

# Parity Violating In Medium Similarity Renormalization Group

ESNT Workshop

Antoine Belley

26 June 2025



# Acknowledgement



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



- Ragnar Stroberg



- Takayuki Miyagi



- Jon Engel
- Beatriz Romeo



- Jason Holt





# Nuclear Theory Challenges

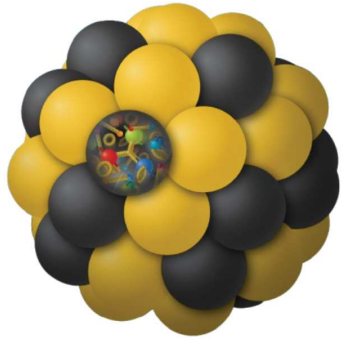
Understanding nuclear structure from microscopic physics



# Nuclear Theory Challenges

Understanding nuclear structure from microscopic physics

Nuclear Interactions



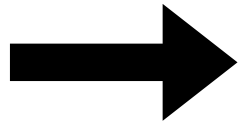
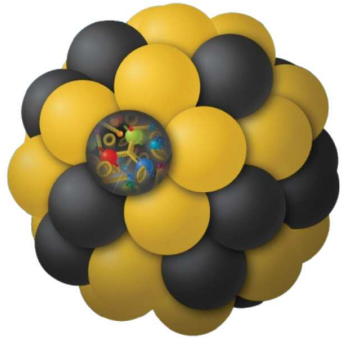


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Understanding nuclear structure from microscopic physics

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Wave functions



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



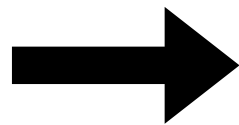
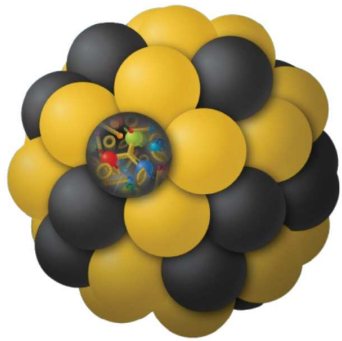
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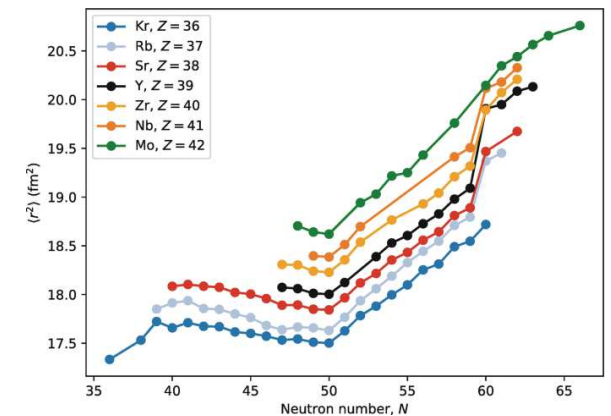
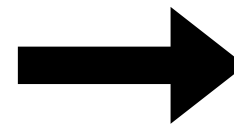
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Figures courtesy of J. Muñoz 3



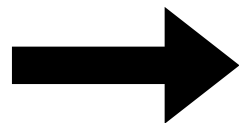
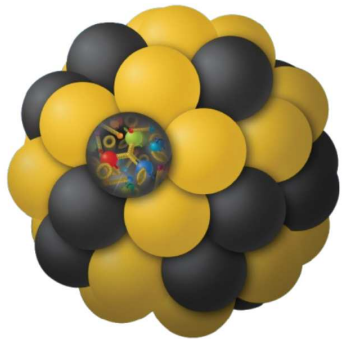
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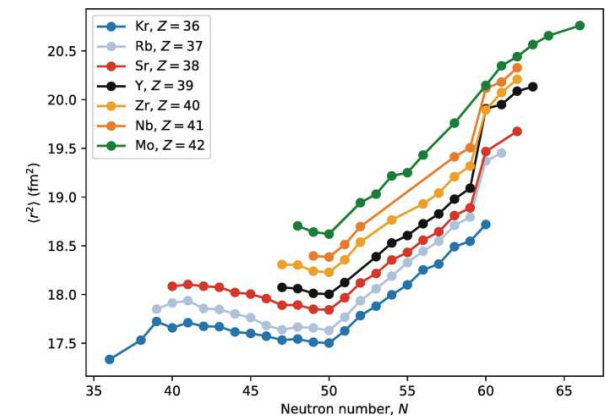
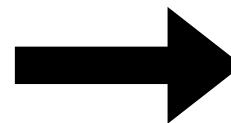
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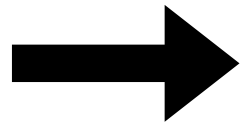
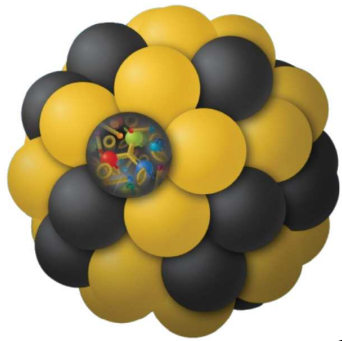
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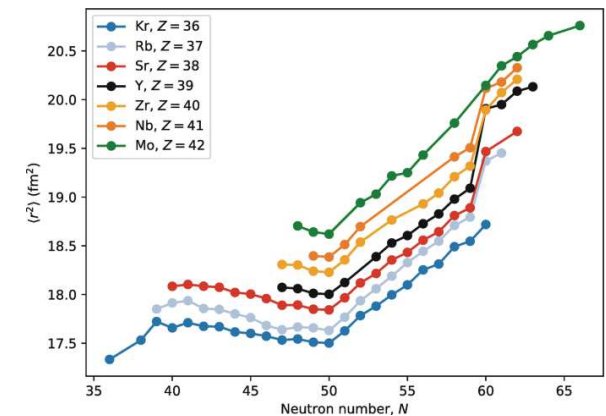
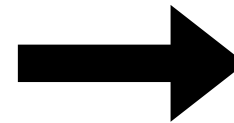
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$$\boxed{H} |\Psi\rangle = E |\Psi\rangle$$



$$H = H_0 + V_{PV}$$

Figures courtesy of J. Muñoz 3





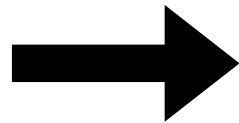
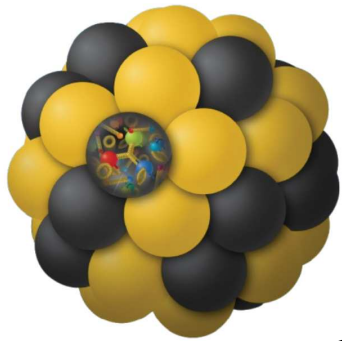
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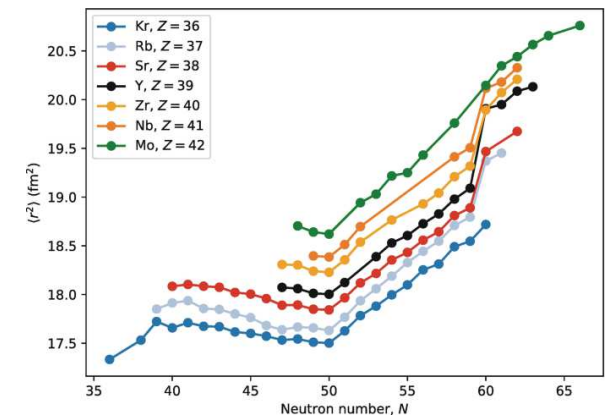
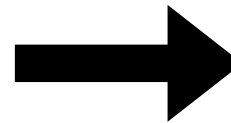
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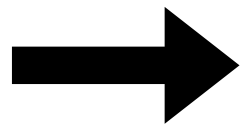
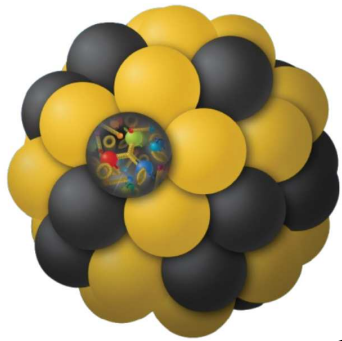
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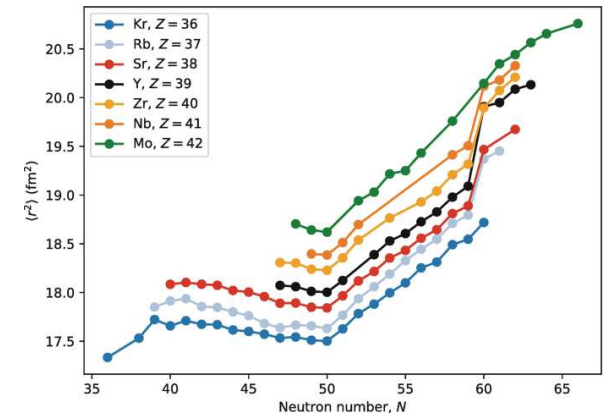
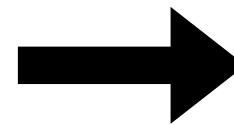
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$$\boxed{H} \boxed{|\Psi\rangle} = E \boxed{|\Psi\rangle}$$



$$H = H_0 + V_{PV}$$

$$|\Psi_{gs}J\rangle = |\Psi_{gs}J^\pi\rangle + \sum_k |\Psi_k J^{-\pi}\rangle \frac{1}{E_{gs} - E_k} \langle \Psi_k J^{-\pi} | V_{PV} | \Psi_{gs} J^\pi \rangle$$

Figures courtesy of J. Muñoz 3



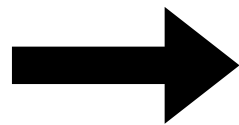
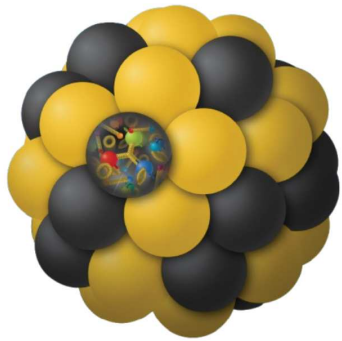
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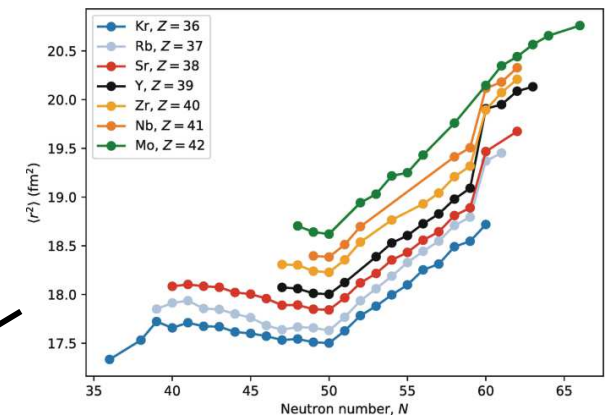
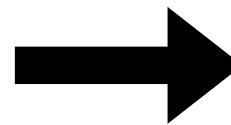
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$$\langle O_{PV} \rangle \propto \sum_k \frac{\langle \Psi_{gs} J^\pi | O_{PV} | \Psi_k J^{-\pi} \rangle \langle \Psi_k J^{-\pi} | V_{PV} | \Psi_{gs} J^\pi \rangle}{E_{gs} - E_k}$$

Figures courtesy of J. Muñoz



# List of Challenges



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Obtaining a result:

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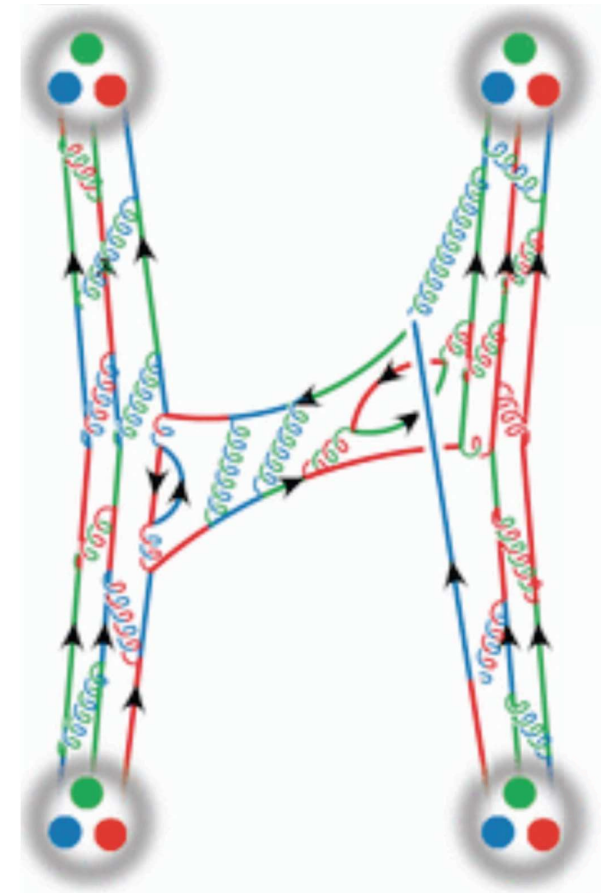
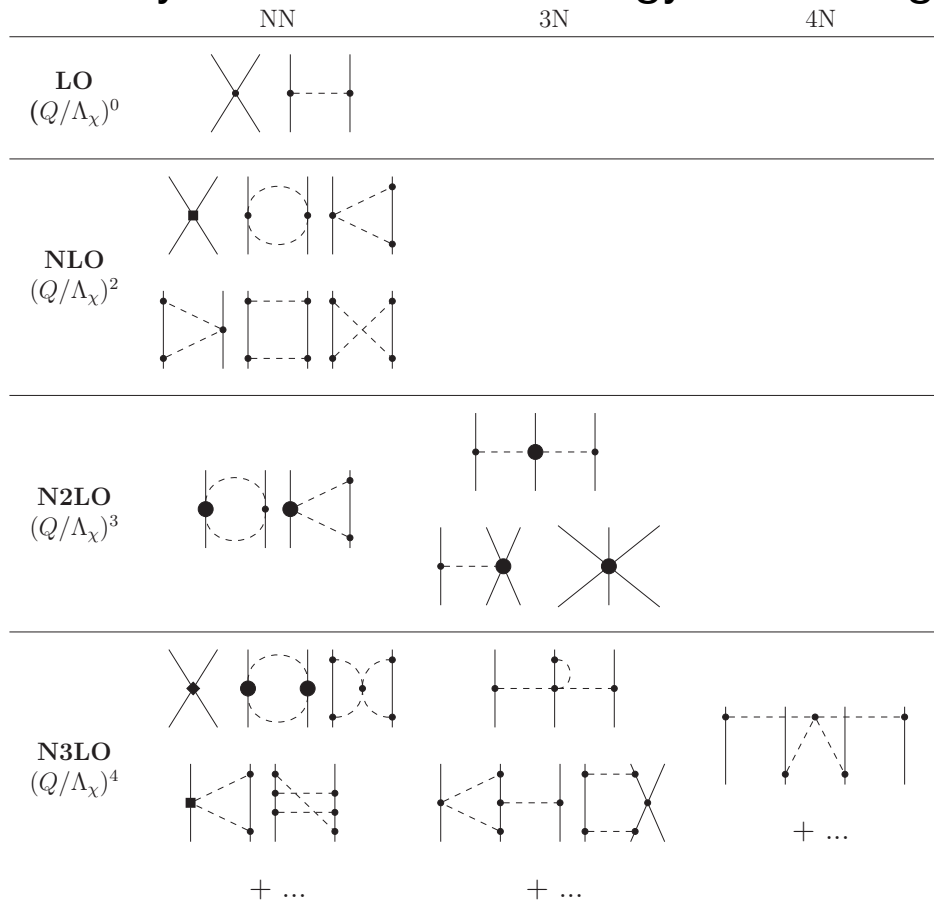
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# Expansion order by order of the nuclear forces

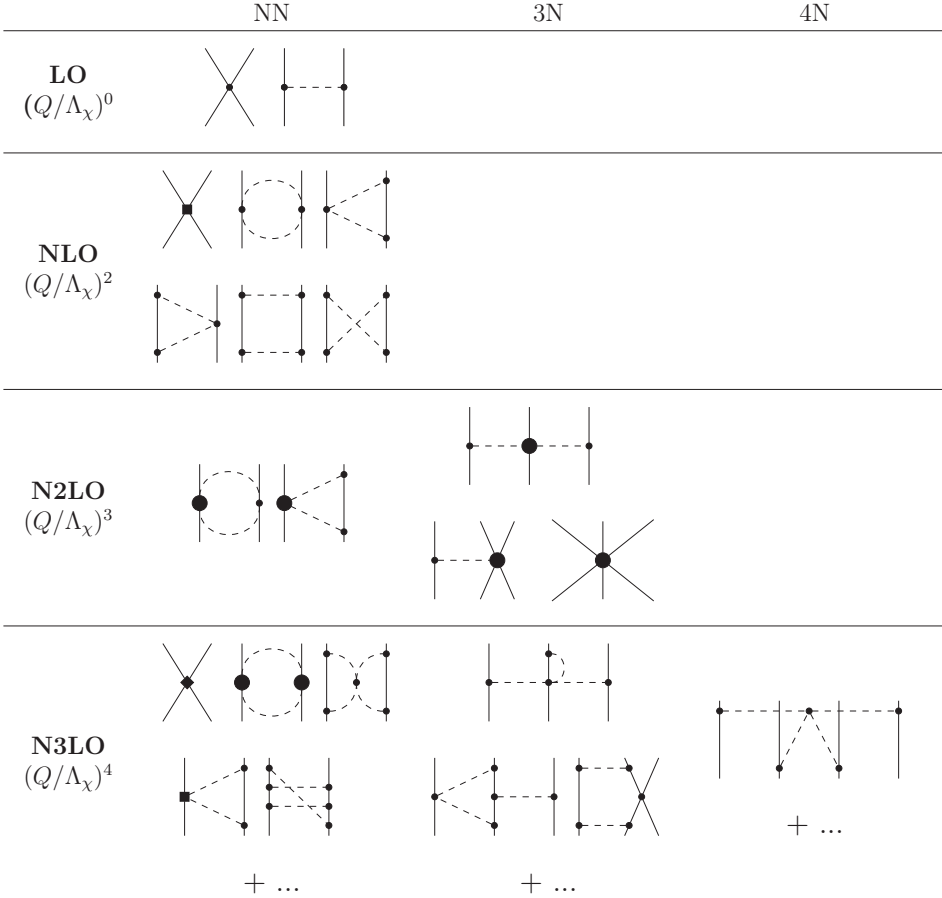
Reproduces symmetries of low-energy QCD using nucleons as fields and pions as force carriers.





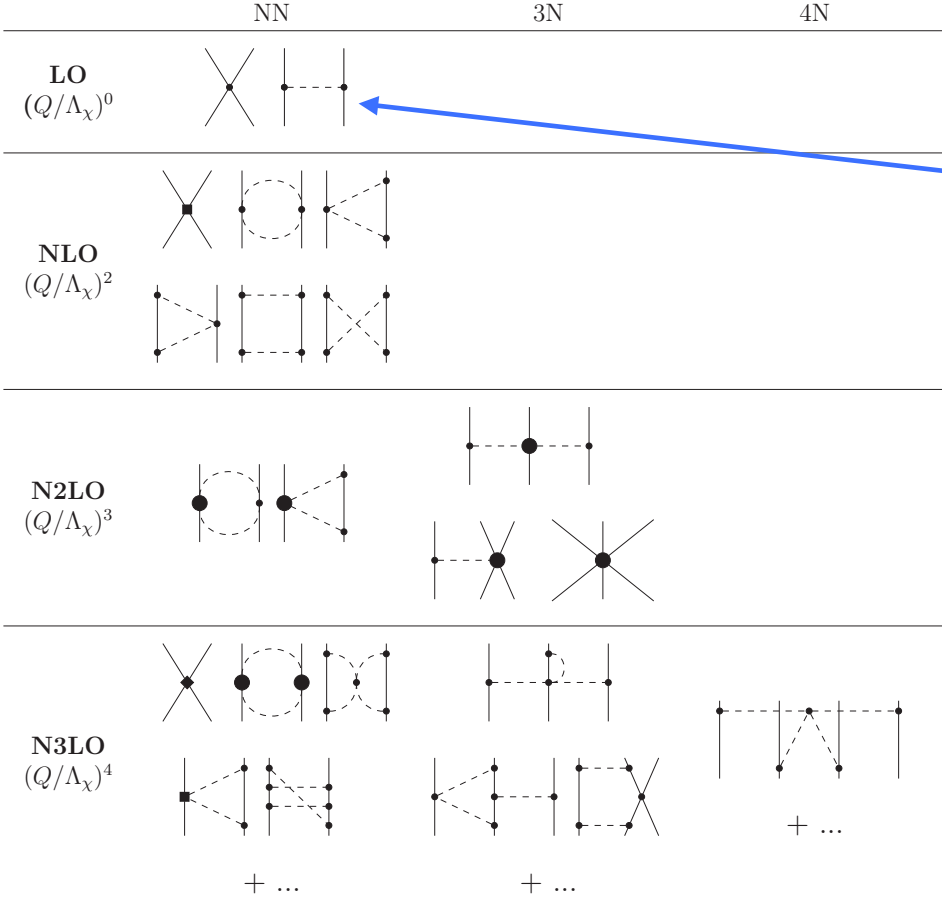
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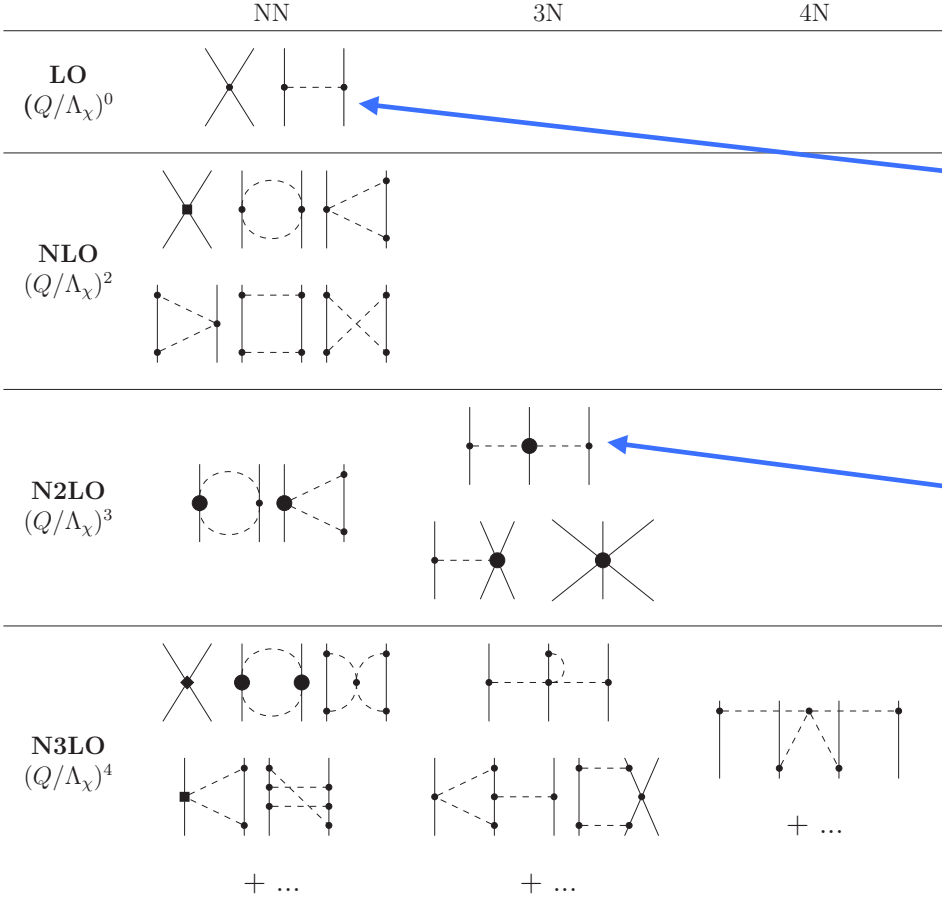
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Reproduces symmetries of low-energy QCD using nucleons as fields and pions as force carriers.



The different low energy coupling constants (LECs) are fitted to few-nucleon data to absorb the effect of higher order terms

Three- (and higher-)body forces needed



## List of Challenges

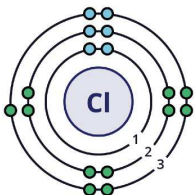
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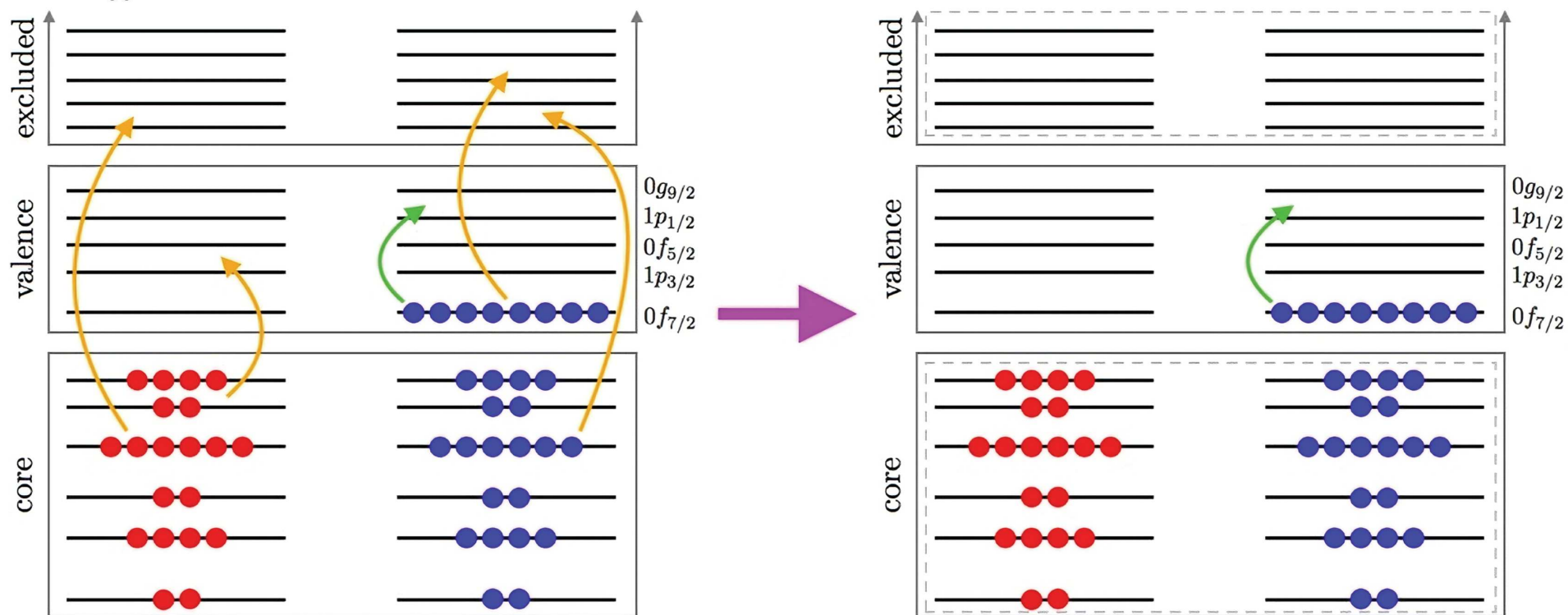


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# The VS-IMSRG

## Valence Space In Medium Similarity Renormalization Group

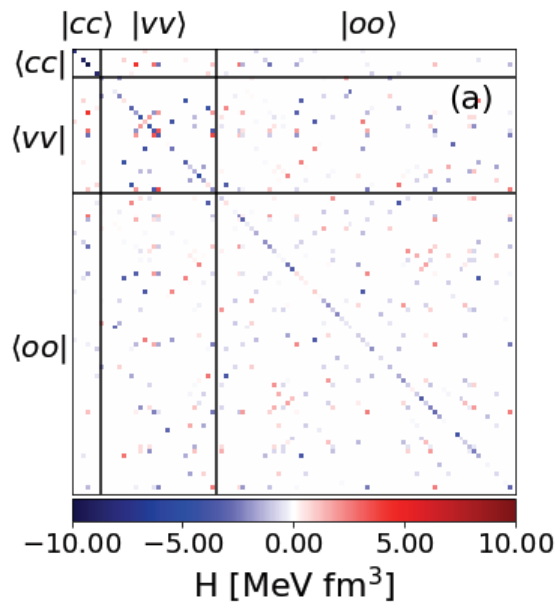


Charlie Payne, Master's Thesis, UBC (2018)



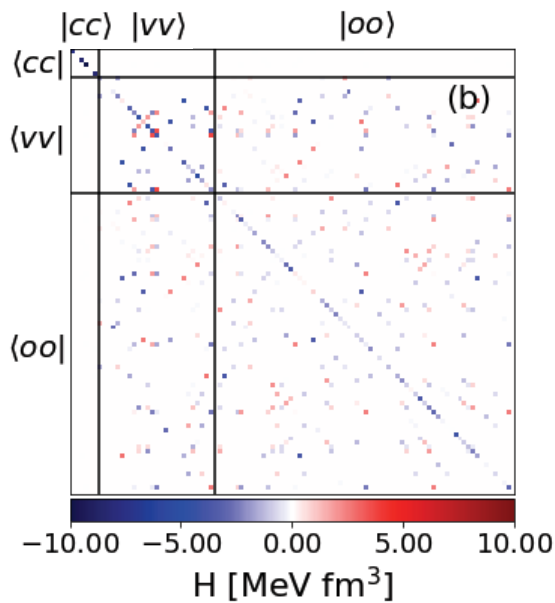
# The VS-IMSRG

## Valence Space In Medium Similarity Renormalization Group



Bare Hamiltonian

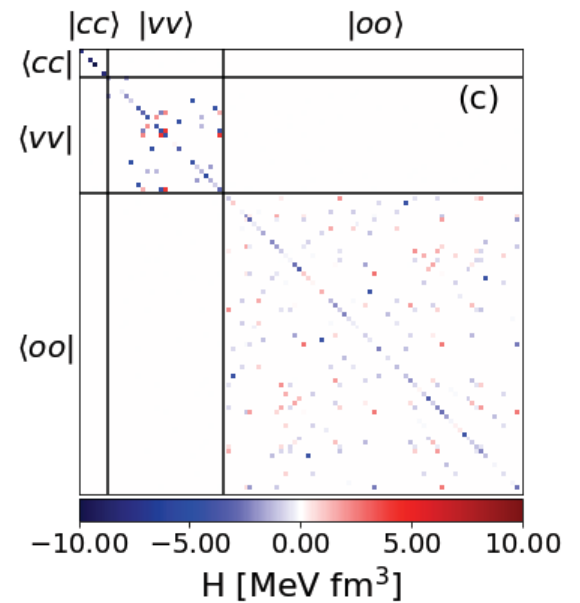
$$\hat{H}(0)$$



Core is decoupled

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

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

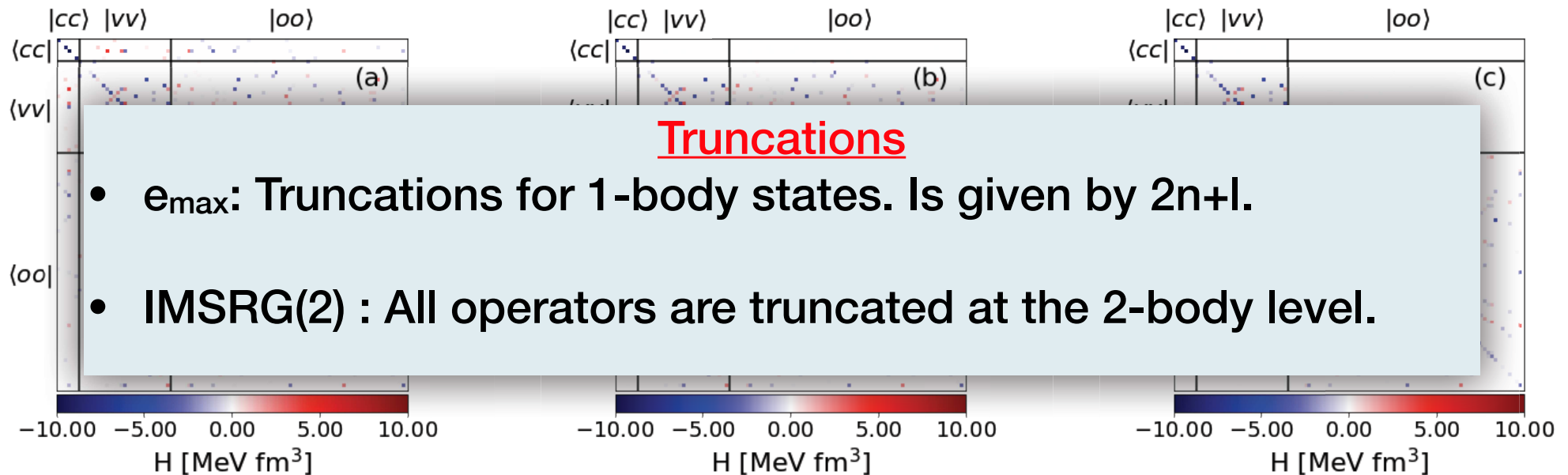


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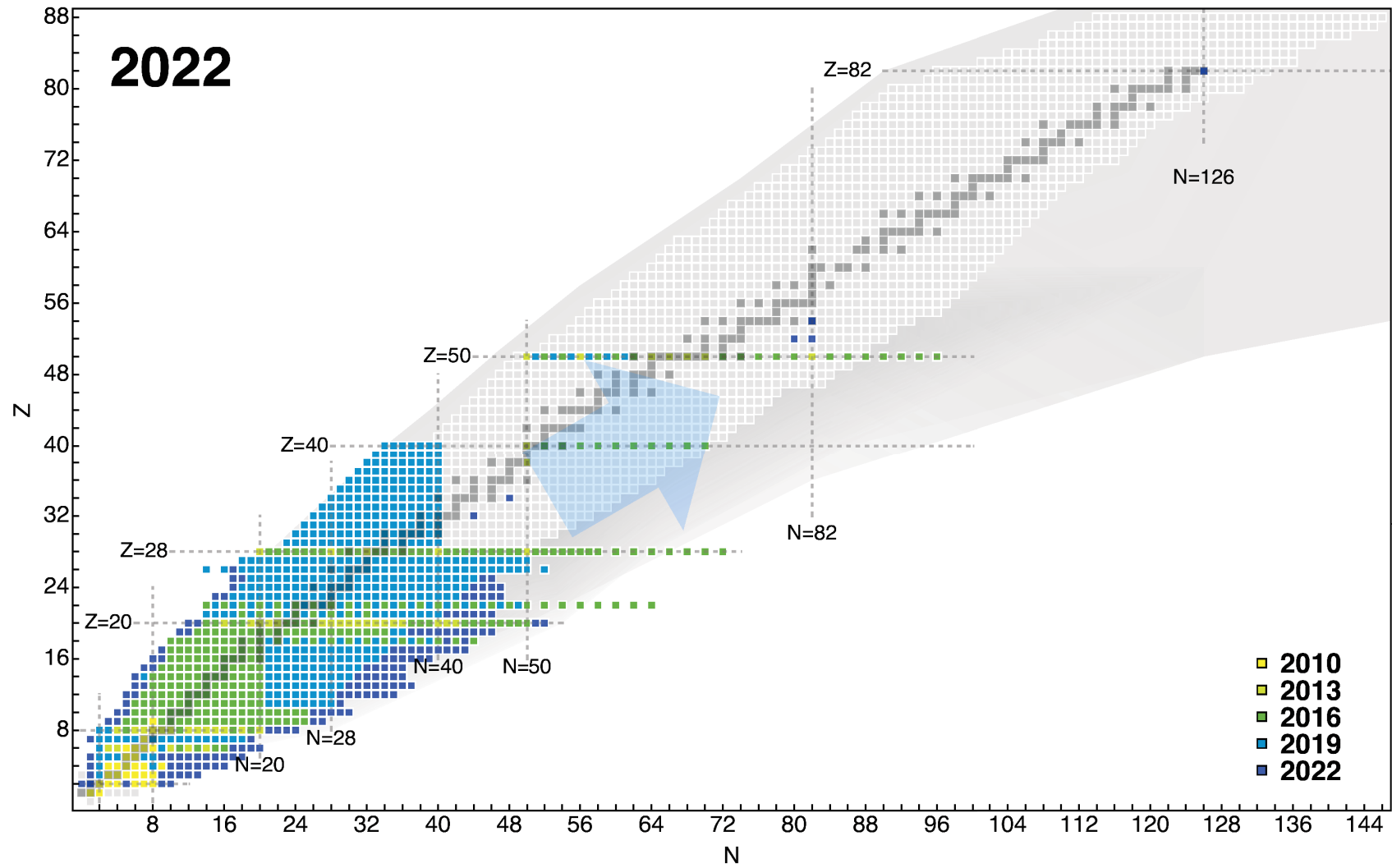
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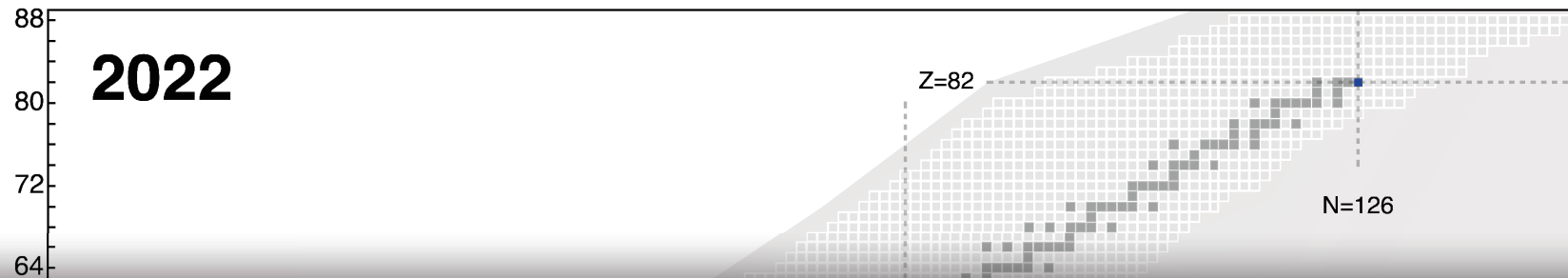
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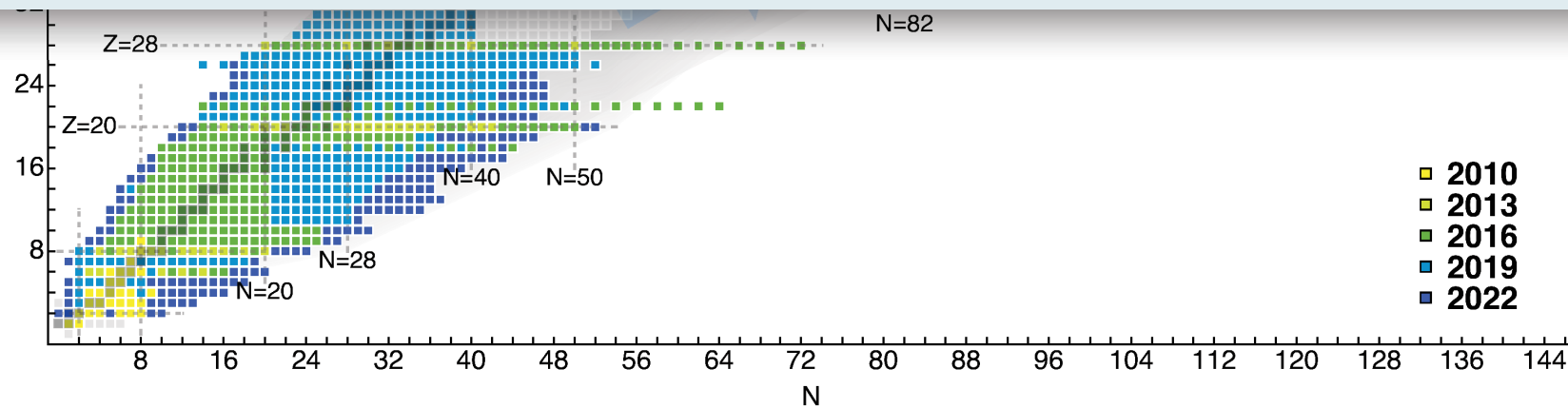


# Ab initio Revolution





e.g. Jason's talk yesterday.





## List of Challenges

Obtaining a result:

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## Valence Space Issue

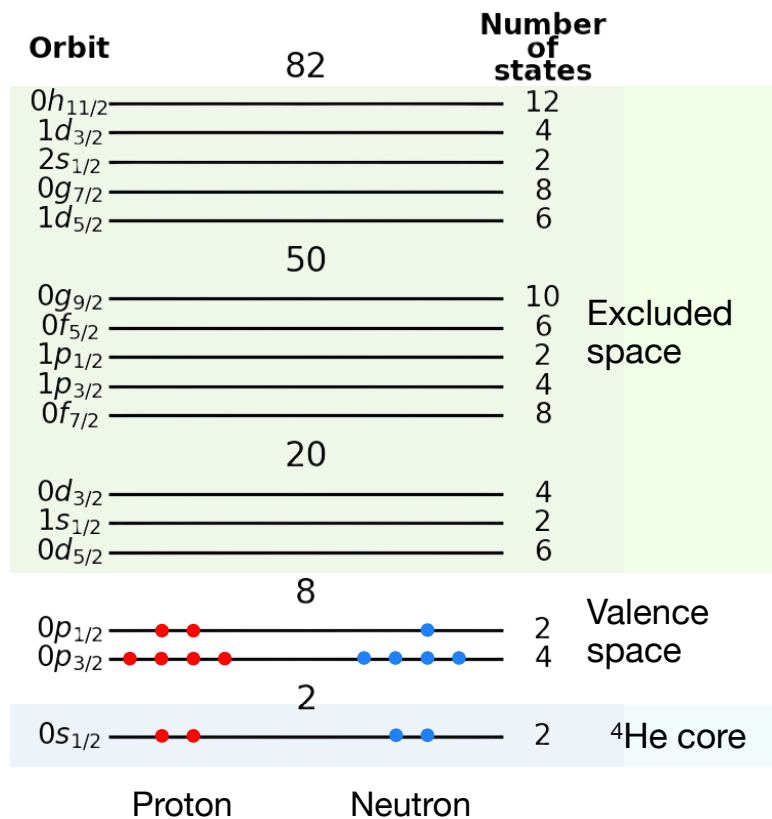
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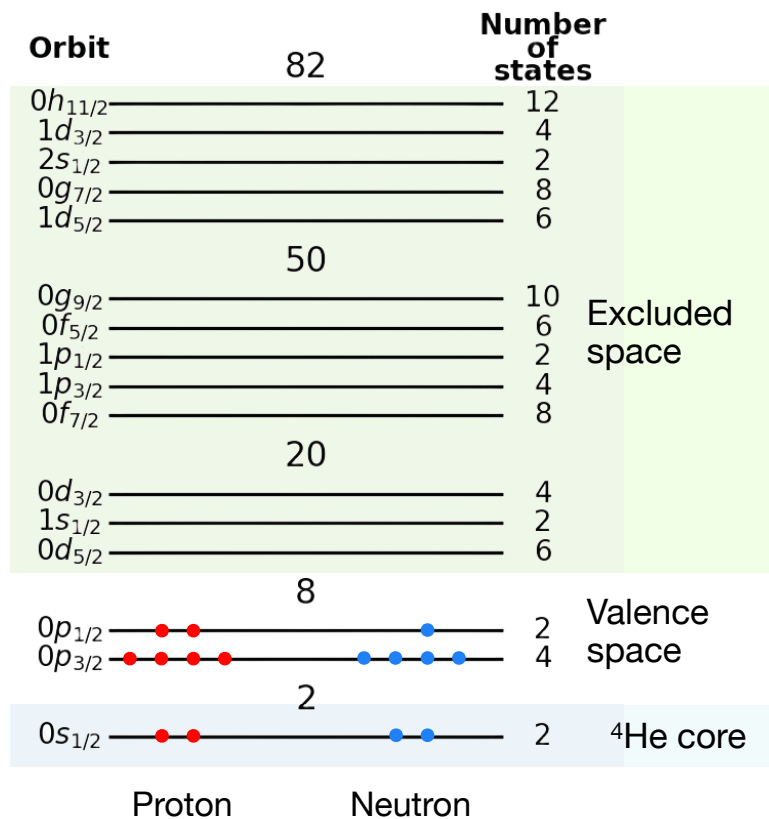
$^{15}\text{N}$



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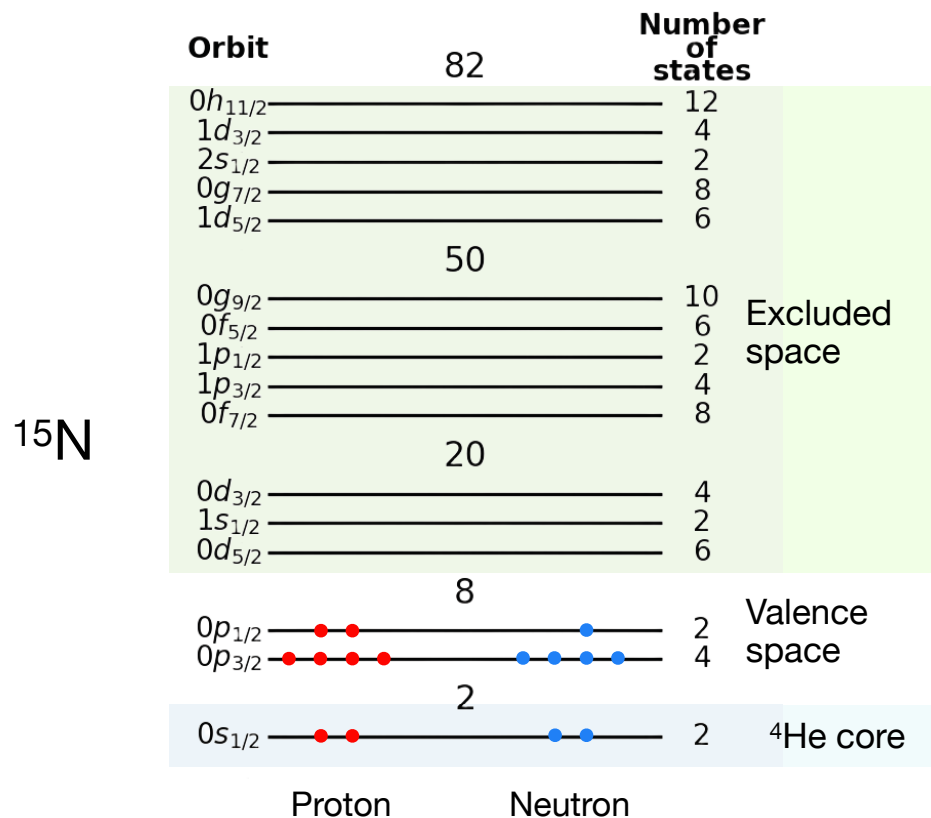


Ground state wave function can be computed in the valence space.



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Ground state wave function can be computed in the valence space.

Opposite parity states are absent from the valence space!



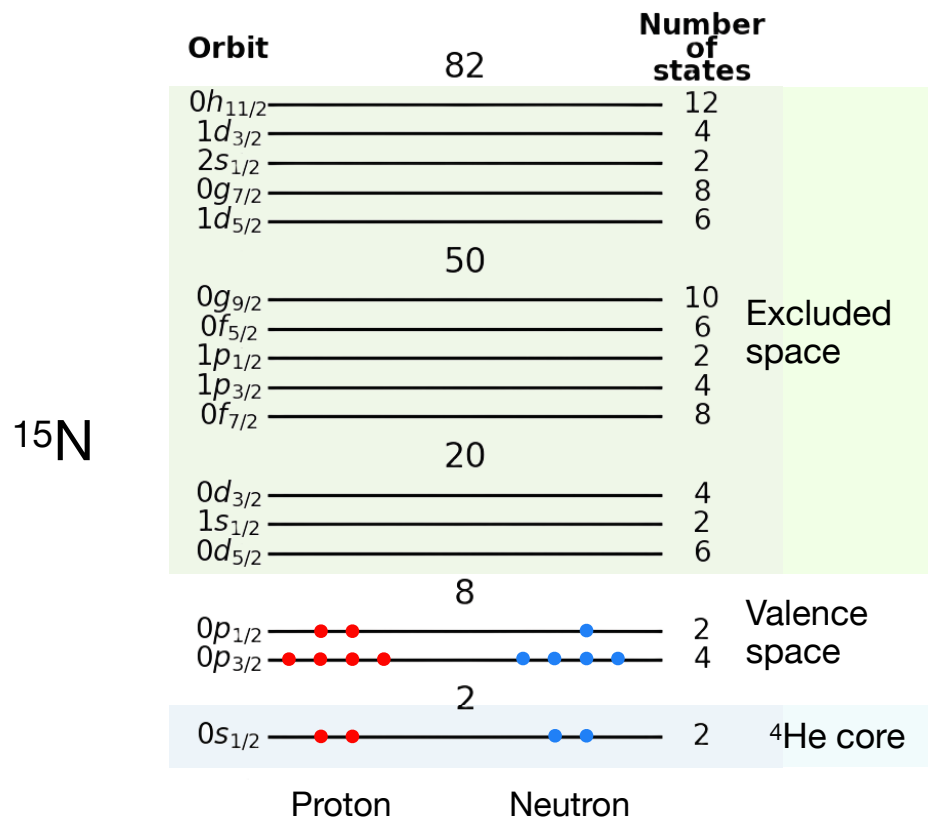


# Solutions to Valence Space



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## 1. Multi-shell valence space

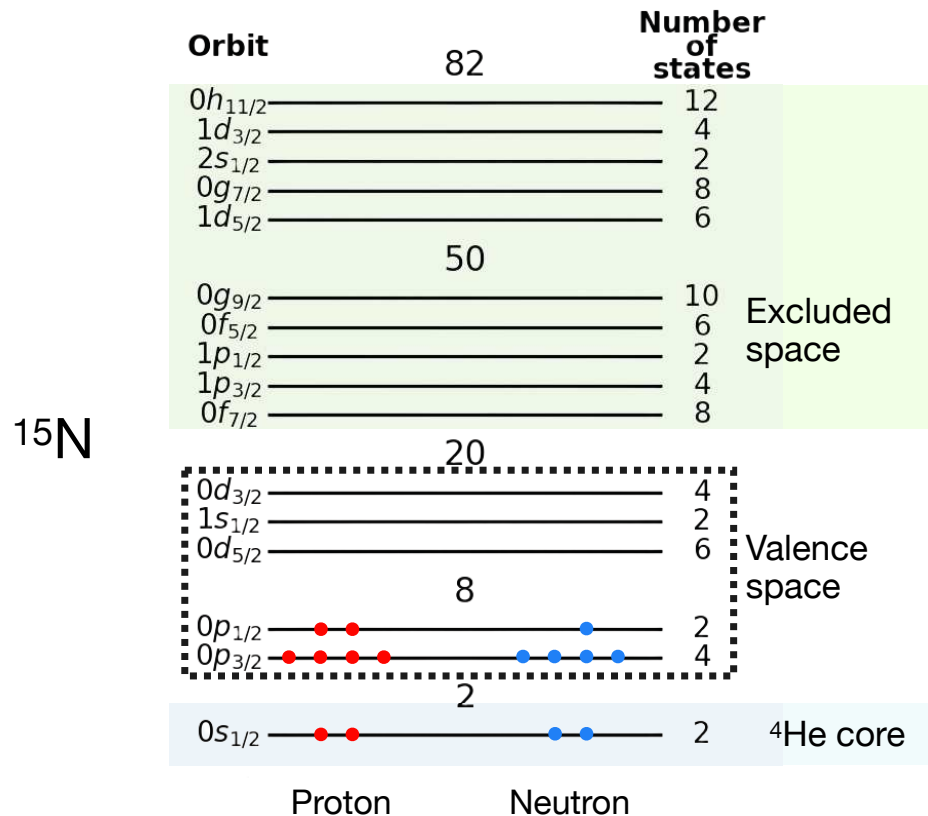


Miyagi et al., Phys. Rev. C 102, 034320 (2020).



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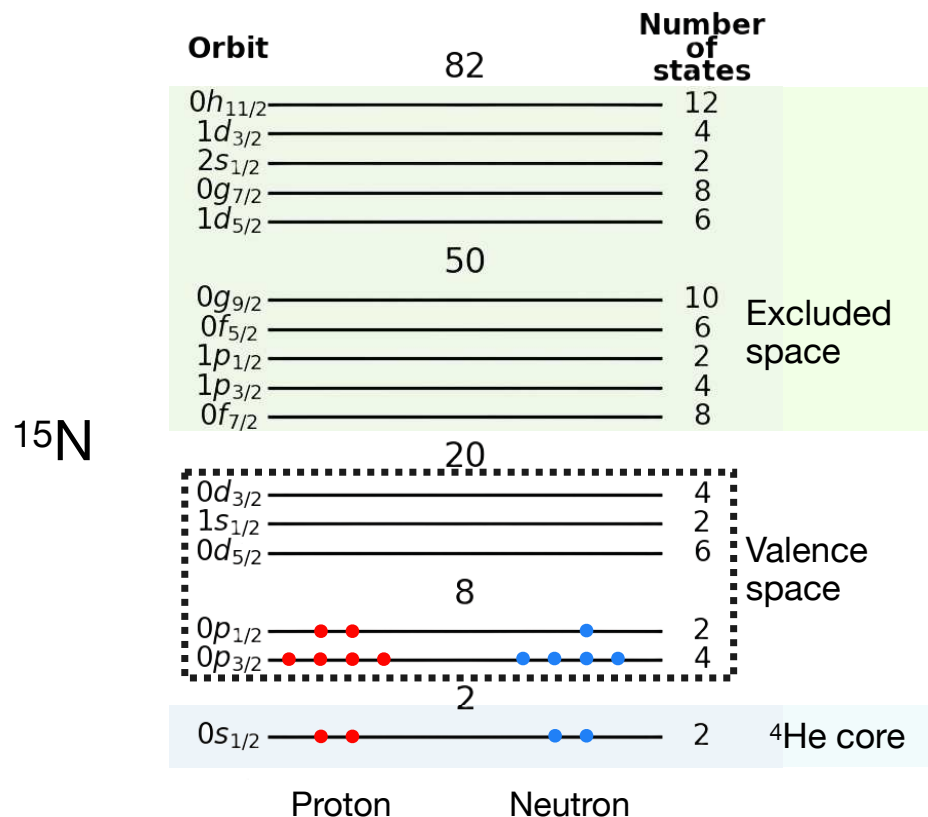


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# Solutions to Valence Space

## 1. Multi-shell valence space



Miyagi et al., Phys. Rev. C 102, 034320 (2020).

## Cons

- Valence space is harder to diagonalize (problematic for heavier nuclei).
- Need to compute many intermediate states to converge.
- Intermediate states are harder to compute correctly in the IMSRG(2).



# Solutions to Valence Space



# Solutions to Valence Space

## 2. Parity violating IMSRG



# Solutions to Valence Space

## **2. Parity violating IMSRG**

Use IMSRG to decouple PV part of interaction, inducing a PC operator.



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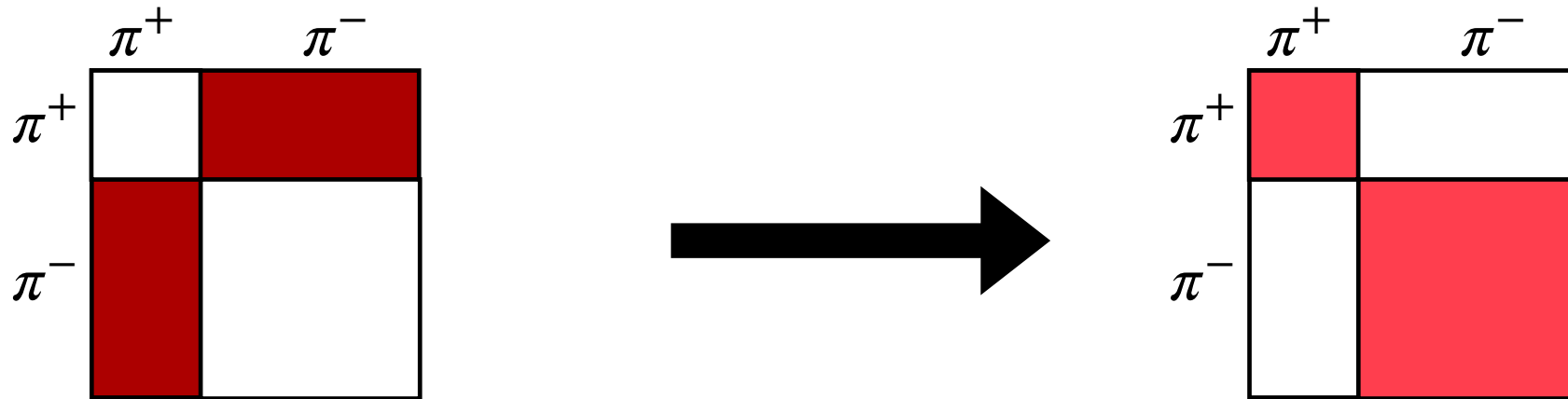
	$\pi^+$	$\pi^-$
$\pi^+$		
$\pi^-$		

$$\langle O \rangle = \langle O_{PV} \rangle \propto \sum_k \frac{\langle \Psi_{gs} J^\pi | O_{PV} | \Psi_k J^{-\pi} \rangle \langle \Psi_k J^{-\pi} | V_{PV} | \Psi_{gs} J^\pi \rangle}{E_{gs} - E_k}$$



## 2. Parity violating IMSRG

Use IMSRG to decouple PV part of interaction, inducing a PC operator.



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$$\langle O \rangle = \langle O_{PC} \rangle = \langle \Psi_{gs} J^\pi | O_{PC} | \Psi_{gs} J^\pi \rangle$$



# IMSRG flow



Normal Ordered Two-Body approximation

**IMSRG flow**



# IMSRG flow

Normal Ordered Two-Body approximation

$$H(s) = E(s) + \sum_{ij} f_{ij}(s) \{a_i^\dagger a_j\} + \frac{1}{4} \sum_{ijkl} \Gamma_{ijkl} \{a_i^\dagger a_j a_l a_k\}$$



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0-body                  1-body



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0-body                  1-body                  2-body



### Normal Ordered Two-Body approximation

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0-body                  1-body                  2-body

## IMSRG flow

$$\eta(s) = \sum_{ij} \eta_{ij}(s) \{a_i^\dagger a_j\} + \sum_{ijkl} \eta_{ijkl}(s) \{a_i^\dagger a_j^\dagger a_l a_k\}$$





### Normal Ordered Two-Body approximation

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0-body                      1-body                      2-body

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e.g.



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## IMSRG flow

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e.g.

$$\eta_{ij} = \frac{f_{ij}}{f_{ii} - f_{jj}}, \dots$$



### Normal Ordered Two-Body approximation

$$H(s) = E(s) + \sum_{ij} f_{ij}(s) \{a_i^\dagger a_j\} + \frac{1}{4} \sum_{ijkl} \Gamma_{ijkl} \{a_i^\dagger a_j a_l a_k\}$$

0-body                      1-body                      2-body

## IMSRG flow

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e.g.

matrix elements we  
want to suppress

$$\eta_{ij} = \frac{f_{ij}}{f_{ii} - f_{jj}}, \dots$$



### Normal Ordered Two-Body approximation

$$H(s) = E(s) + \sum_{ij} f_{ij}(s) \{a_i^\dagger a_j\} + \frac{1}{4} \sum_{ijkl} \Gamma_{ijkl} \{a_i^\dagger a_j a_l a_k\}$$

0-body                      1-body                      2-body

$$\frac{dH(s)}{ds} = [\eta(s), H(s)]$$

## IMSRG flow

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e.g.

matrix elements we  
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$$\begin{aligned} \frac{dH(s)}{ds} &= [\eta(s), H(s)] \\ &= [\eta(s), H(s)]_{0B} + [\eta(s), H(s)]_{1B} + [\eta(s), H(s)]_{2B} + [\eta(s), H(s)]_{3B} + \dots \end{aligned}$$



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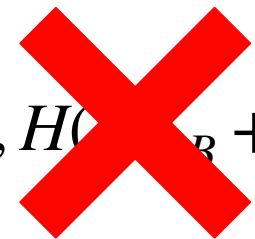
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For operators:  $\frac{dO(s)}{ds} = [\eta(s), O(s)]$



**IMSRG**

**PV-IMSRG flow**





## PV-IMSRG flow

### IMSRG

Operators  $\left\{ \begin{array}{l} H(s) \\ \eta(s) \\ O(s) \end{array} \right.$



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### PV-IMSRG

$$H(s) = H_0(s) + \lambda V_{PV}(s)$$

$$\eta(s) = \eta_{pc}(s) + \lambda \eta_{pv}(s)$$

$$O(s) = O_{PC}(s) + O_{PV}(s)$$



# PV-IMSRG flow

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$$\frac{dH_0}{ds} = [\eta_{PC}, H_0] + \lambda^2 [\eta_{PV}, V_{PV}]$$

$$\frac{dV_{PV}}{ds} = \lambda [\eta_{PC}, V_{PV}] + \lambda [\eta_{PV}, H_0]$$

$$\frac{dO_{PC}}{ds} = [\eta_{PC}, O_{PC}] + \lambda [\eta_{PV}, O_{PV}]$$

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## PV-IMSRG flow



## PV-IMSRG flow

### Remarks:

- At any point in the flow:  
 $\langle O \rangle = \langle O_{PC} \rangle + \langle O_{PV} \rangle$
- For a unitary flow  $\langle O \rangle(s) = \langle O \rangle$  constant
- At  $s=0$  :  $\langle O_{PC} \rangle = 0$  and  
 $\langle O \rangle = \langle O_{PV} \rangle(0)$
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## Pros:

- Only requires grounds state expectation value.
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## Cons:

- Requires 4x the amount of commutator evaluation.
- Extra flow is also truncated, possible truncation errors.

# Results (very preliminary)



# Preservation of Unitarity: Schiff Moment

Exact sum and PV-IMSRG results in small model space ( $e_{\text{max}} = 1$ , all orbit in sp-shell).



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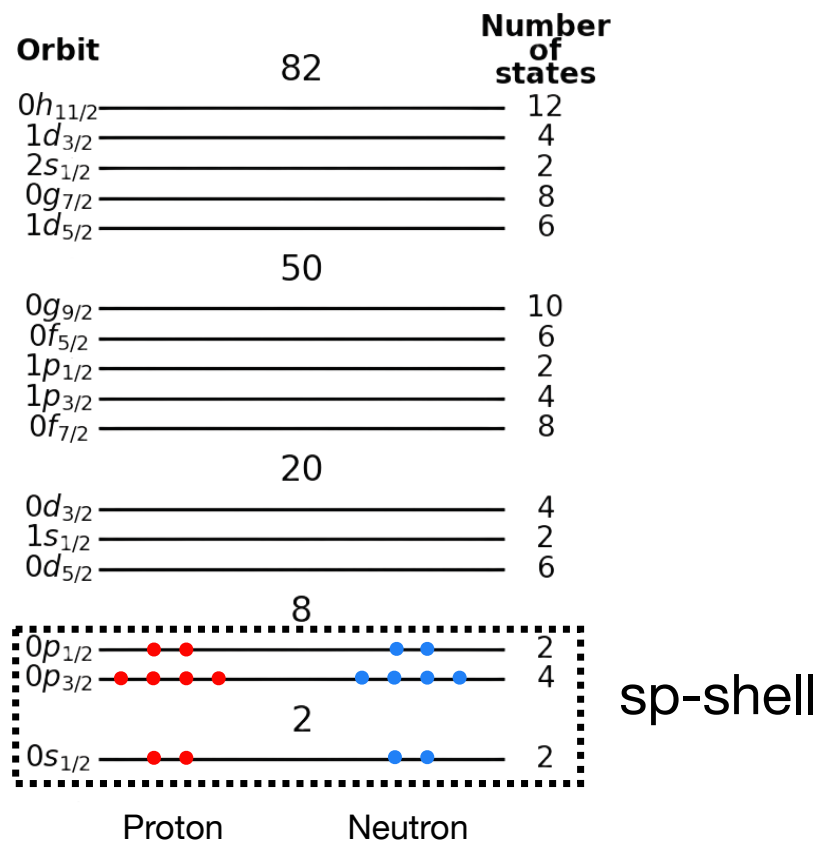
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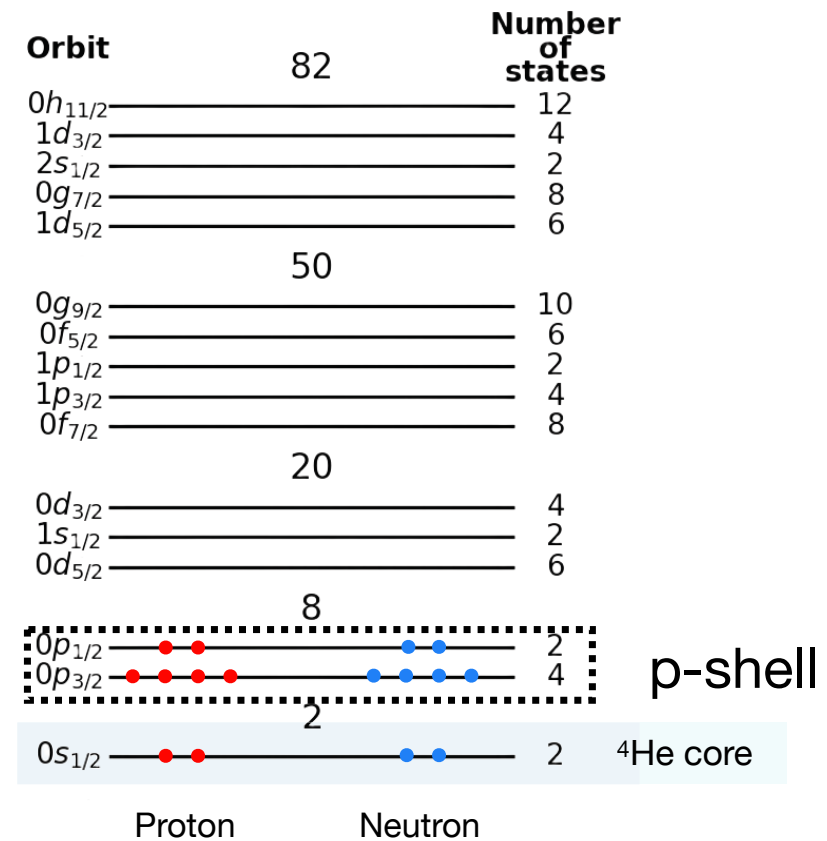
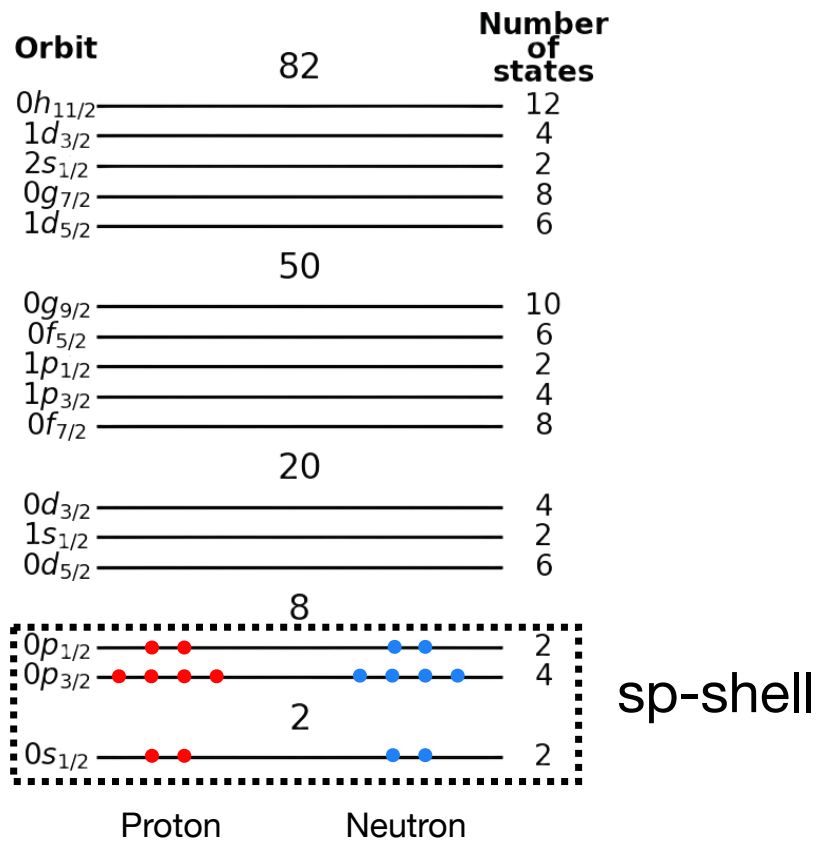
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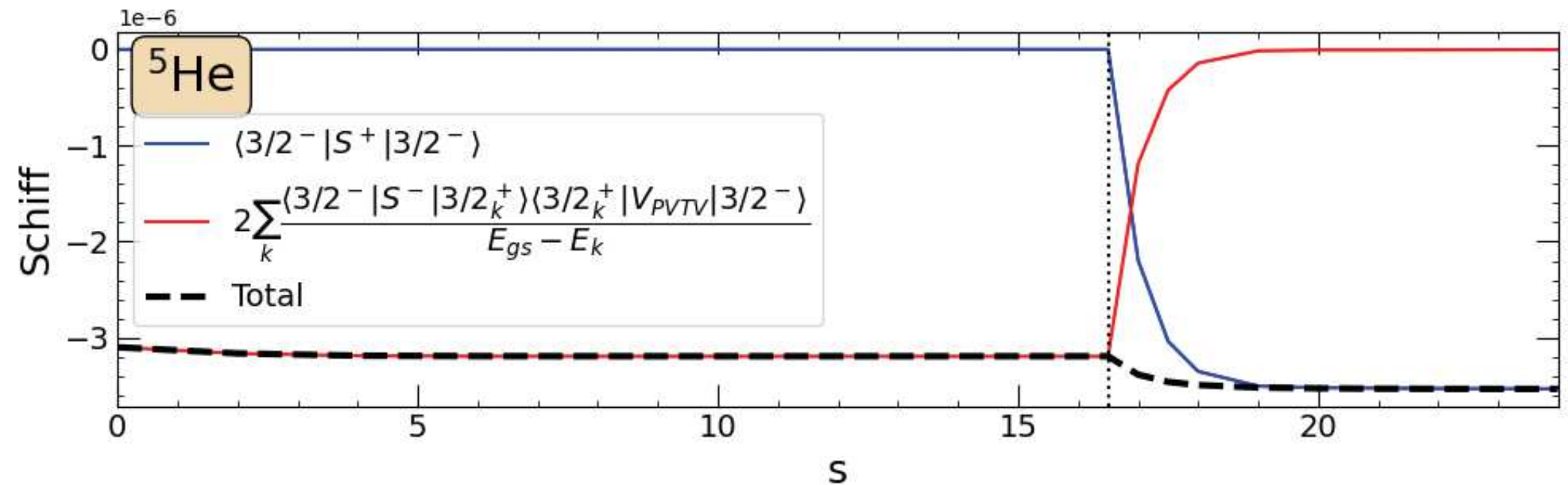


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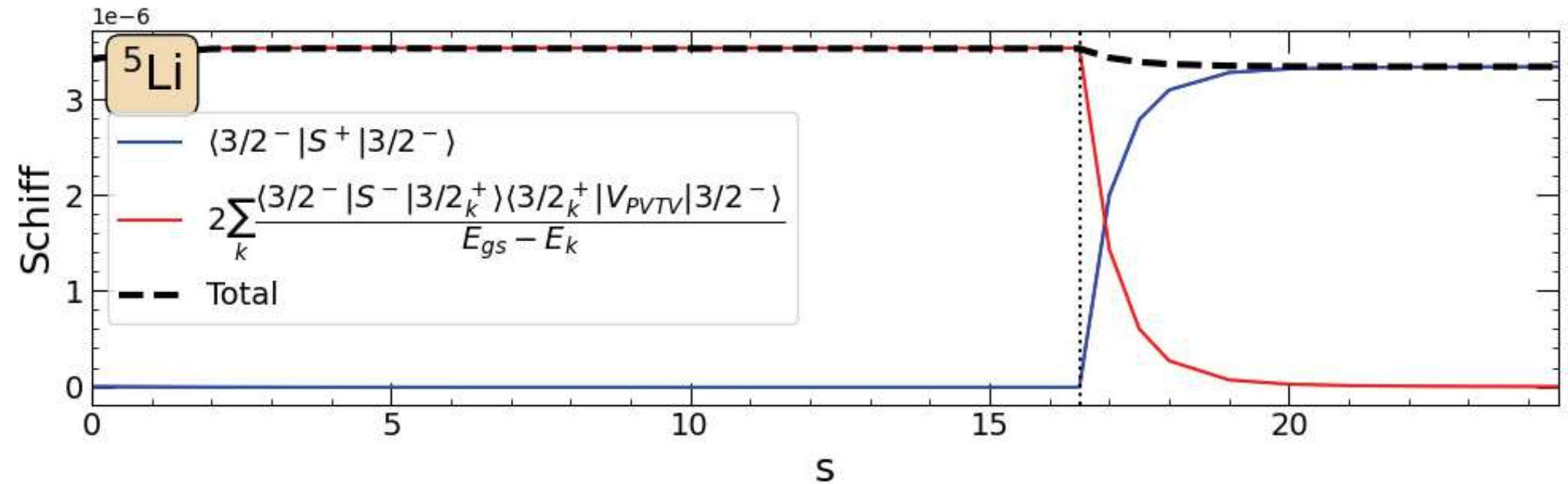


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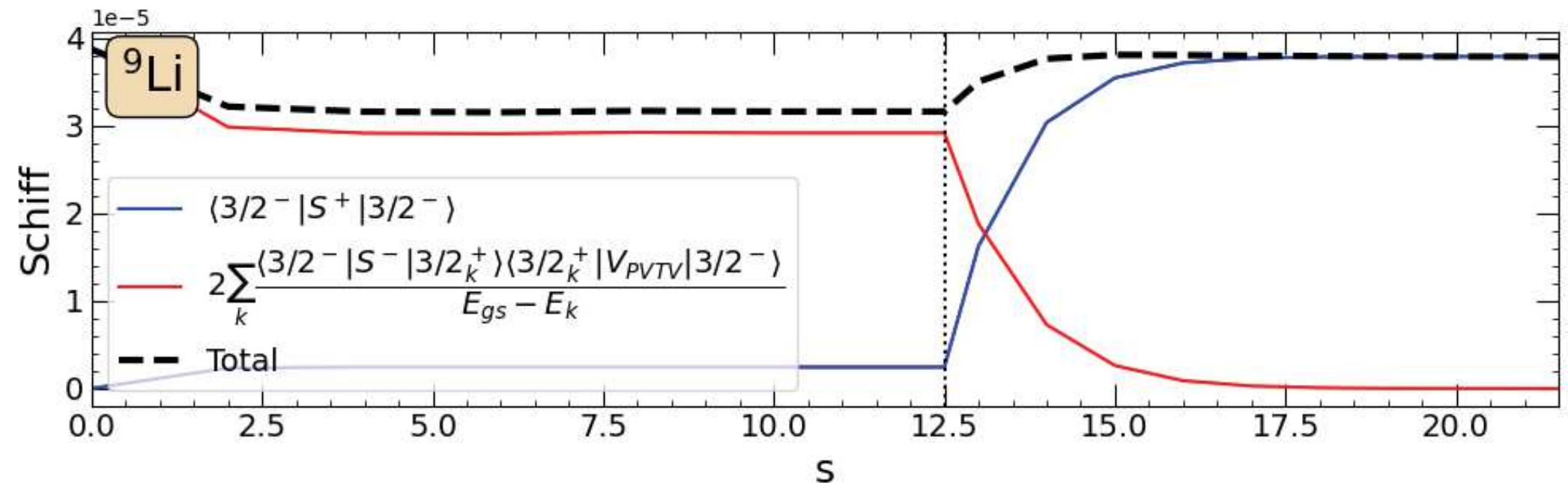


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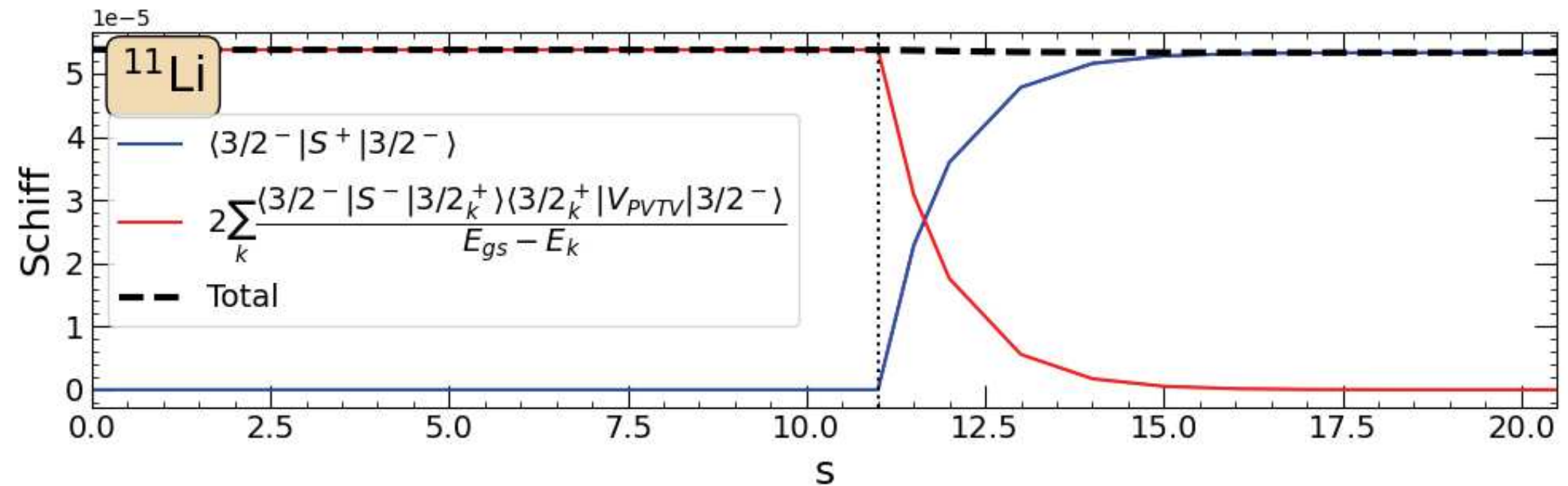


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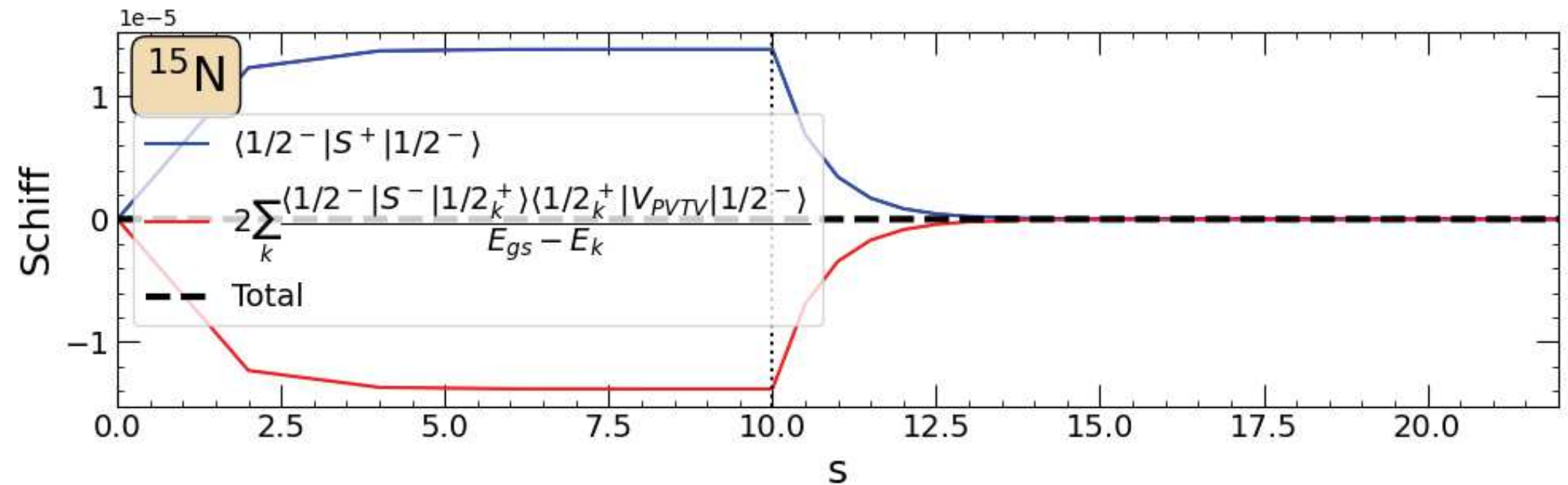


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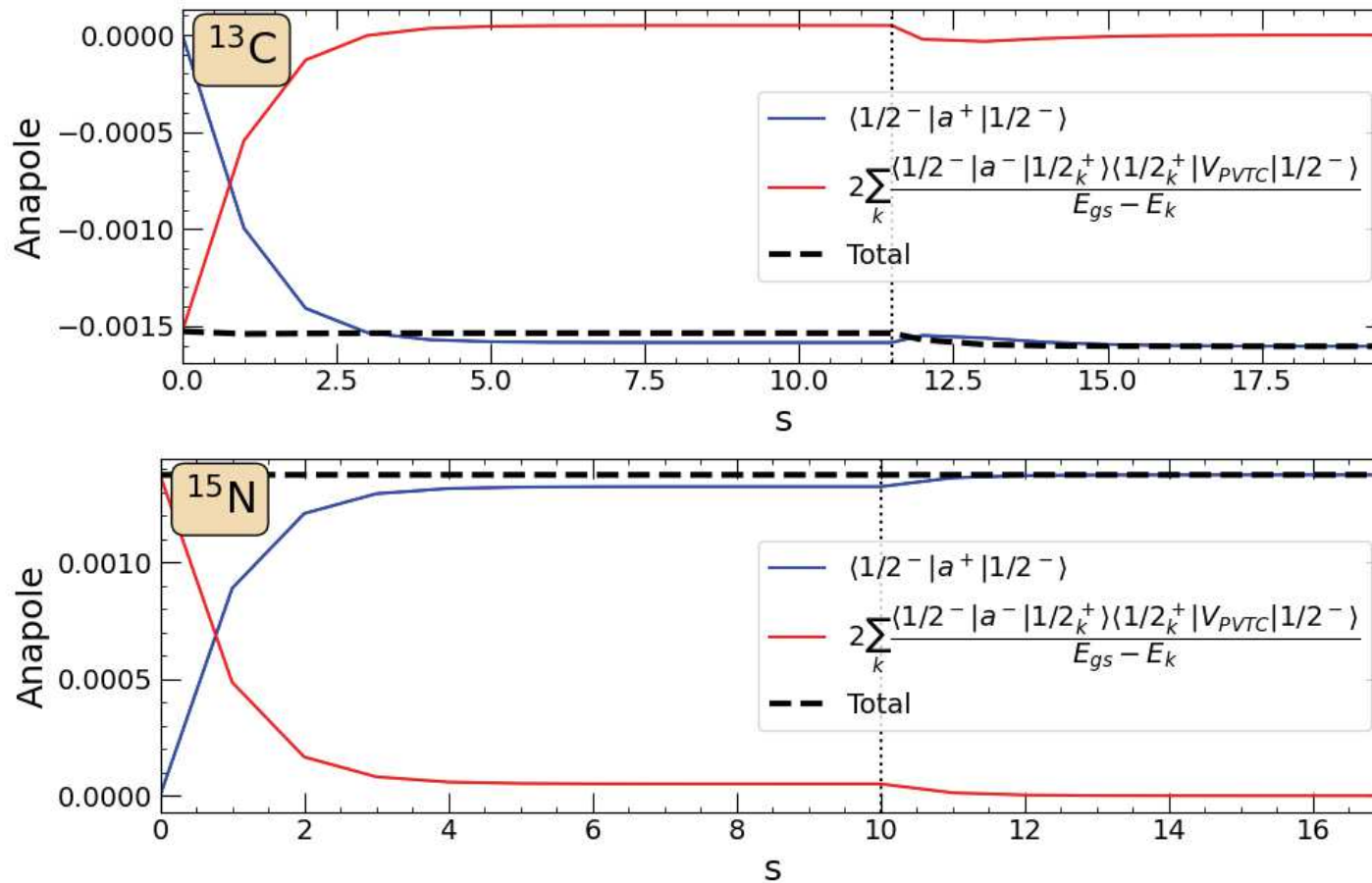
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# Preservation of Unitarity: Anapole Moment

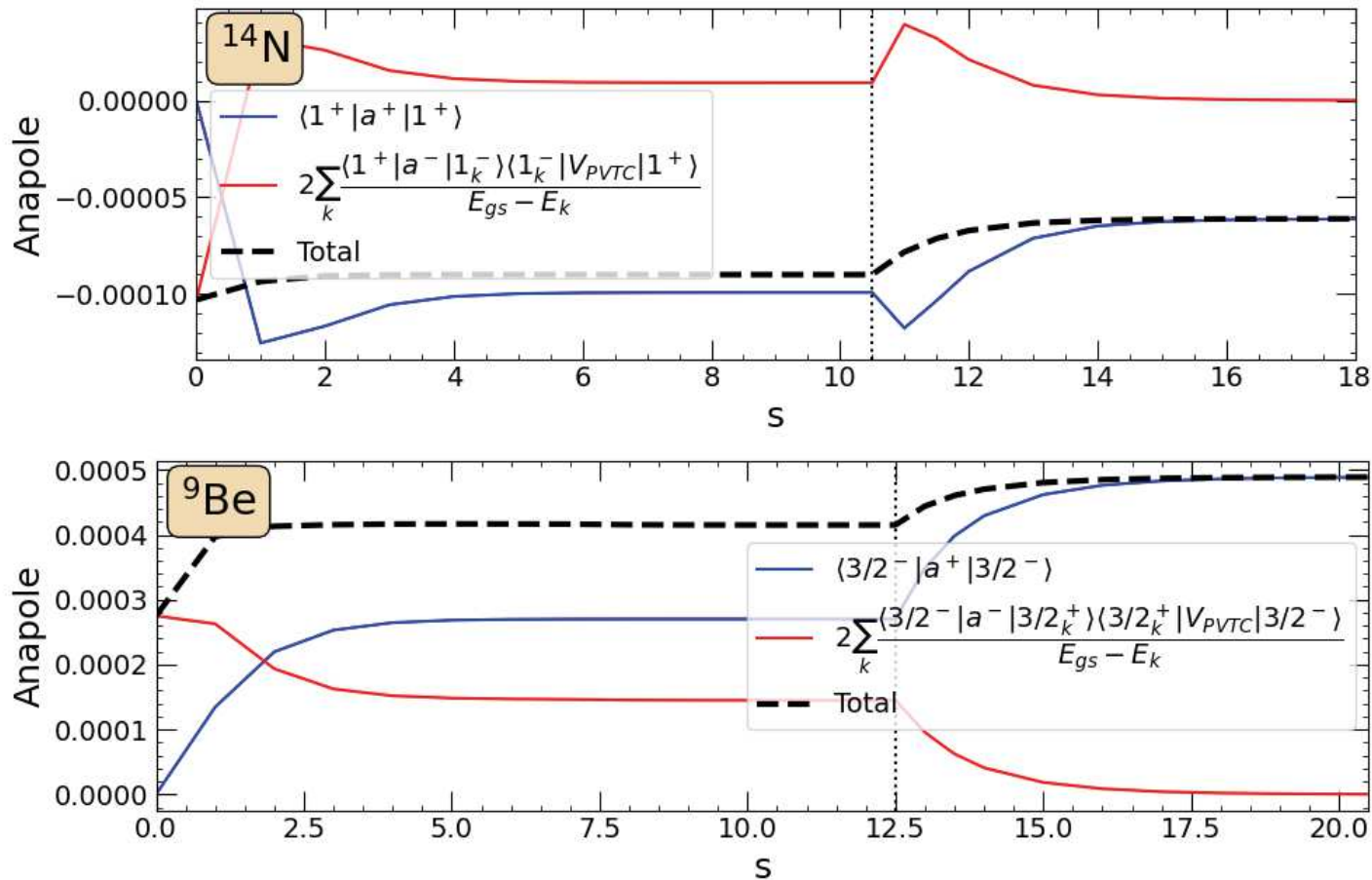
Can do the same test with anapole moments.





# Preservation of Unitarity: Anapole Moment

Seems to be a bug for different values of J ...





# Summary





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- PV IMSRG is a new many-body method for parity-violating observables.



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- Initial test in small model-spaces show that unitarity is conserved.
- Bug is still present for anapole moments.
- Need to benchmark calculation with NCSM results in larger model-spaces before scaling to heavier nuclei.

# Uncertainty quantification



## Propagating the LECs Error

Recall that the nuclear potential depends on a set of LECs  $\alpha$ :

$$O(\alpha) = \langle \psi_f(\alpha) | O | \psi_i(\alpha) \rangle$$

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

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

We read  $\textit{prob}(A | B)$  as  
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The “true” value of  
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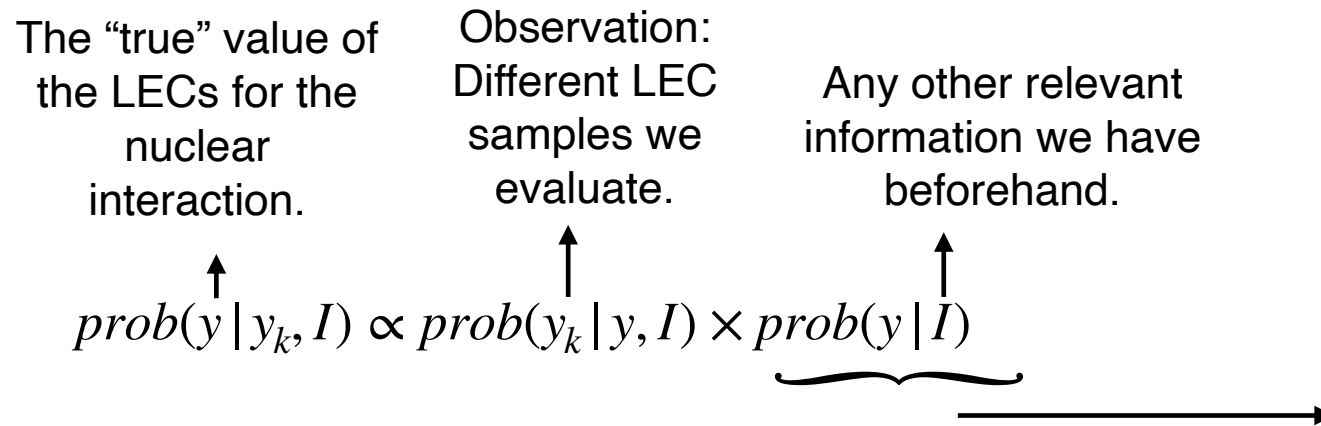
Any other relevant information we have beforehand.

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# Bayesian Approach



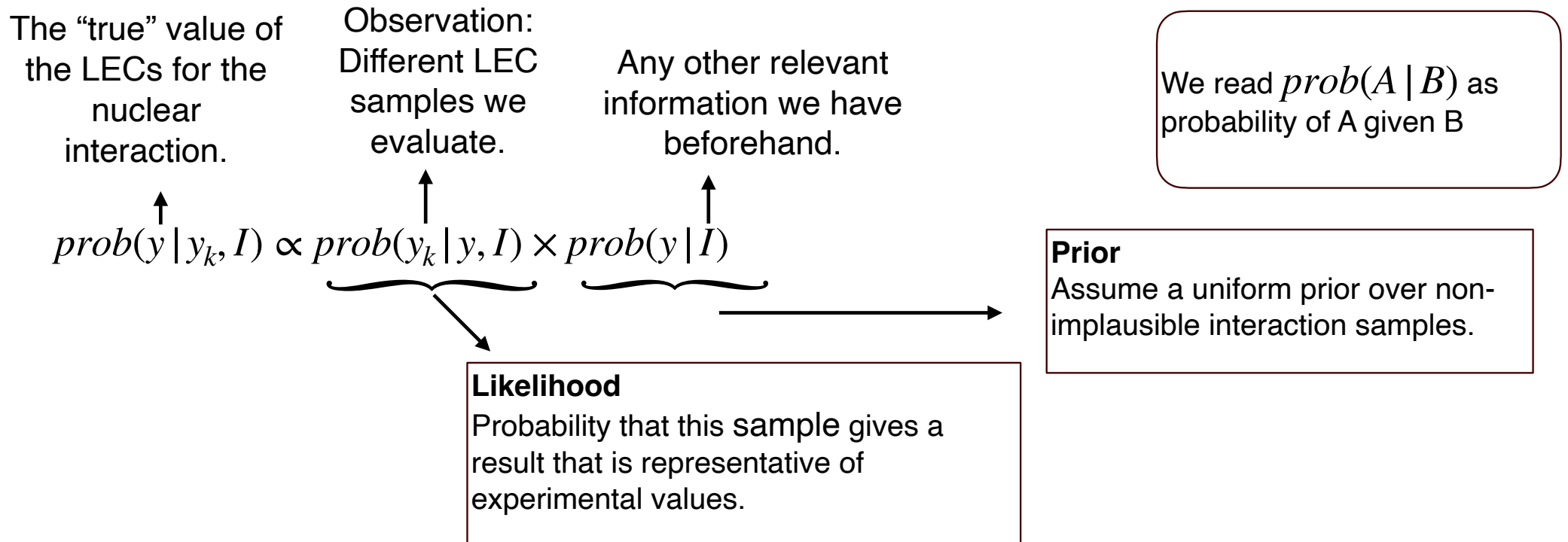
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## Prior

Assume a uniform prior over non-implausible interaction samples.



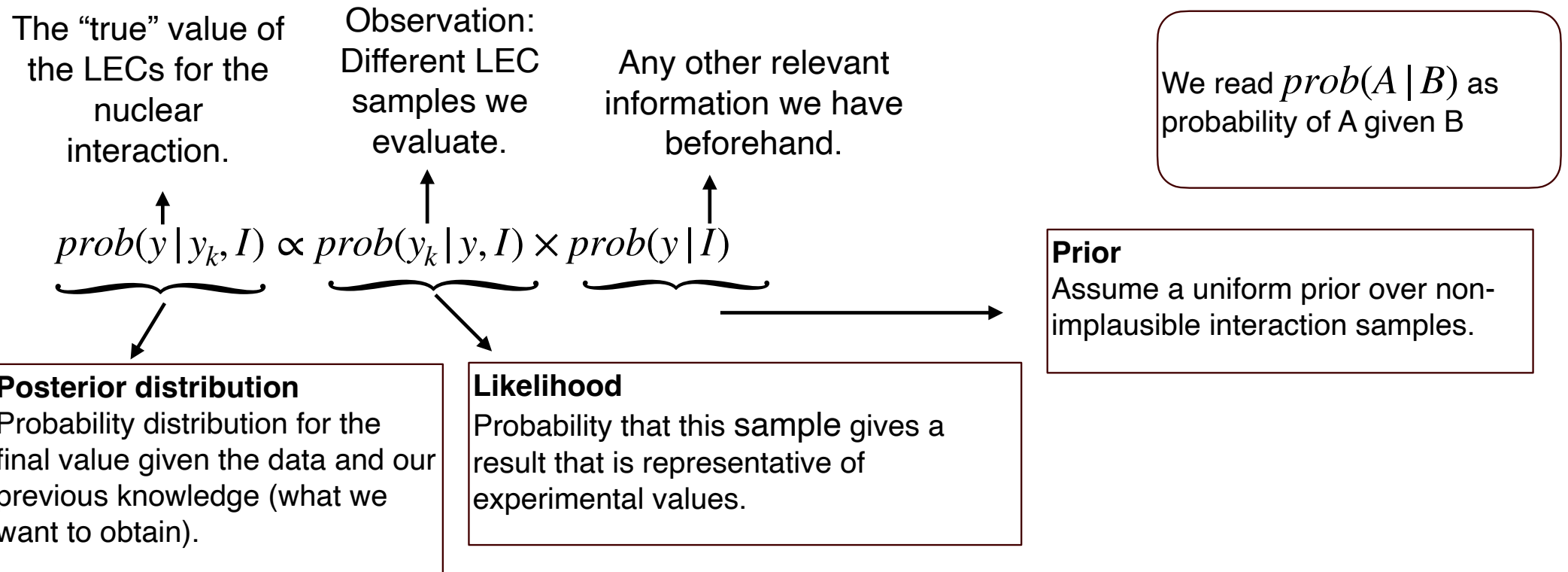
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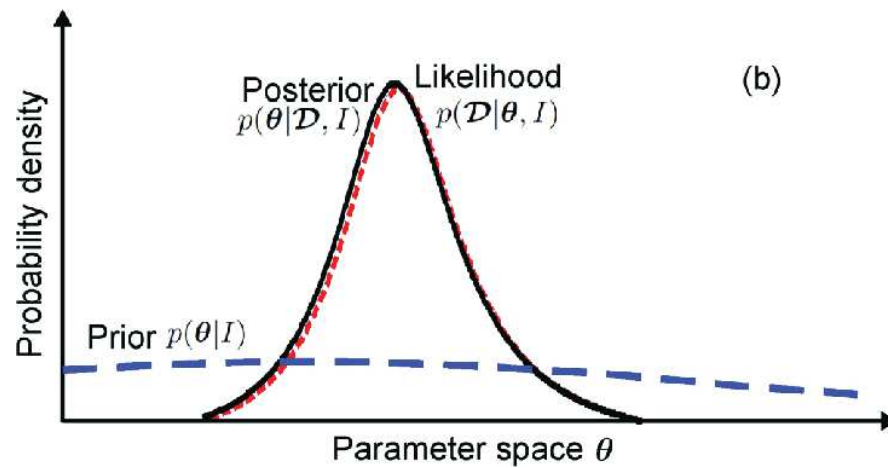
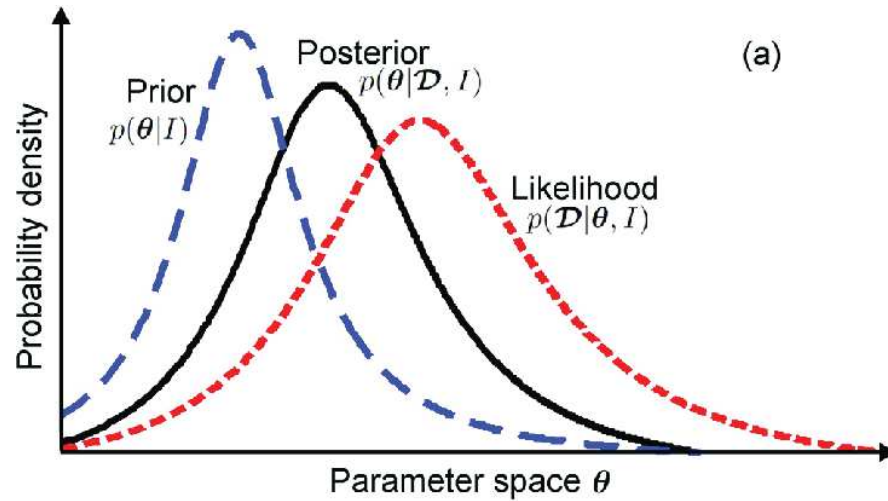


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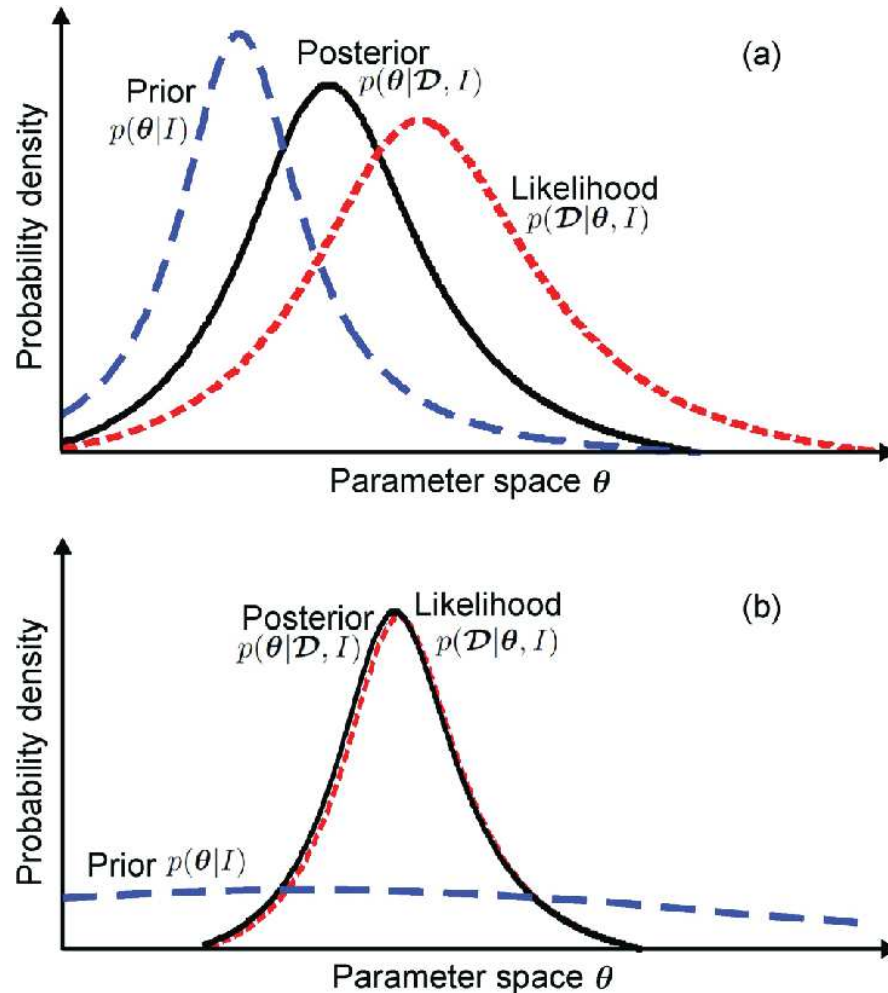


# Procedure for UQ in the Bayesian Approach





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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.
- Cost > \$2 million!
- Huge environmental impact (220 tree-years calculated using [green-algorithms.org](https://green-algorithms.org) v3.0 )

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# Emulators for Many-Body Methods

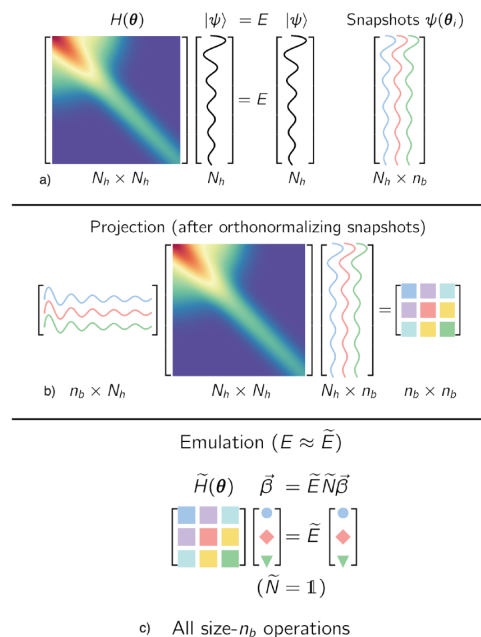
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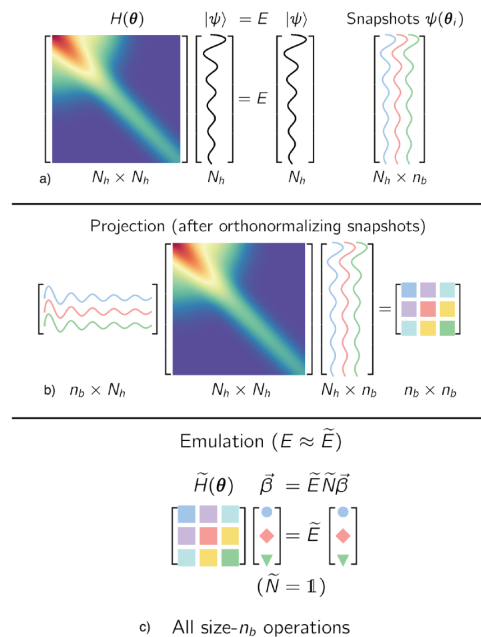


Duguet, et al., Rev. Mod. Phys. **96**, 031002 (2024)

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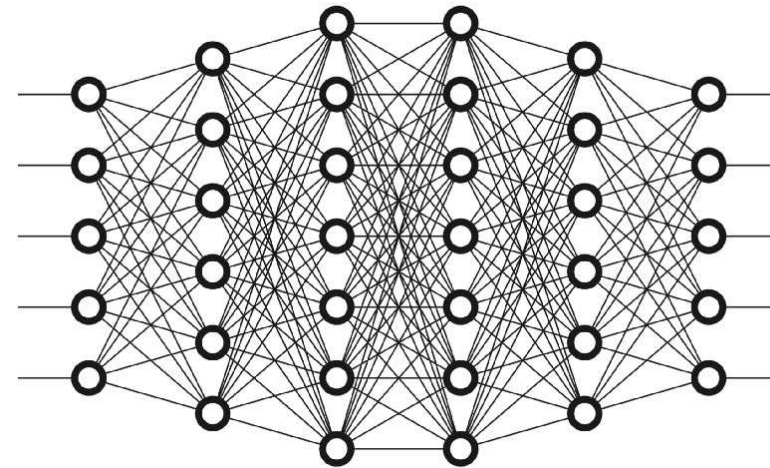
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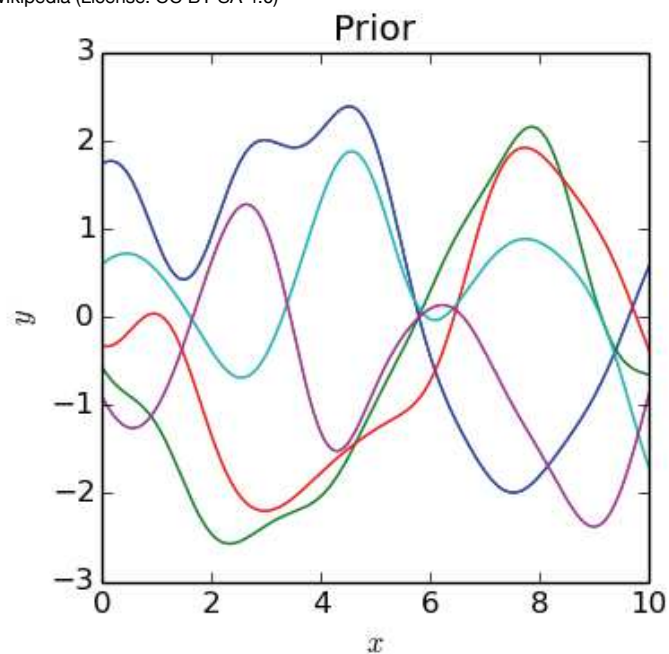
## 2. Data driven





# Using Gaussian Process as an Emulator

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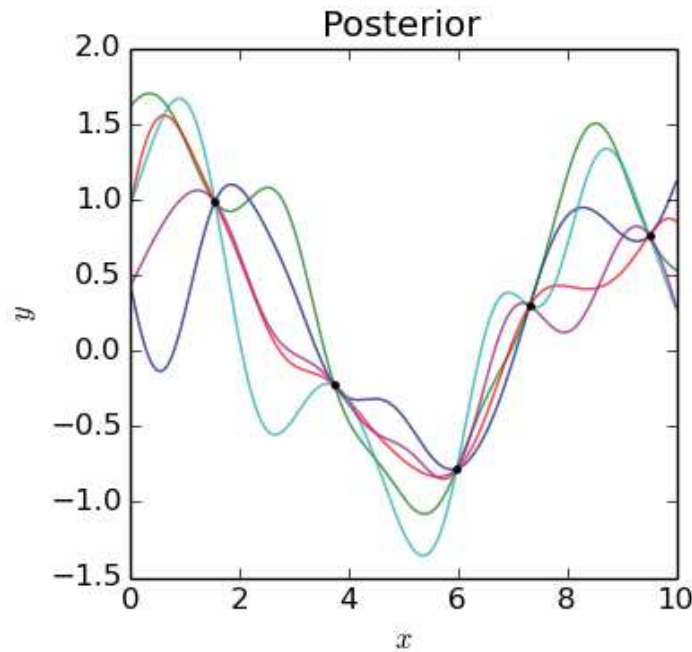
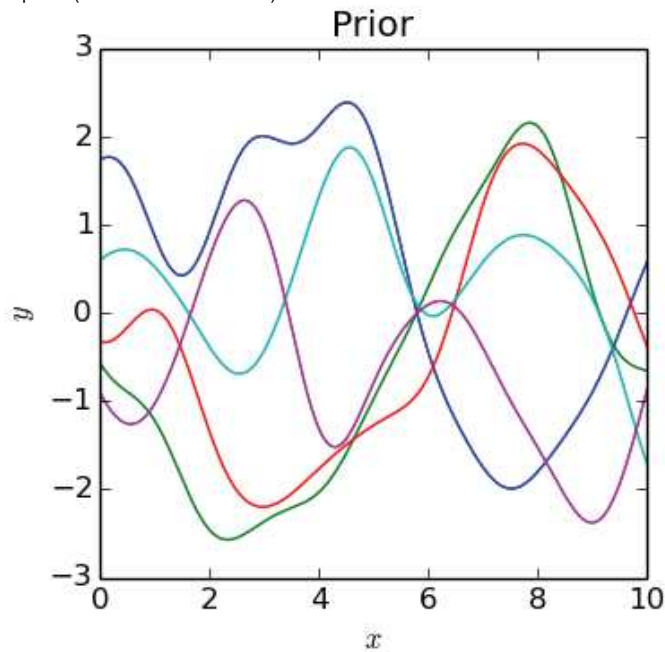
$$f(\mathbf{x}) = \mathcal{N}(\mu, K(\mathbf{x}, \mathbf{x}))$$





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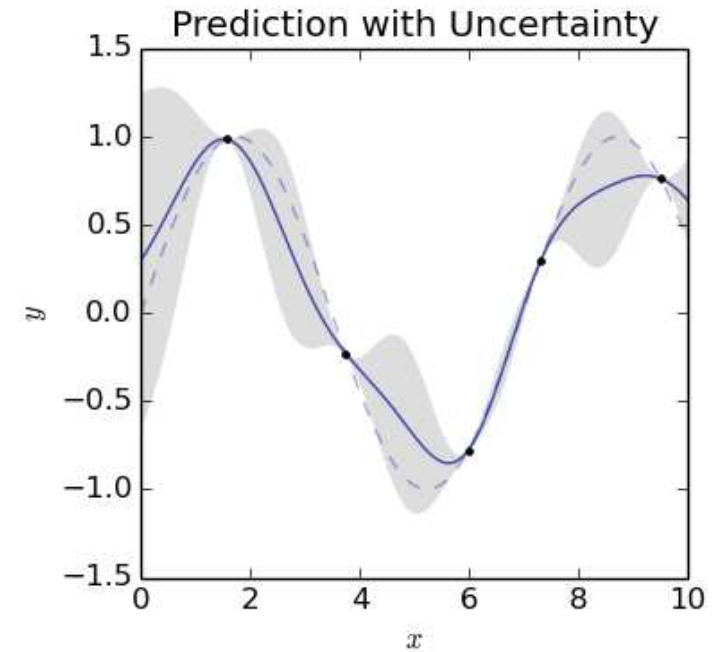
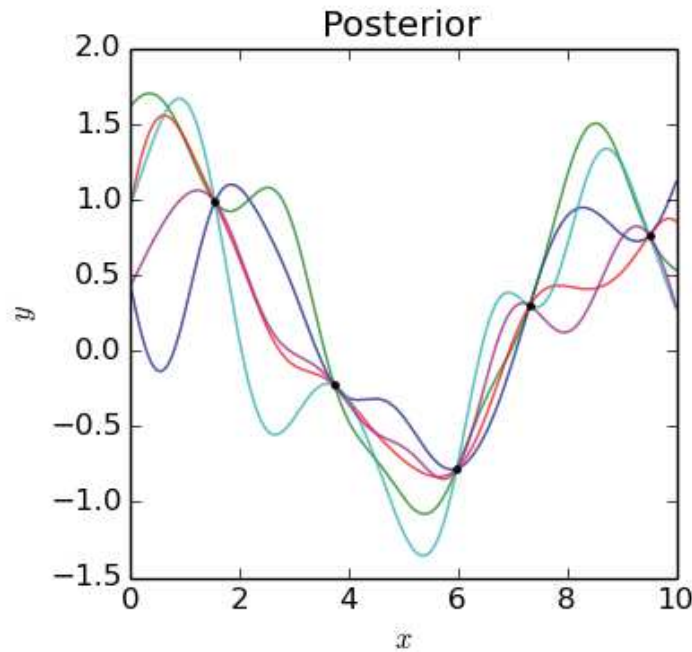
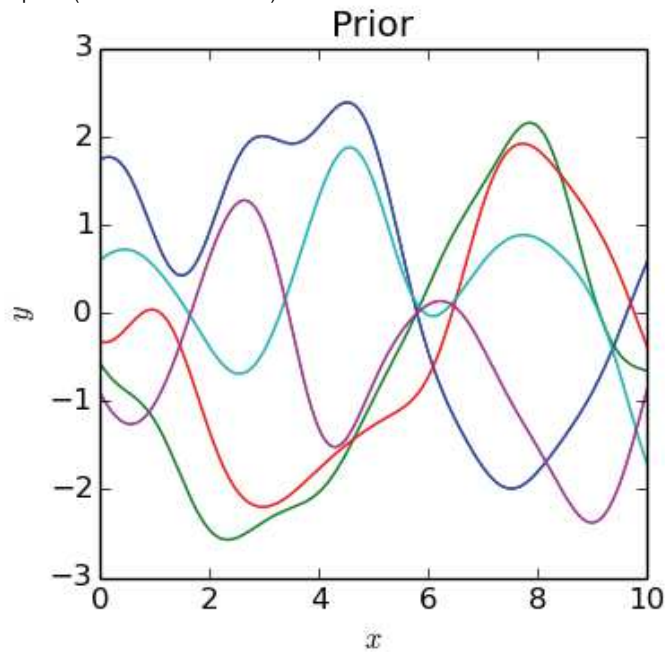
$$f(\mathbf{x}) = \mathcal{N}(\mu, K(\mathbf{x}, \mathbf{x}))$$

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



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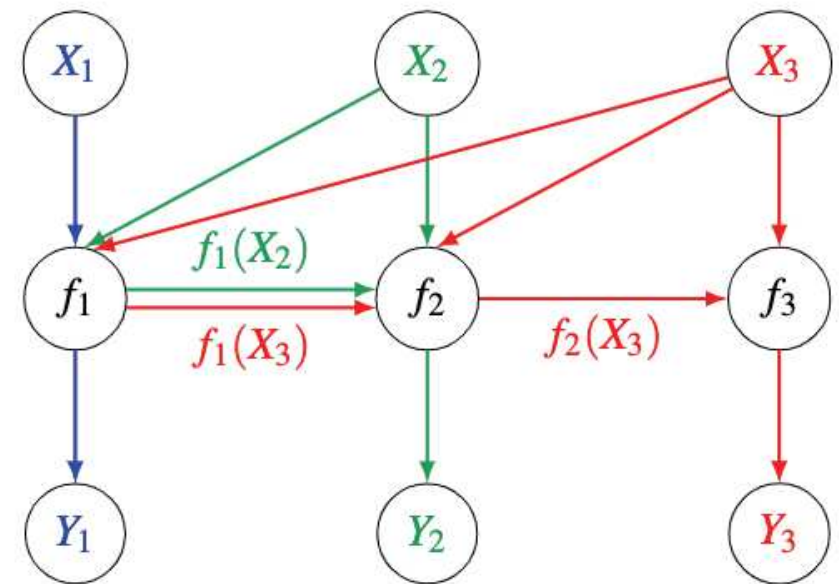
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# The MM-DGP Algorithm

- **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)**.

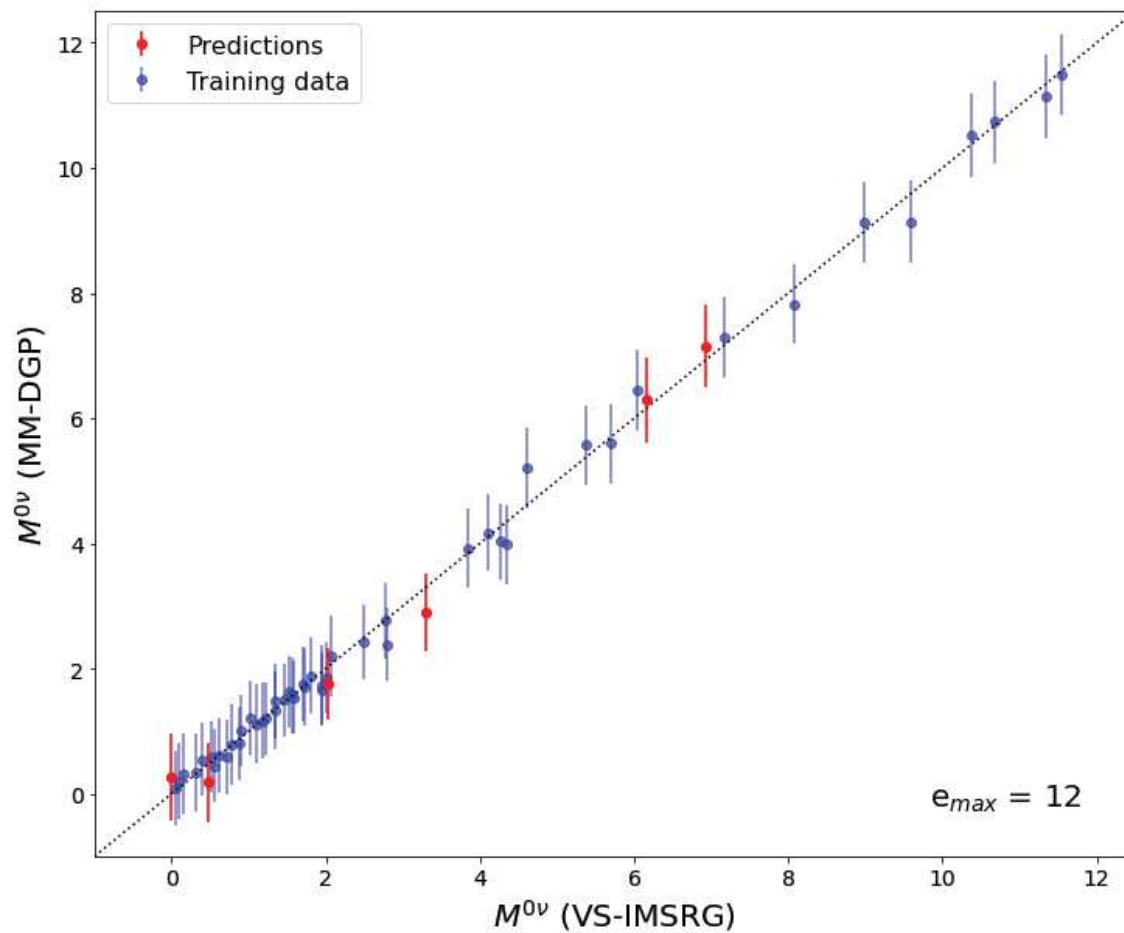




# The MM-DGP Algorithm: $0\nu\beta\beta$ NMEs

Using  $\Delta$ -full chiral EFT interactions at N2LO:

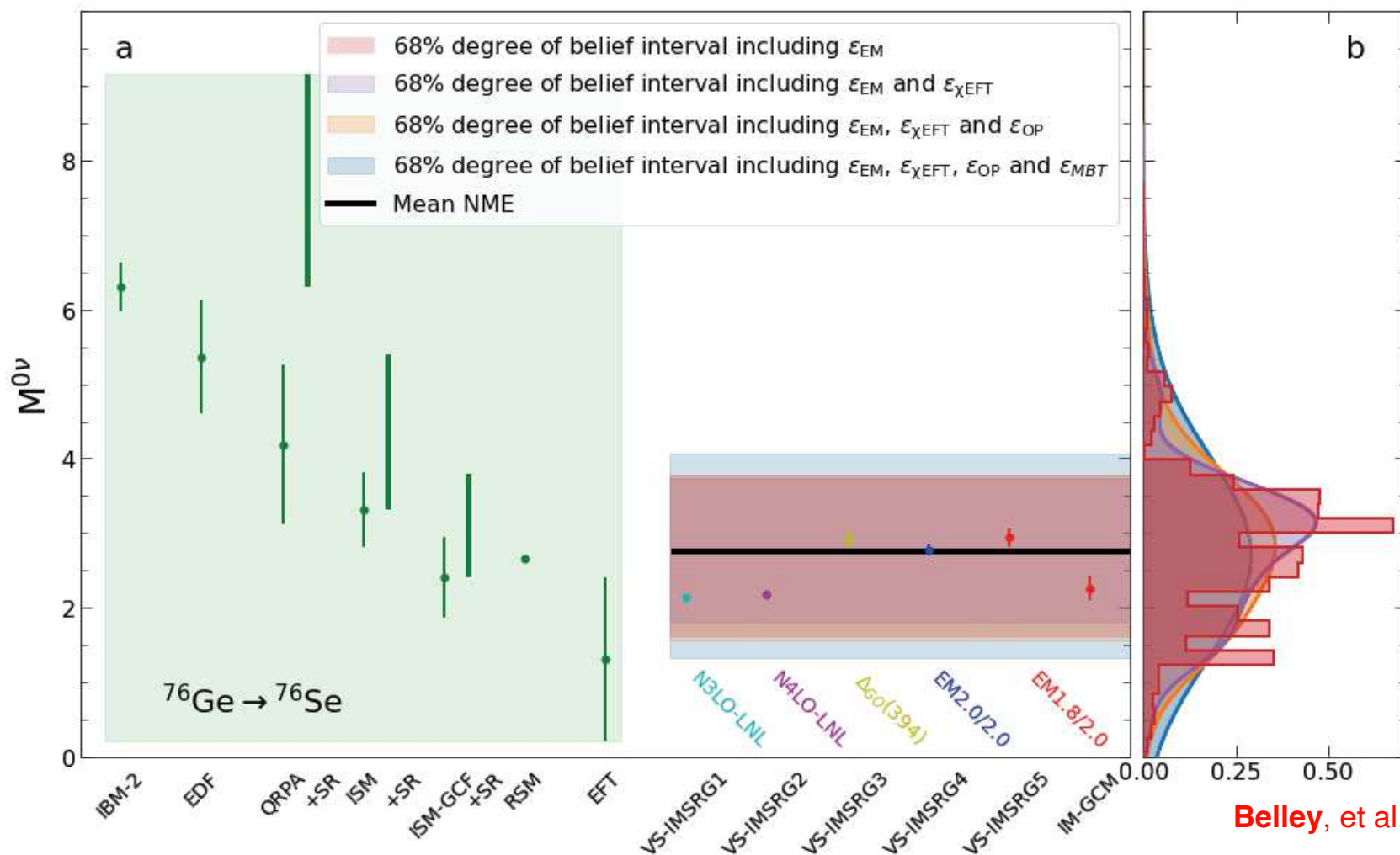
50 training points



Root Mean Square  
Error = 0.13



# Combining All Sources of Uncertainty

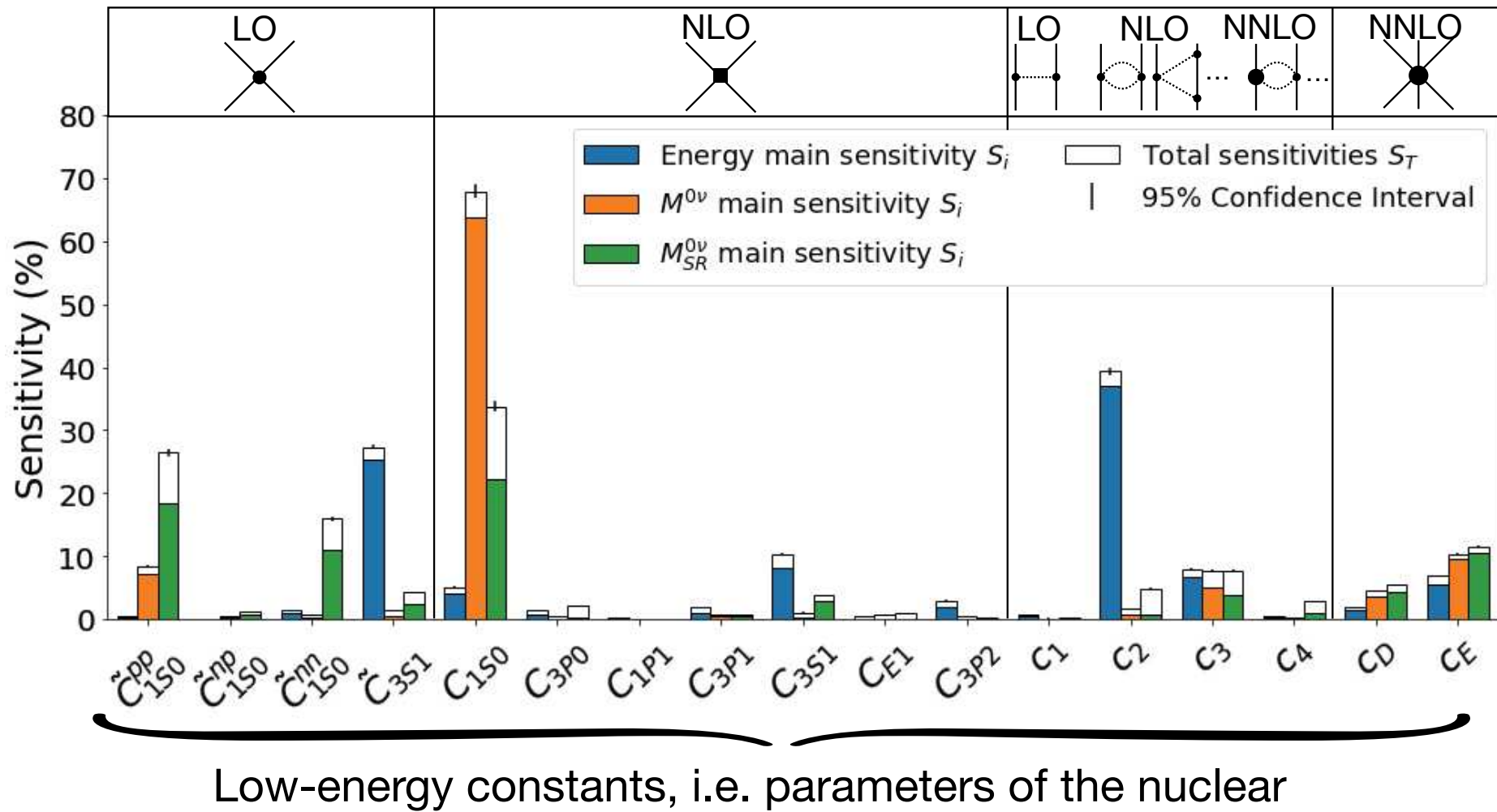


$$M^{0\nu\beta\beta} = 2.60^{+1.28}_{-1.36}$$

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

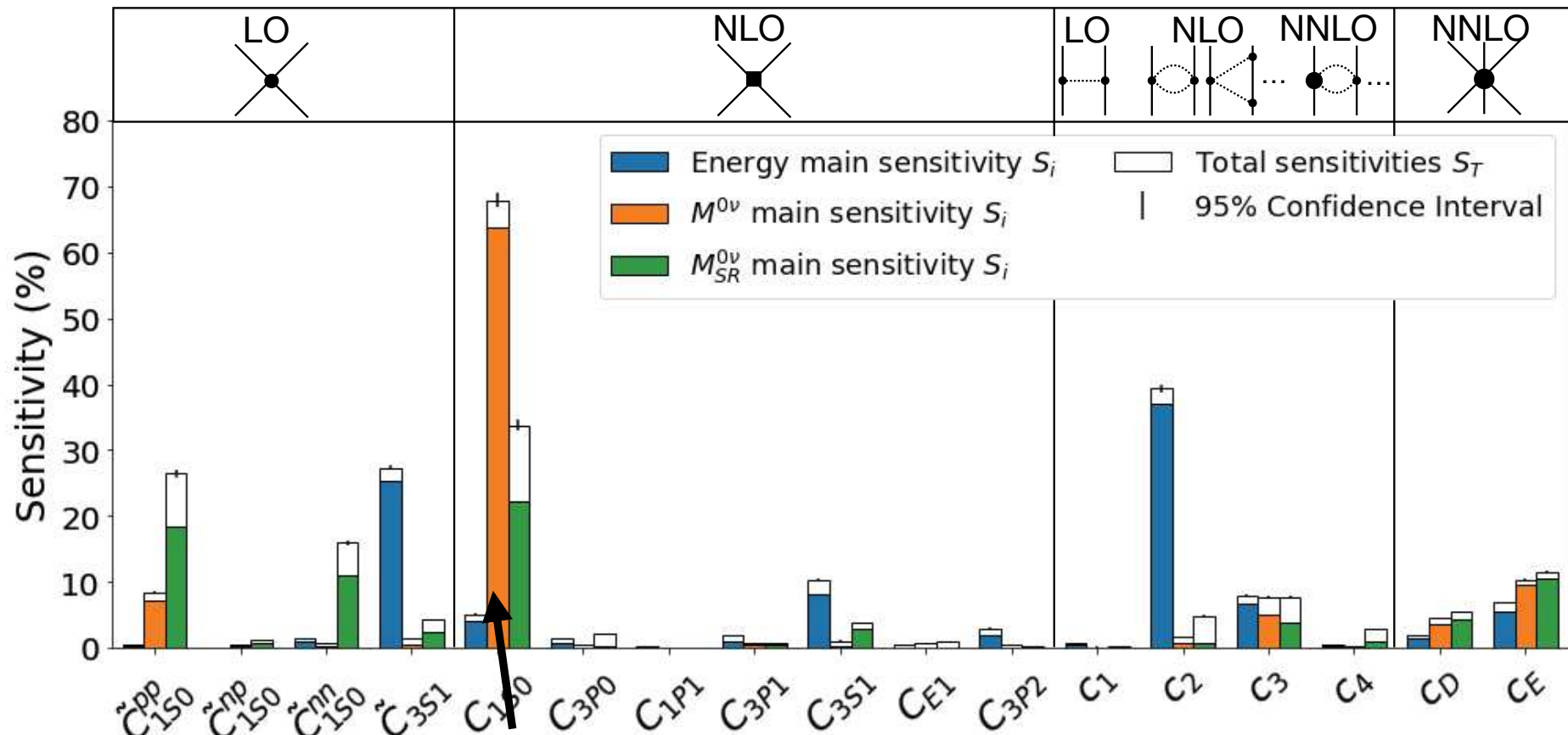
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Belley, et al., arXiv:2408.02169 (2024)



# The MM-DGP Algorithm: GSA

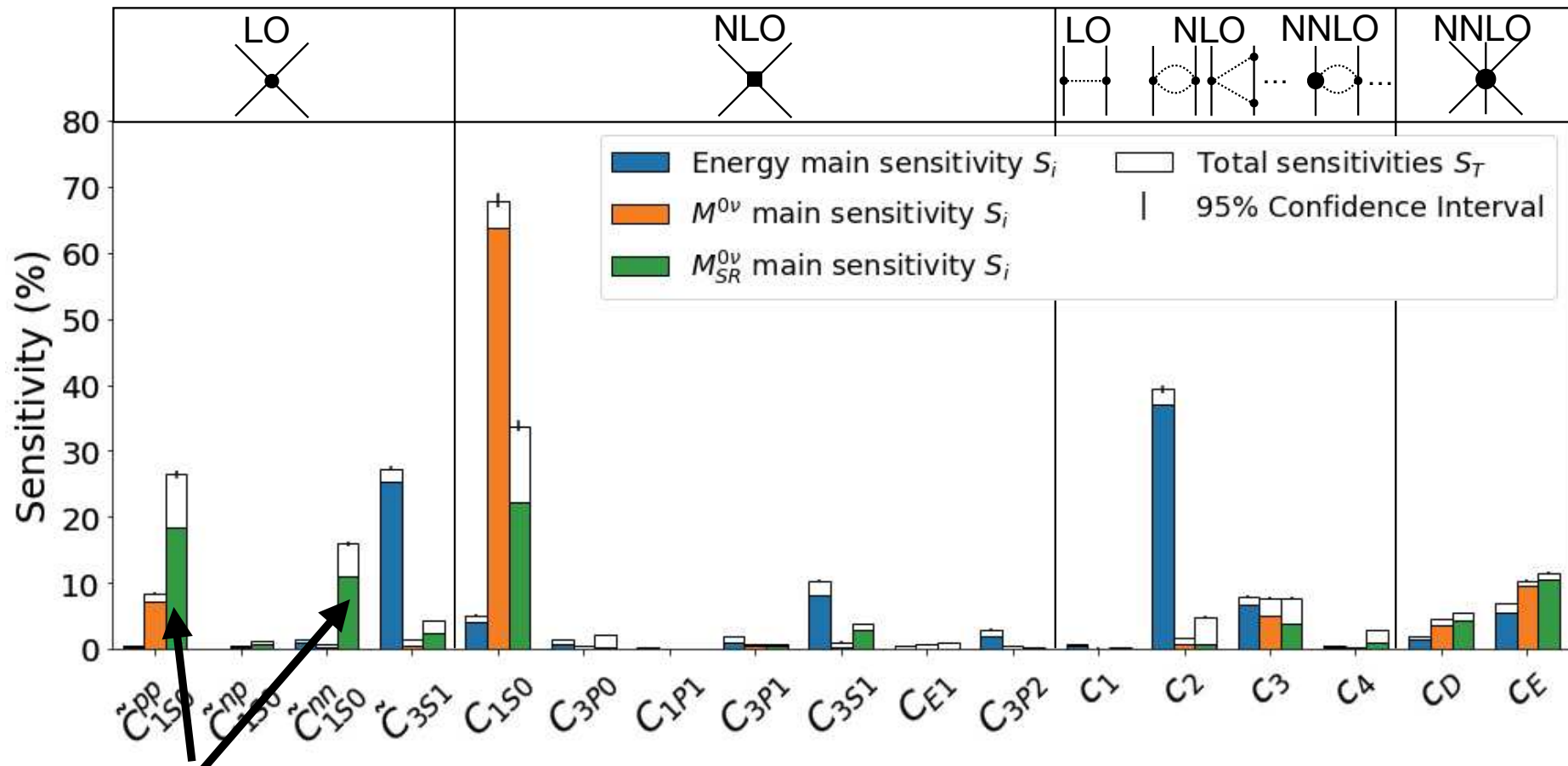
Belley, et al., arXiv:2408.02169 (2024)



The total matrix element mostly depends on one LEC!

# The MM-DGP Algorithm: GSA

Belley, et al., arXiv:2408.02169 (2024)

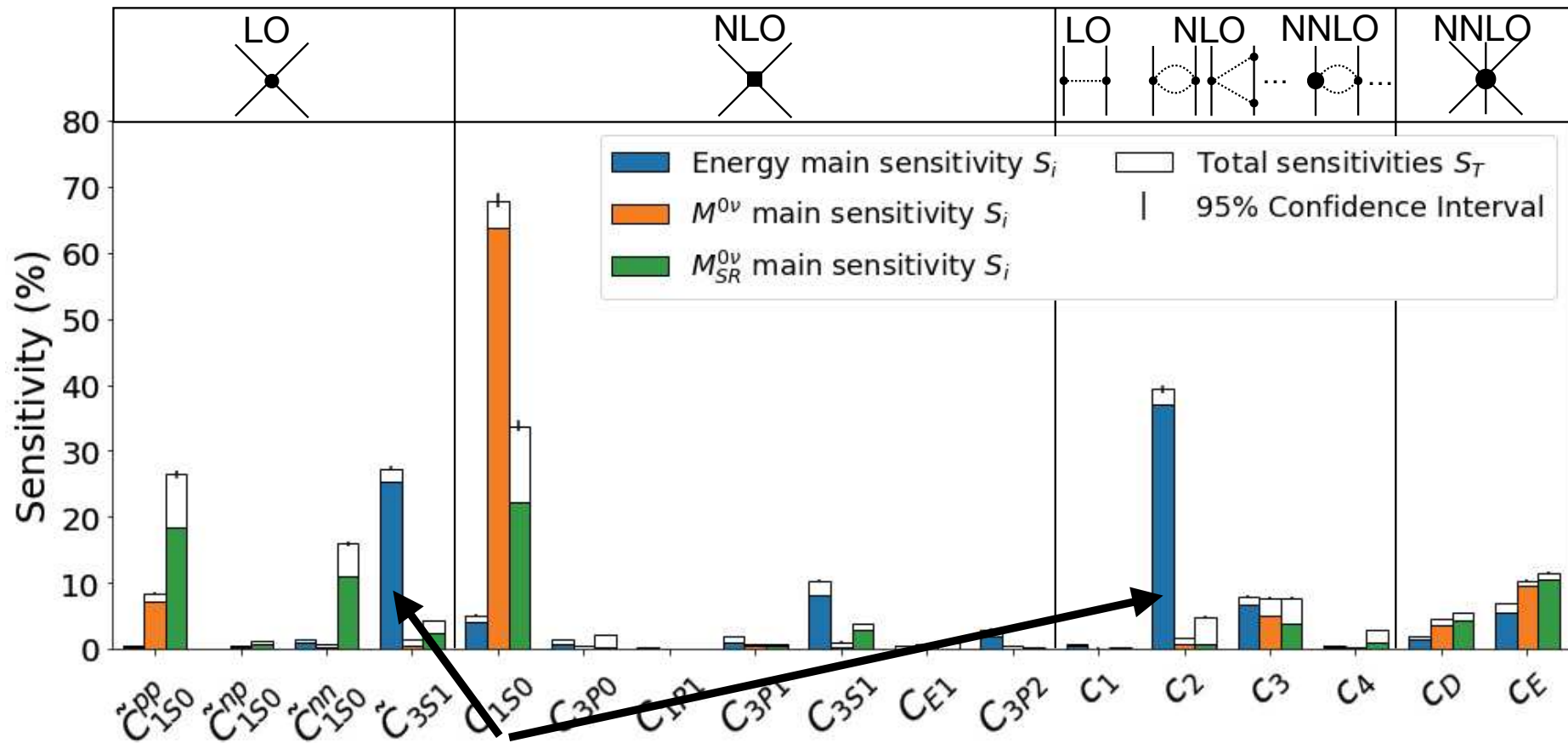


The short-range matrix element however sees other contributions from LECs associated to the short-range nuclear interaction.



# The MM-DGP Algorithm: GSA

Belley, et al., arXiv:2408.02169 (2024)



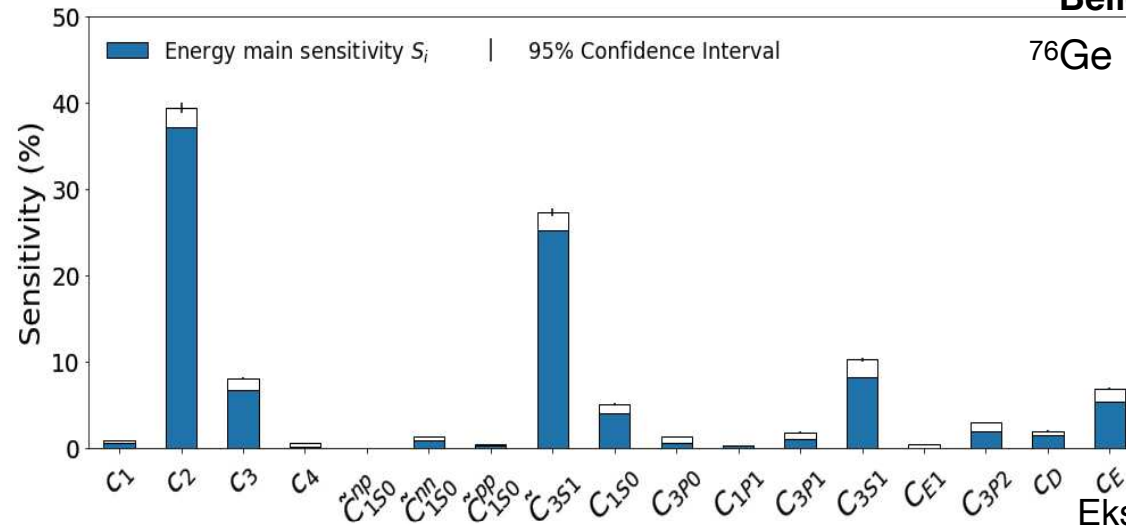
Results for energies are consistent with results of physics-based emulators of the coupled cluster method.



# The MM-DGP Algorithm: GSA

Belley, et al., arXiv:2408.02169 (2024)

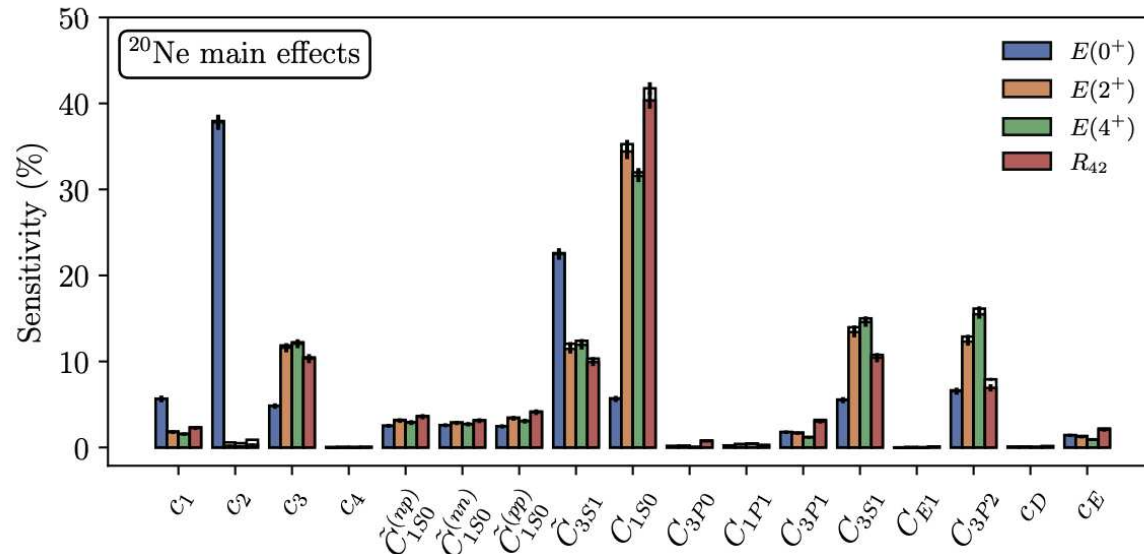
Data driven  
MM-DGP



VS

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

Physics  
Driven



# Global emulation



# Emulators for Nuclear Physics



# Emulators for Nuclear Physics

- Emulators are emerging tools in nuclear physics to allow to quickly sample parameters space of costly calculations.



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- They are required to correctly interpret results of experiments.



## Emulators for Nuclear Physics

- Emulators are emerging tools in nuclear physics to allow to quickly sample parameters space of costly calculations.
- Essential for robust uncertainty quantification of theoretical results.
- They are required to correctly interpret results of experiments.
- Current emulators have to be trained individually per nucleus.

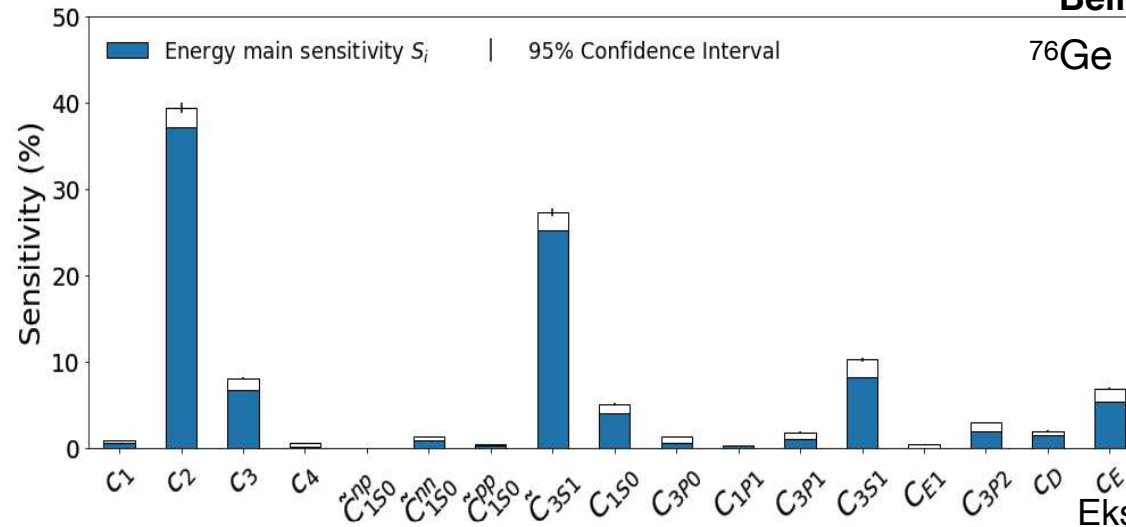




# The MM-DGP Algorithm: GSA

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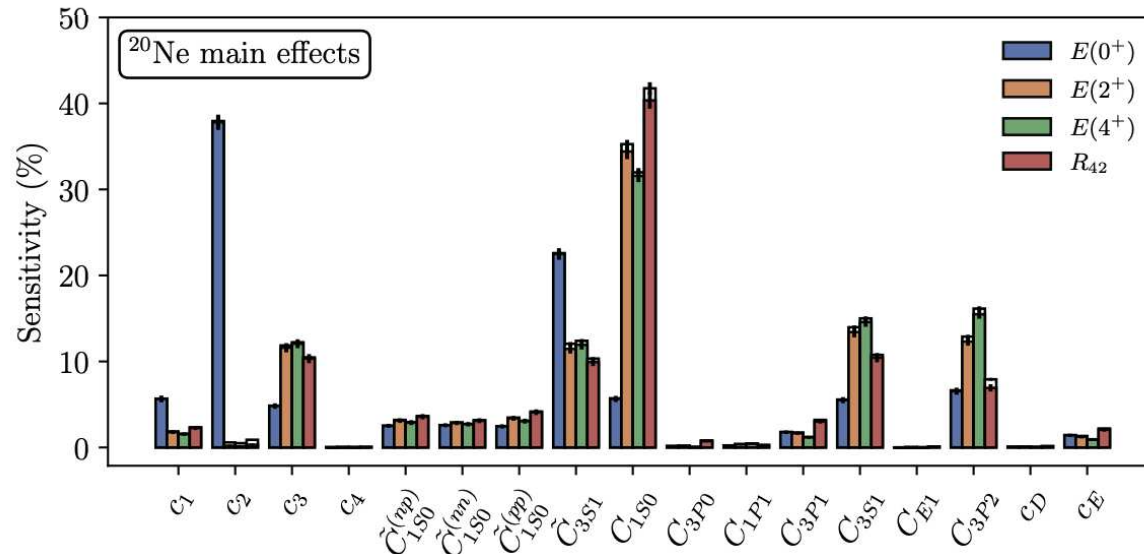
Data driven  
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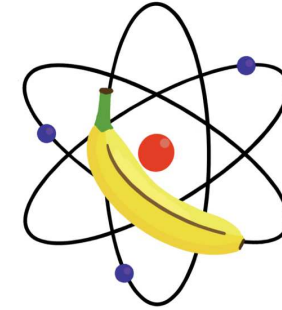
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Physics  
Driven

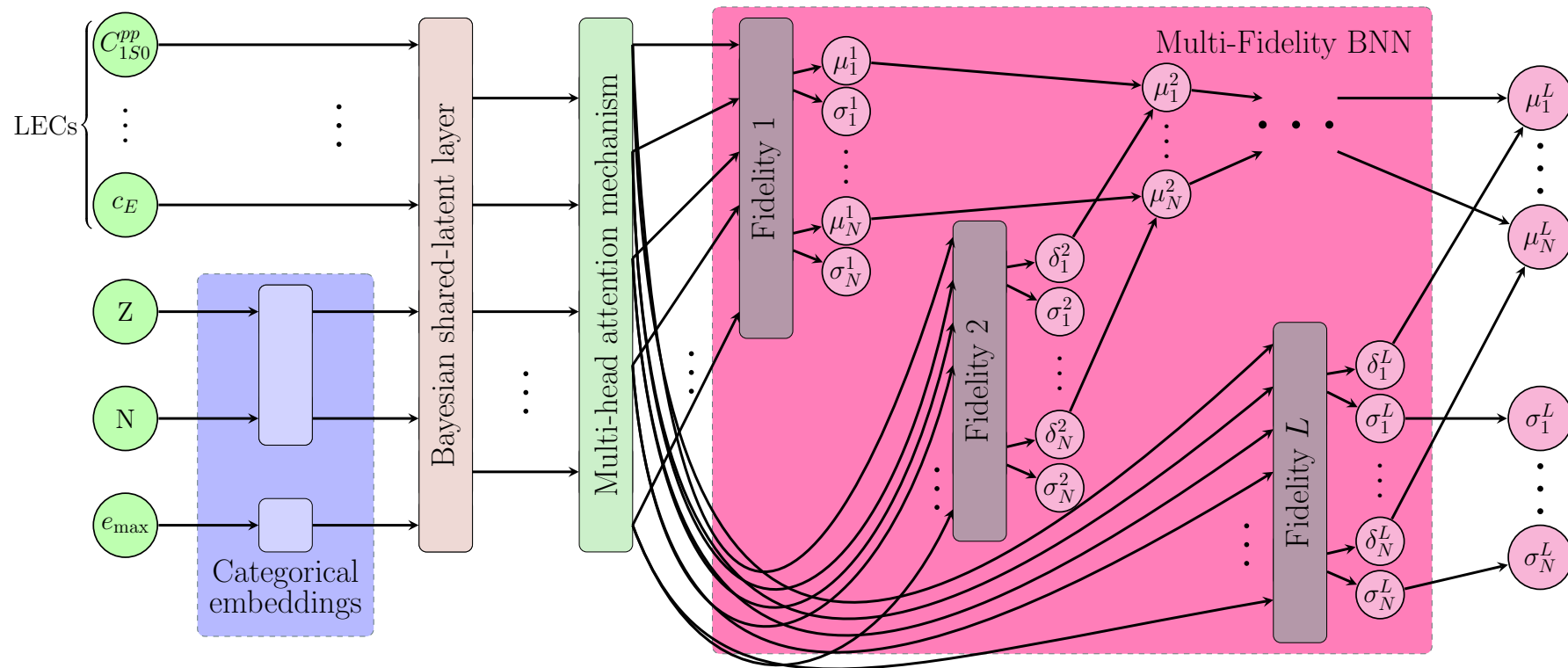


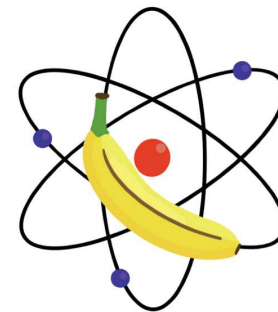


Jose Miguel Muñoz Arias

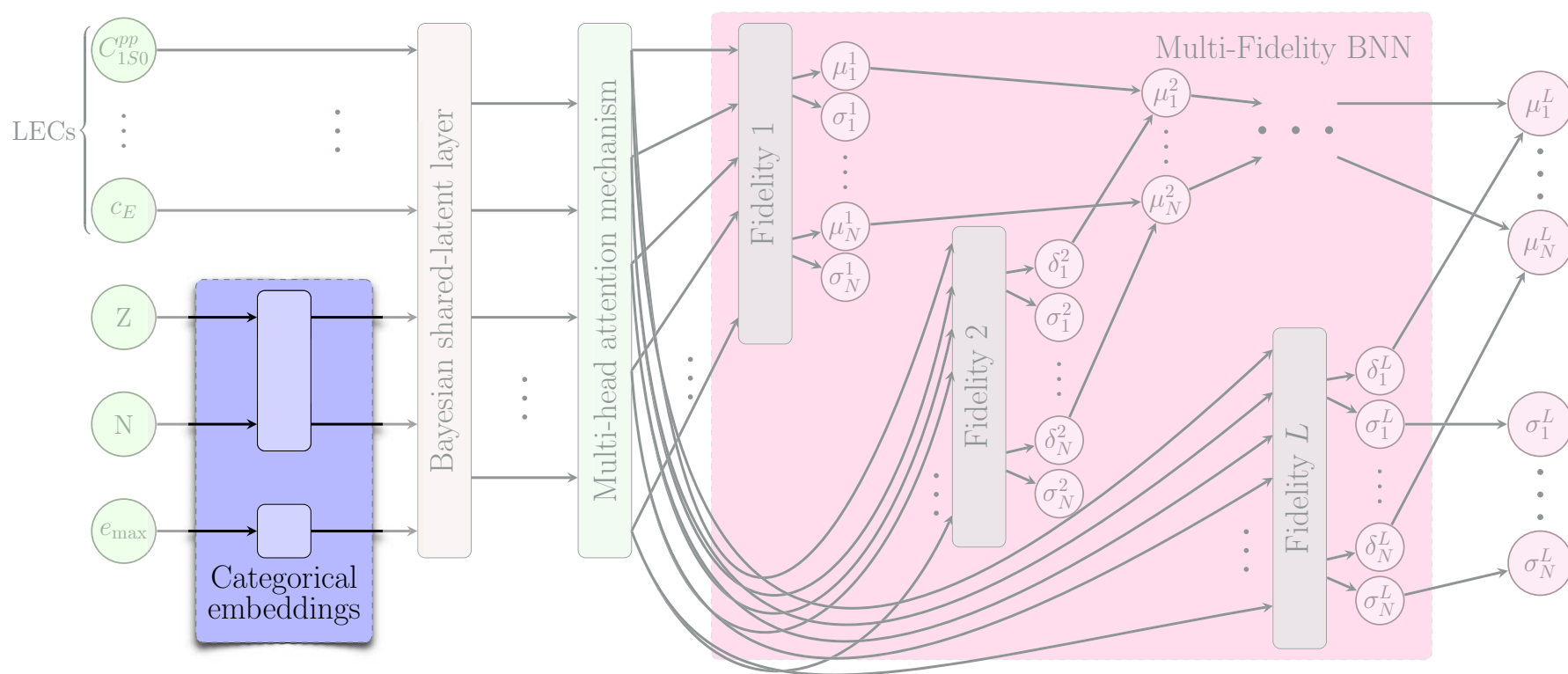


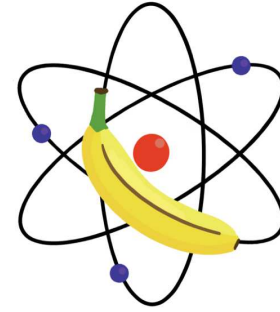
## BAYesian Neural Network for Atomic Nuclei Emulation





## BAYesian Neural Network for Atomic Nuclei Emulation

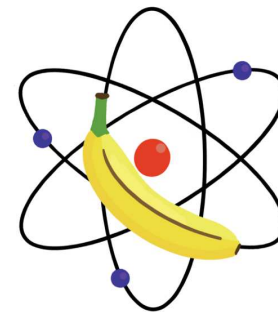




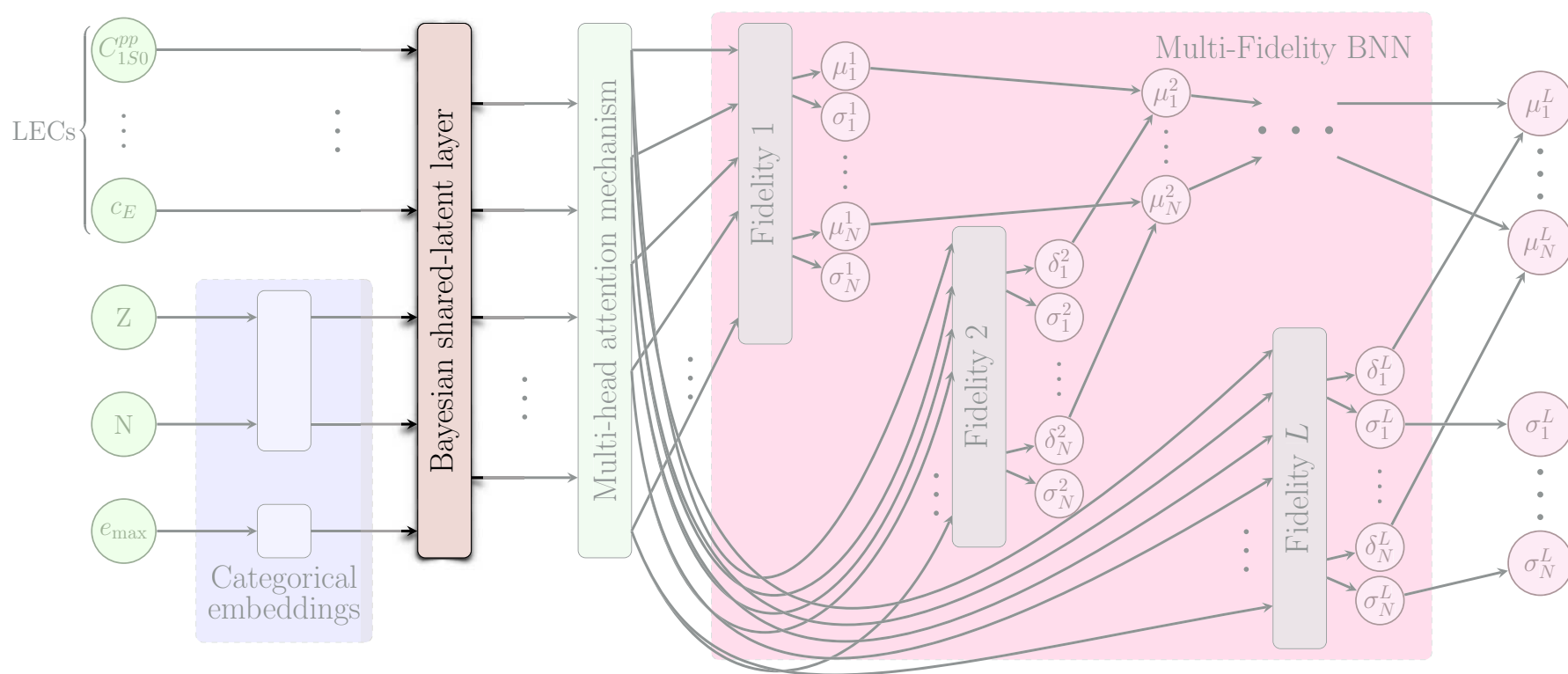
# Embeddings

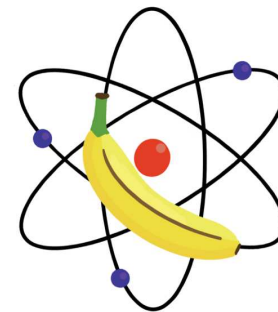
**Encodes discrete data into a vector space, while learning their relative positions, e.g.**

- $e_{max} = 4 \rightarrow 6 \rightarrow 8 \rightarrow 10$
- **Positions in the nuclear chart: ordering of N and Z**

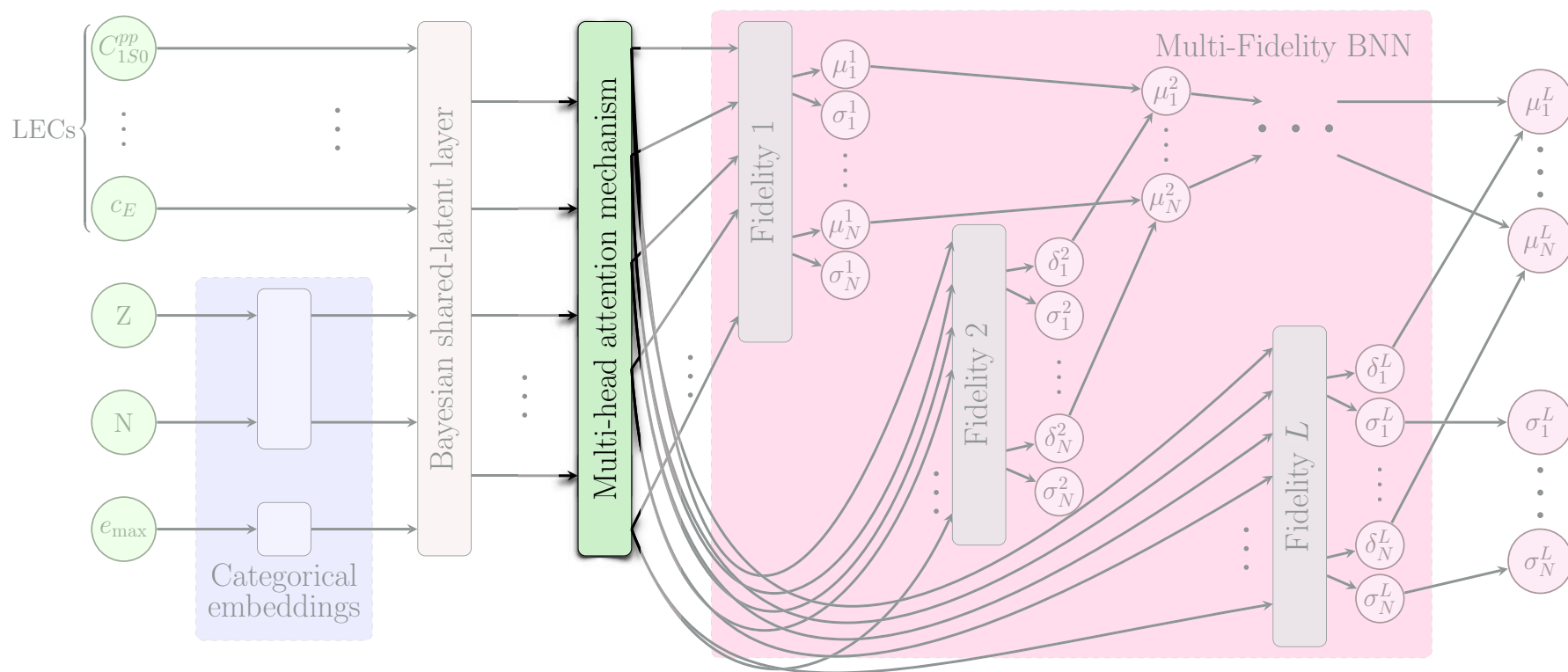


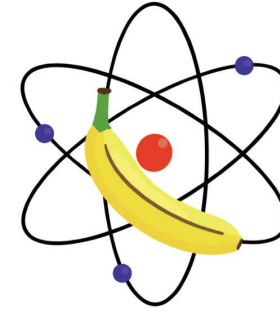
## BAYesian Neural Network for Atomic Nuclei Emulation





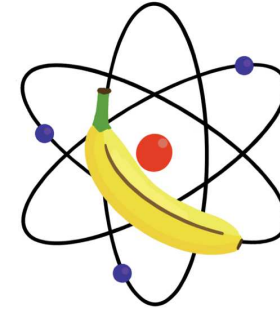
## BAYesian Neural Network for Atomic Nuclei Emulation





**Attention!**

- **Attention Mechanisms** learns how the embeddings need to be adapted due to other inputs
- **Responsible to** for the improvements of large language models in recent years!



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## Attention Is All You Need

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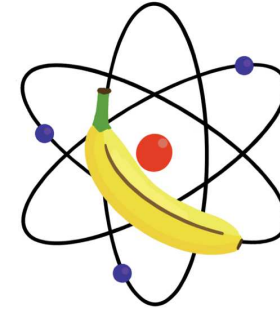
Ashish Vaswani*	Noam Shazeer*	Niki Parmar*	Jakob Uszkoreit*
Google Brain	Google Brain	Google Research	Google Research
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Illia Polosukhin\* ‡  
illia.polosukhin@gmail.com

186, 030 citations





# Attention!

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## Attention Is All You Need

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Ashish Vaswani* Google Brain avaswani@google.com	Noam Shazeer* Google Brain noam@google.com	Niki Parmar* Google Research nikip@google.com	Jakob Uszkoreit* Google Research usz@google.com
Llion Jones* Google Research llion@google.com	Aidan N. Gomez* <sup>†</sup> University of Toronto aidan@cs.toronto.edu	Lukasz Kaiser* Google Brain lukaszkaiser@google.com	
Illia Polosukhin* <sup>‡</sup> illia.polosukhin@gmail.com			

186, 030 citations

## Highly accurate protein structure prediction with AlphaFold

[John Jumper](#) ✉, [Richard Evans](#), [Alexander Pritzel](#), [Tim Green](#), [Michael Figurnov](#), [Olaf Ronneberger](#), [Kathryn Tunyasuvunakool](#), [Russ Bates](#), [Augustin Židek](#), [Anna Potapenko](#), [Alex Bridgland](#), [Clemens Meyer](#), [Simon A. A. Kohl](#), [Andrew J. Ballard](#), [Andrew Cowie](#), [Bernardino Romera-Paredes](#), [Stanislav Nikolov](#), [Rishub Jain](#), [Jonas Adler](#), [Trevor Back](#), [Stig Petersen](#), [David Reiman](#), [Ellen Clancy](#), [Michal Zielinski](#), ... [Demis Hassabis](#) ✉

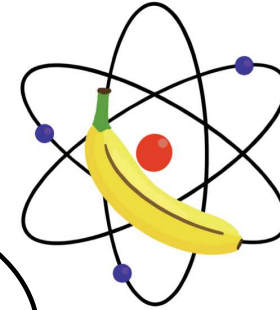
+ Show authors



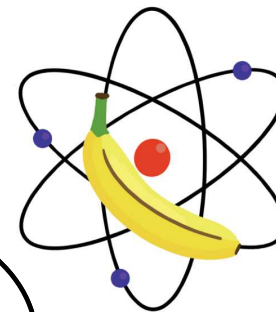
36, 760 citations



I am going  
completely bananas!

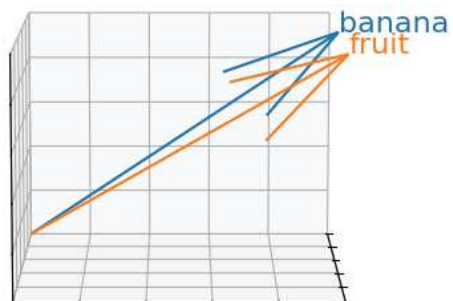
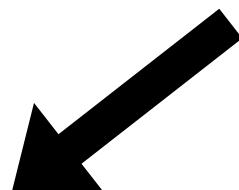


**Attention!**

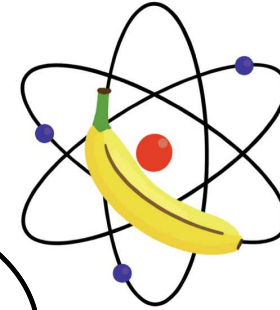


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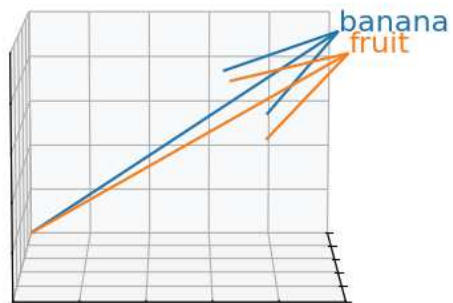
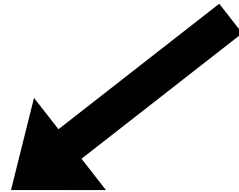
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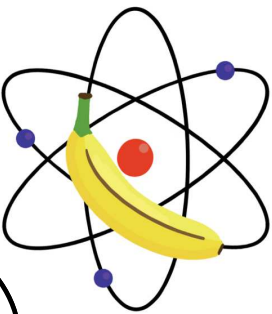
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ChatGPT:



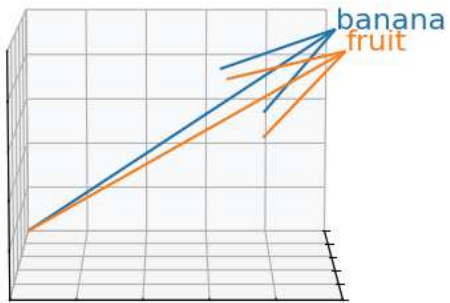
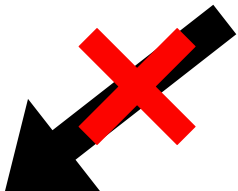
Attention!



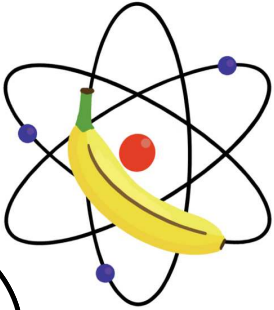
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ChatGPT:

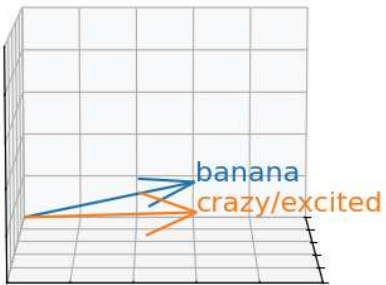
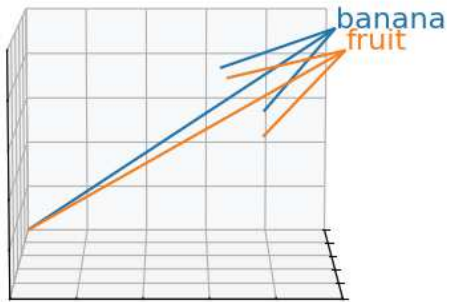
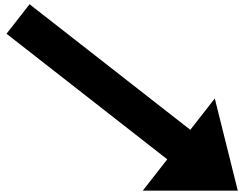


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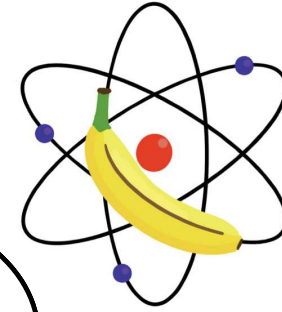


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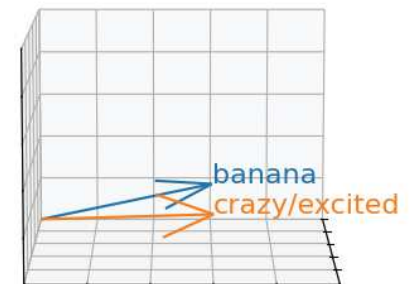
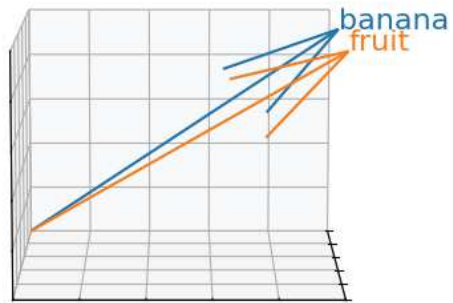


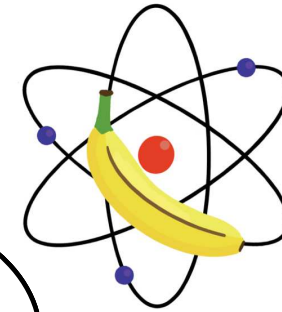




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ChatGPT:



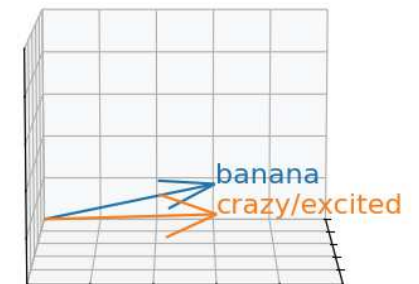
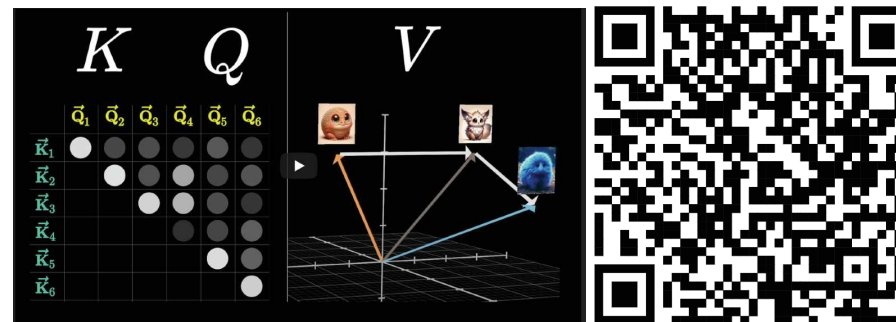
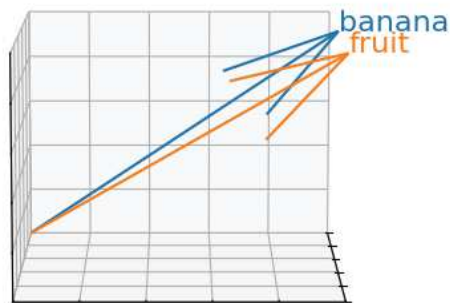


Attention!

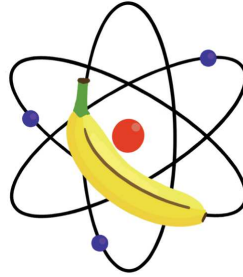
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3Blue1Brown:

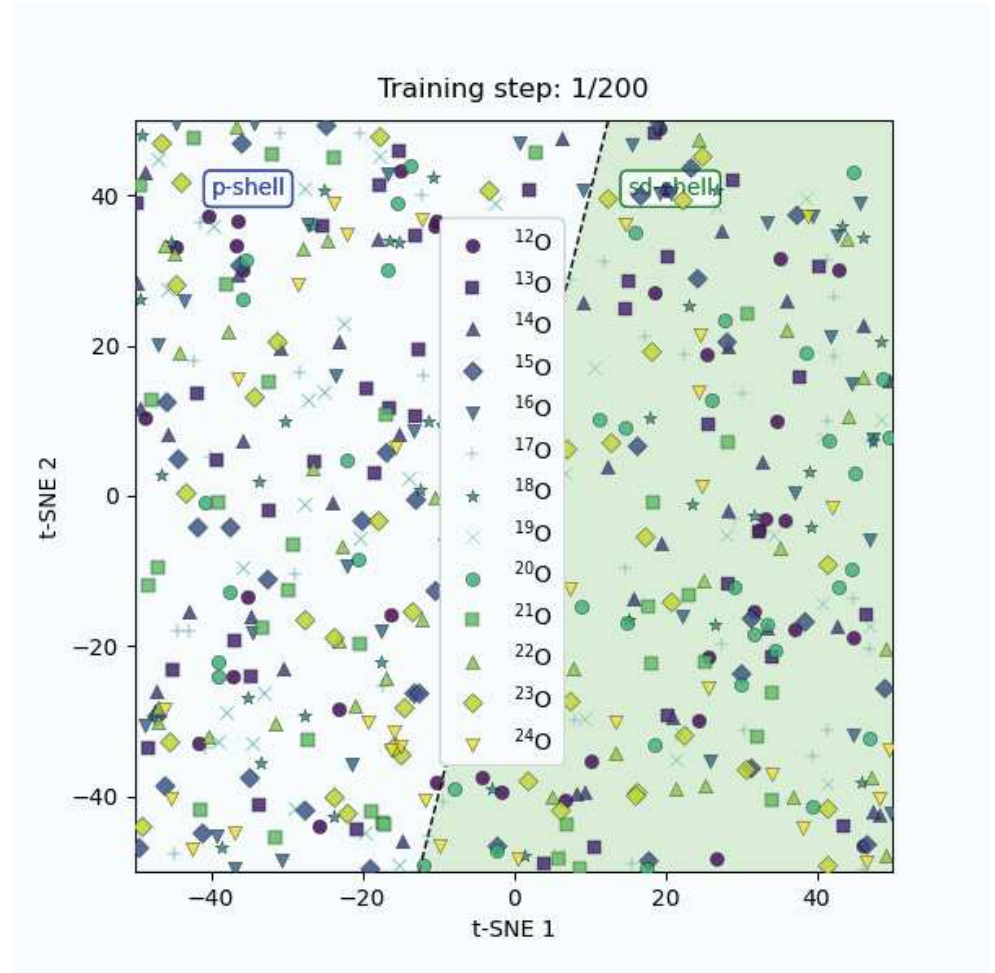
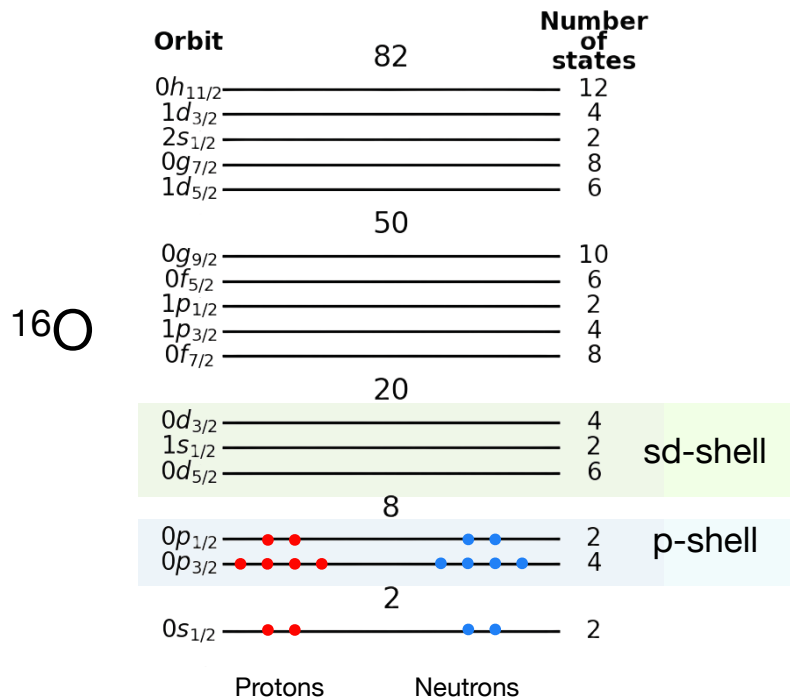


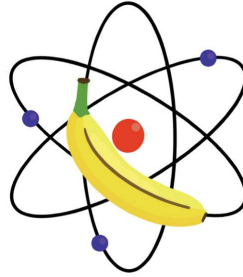




# Visualizing the Embeddings

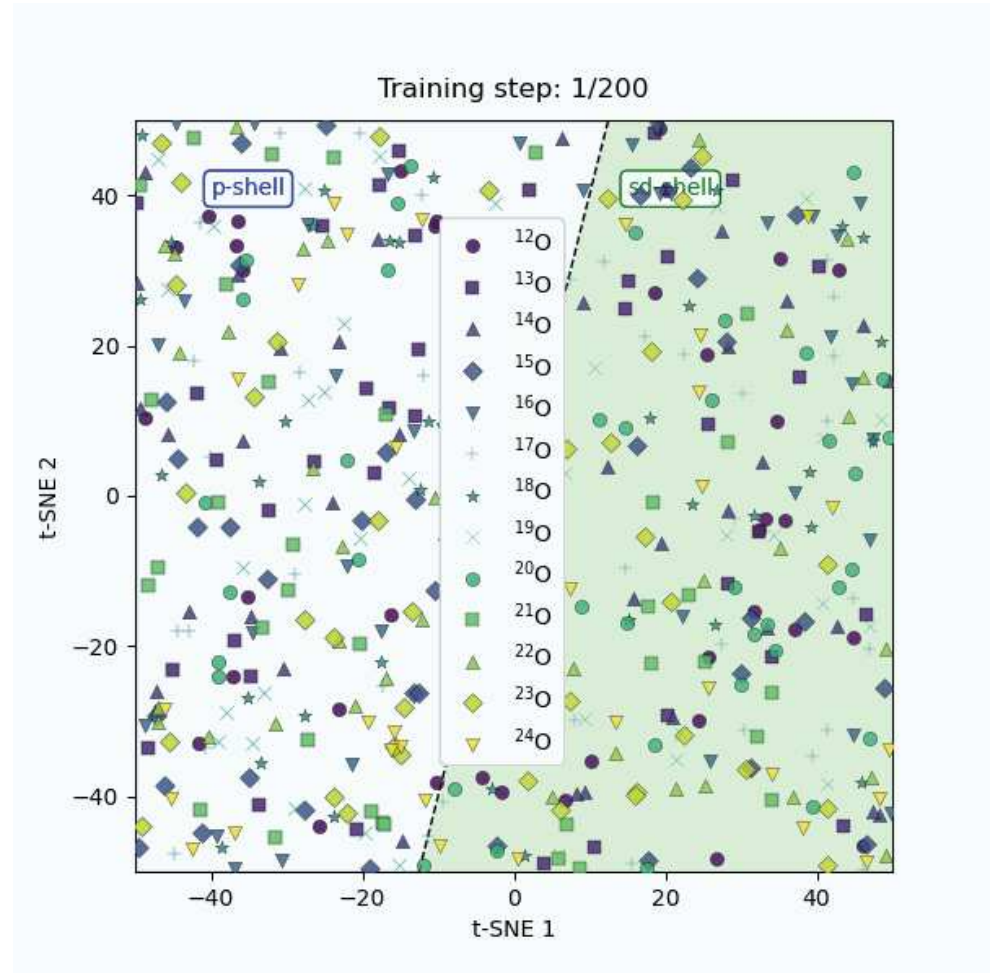
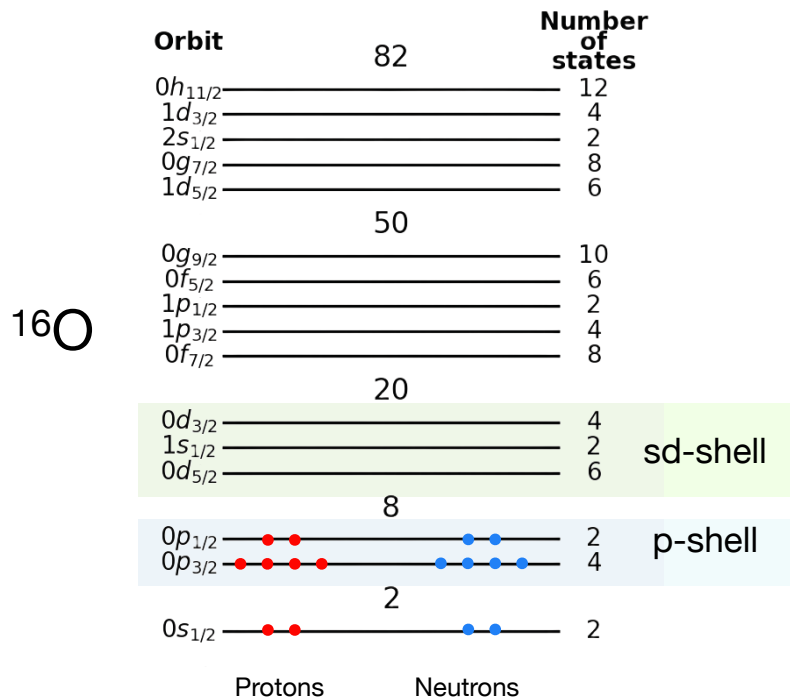
- Projection of embeddings from the attention mechanism.
- Model is learning nuclear shells!

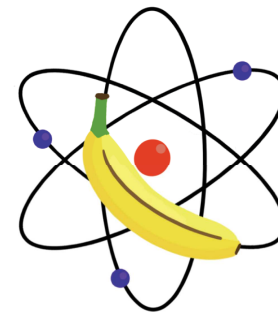




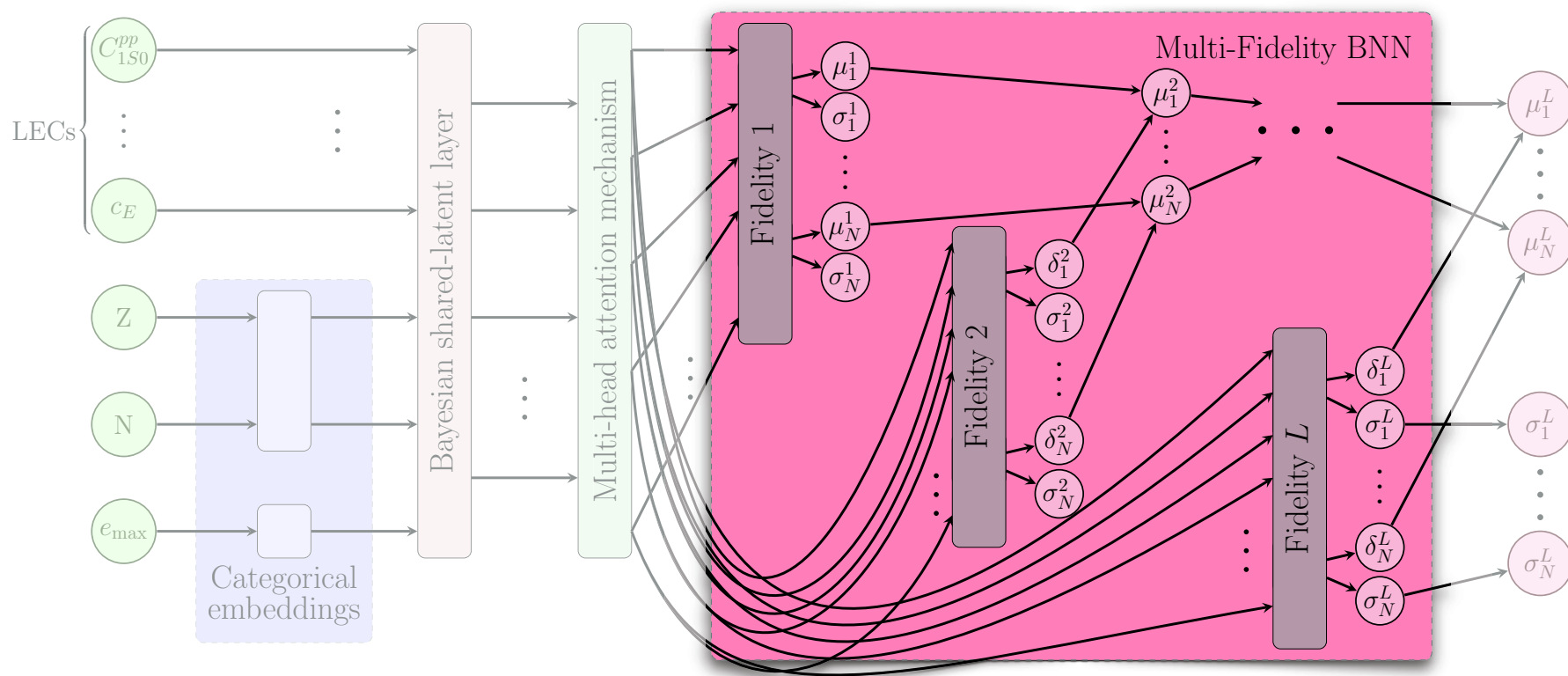
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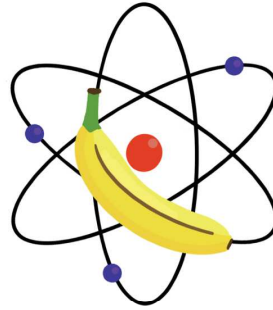




## BAYesian Neural Network for Atomic Nuclei Emulation

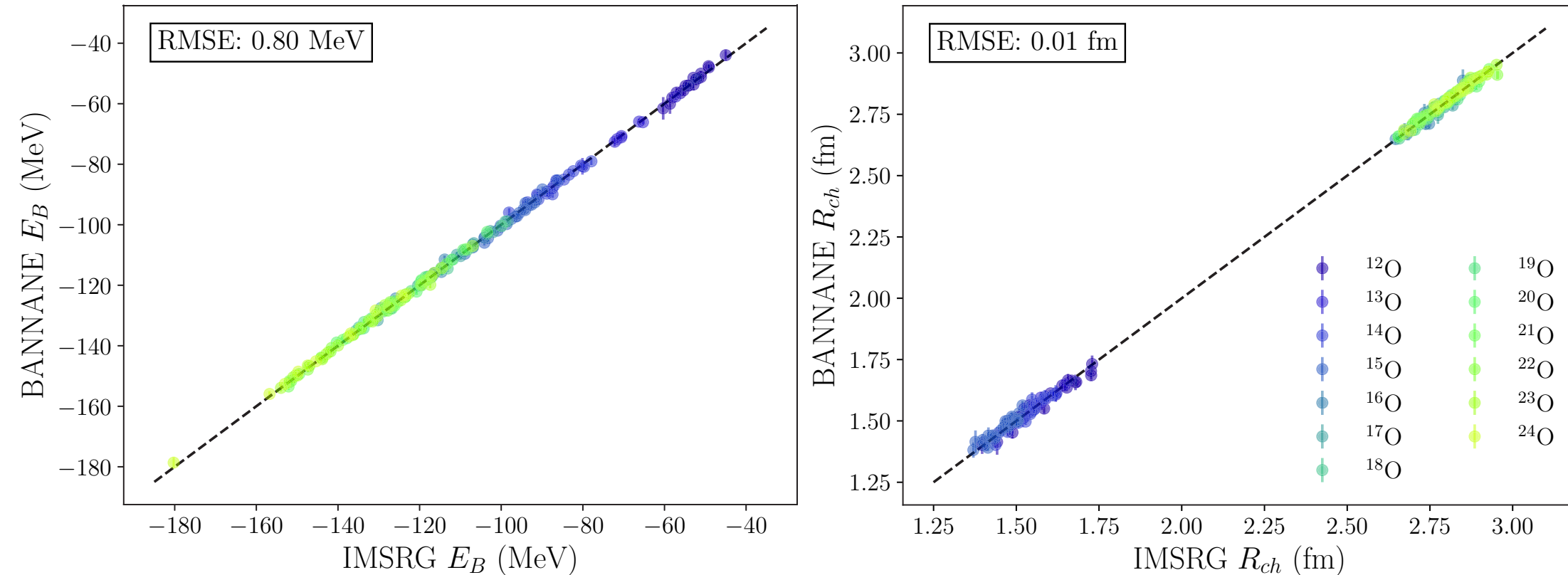


# Results

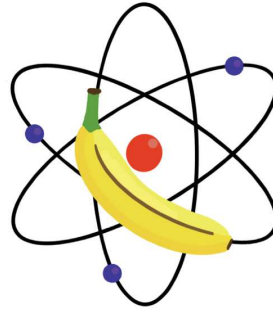


# Emulating Multiple Isotopes

Belley, Munoz, García., arxiv:2502.20363



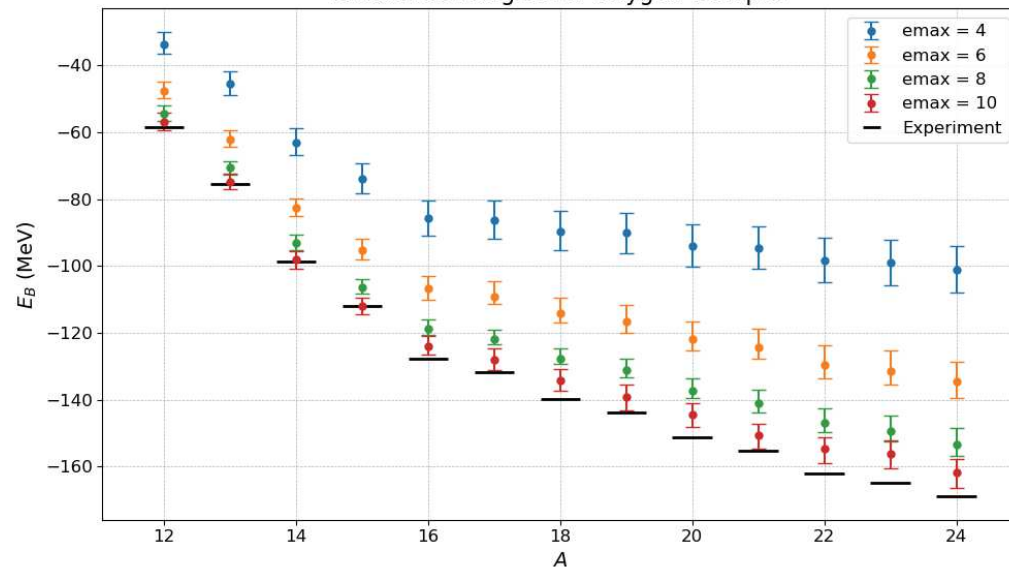
BANNANE achieves state-of-the-art emulation, with smaller errors than other emulators while emulating over a full isotopic chain.



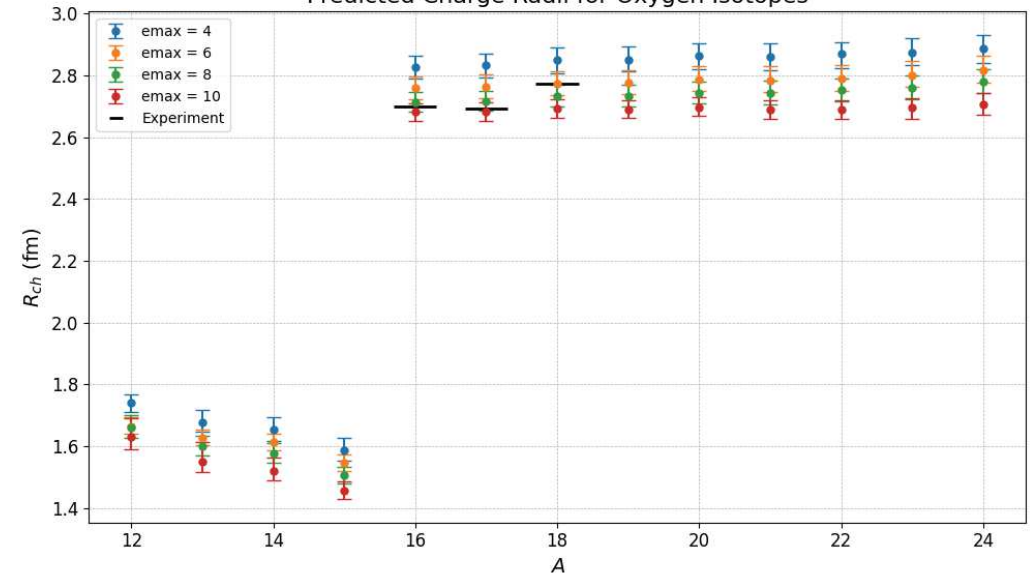
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Belley, Munoz, Garcia., arxiv:2502.20363

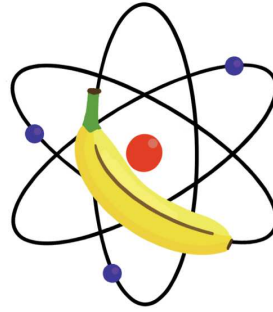
Predicted Binding Energies for Oxygen Isotopes



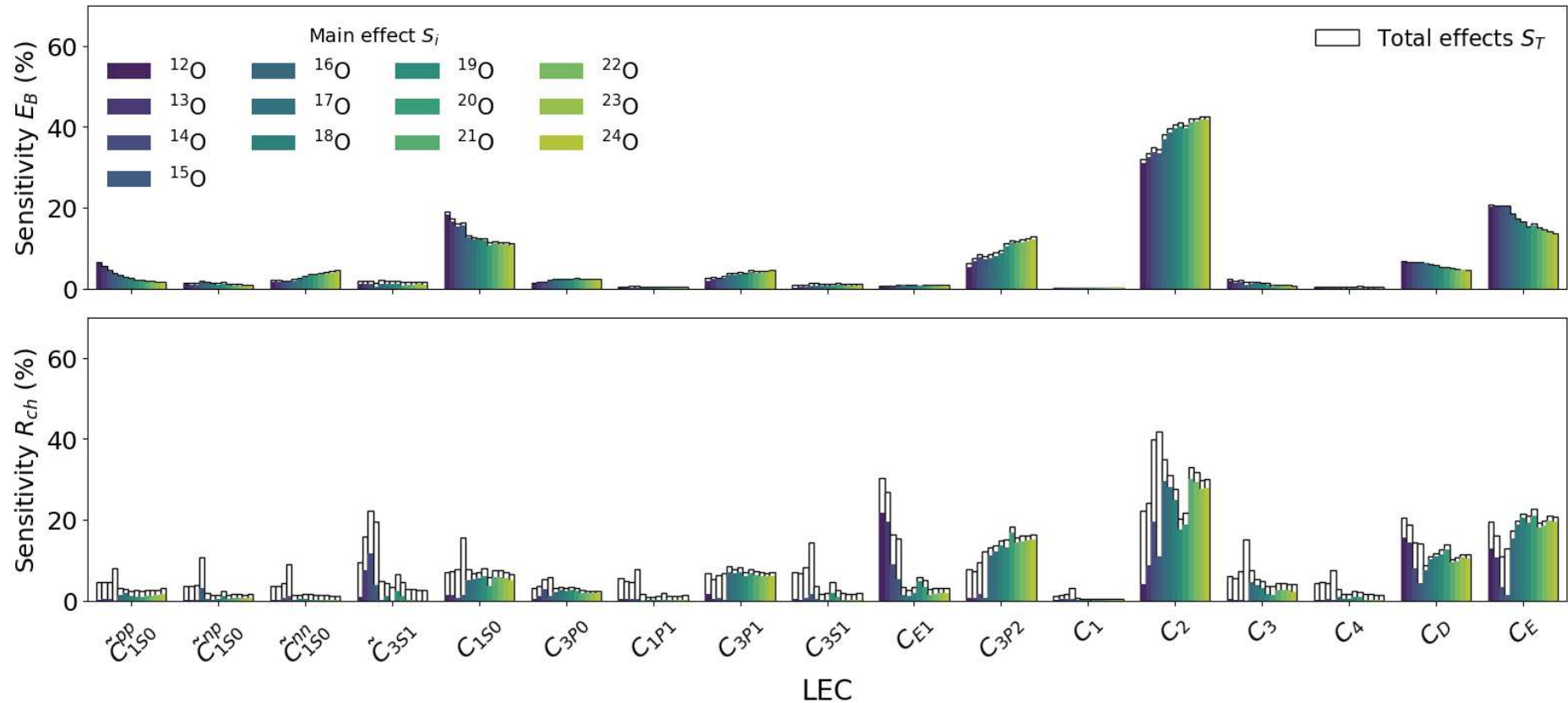
Predicted Charge Radii for Oxygen Isotopes



Combining this with UQ technique, we can predict observables with associated uncertainties over the full isotopic chains in a few minutes.

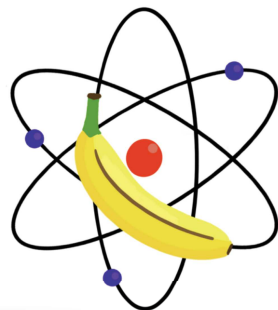


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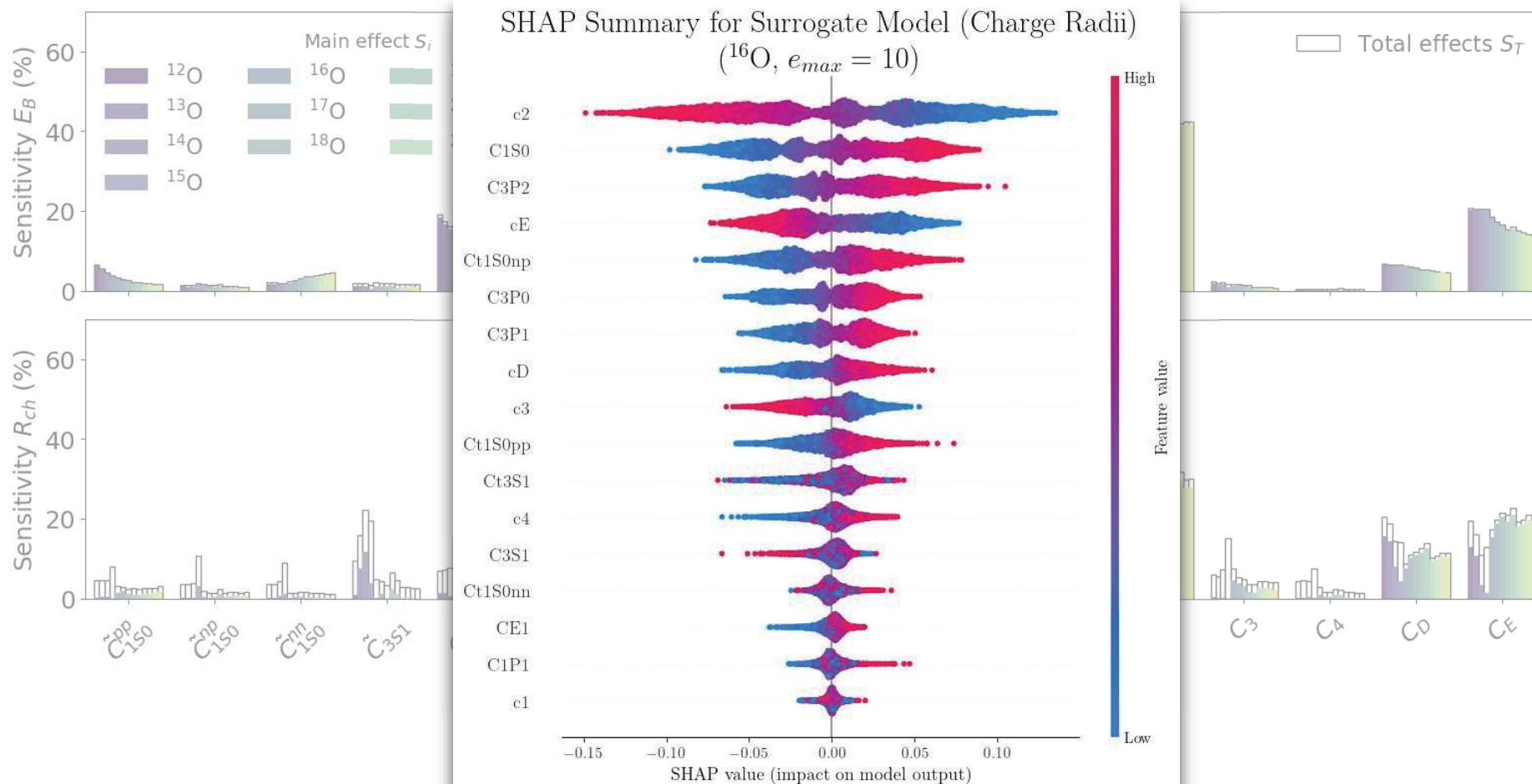


Global sensitivity analysis is consistent with other emulators!

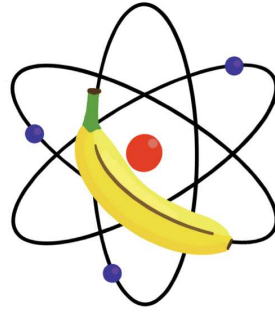




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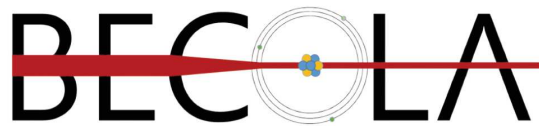
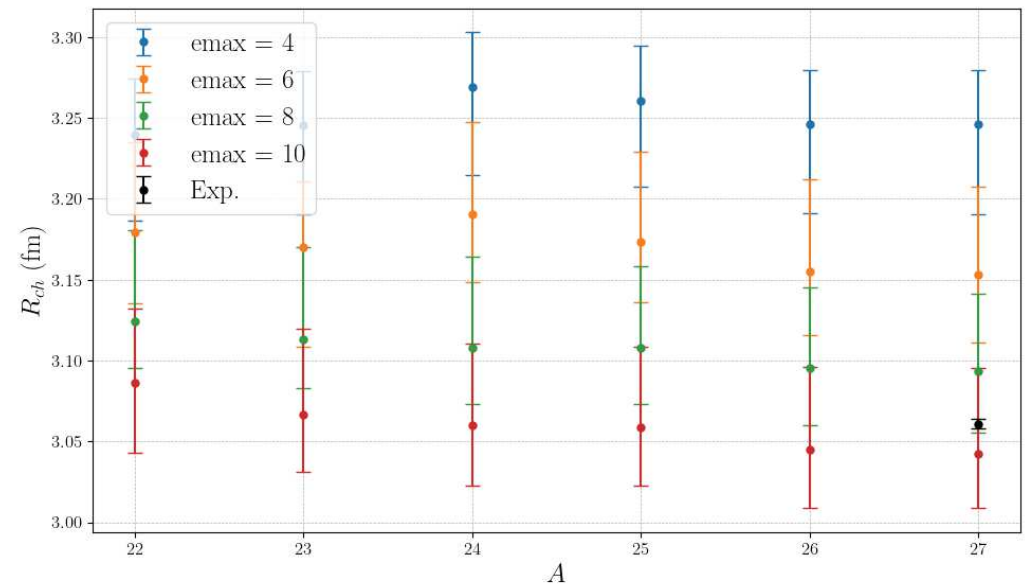


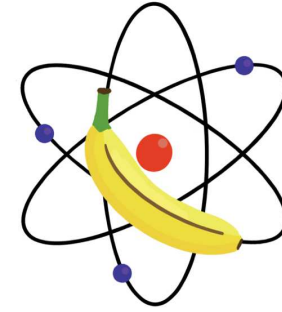


# BANNANE with Experiments

Collaboration with the Resonant ionization Spectroscopy Experiment (RiSE) at BECOLA facility at FRIB

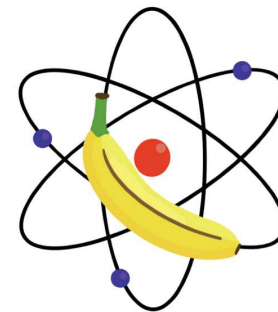
- Study charge radii of Aluminum isotopes.
- BANNANE is used to understand the trends across the isotopic chain from theory point of view.
- Results soon available.





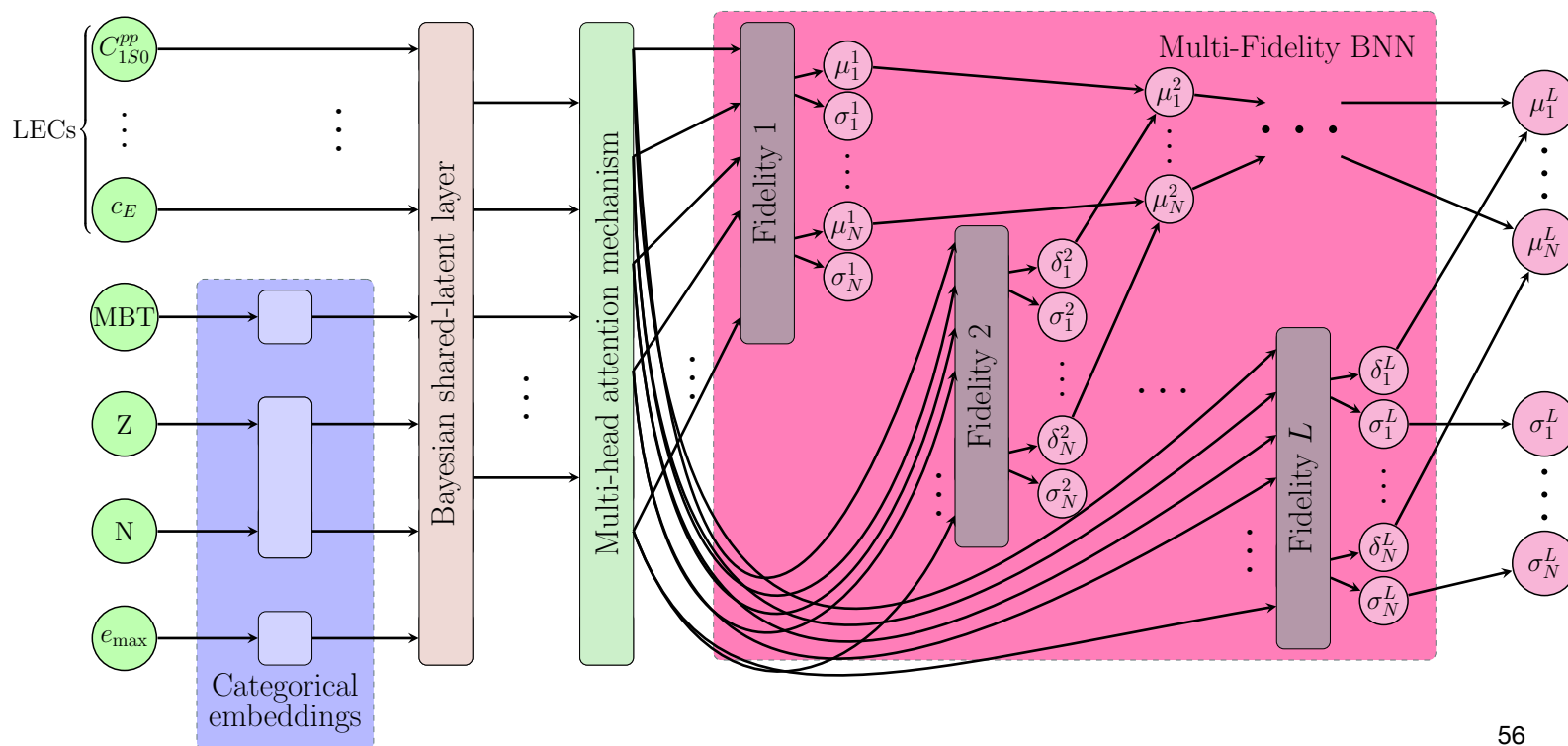
**BANNANE**

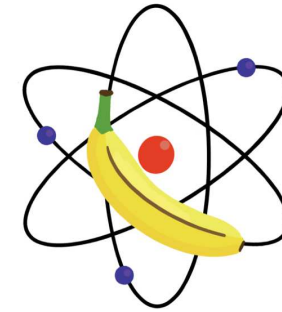
- **BANNANE architecture is extremely flexible! Categorical embeddings allow to encode a lot more: e.g.**



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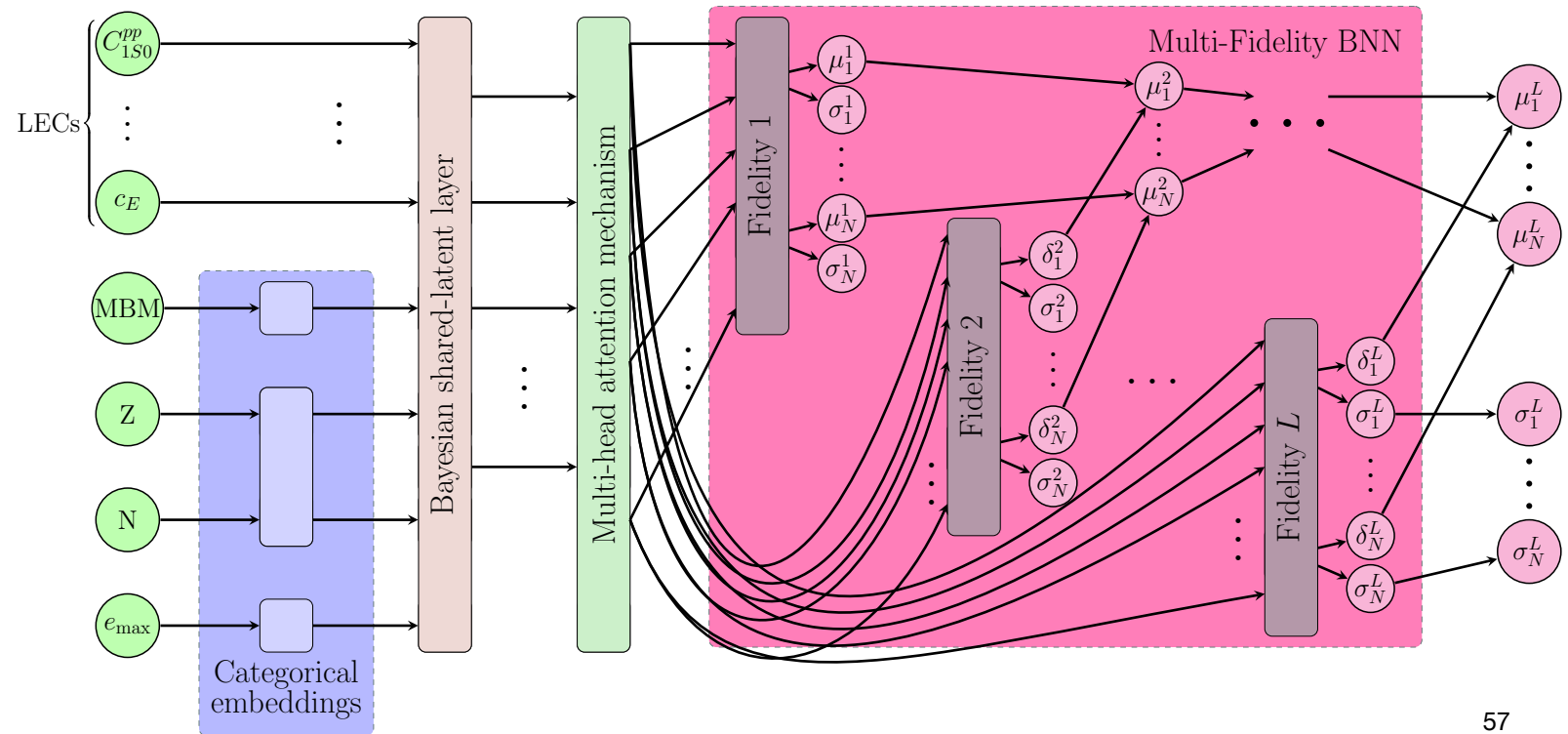
Can encode results from different truncation schemes as well, e.g.  
 HF, IMSRG(2), IMSRG(3f2), IMSRG(3), ...  
 or  
 CCS, CCSD, CCSDT1, ...

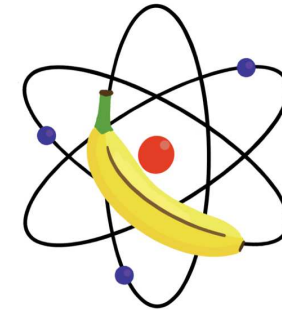




- **BANNANE architecture is extremely flexible! Categorical embeddings allow to encode a lot more: e.g.**

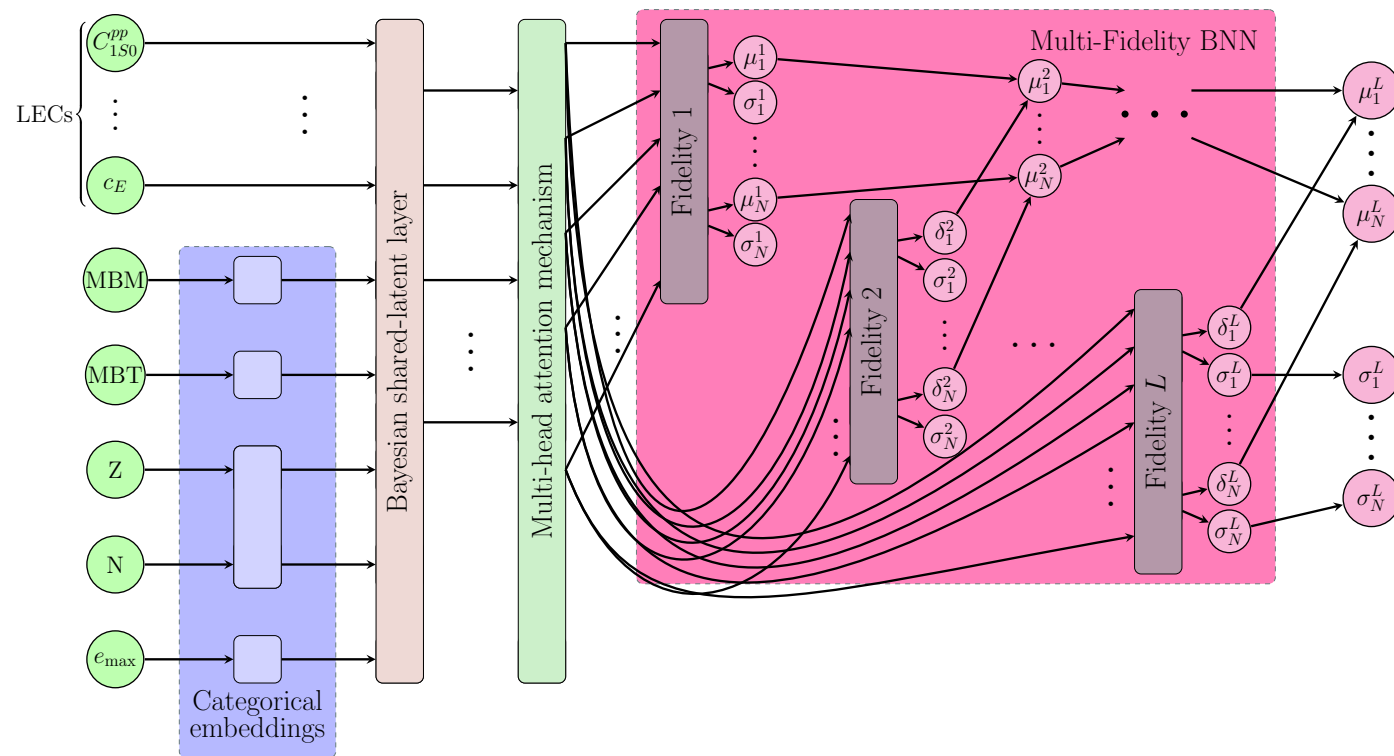
Can encode results from different many-body methods to be modelled simultaneously!





- **BANNANE architecture is extremely flexible! Categorical embeddings allow to encode a lot more: e.g.**

Can do both at the same time!





**Summary ...**

**Thank you!**



## Summary ...

- Developed new many-body method for PV observables.

**Thank you!**



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## Summary ...

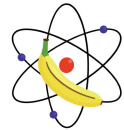
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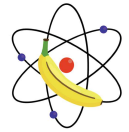


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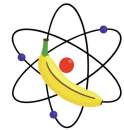
## ... and Outlook

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## ... and Outlook

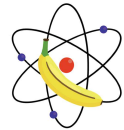
- Benchmark the PV-IMSRG with NCSM if light nuclei for multiple parity-violating observables.

**Thank you!**



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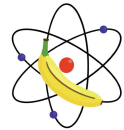
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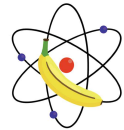
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