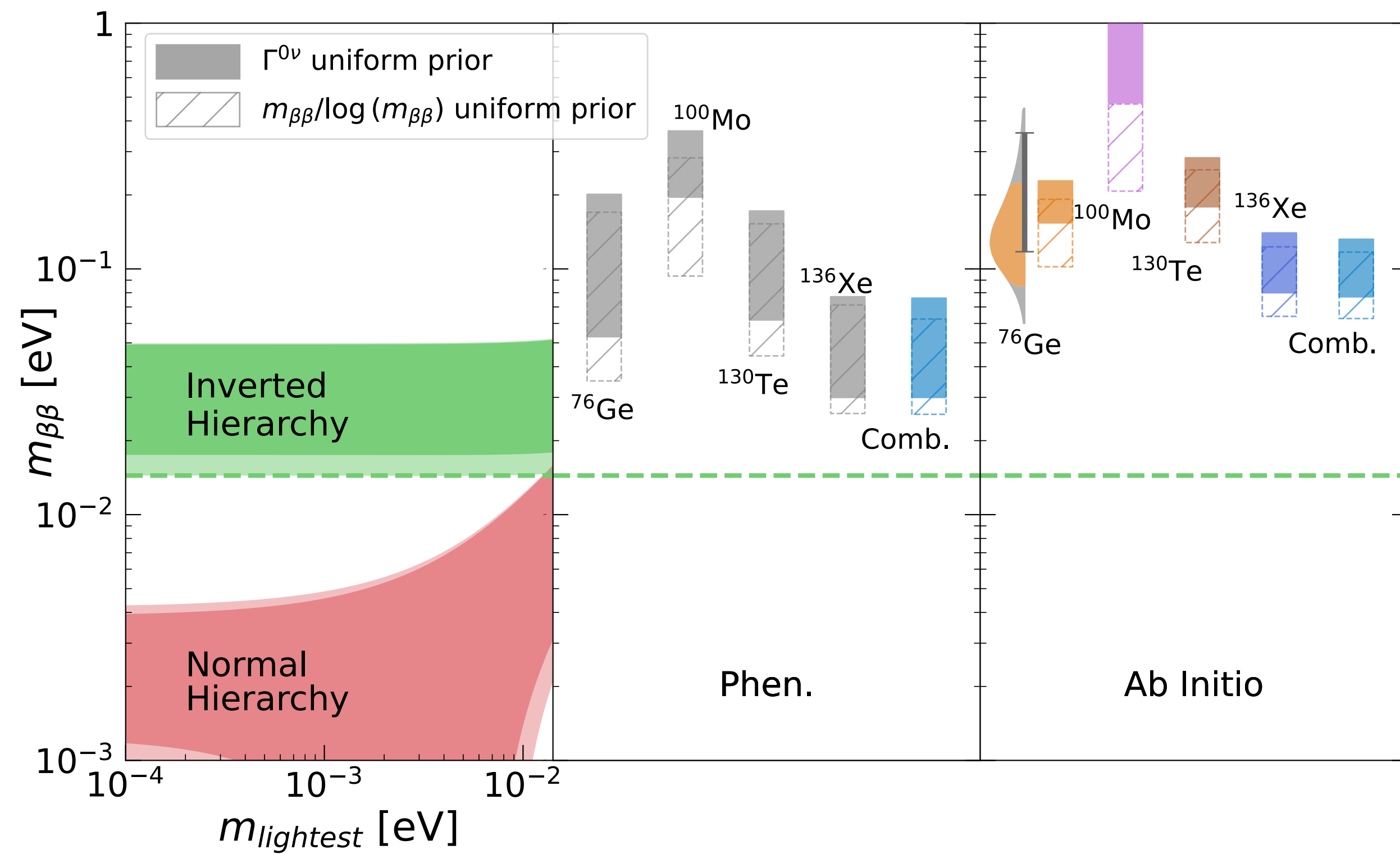


Current

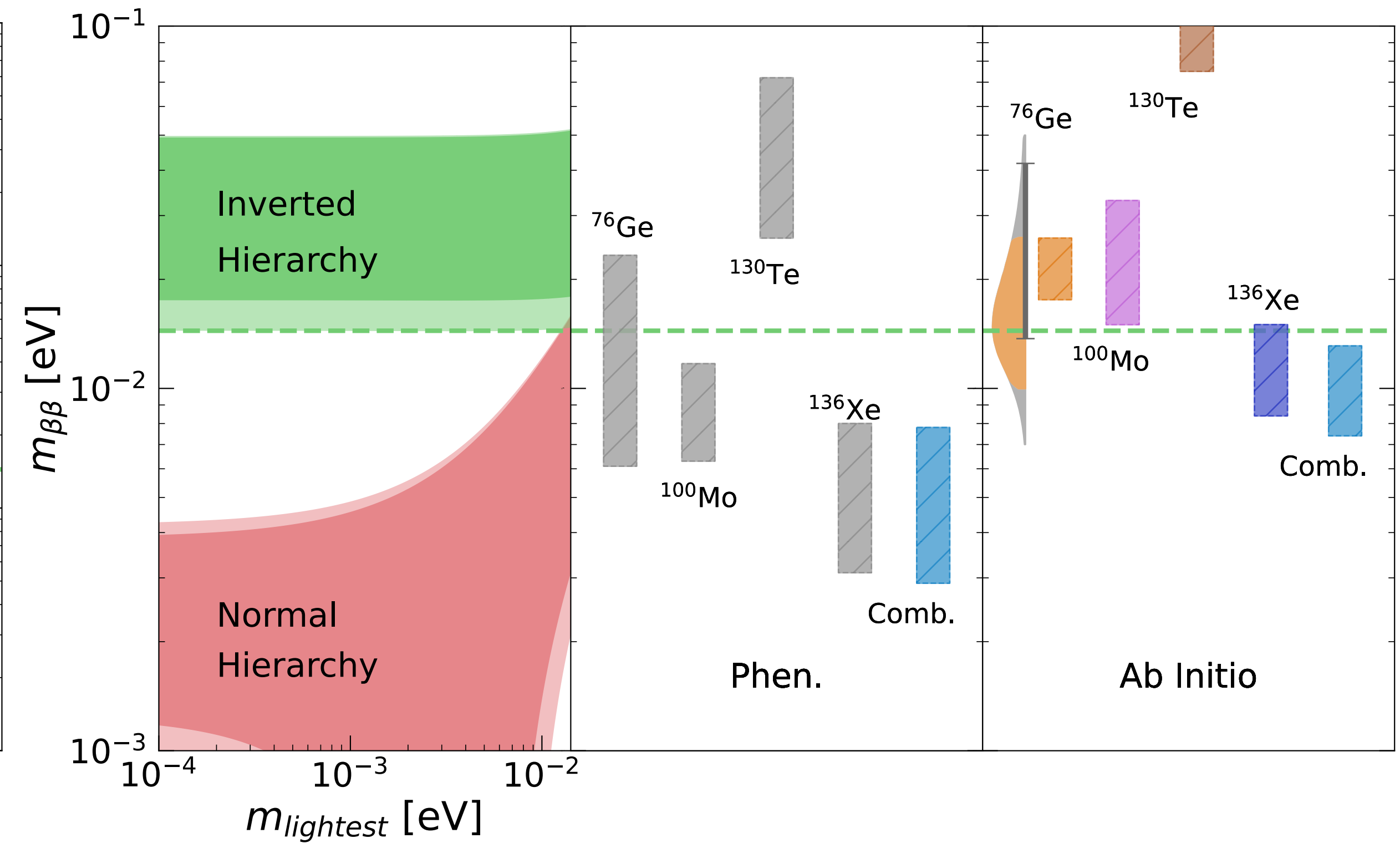


Taiki Shickele

Combining Limits of Different Isotopes



Current



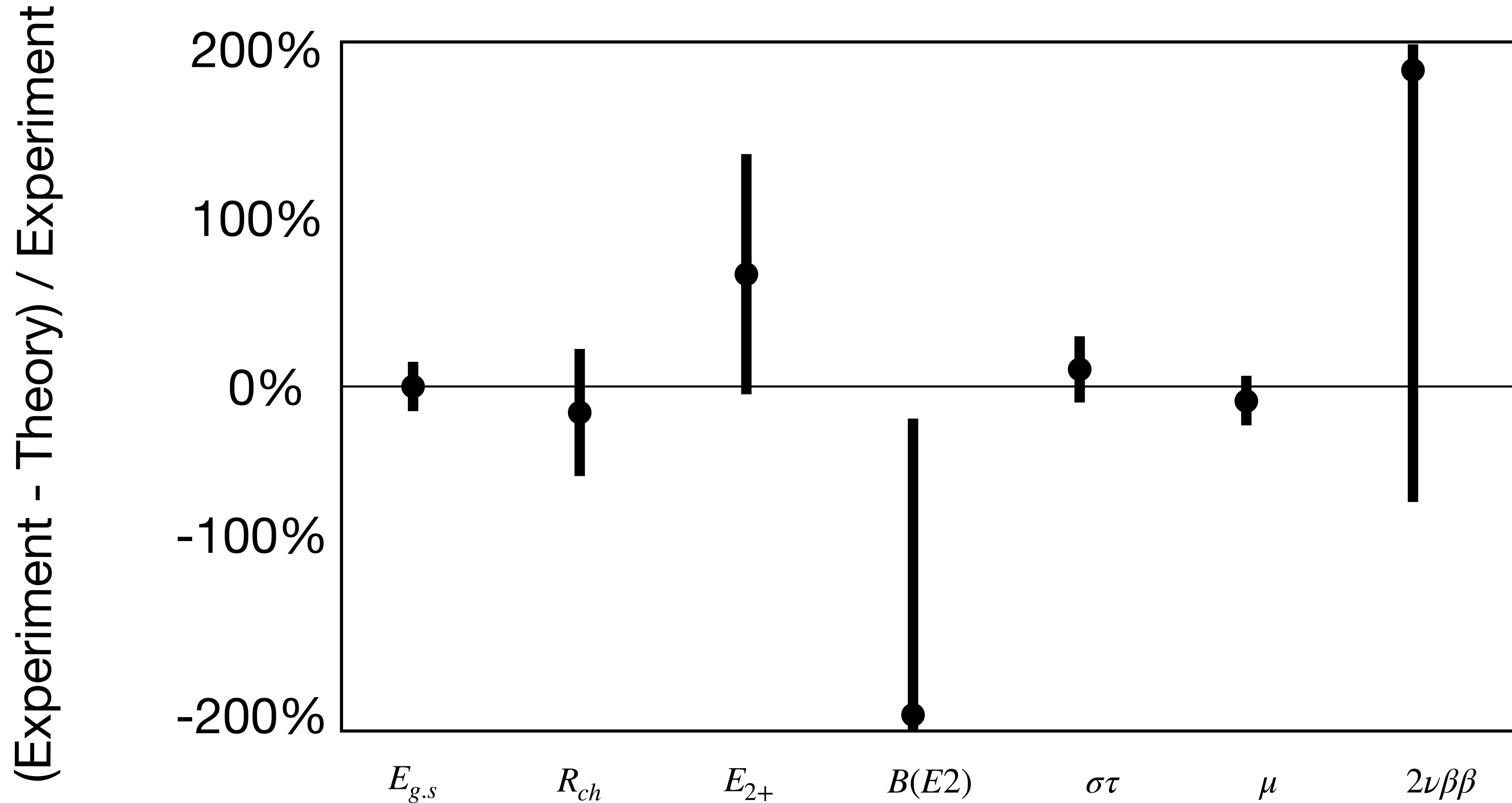
Future

Experimental limits: **GERDA (^{76}Ge)** Phys. Rev. Lett. 125, 252502, **CUPID-Mo (^{100}Mo)** Eur. Phys. J. C 82 11, 1033, **CUORE(^{130}Te)** arXiv:2404.04453, **EXO(^{136}Xe)** Phys. Rev. Lett. 123, 161802 and **Kamland Zen (^{136}Xe)** arXiv:2406.11438

Expected limits: **LEGEND (^{76}Ge)** arXiv:2107.11462, **CUPID-1T (^{100}Mo)** arXiv:2203.08386, **AMoRE (^{100}Mo)** arXiv:2406.09698, **SNO+(^{130}Te)** arXiv:2104.11687, **NEXT (^{136}Xe)** JHEP09(2023)190 and **nEXO (^{136}Xe)** J. Phys. G 49 1, 015104.



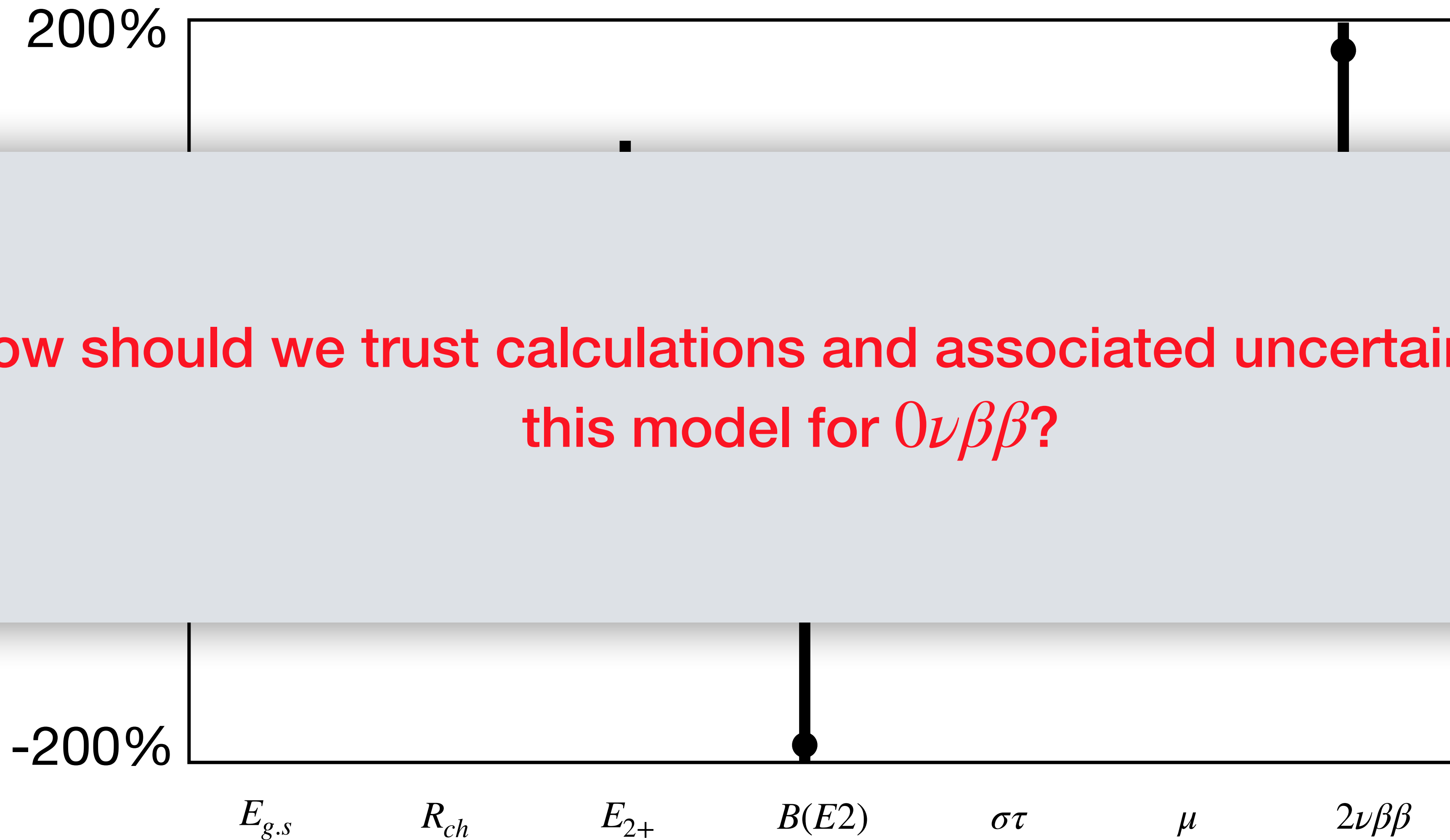
Using other observables





Using other observables

(Experiment - Theory) / Experiment



Now should we trust calculations and associated uncertainties of this model for $0\nu\beta\beta$?

How to improve uncertainty models?

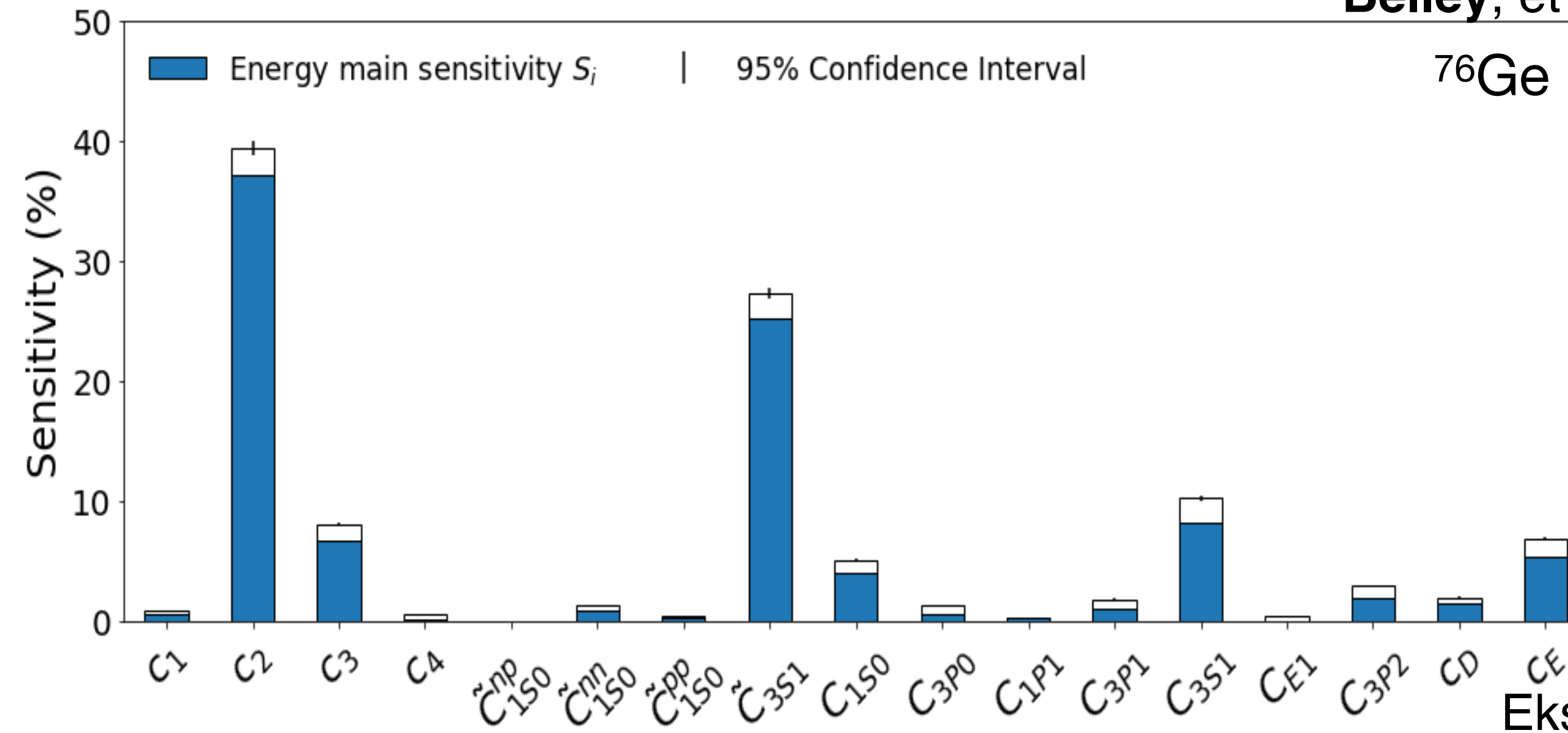


Weakness of uncertainty model

1. Theoretical uncertainty are somewhat double counted since they are included in the likelihood.
2. Correlations between the different sources of uncertainty are not included.
3. Uncertainty limited to one many-body method.
4. Choice of observables used in the likelihood might not constrain the LECs optimally for $0\nu\beta\beta$.
5. Not considering correlation between the different isotopes.

Global emulation for nuclear structure

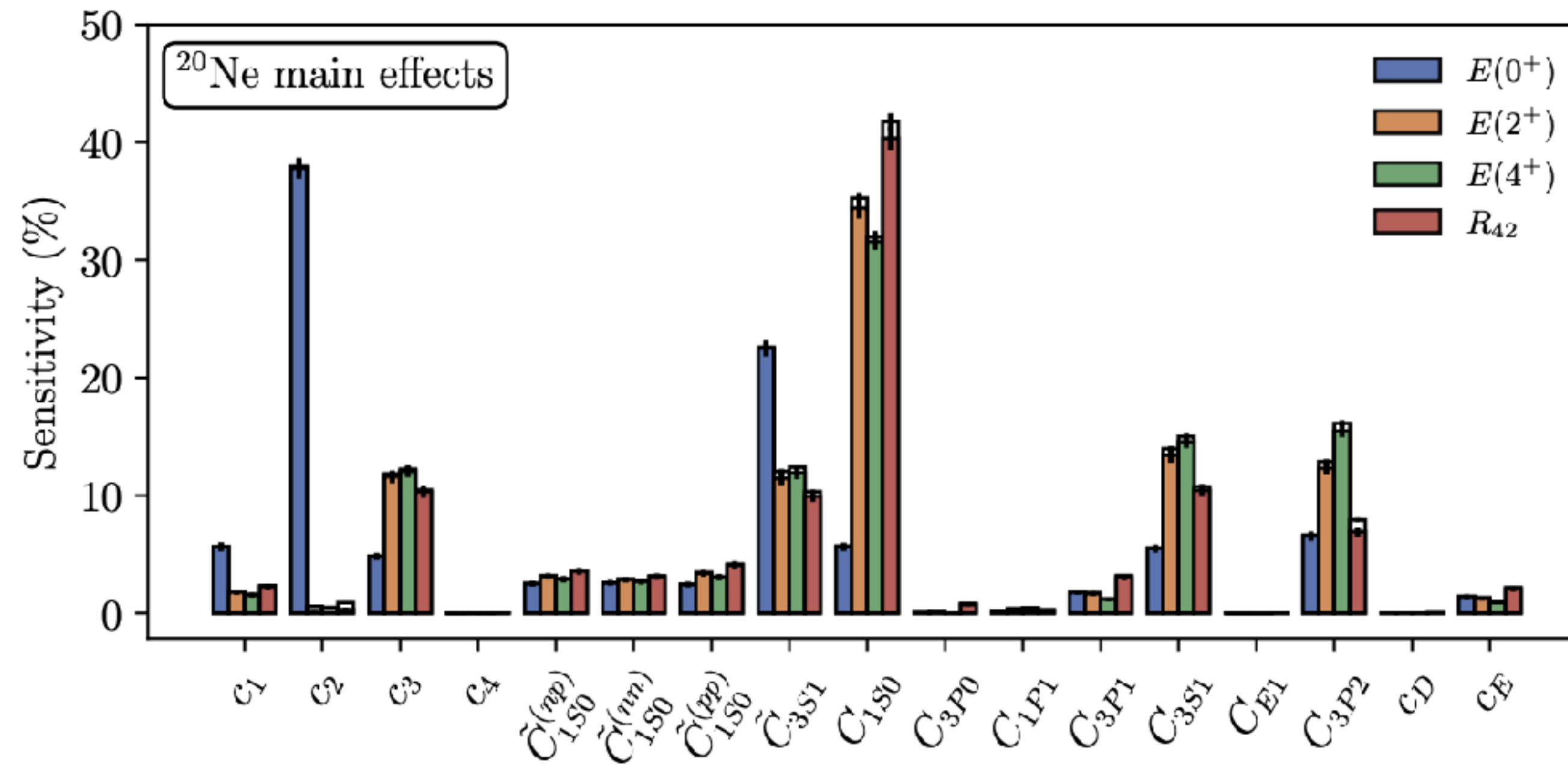
Data driven
MM-DGP



Ekström, et al., arXiv:2305.06955 (2023)

VS

Physics
Driven





Emulators for Many-Body Methods

There are two? ways to build an emulator for nuclear physics:

Physics driven

Data driven





Emulators for Many-Body Methods

There are two? ways to build an emulator for nuclear physics:

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Data driven



Reduce Basis Methods



Emulators for Many-Body Methods

There are two? ways to build an emulator for nuclear physics:

Physics driven

Data driven



Reduce Basis Methods

NN, GPs



Emulators for Many-Body Methods

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Reduce Basis Methods

PMMs

NN, GPs



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Emulators for Many-Body Methods

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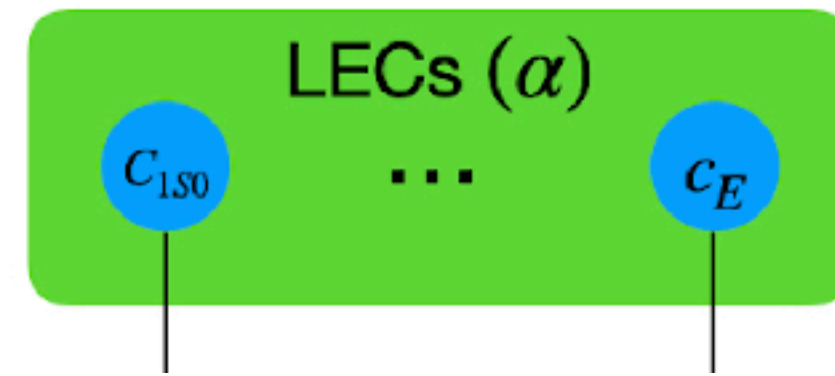
PINNs

NN, GPs



Jose Miguel Muñoz Arias

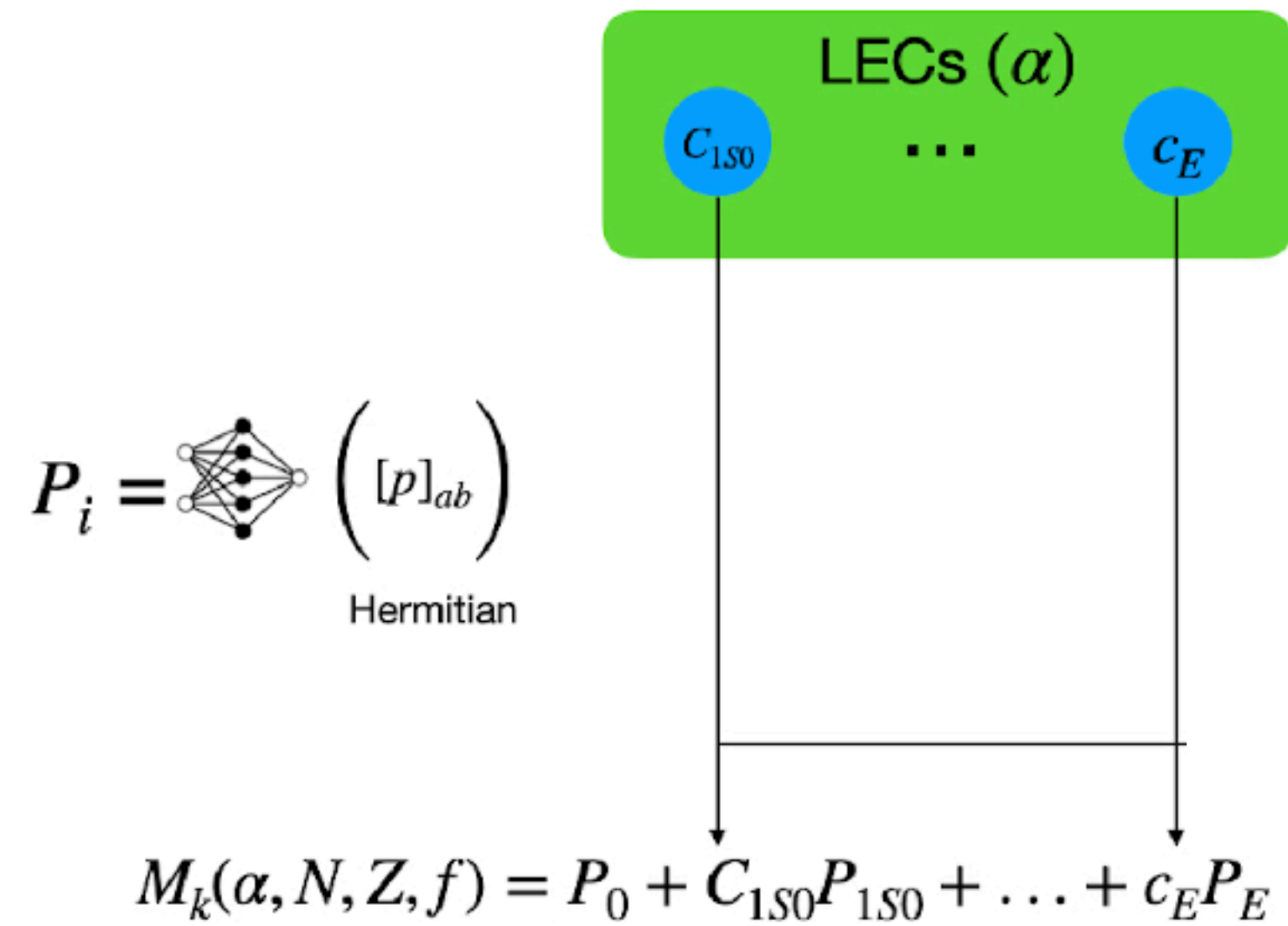
Physics Driven Global Emulation





Jose Miguel Muñoz Arias

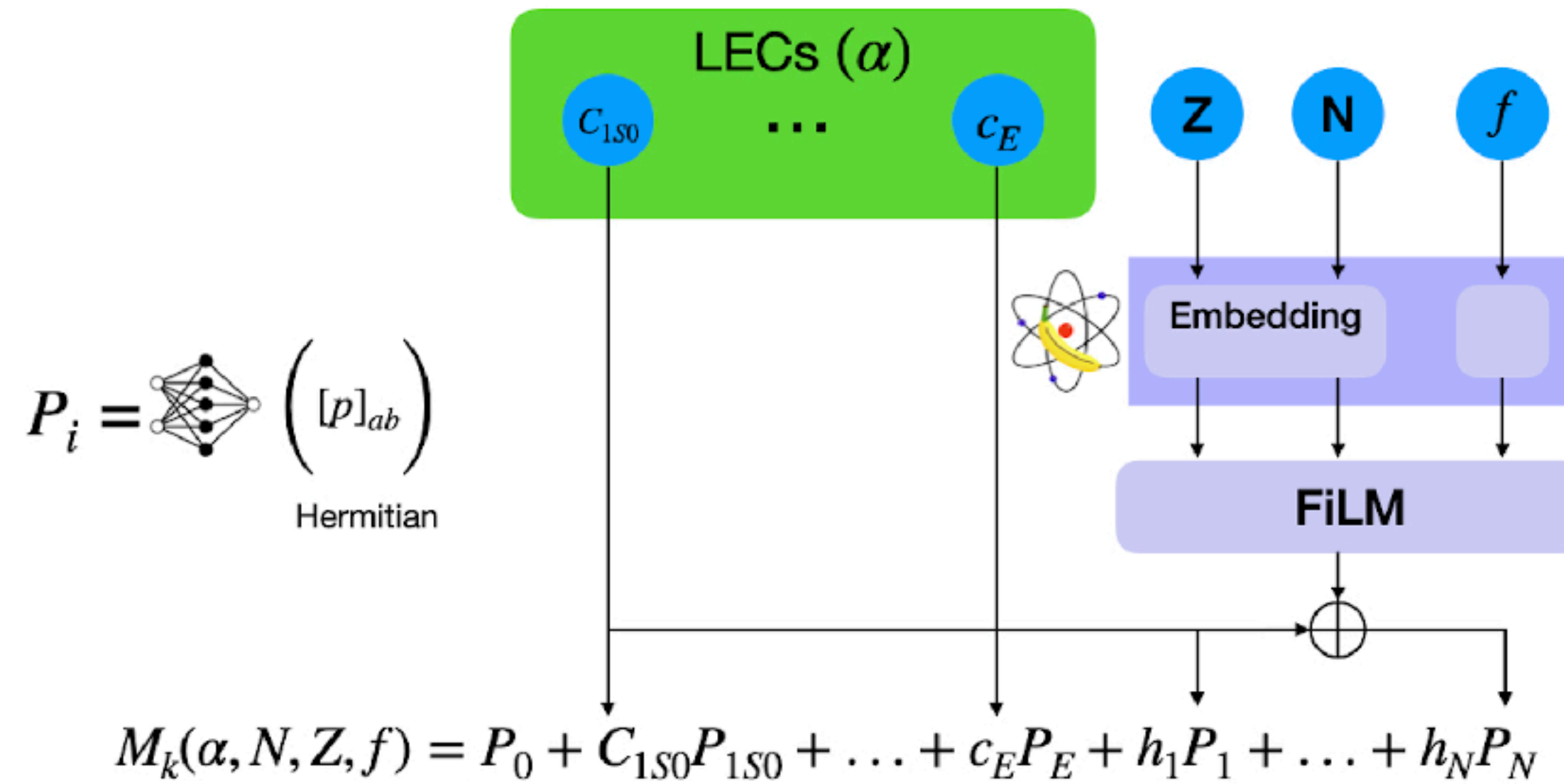
Physics Driven Global Emulation





Jose Miguel Muñoz Arias

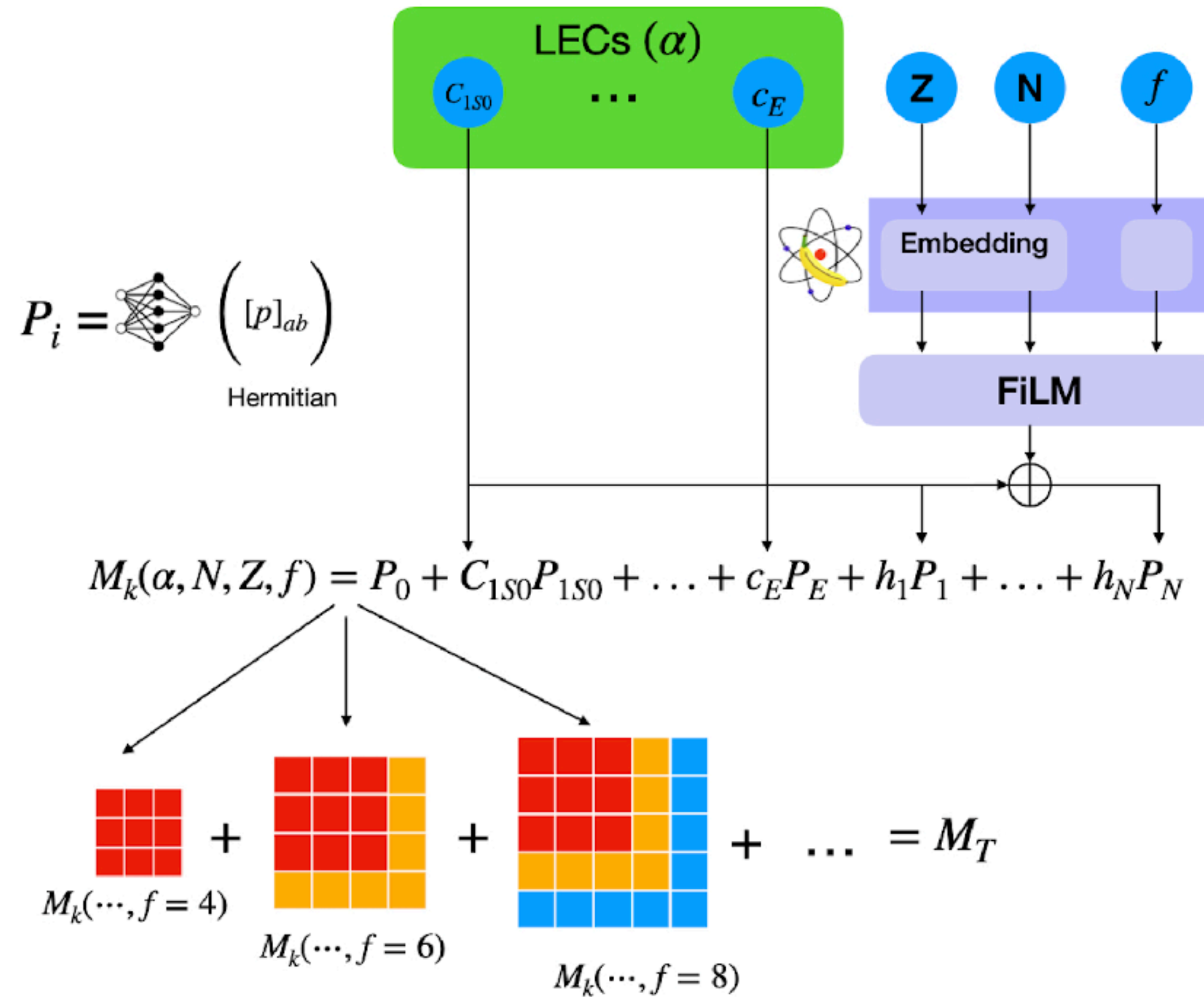
Physics Driven Global Emulation





Jose Miguel Muñoz Arias

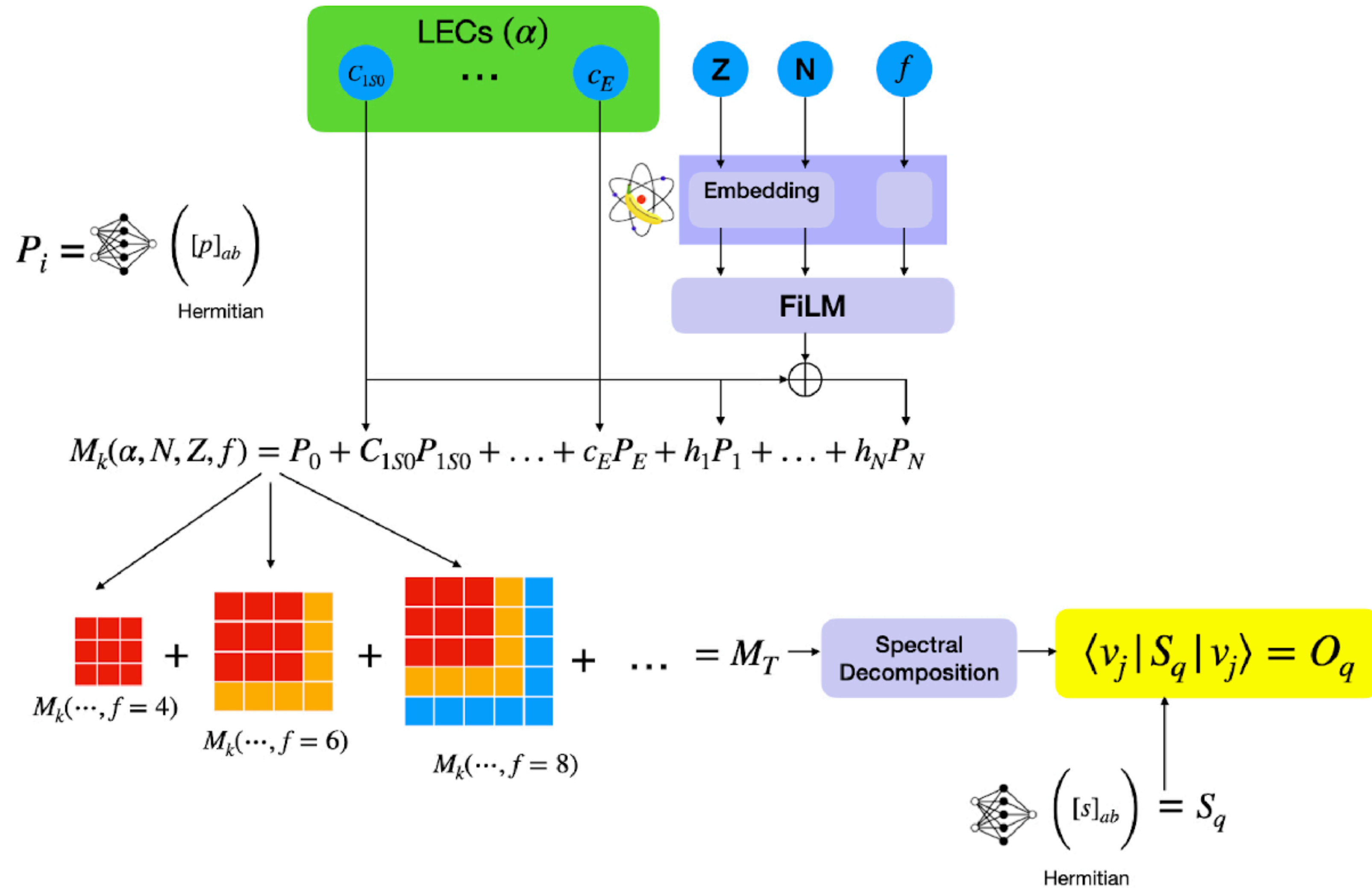
Physics Driven Global Emulation





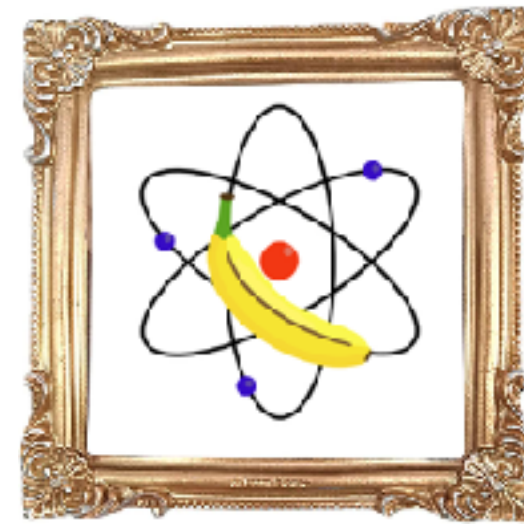
Jose Miguel Muñoz Arias

Physics Driven Global Emulation



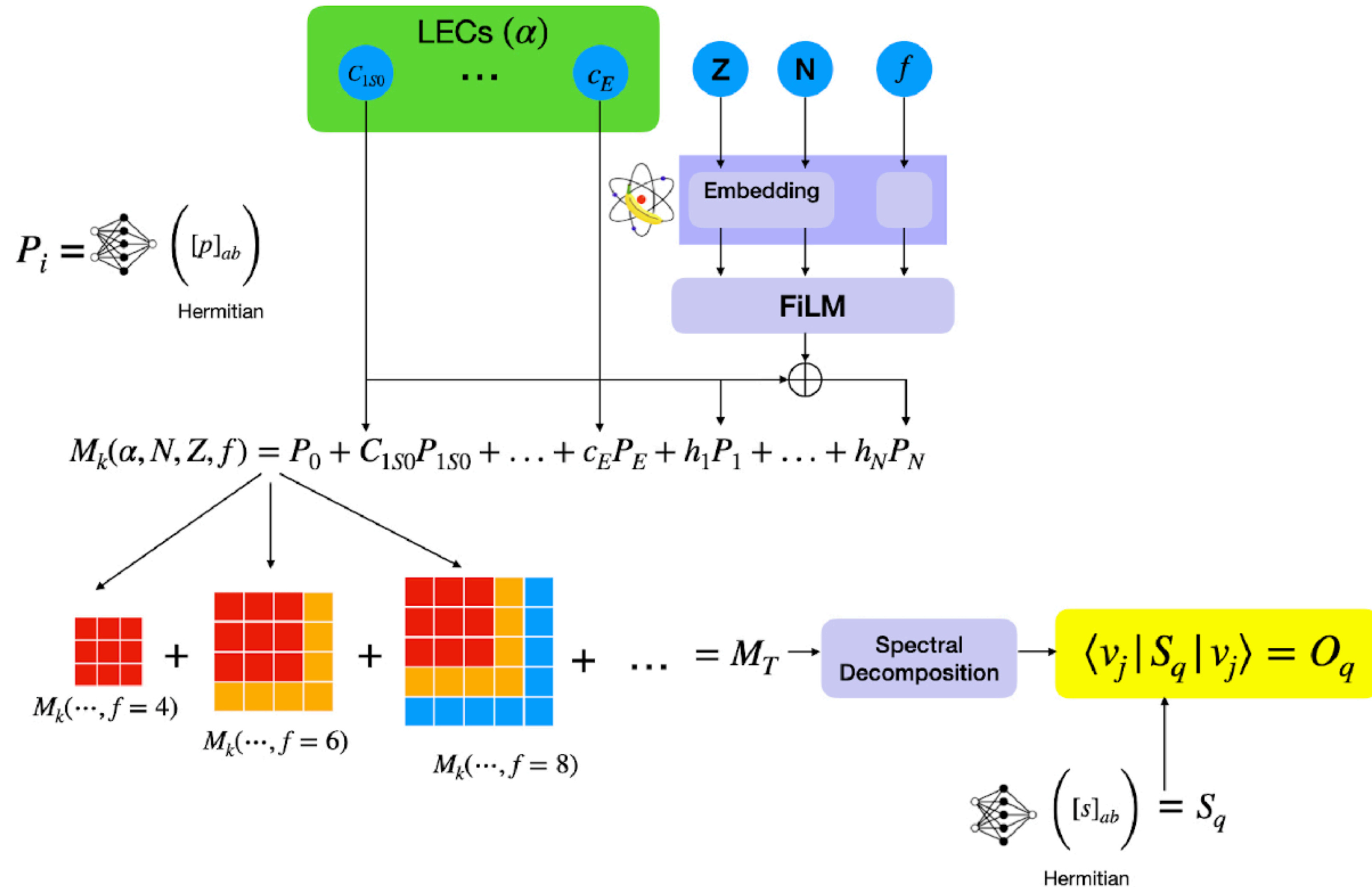


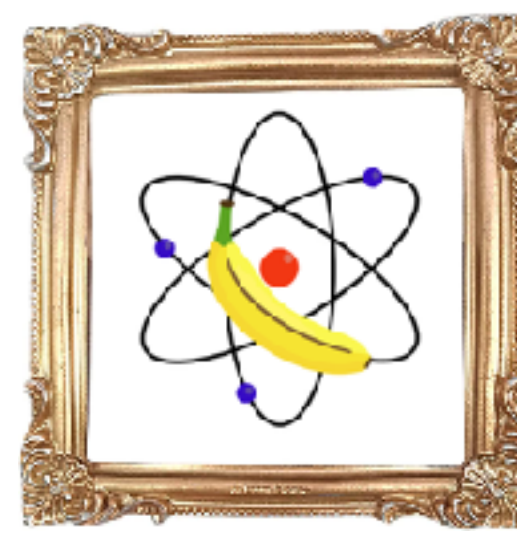
Jose Miguel Muñoz Arias



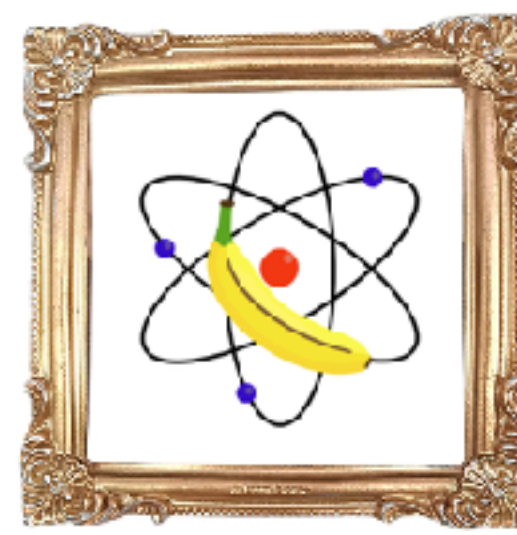
Physics Driven Global Emulation

Feature Resolved Affine Matrix Emulator (FRAME)



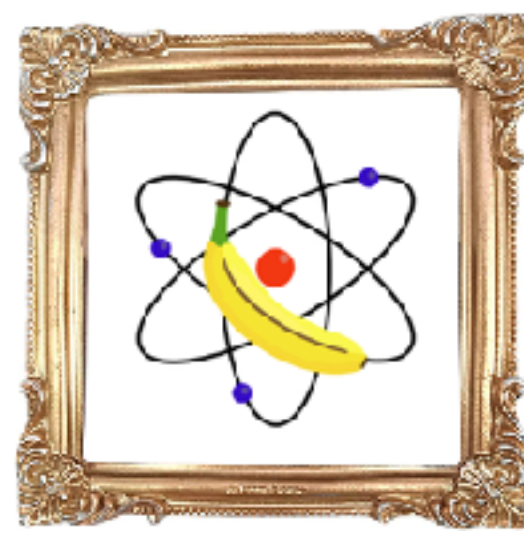


Anchor and Refinement



Anchor and Refinement

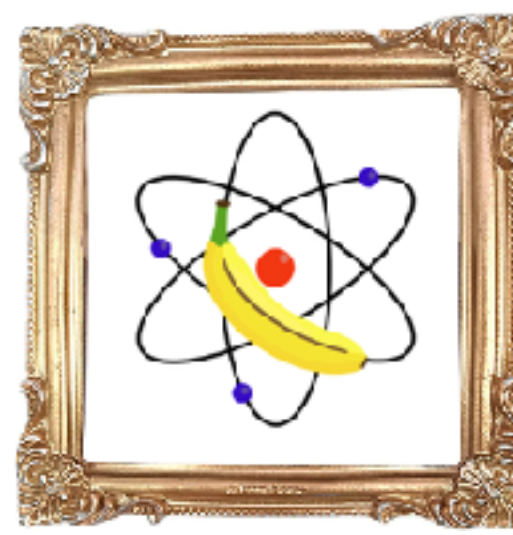
$$M(N, Z, f, \alpha) = [M_{f_{min}} + \sum_{p=1}^f \xi(f; N, Z, \alpha) \Delta M_p]$$



Anchor and Refinement

$$M(N, Z, f, \alpha) = [M_{f_{min}} + \sum_{p=1}^f \xi(f; N, Z, \alpha) \Delta M_p]$$

Anchor: Matrix at the lowest fidelity

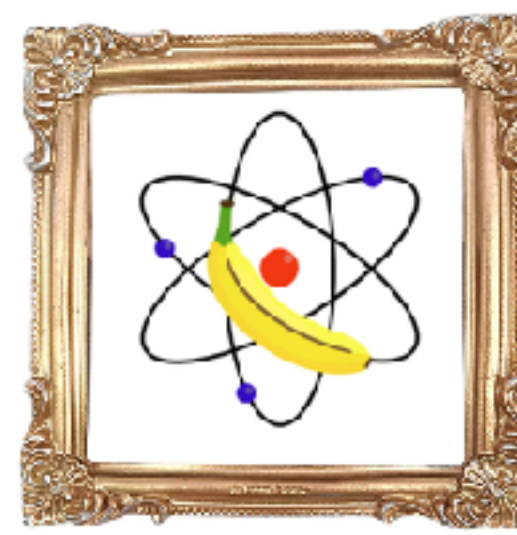


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$$M(N, Z, f, \alpha) = [M_{f_{min}} + \sum_{p=1}^f \xi(f; N, Z, \alpha) \Delta M_p]$$

Anchor: Matrix at the lowest fidelity

Refinement: Corrections from higher fidelities



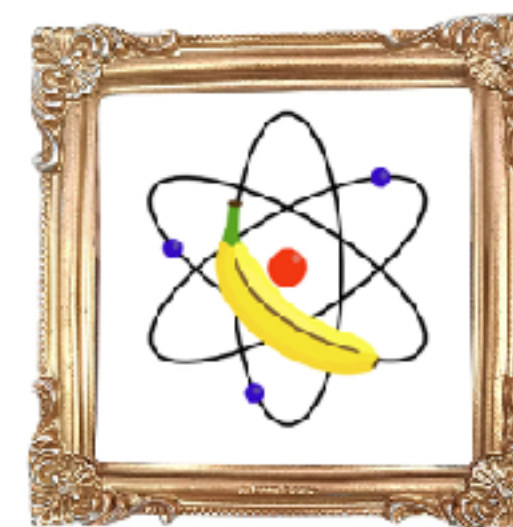
Anchor and Refinement

$$M(N, Z, f, \alpha) = [M_{f_{min}} + \sum_{p=1}^f \xi(f; N, Z, \alpha) \Delta M_p]$$

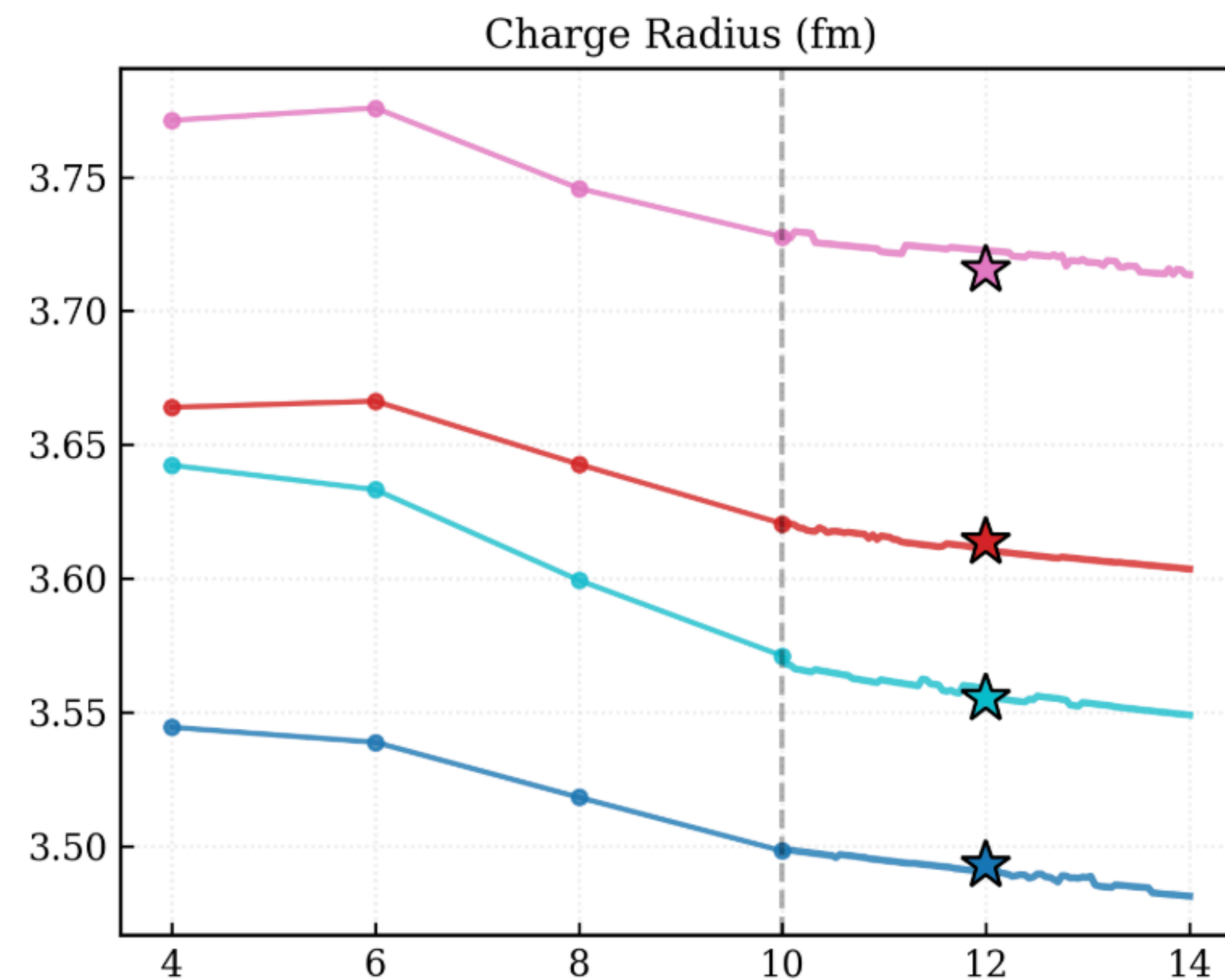
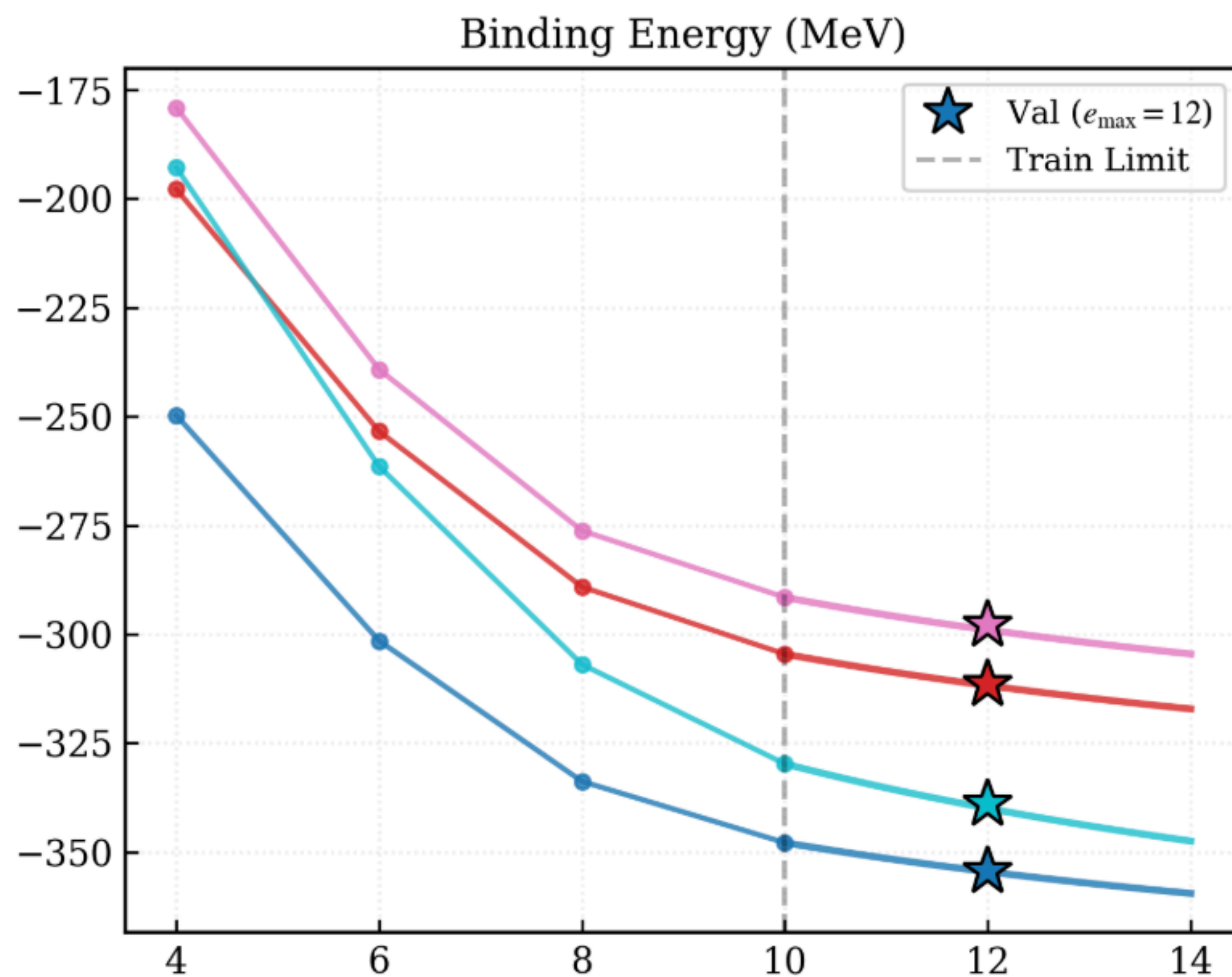
Anchor: Matrix at the lowest fidelity

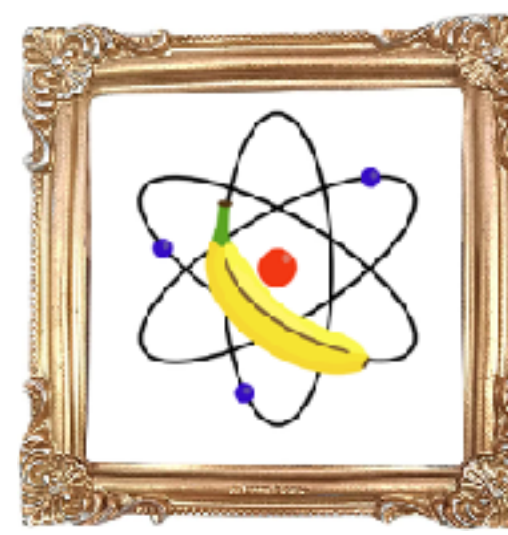
Refinement: Corrections from higher fidelities

<https://frame-architecture-explorer-553167399436.us-west1.run.app/>

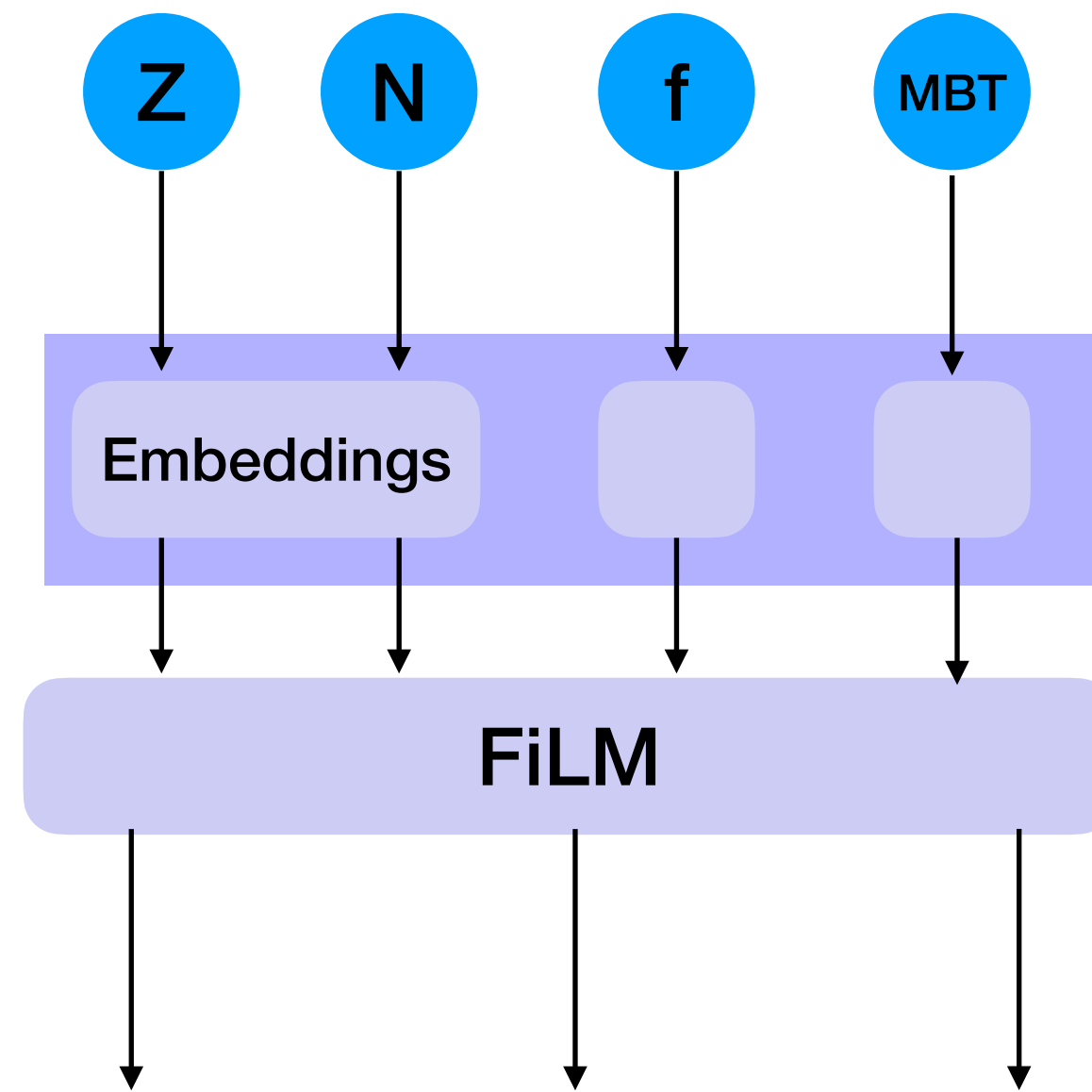


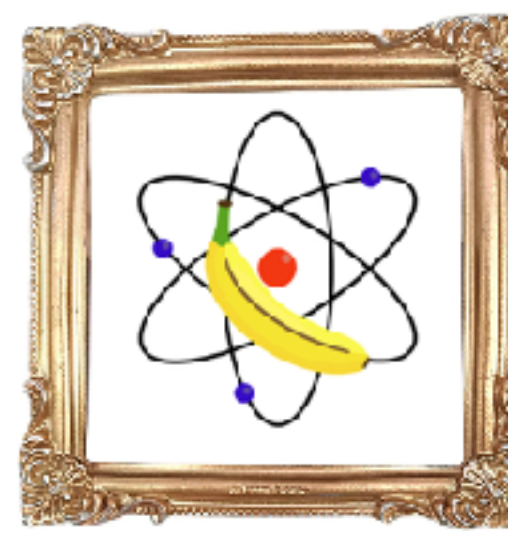
Extrapolating in $e_{\max}$



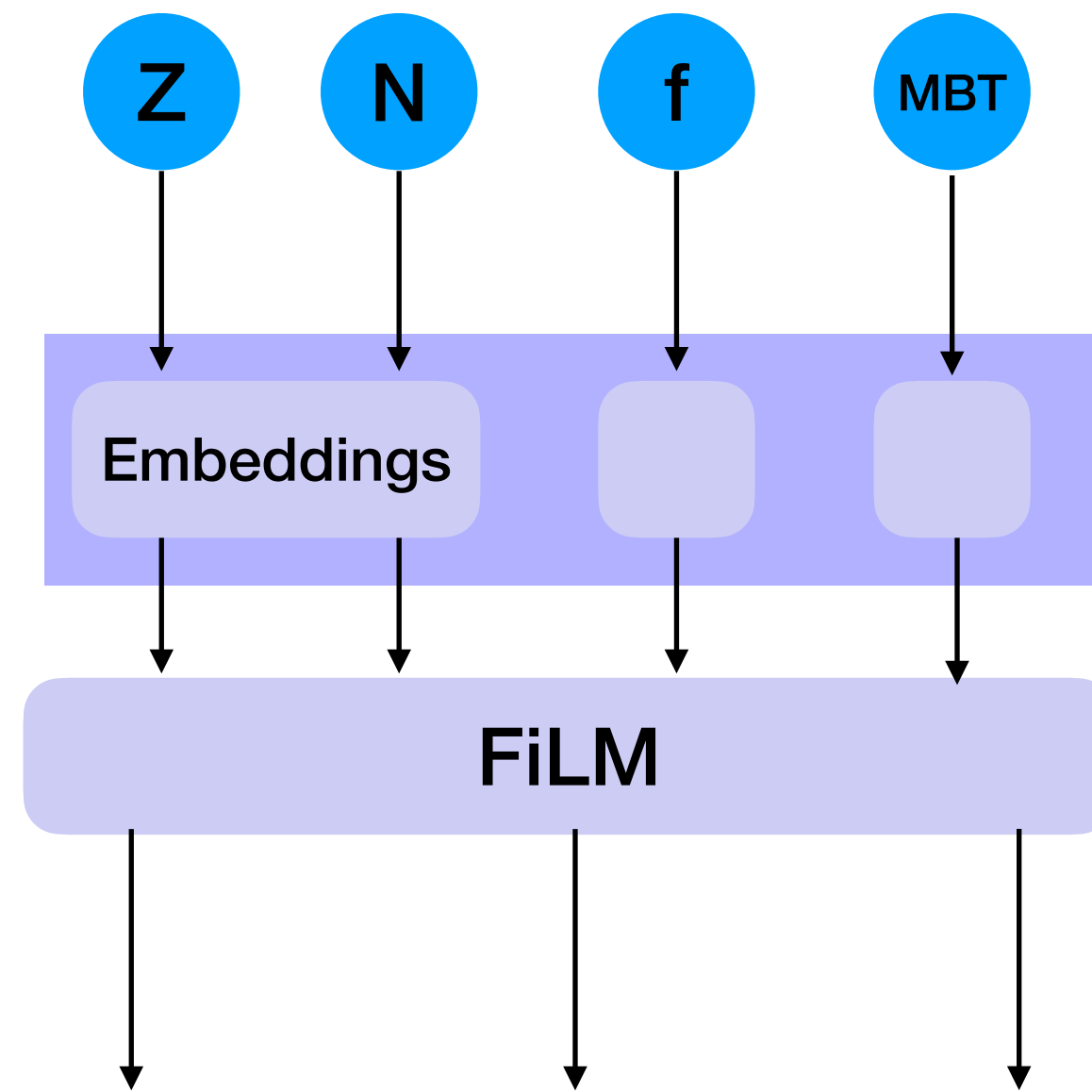


Extrapolating to IMSRG(3)

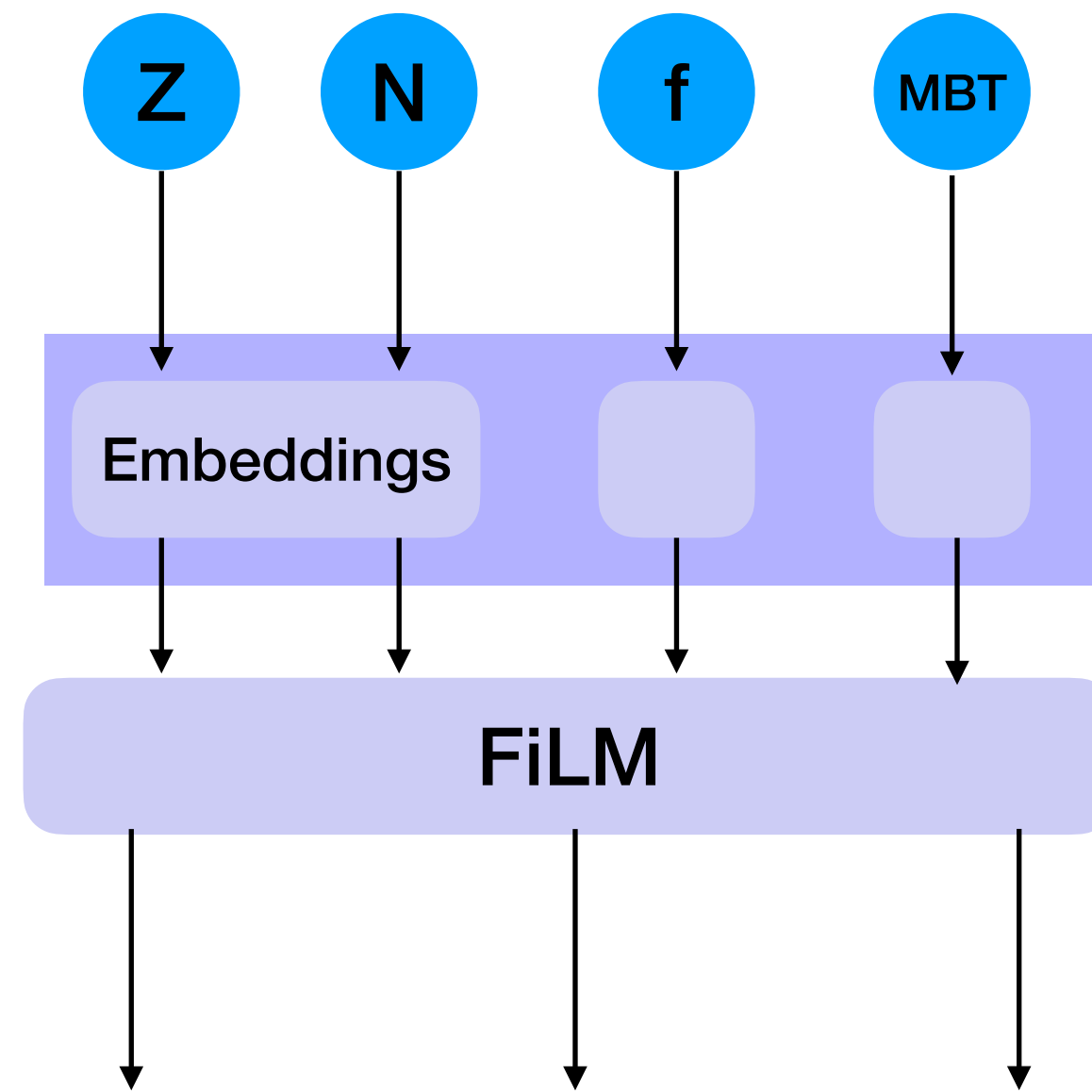




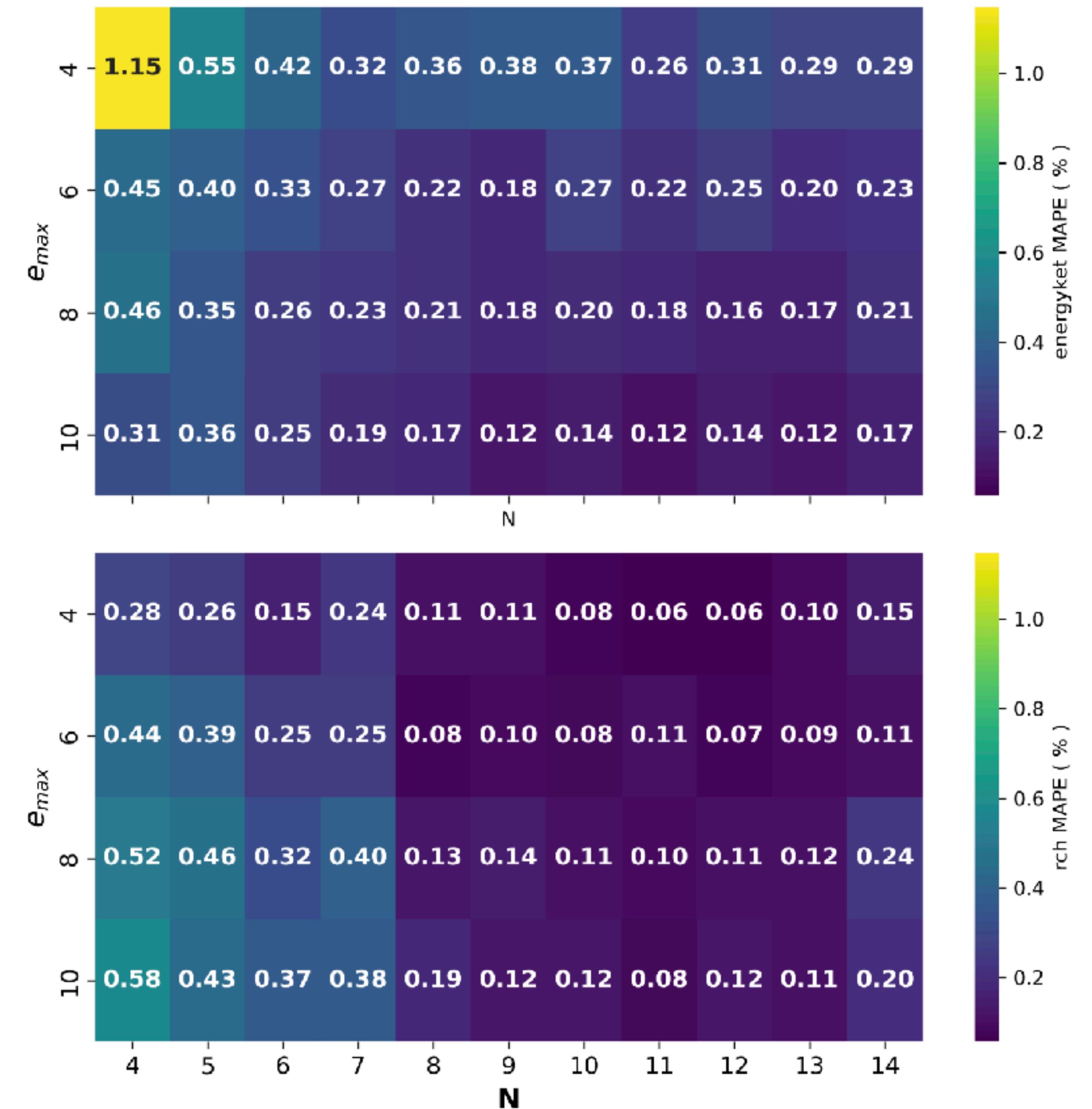
Extrapolating to IMSRG(3)



Difference with model and calculation of IMSRG(3f2) when no IMSRG(3f2) is used to train in a specific isotope.



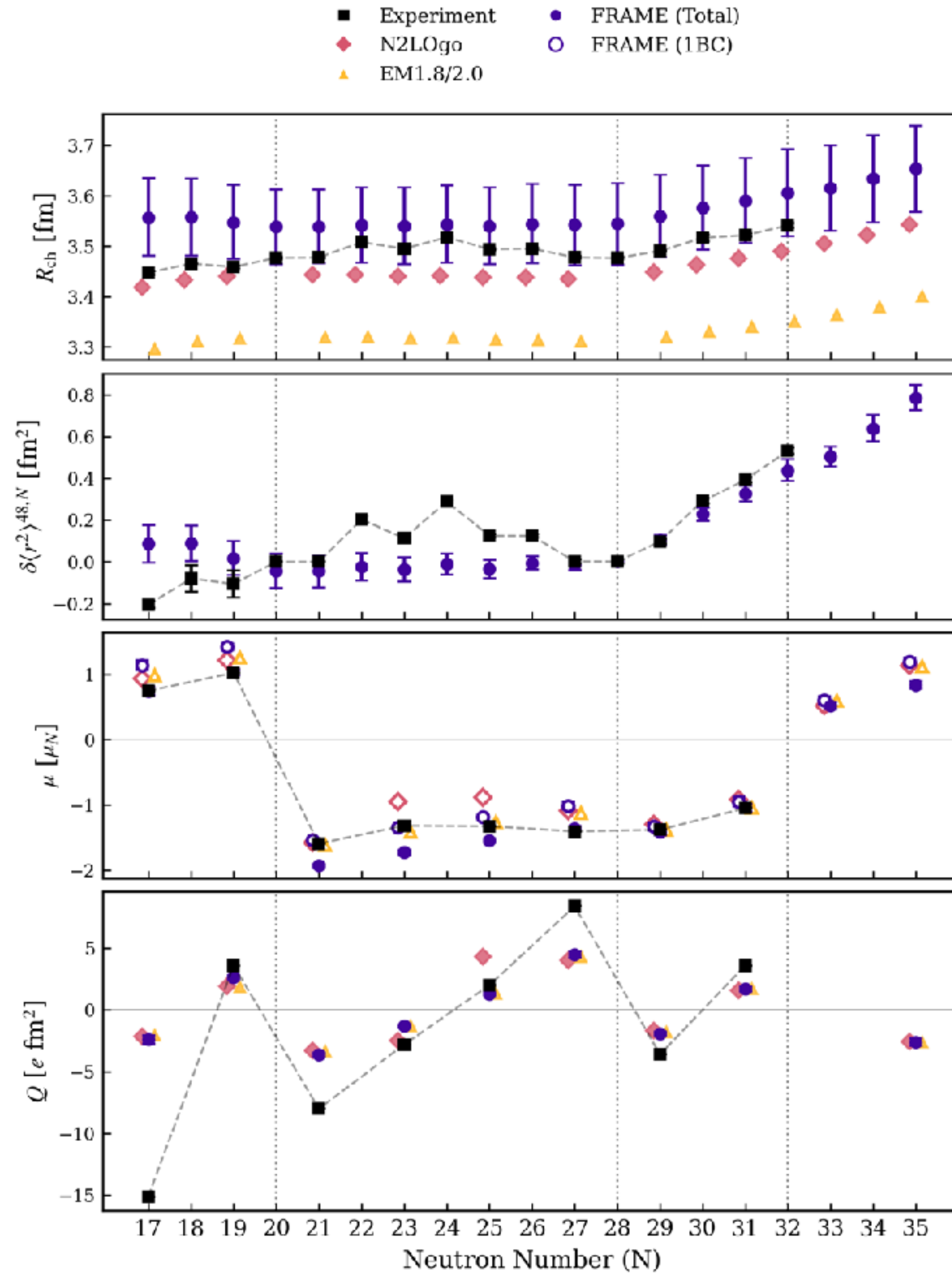
Difference with model and calculation of IMSRG(3f2) when no IMSRG(3f2) is used to train in a specific isotope.



Case study: EM Moments of Ca isotopes

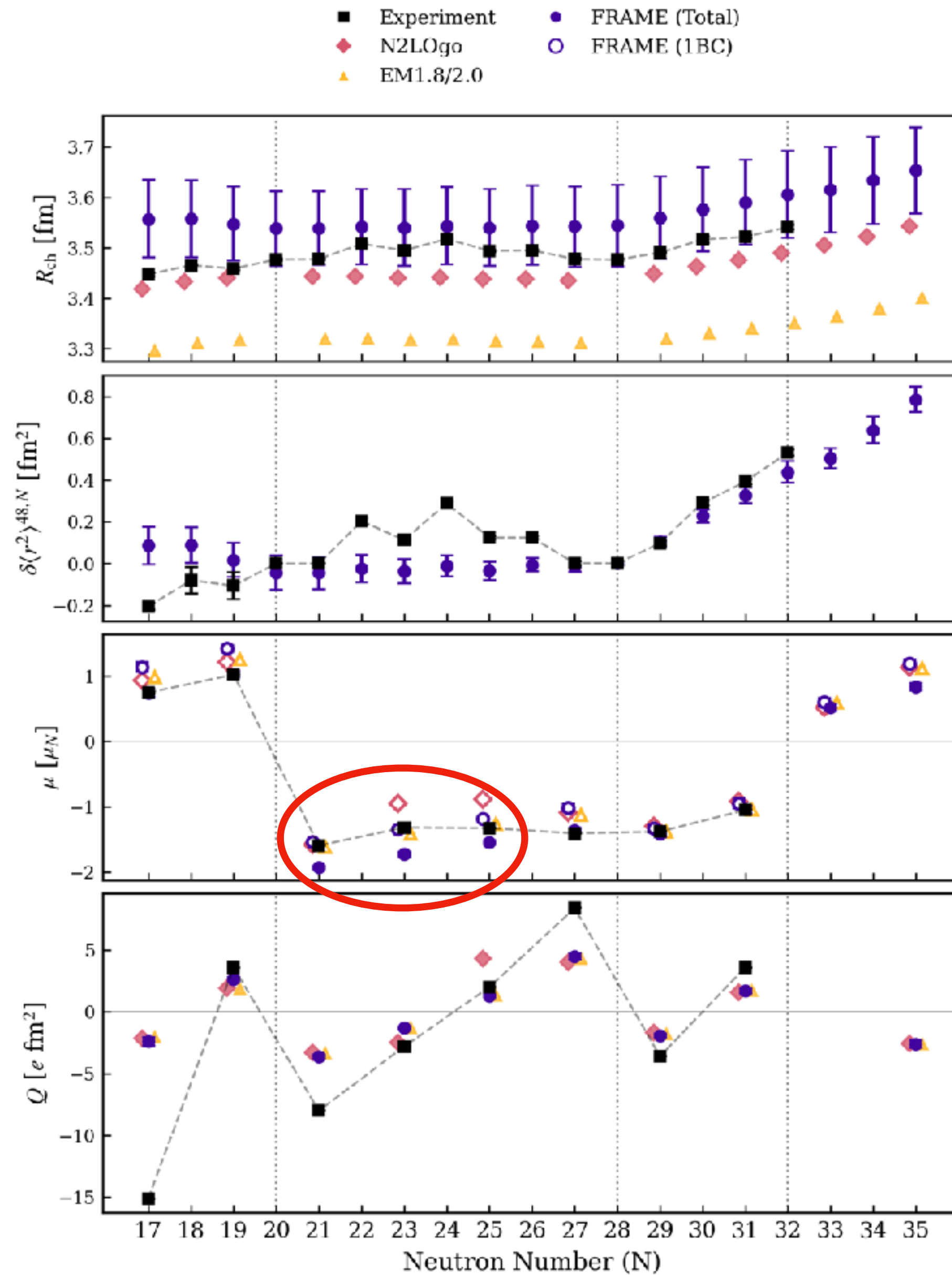


EM Moments of Ca Isotopes



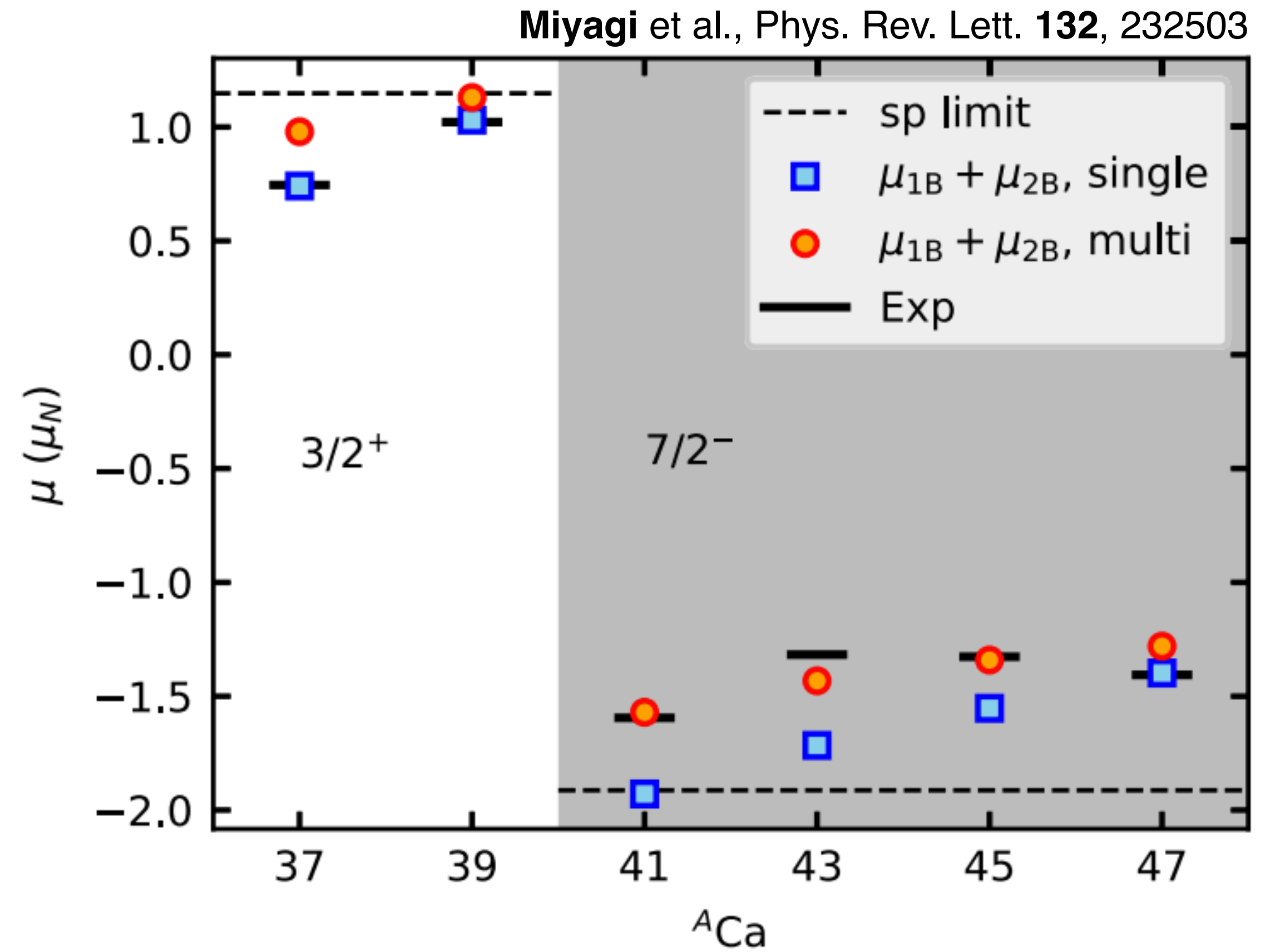
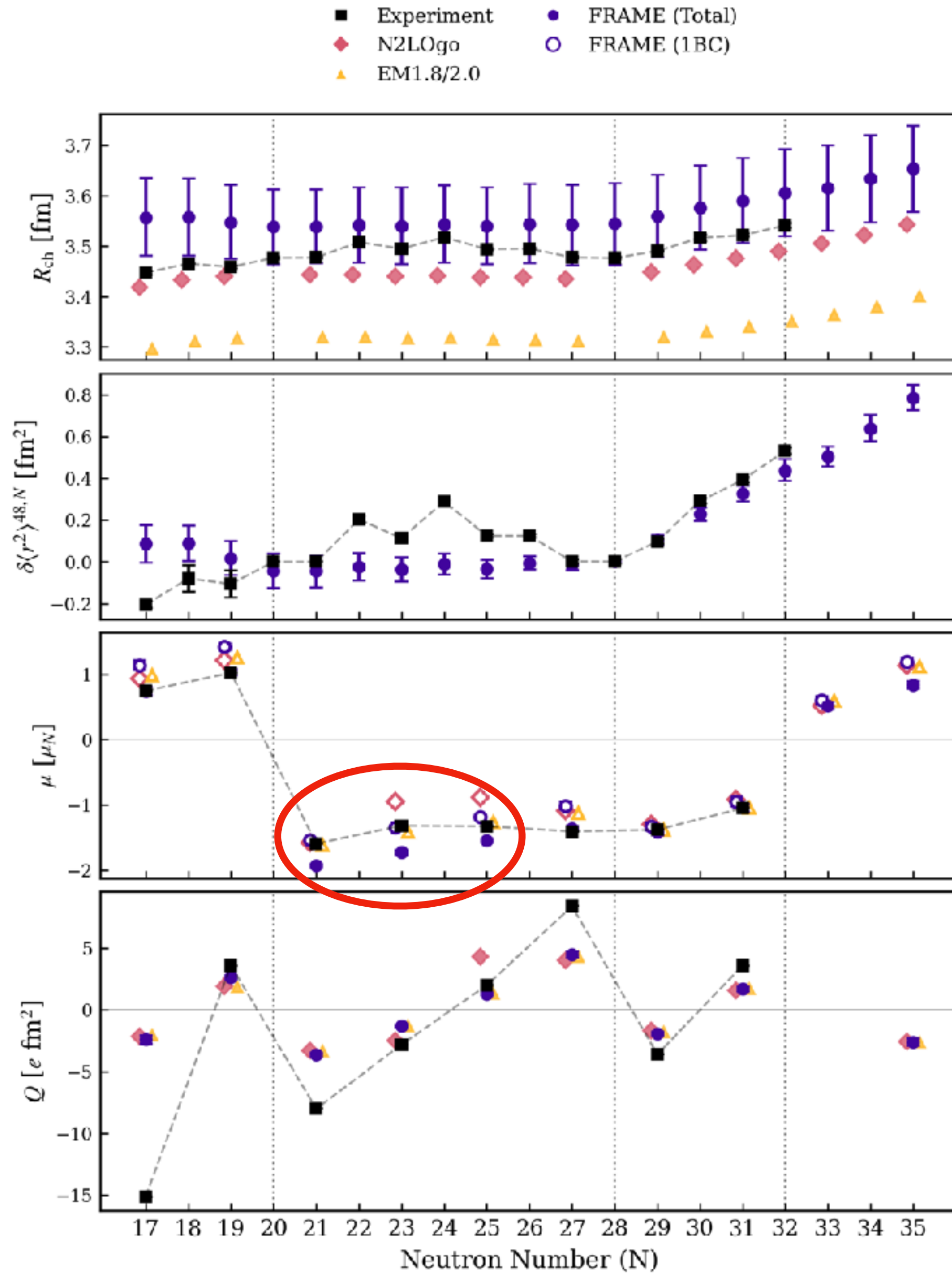


EM Moments of Ca Isotopes



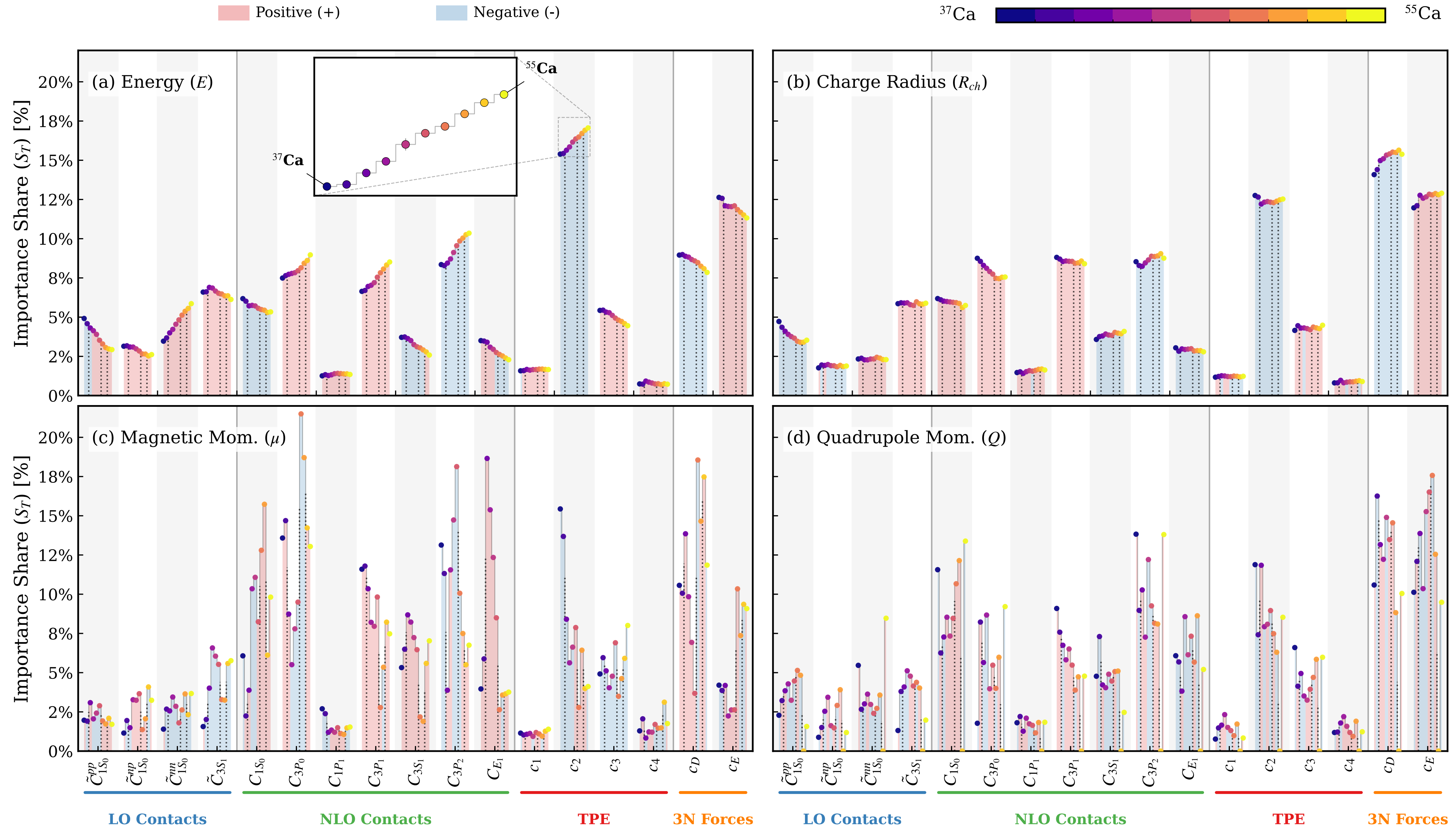


EM Moments of Ca Isotopes



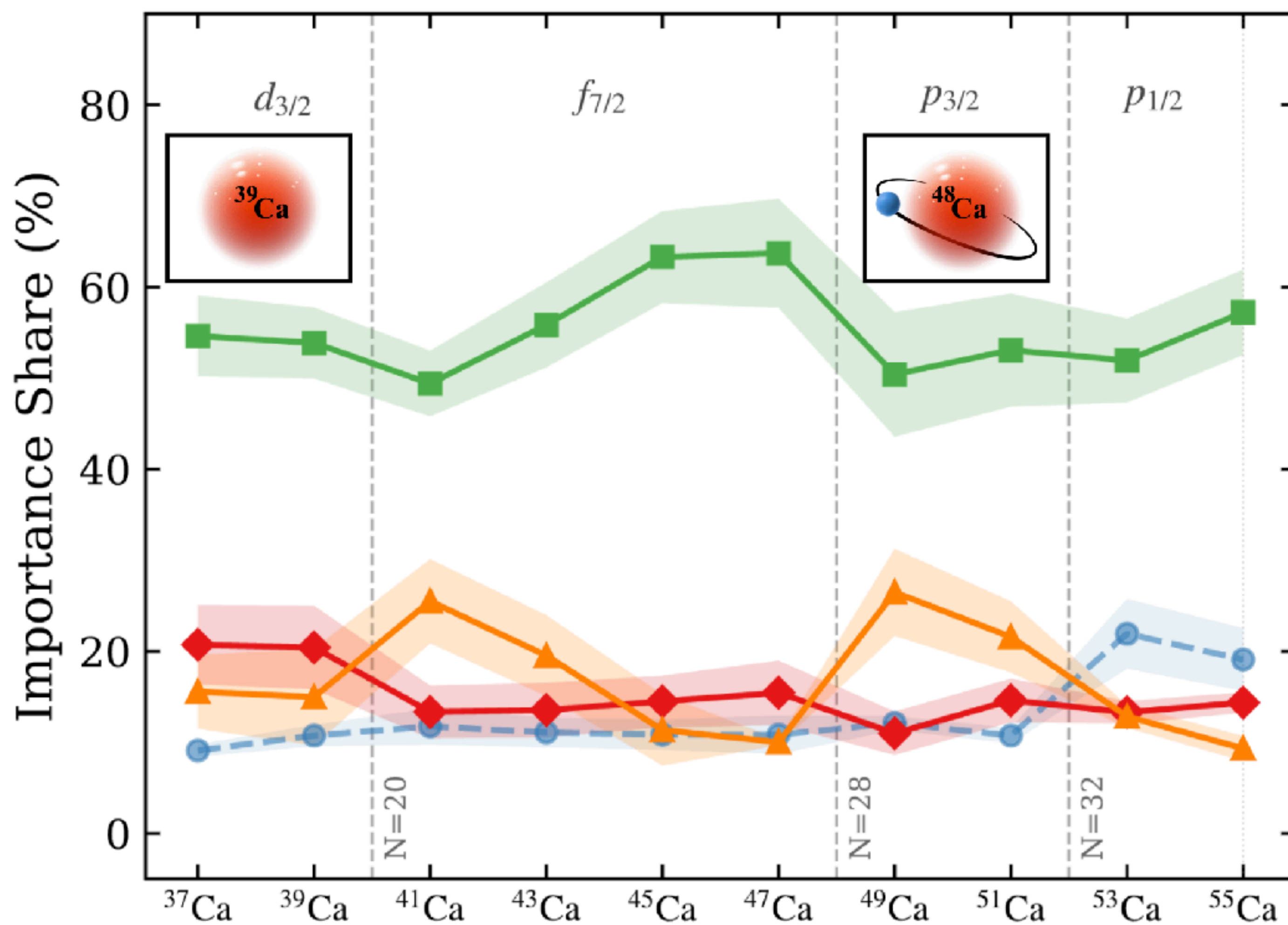
SHAP values in Ca Isotopes

Munoz, **Belley**, et al., arXiv: 2603.26905 (2026)

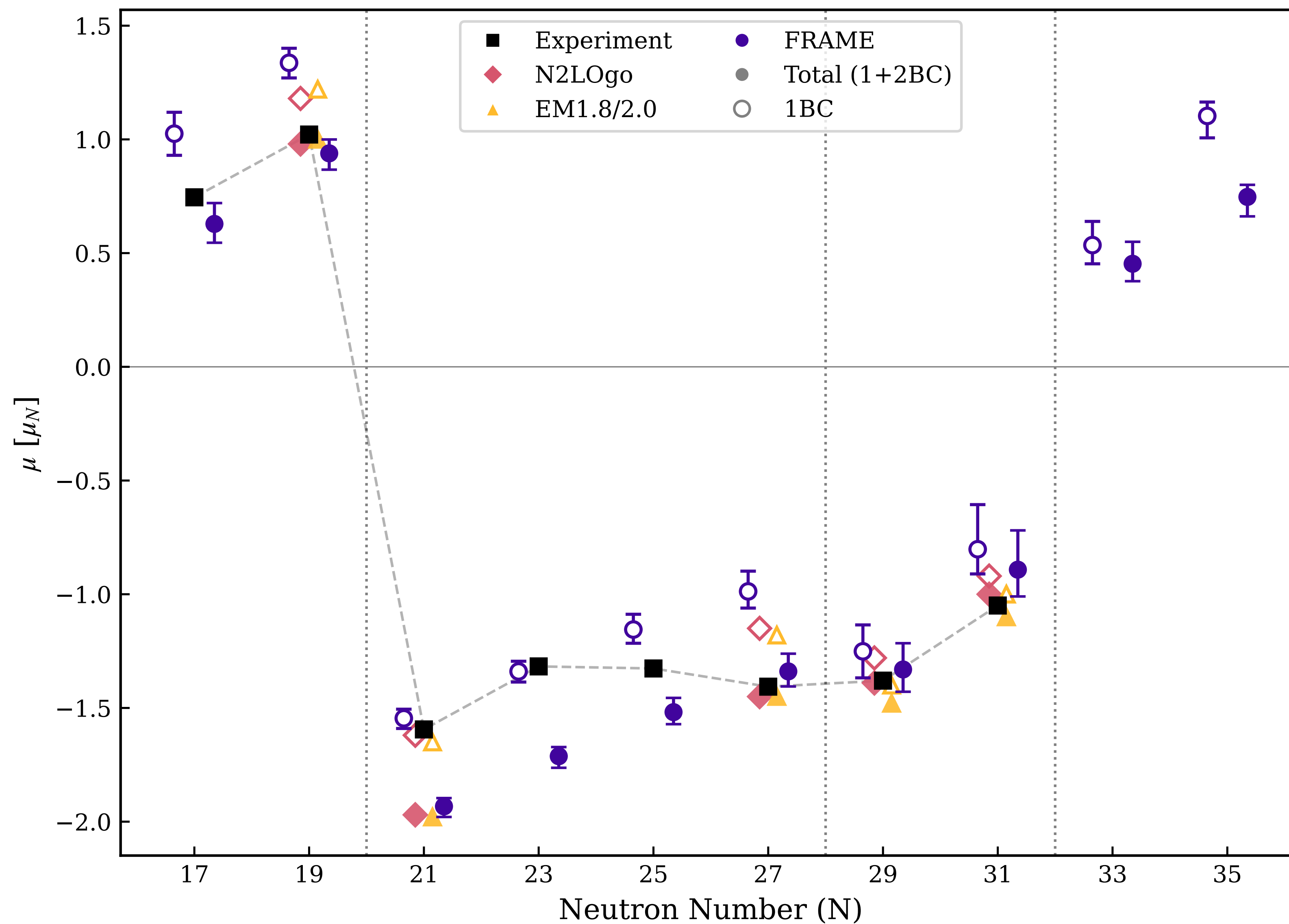


Forces Through the Shells

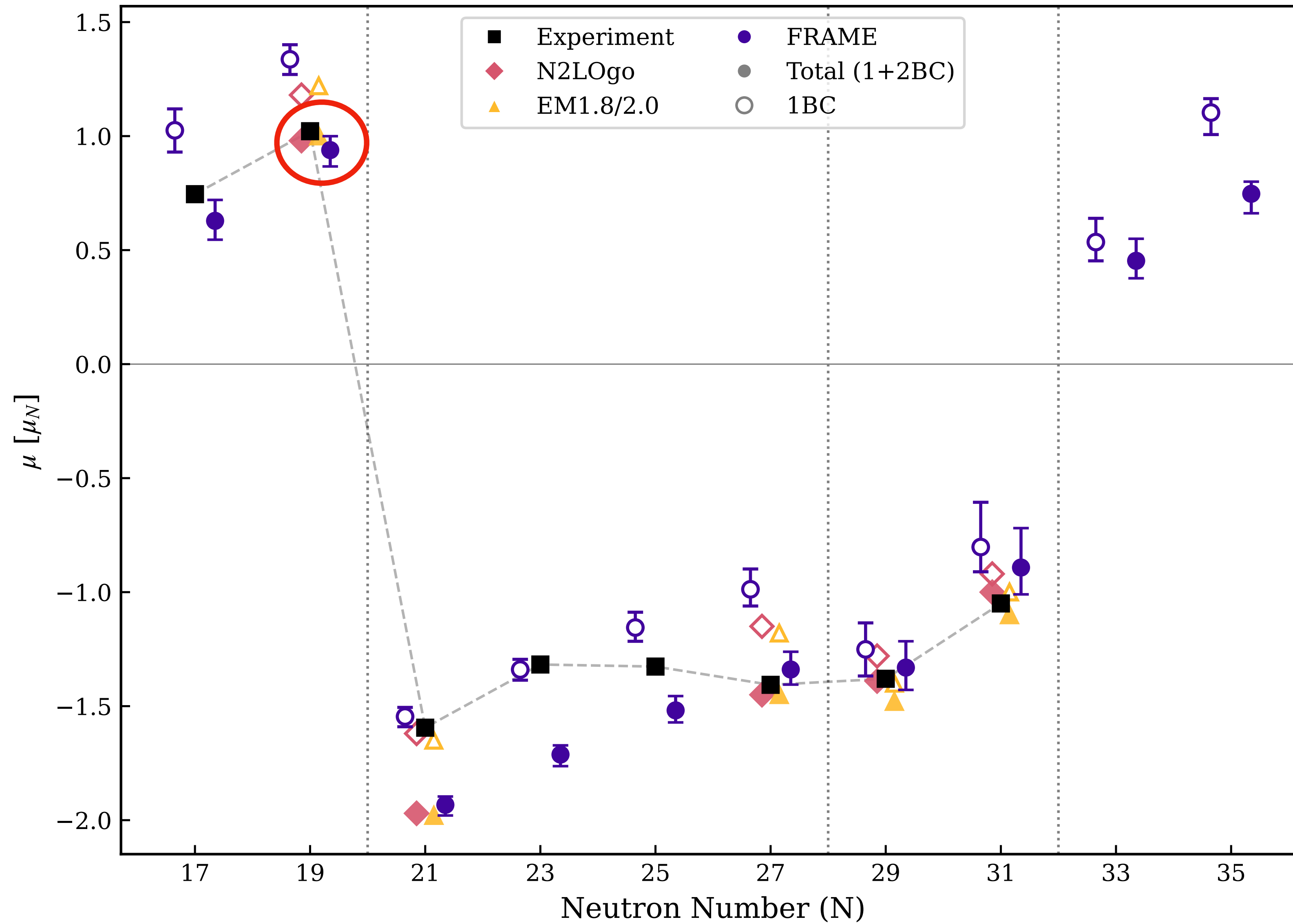
▲ 3N Forces (c_D, c_E)
 ■ NLO Contacts ($C_{S,P}$)
 ◆ πN TPE (c_i)
 ● LO Contacts ($\tilde{C}$)



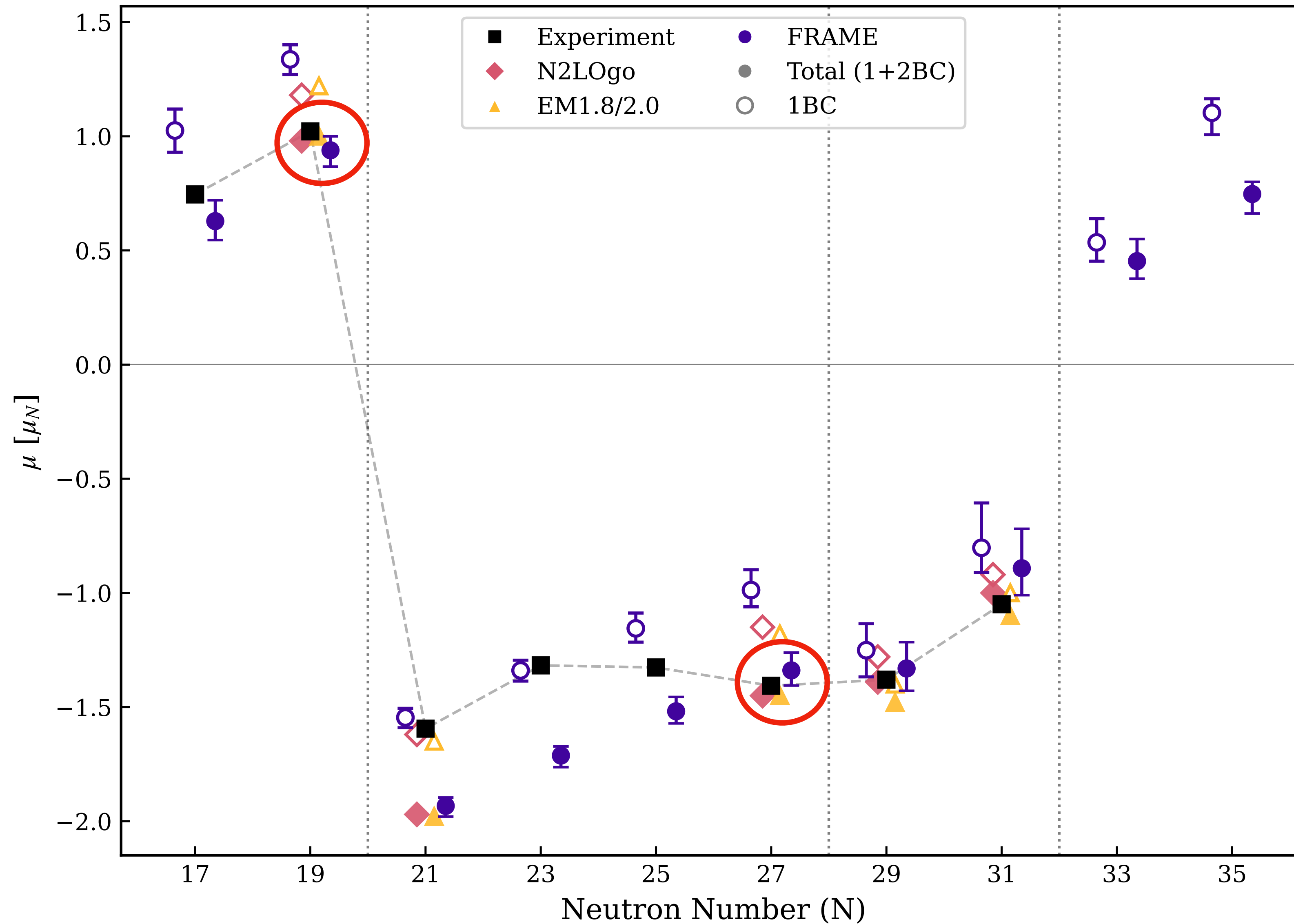
Using Emulators to Constrain Forces



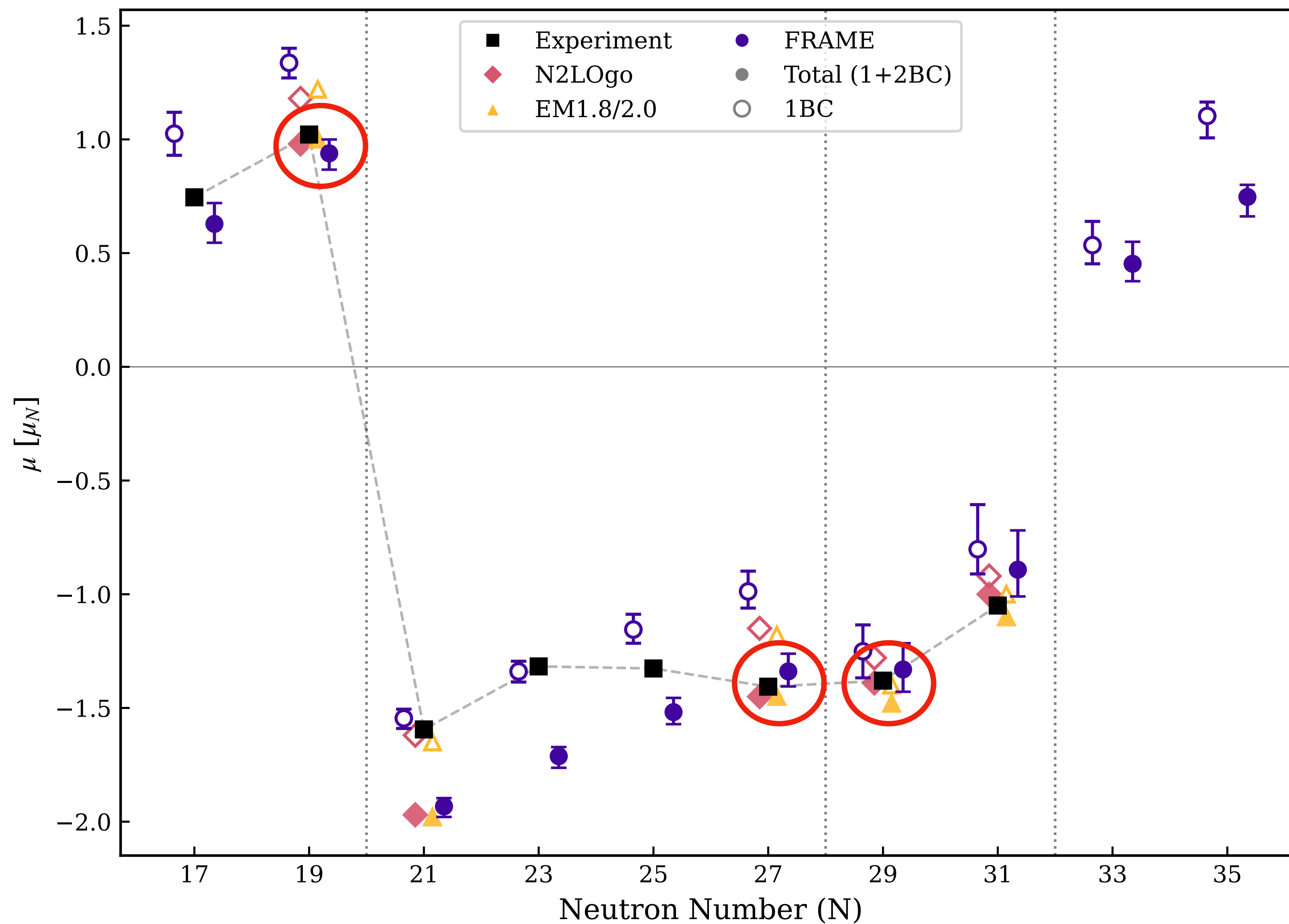
Using Emulators to Constrain Forces



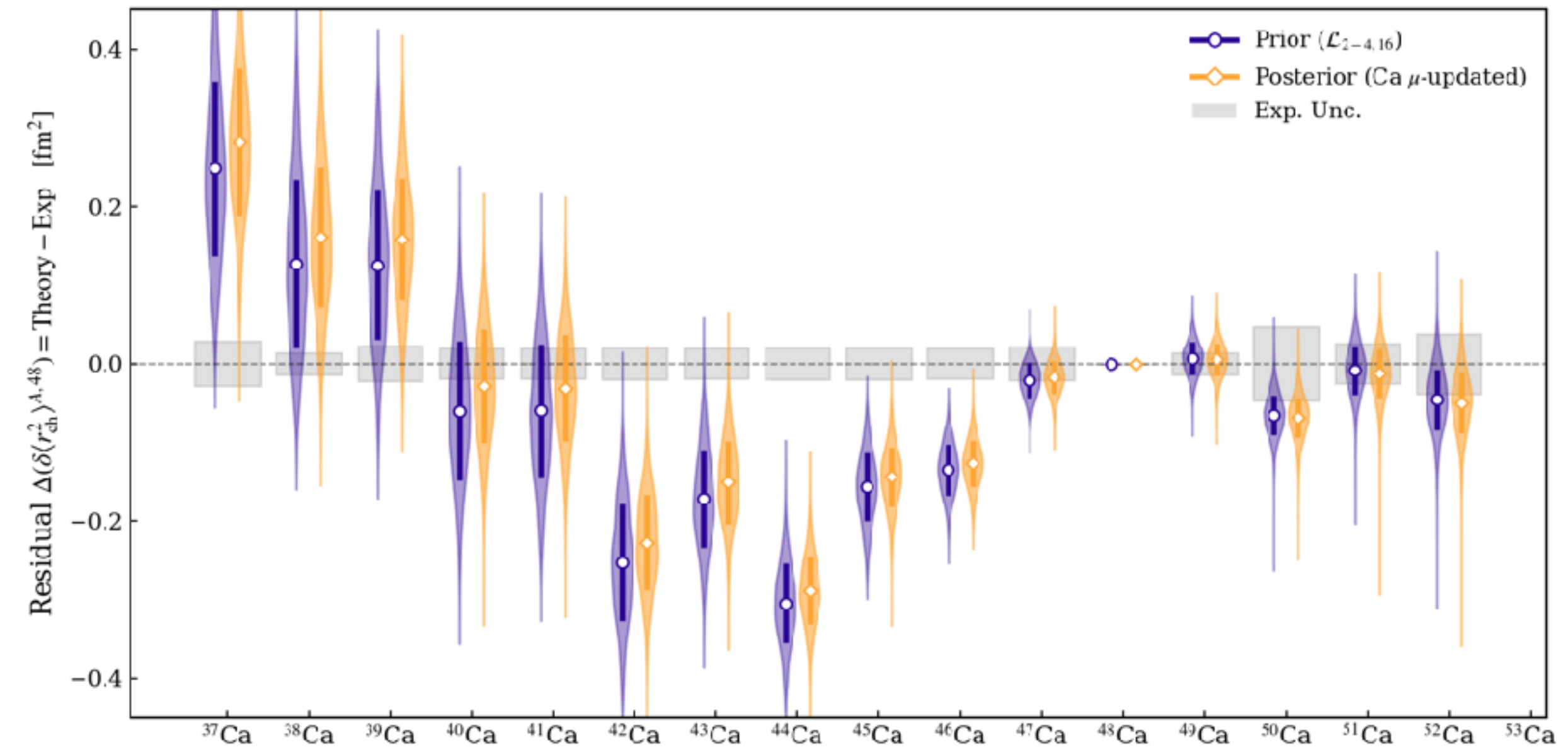
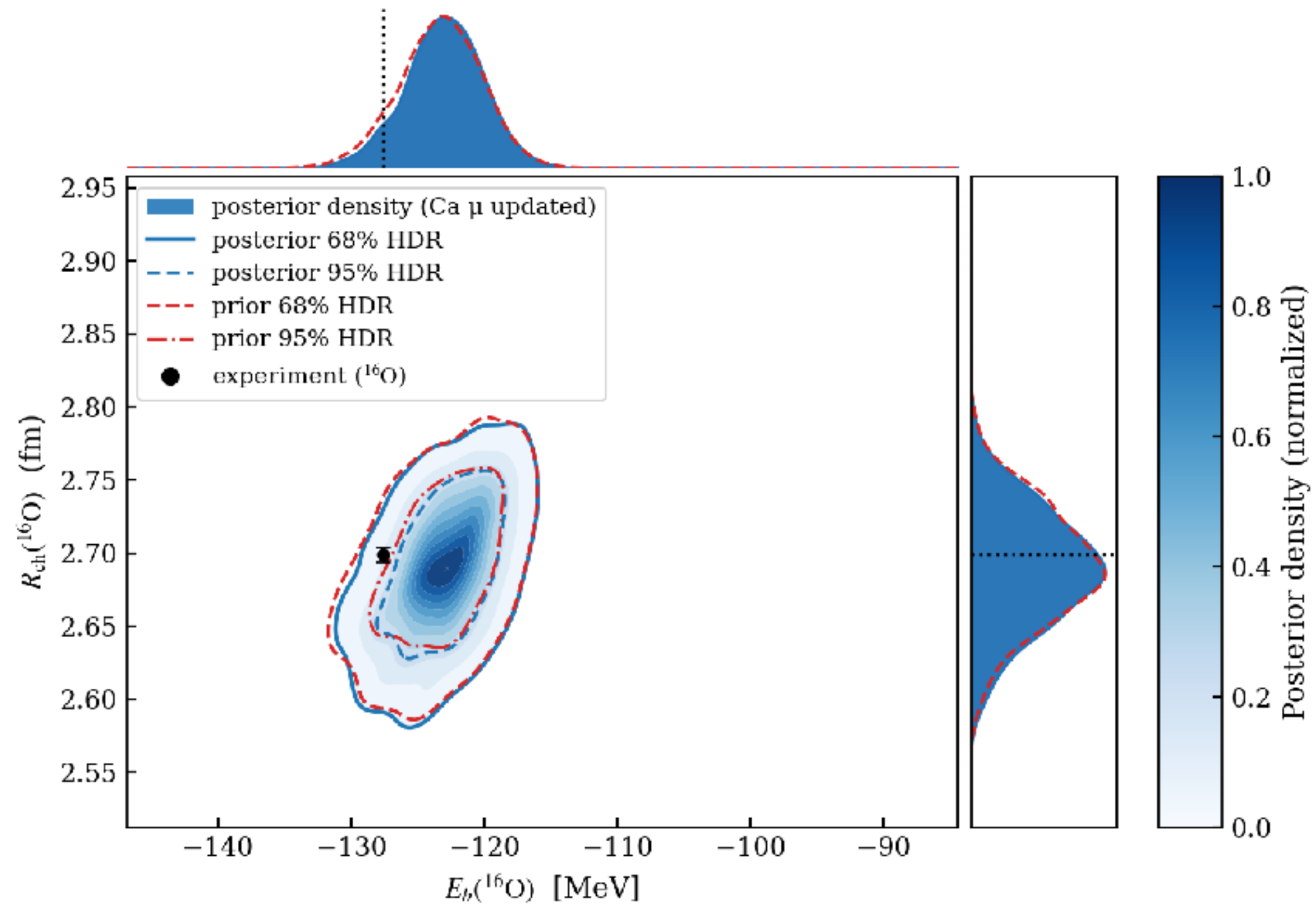
Using Emulators to Constrain Forces

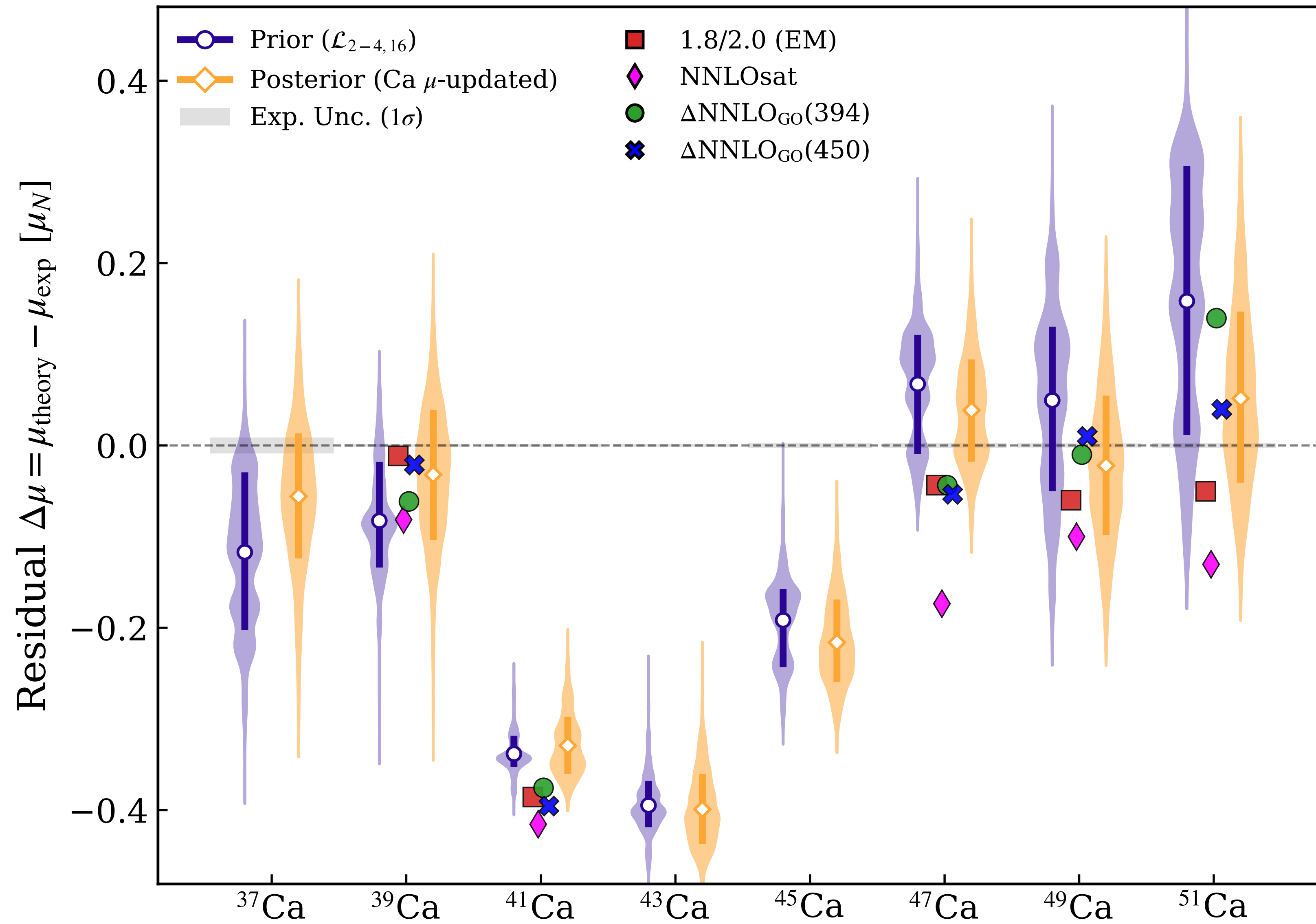


Using Emulators to Constrain Forces

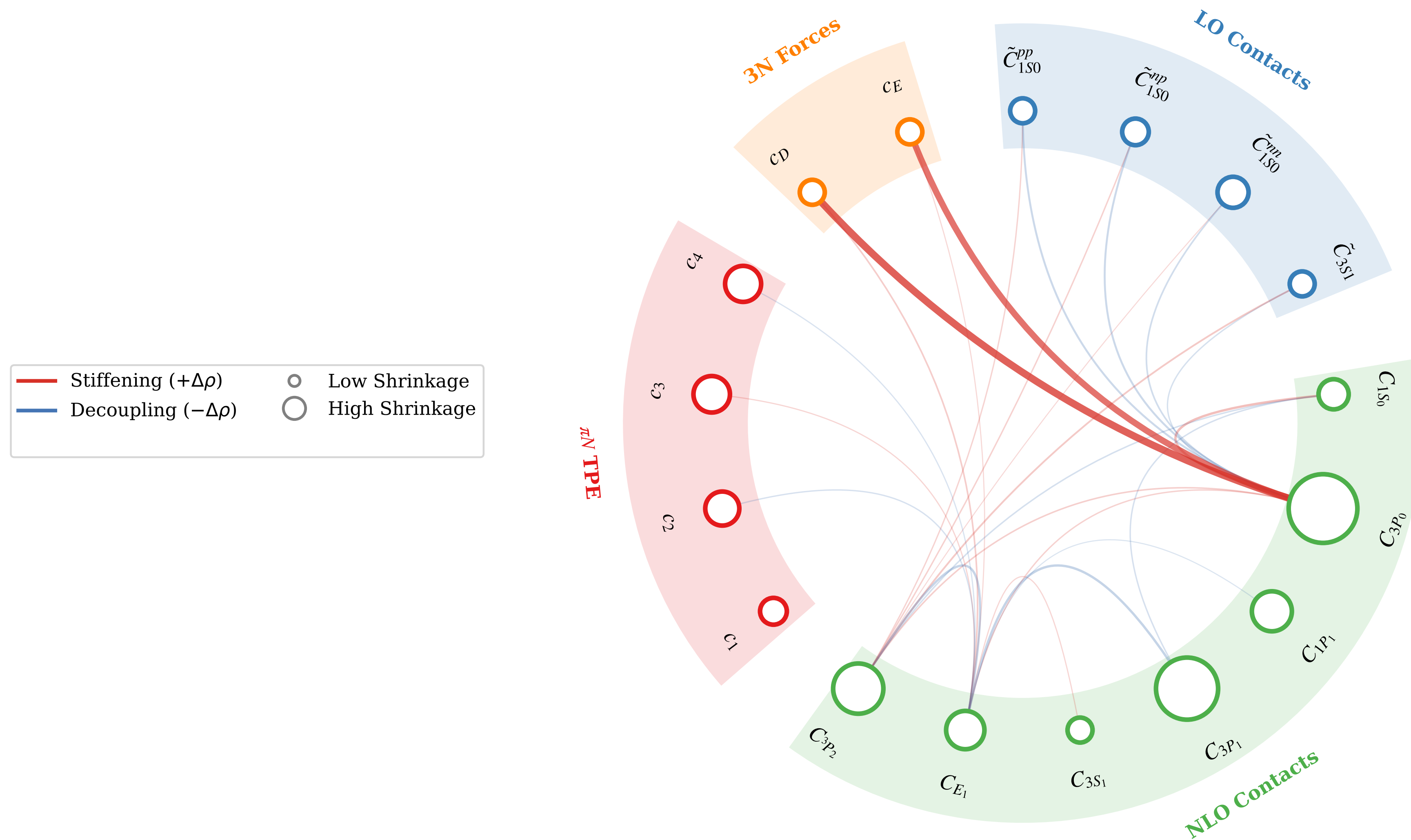


Changes to Likelihood



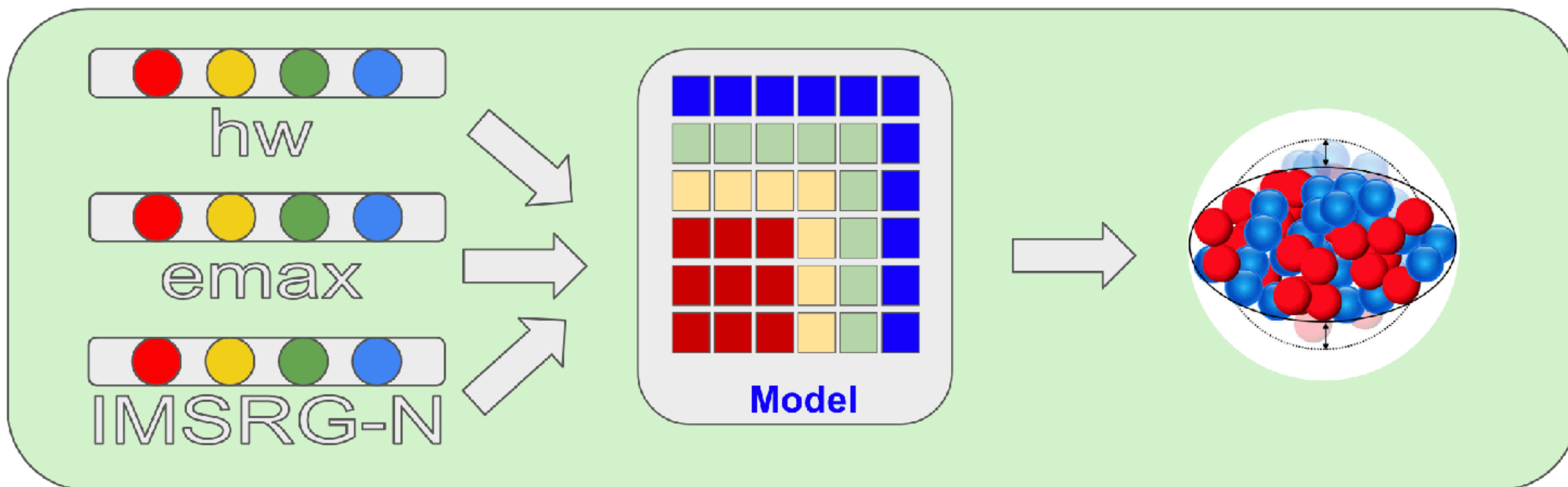
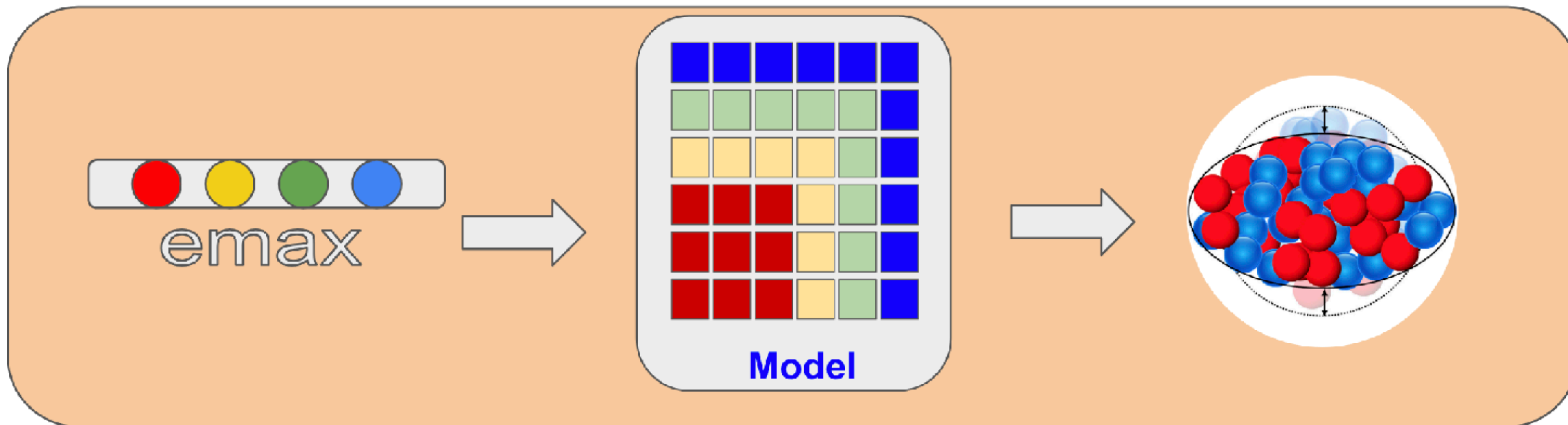


Changes to Likelihood

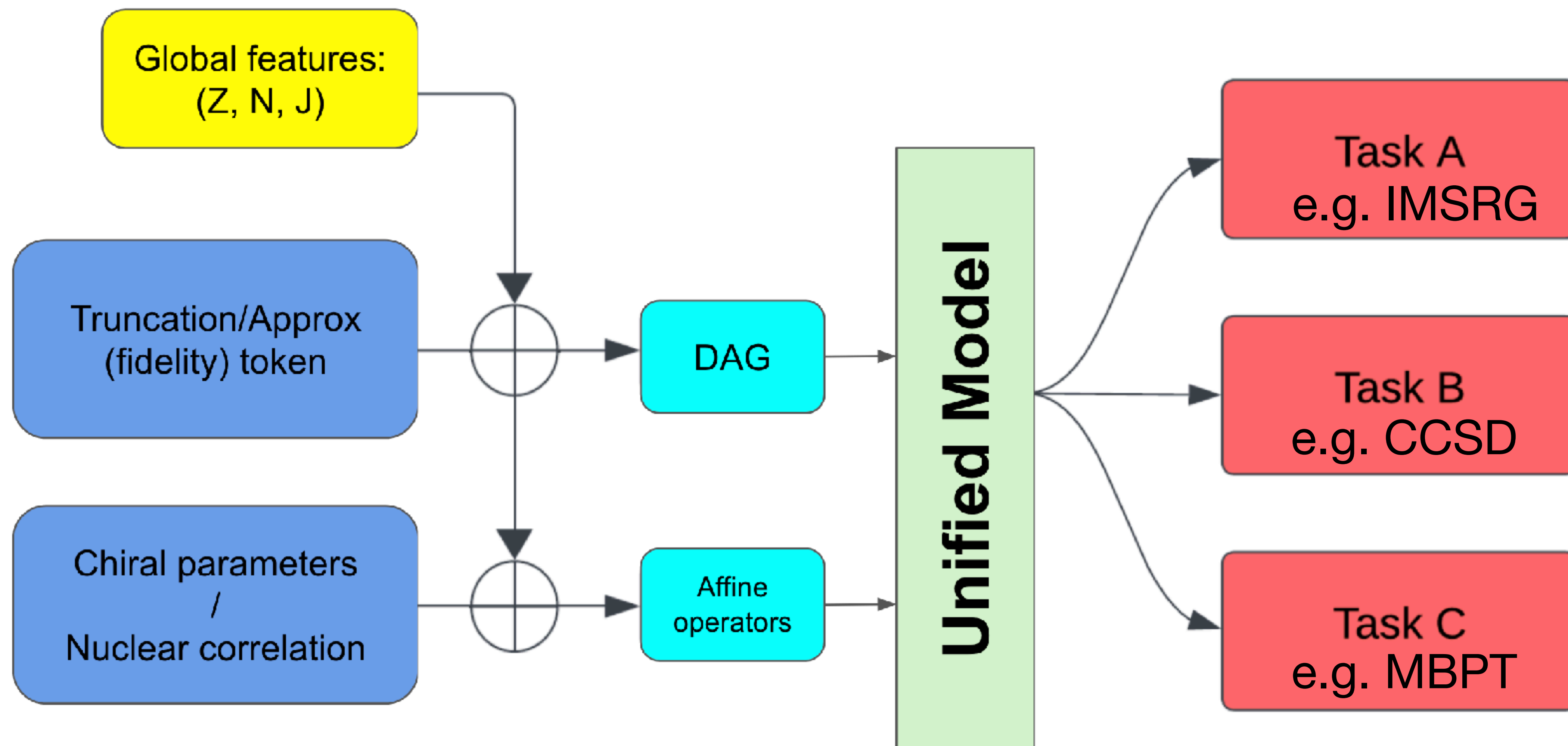


How to improve uncertainty models?

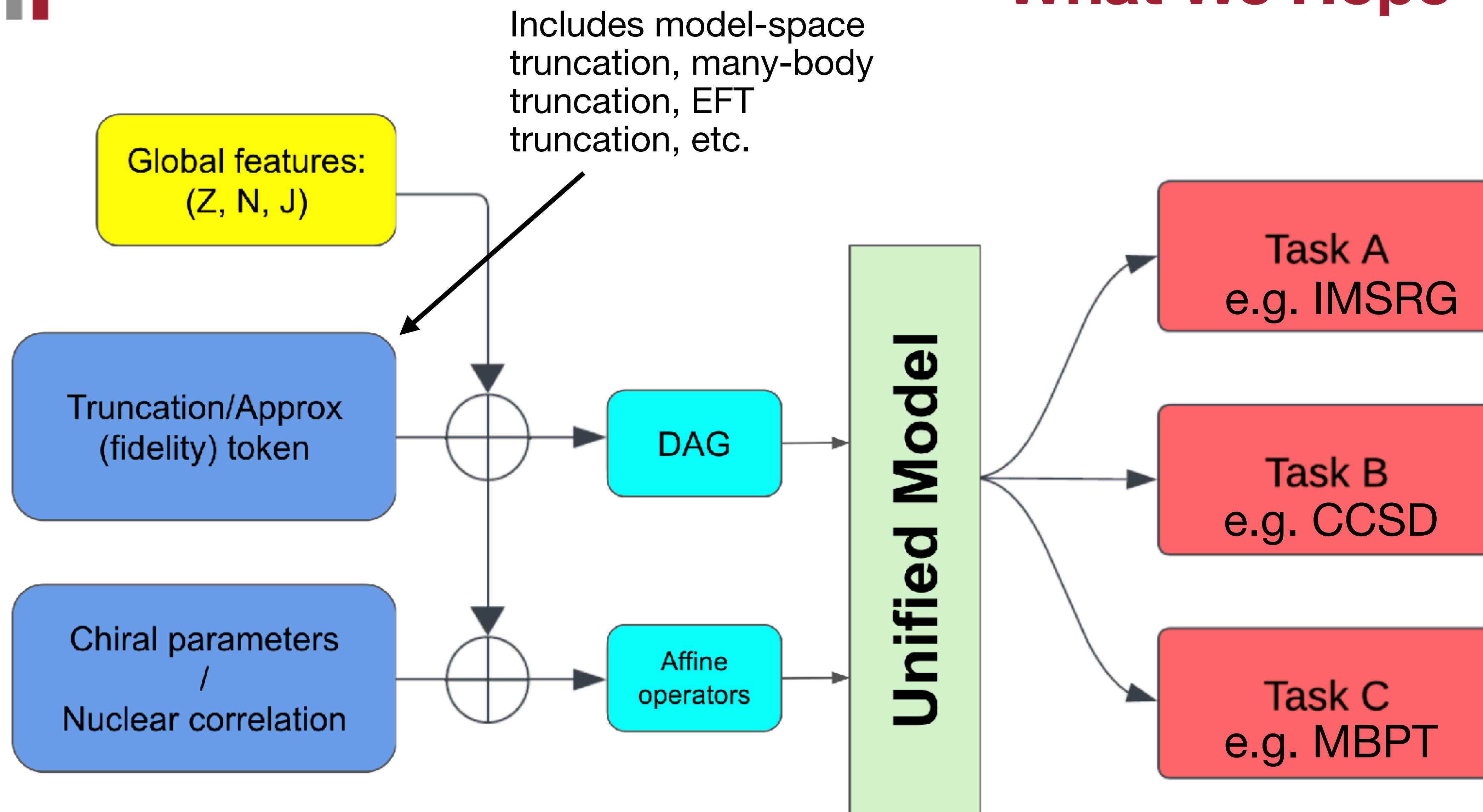
What We Currently Have



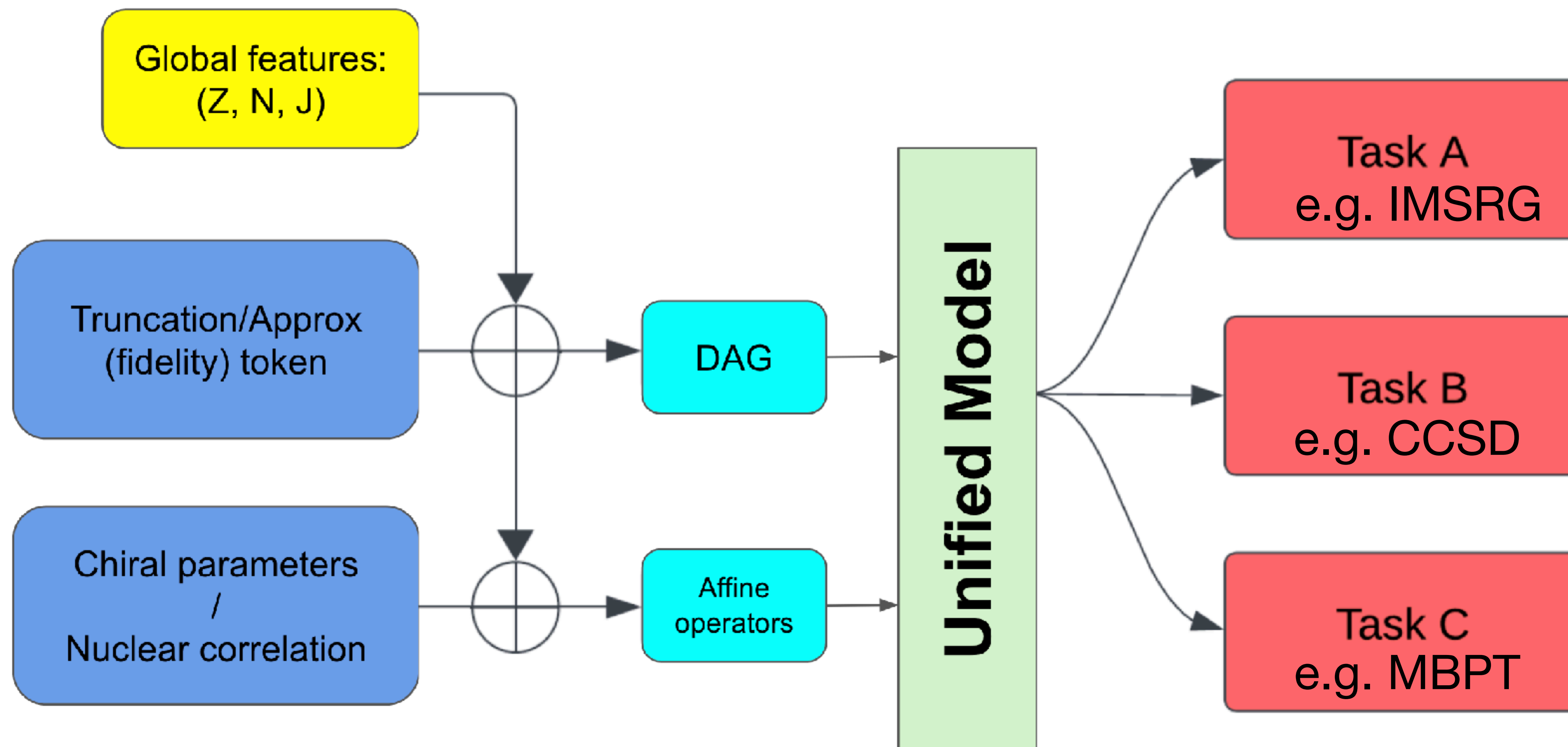
What We Hope To Get

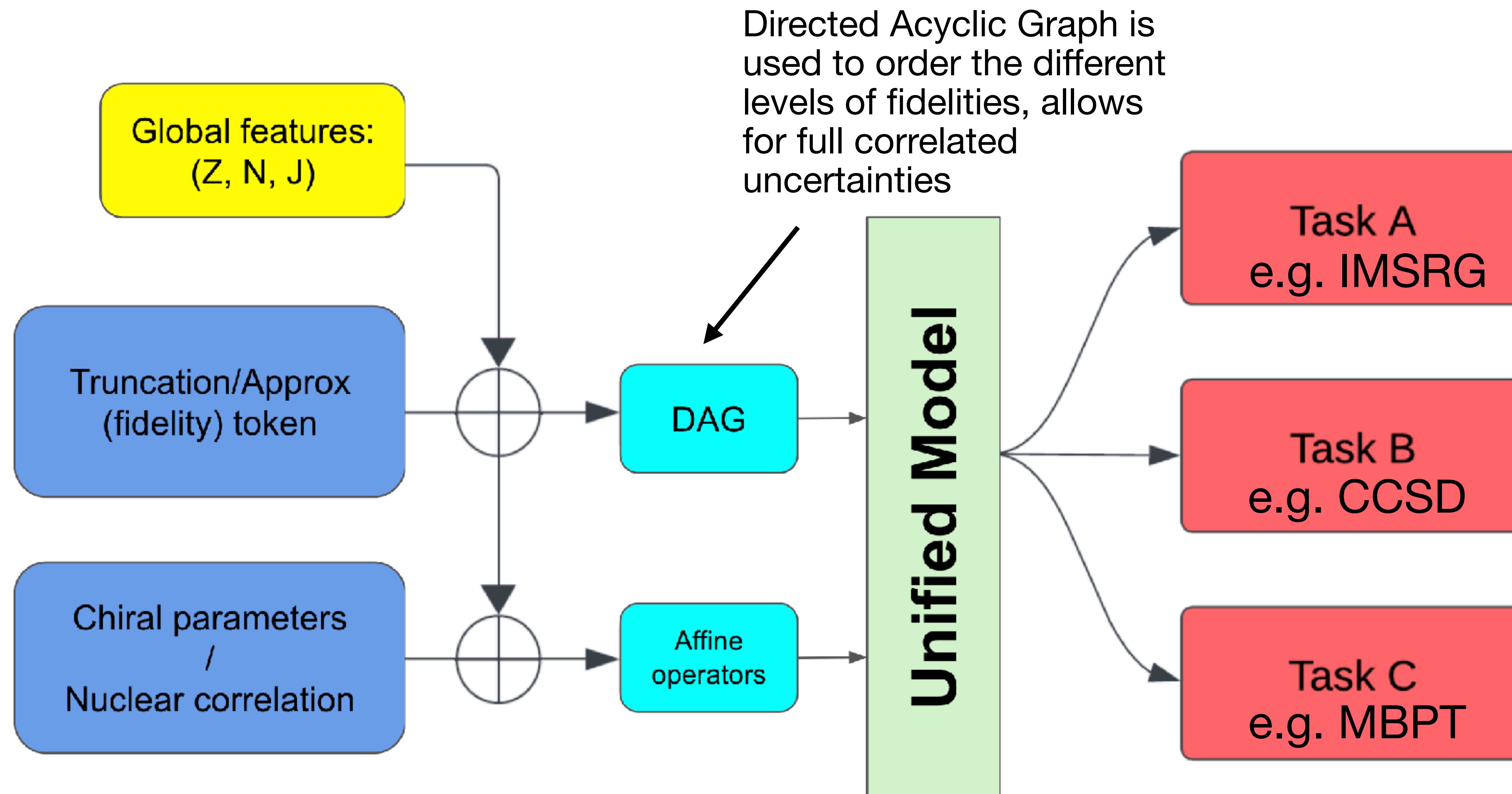


What We Hope To Get

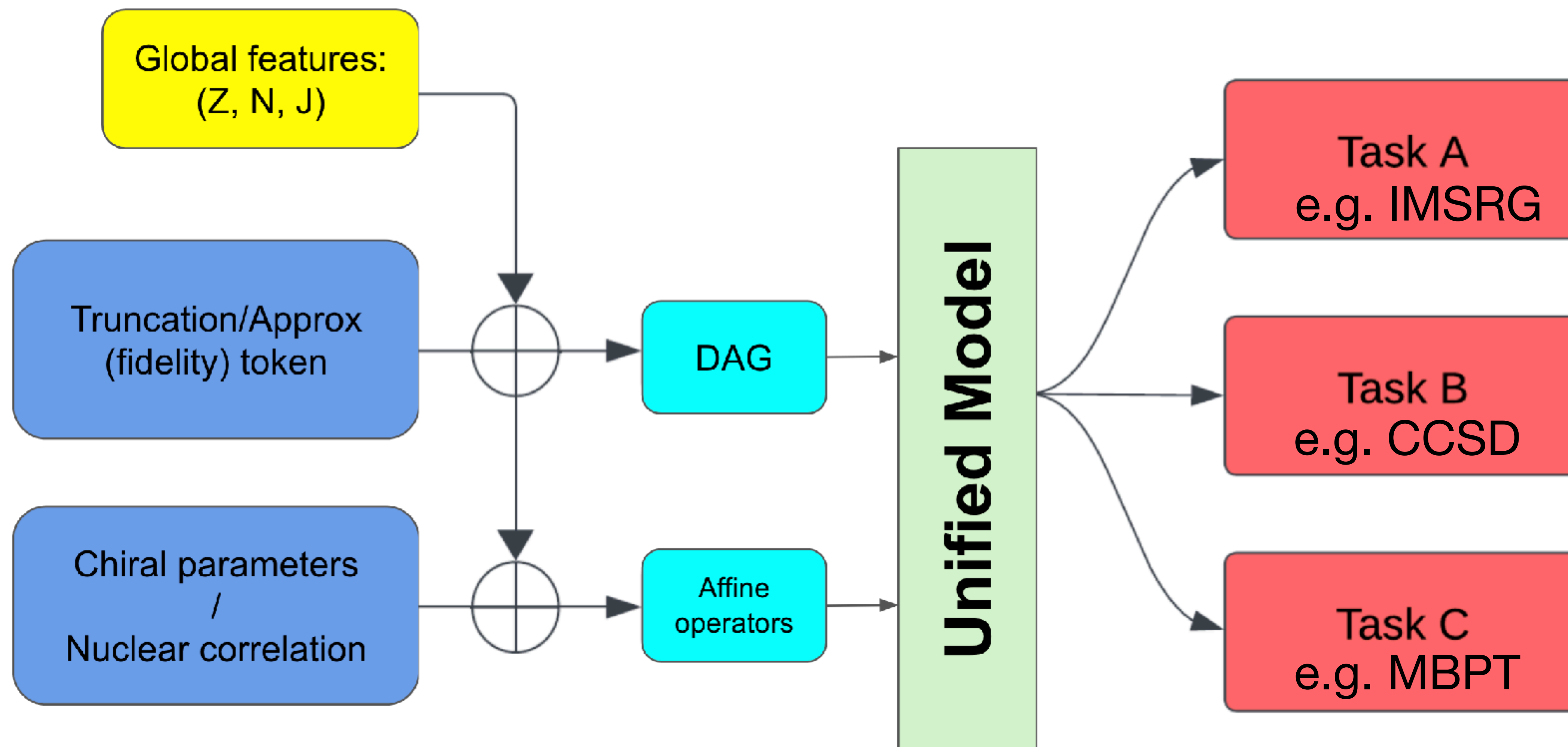


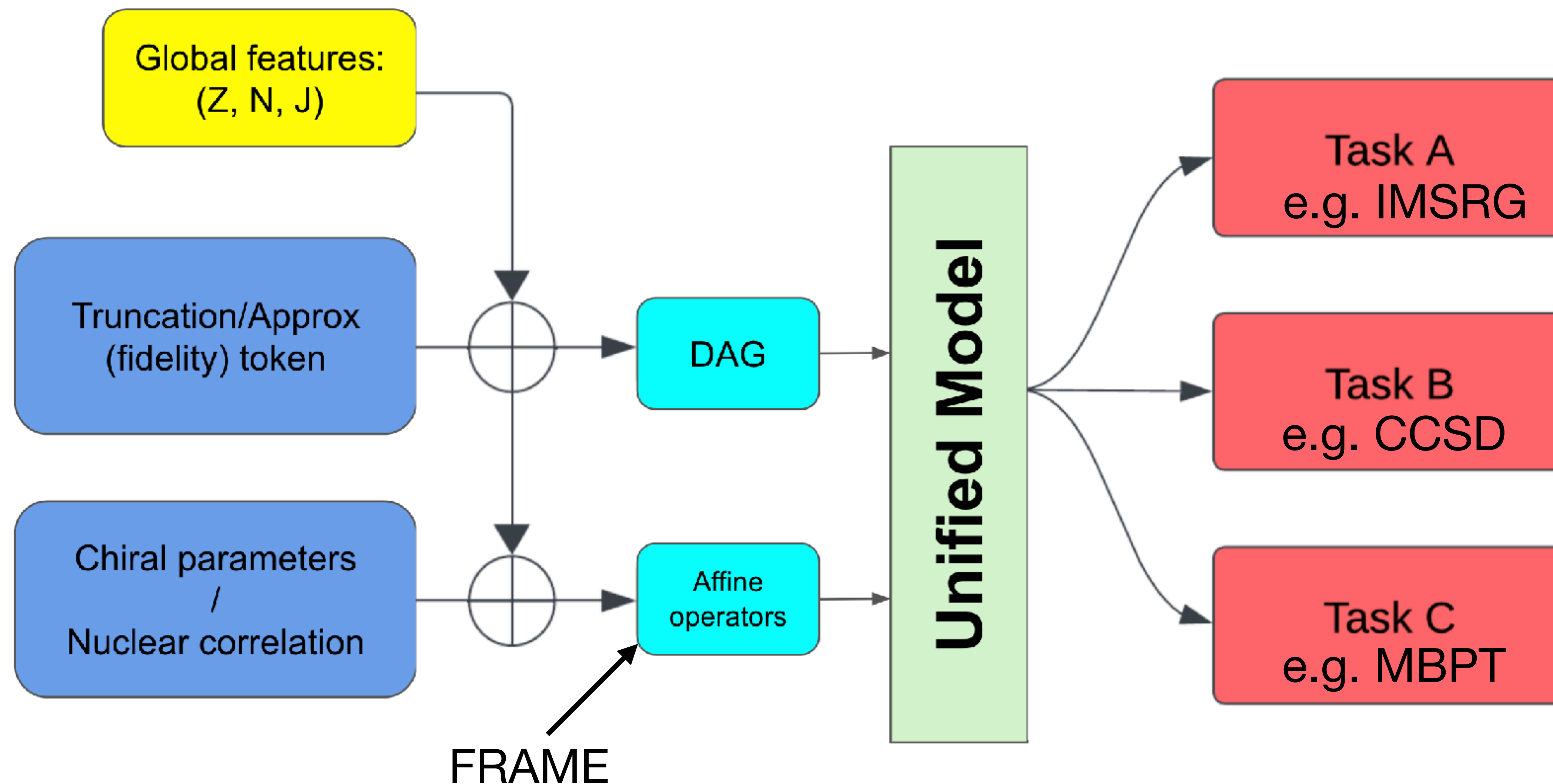
What We Hope To Get



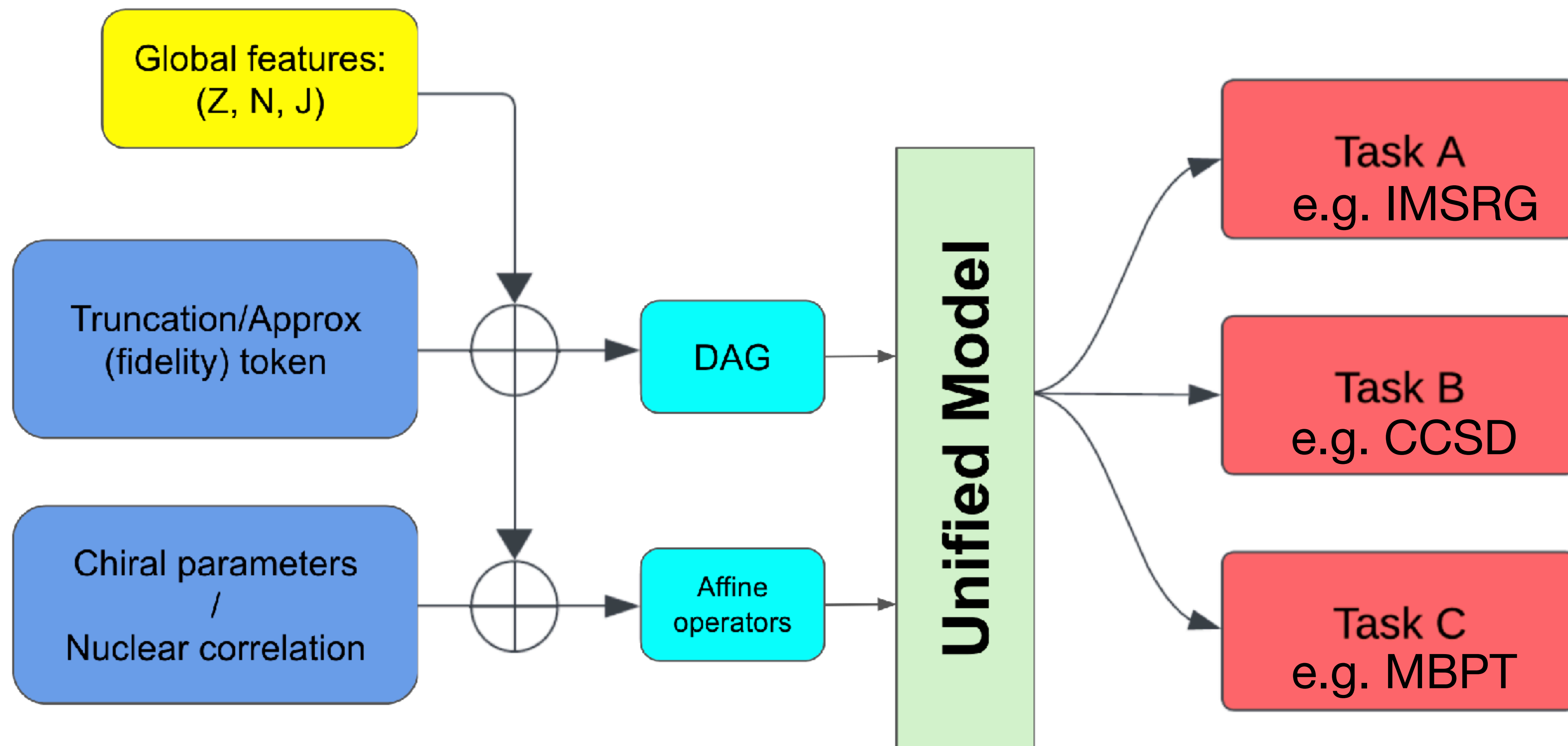


What We Hope To Get





What We Hope To Get





Summary ...

- Emulators are required to obtain uncertainty quantification of nuclear theory observables required for searches of new physics.
- Emulator further allows the use of other statistical tools like global sensitivity analysis.
- Many-body uncertainty is the main source of uncertainty in current calculations.

... and Outlook

- Improving the emulator with other machine learning models.
- Reducing the many-body error using methods that probe the IMSRG(3).
- Computing other observables for BSM searches with uncertainties.
- Building foundation model to obtain full correlated uncertainties.

Thank you!



Questions?

abelley@mit.edu