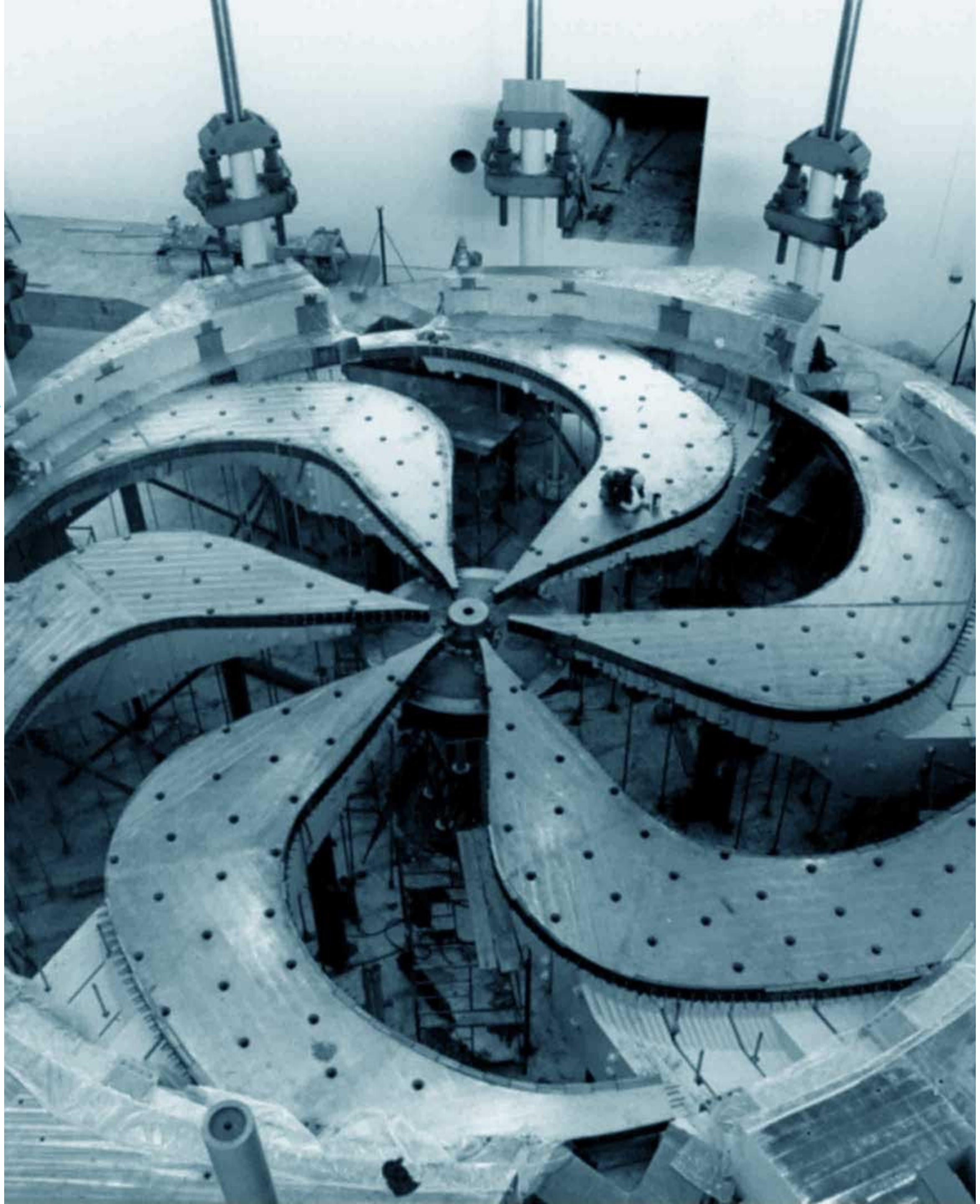
Ab initio theory towards reliable neutrinoless double beta decay nuclear matrix elements

Antoine Belley
TRIUMF PAINT 2024

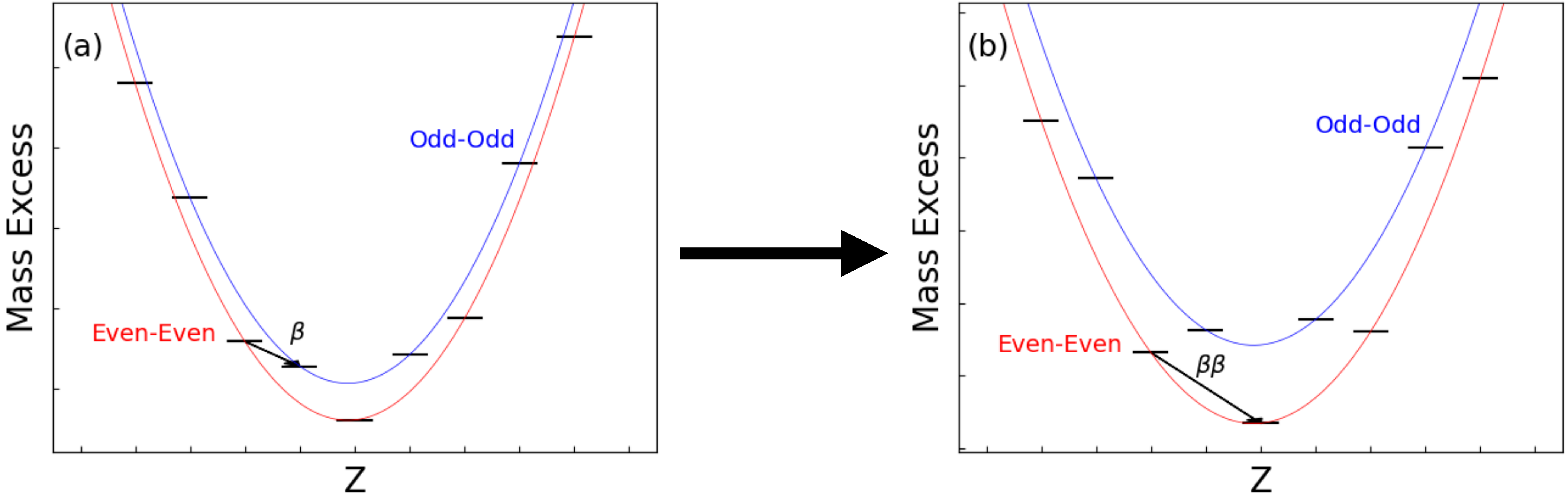
Collaborators: **Jack Pitcher**, Takayuki Miyagi, Ragnar Stroberg, Jason Holt



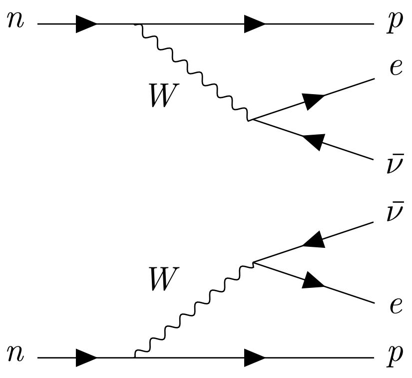
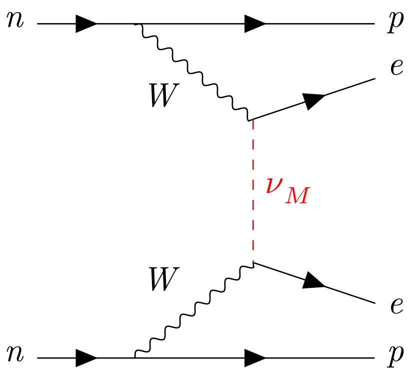
Discovery, accelerated

Second order weak process

Only possible when single beta decay is energetically forbidden (or strongly disadvantaged).

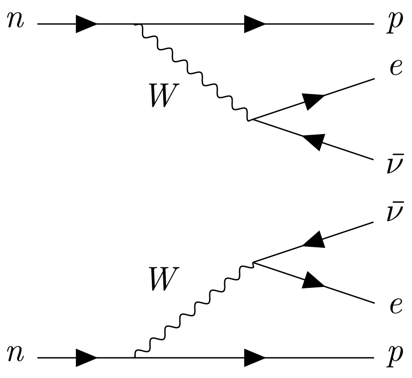
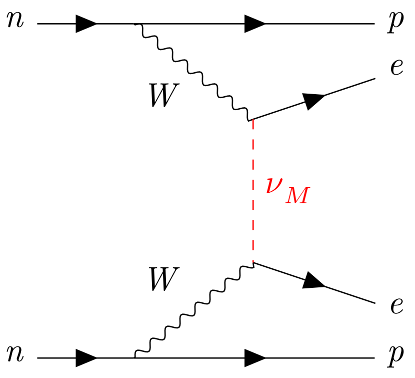


$2\nu\beta\beta$ vs $0\nu\beta\beta$

Decay	$2\nu\beta\beta$	$0\nu\beta\beta$
Diagram		
Half-life Formula	$[T^{2\nu}_{1/2}]^{-1} = G^{2\nu}\|M^{2\nu}\|^2$	$[T^{0\nu}_{1/2}]^{-1} = G^{0\nu}\|M^{0\nu}\|^2\left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2$
NME Formula	$M^{2\nu} \approx M^{2\nu}_{GT}$	$M^{0\nu} = M^{0\nu}_{GT} - (\frac{g_v}{g_a})^2 M^{0\nu}_F + M^{0\nu}_T - 2g_{\nu\nu}M^{0\nu}_{CT}$
LNV	No	Yes!
Observed	Yes	No

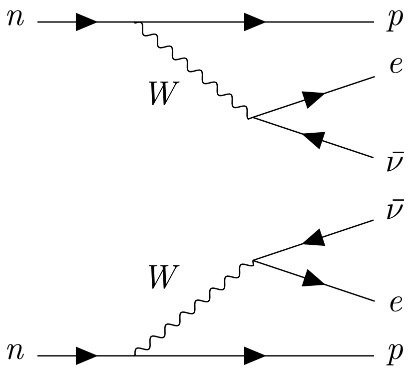
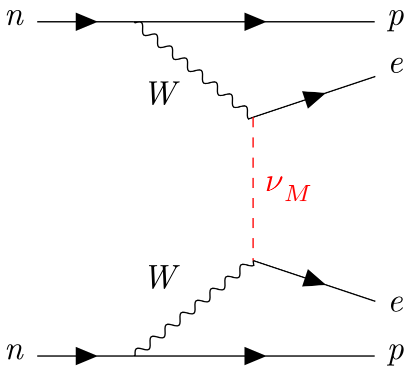
*NME : Nuclear matrix elements
**LNV : Lepton number violation

2νββ vs 0νββ

Decay	$2\nu\beta\beta$	$0\nu\beta\beta$
Diagram		
Half-life Formula	$[T^{2\nu}_{1/2}]^{-1} = G^{2\nu}\|M^{2\nu}\|^2$	$\boxed{[T^{0\nu}_{1/2}]^{-1} = G^{0\nu}\|M^{0\nu}\|^2 \left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2}$
NME Formula	$M^{2\nu} \approx M^{2\nu}_{GT}$	$M^{0\nu} = M^{0\nu}_{GT} - (\frac{g_v}{g_a})^2 M^{0\nu}_F + M^{0\nu}_T - 2g_{\nu\nu}M^{0\nu}_{CT}$
LNV	No	Yes!
Observed	Yes	No

*NME : Nuclear matrix elements

**LNV : Lepton number violation

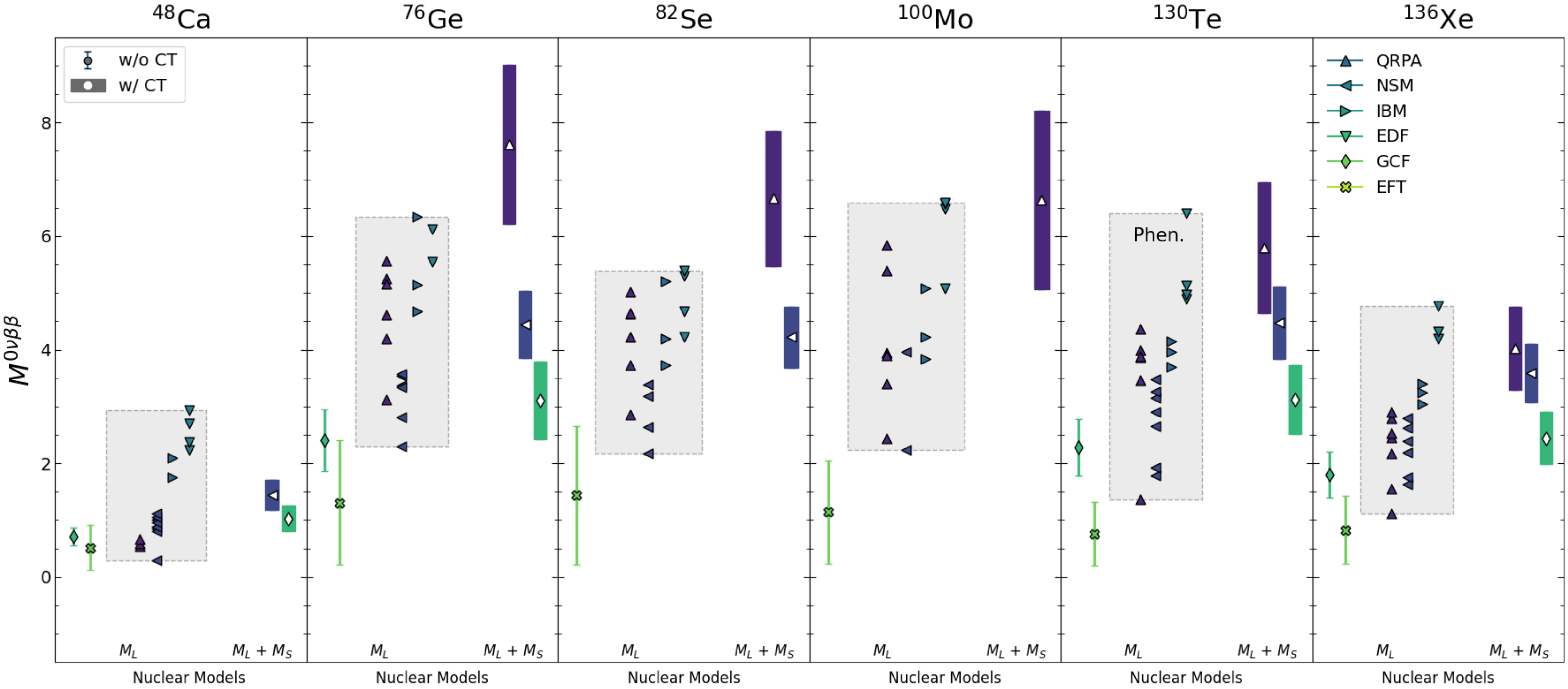
Decay	$2\nu\beta\beta$	$0\nu\beta\beta$
Diagram		
Half-life Formula	$[T^{2\nu}_{1/2}]^{-1} = G^{2\nu}\|M^{2\nu}\|^2$	$[T^{0\nu}_{1/2}]^{-1} = G^{0\nu}\|M^{0\nu}\|^2 \left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2$
NME Formula	$M^{2\nu} \approx M^{2\nu}_{GT}$	$\boxed{M^{0\nu} = M^{0\nu}_{GT} - (\frac{g_v}{g_a})^2 M^{0\nu}_{F} + M^{0\nu}_{T} - 2g_{\nu\nu}M^{0\nu}_{CT}}$
LNV	No	Yes!
Observed	Yes	No

*NME : Nuclear matrix elements
**LNV : Lepton number violation

TRIUMF

Status of 0νββ-decay Matrix Elements

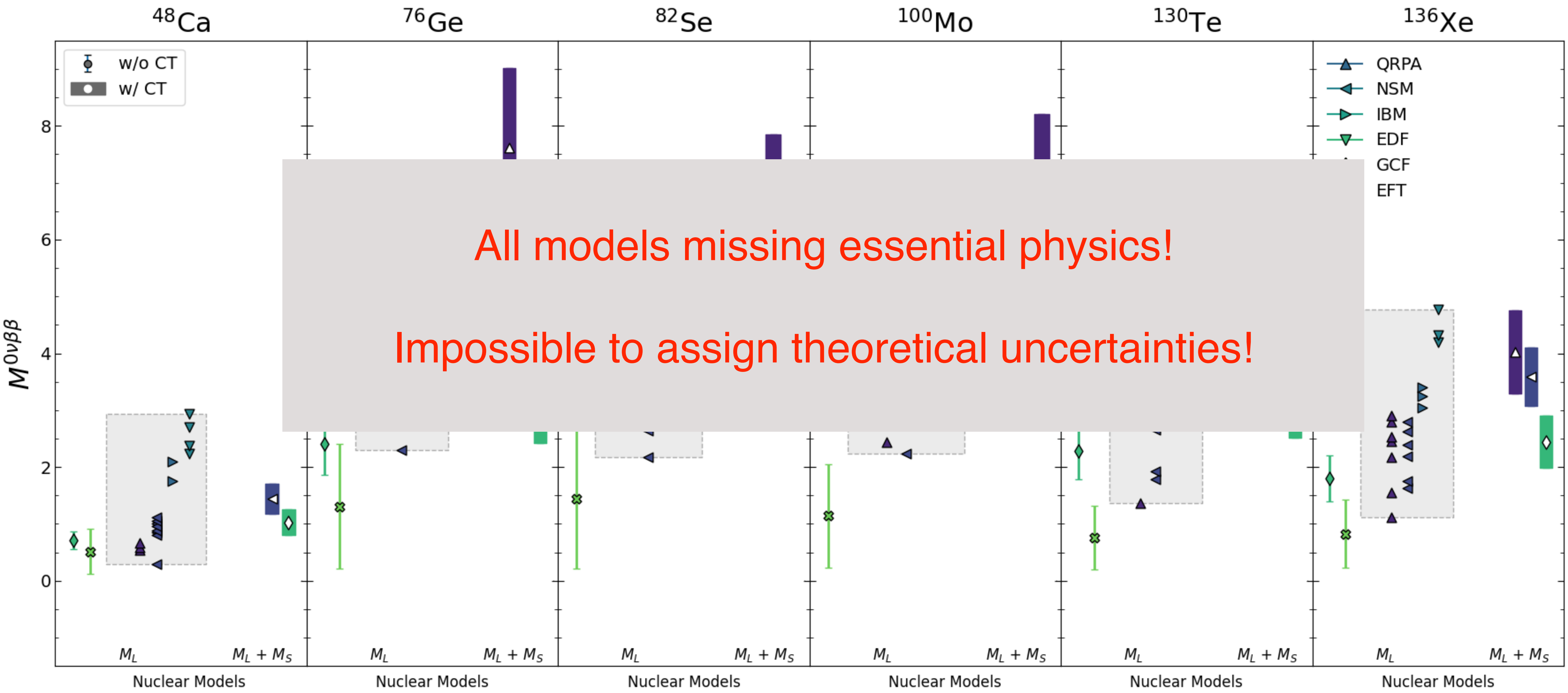
Current calculations from phenomenological models have a large spread in results.



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)

Status of 0νββ-decay Matrix Elements

Current calculations from phenomenological models have large spread in results.



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)

Goal of the talk

Show how by using ab initio methods that rely on systematically improvable expansions, a coherent picture can be achieved for the NMEs.

List of challenges

- Obtaining a result:

- Obtaining a **reliable** result:

List of challenges

- Obtaining a result:

$$NME = \langle \psi_f | O | \psi_i \rangle$$

- Obtaining a **reliable** result:

List of challenges

- Obtaining a result:

$$NME = \langle \psi_f | O | \psi_i \rangle$$

  - Deriving an expression for the nuclear potential
  - Solving the nuclear many-body problem

- Obtaining a **reliable** result:

List of challenges

- Obtaining a result:

$$NME = \langle \psi_f | O | \psi_i \rangle$$

  - Deriving an expression for the nuclear potential
  - Solving the nuclear many-body problem
  - Deriving operators consistent with the nuclear interactions
- Obtaining a **reliable** result:

List of challenges

- Obtaining a result:

$$NME = \langle \psi_f | O | \psi_i \rangle$$

  - Deriving an expression for the nuclear potential
  - Solving the nuclear many-body problem
  - Deriving operators consistent with the nuclear interactions
- Obtaining a **reliable** result:
  - Uncertainty quantification

List of challenges

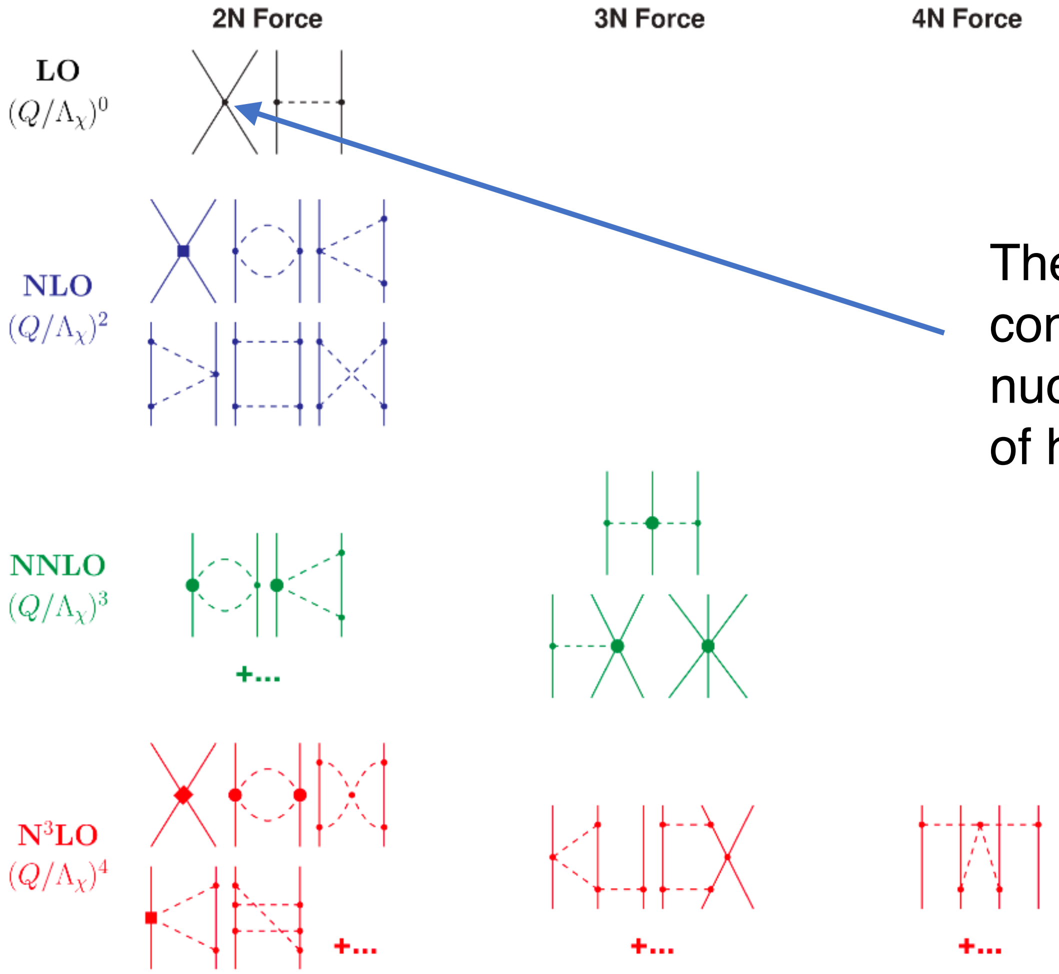
- Obtaining a result:

$$NME = \langle \psi_f | O | \psi_i \rangle$$

  - Deriving an expression for the nuclear potential (χ-EFT)
  - Solving the nuclear many-body problem (VS-IMSRG)
  - Deriving operators consistently with the nuclear interactions (EFTs)
- Obtaining a **reliable** result:
  - Uncertainty quantification

Expansion order by order of the nuclear forces

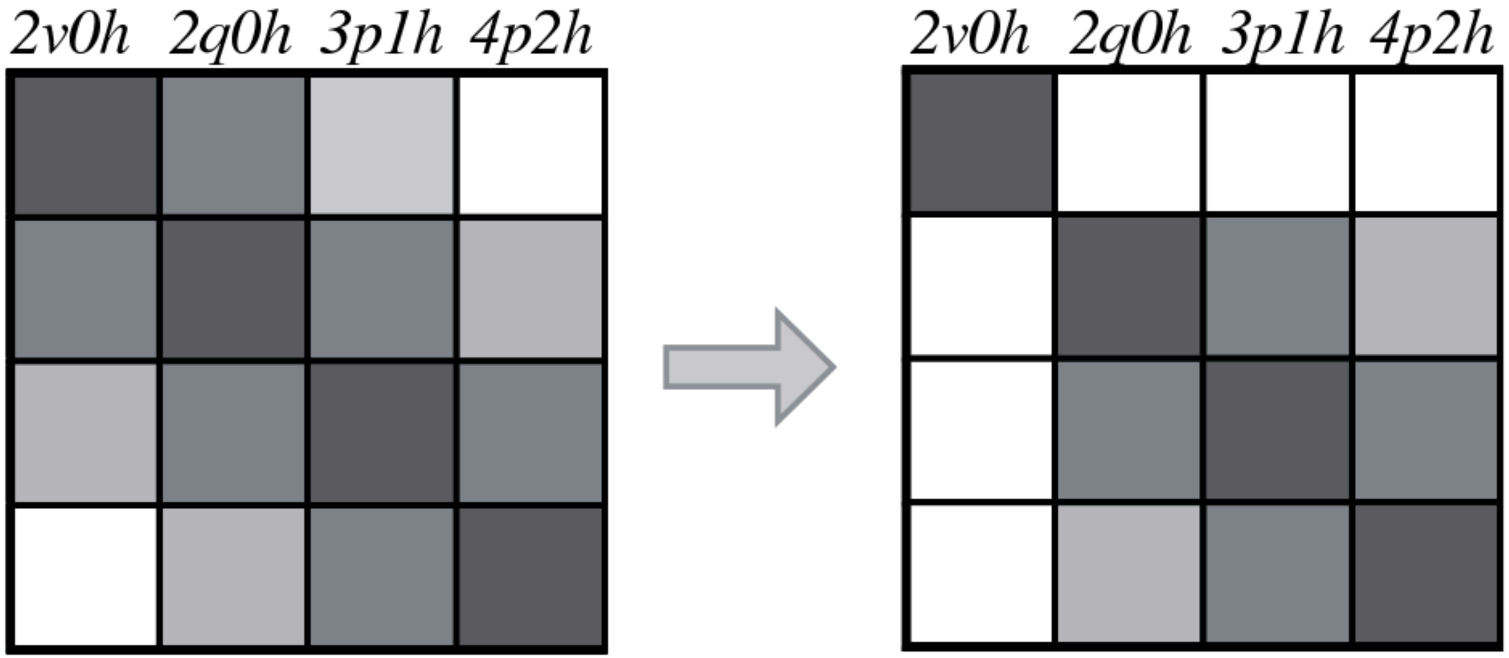
Reproduces symmetries of low-energy QCD using nucleons as fields and mesons as force carriers.



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

Machleidt and Entem, Phys. Rep., vol.503, no.1, pp.1–75 (2011)

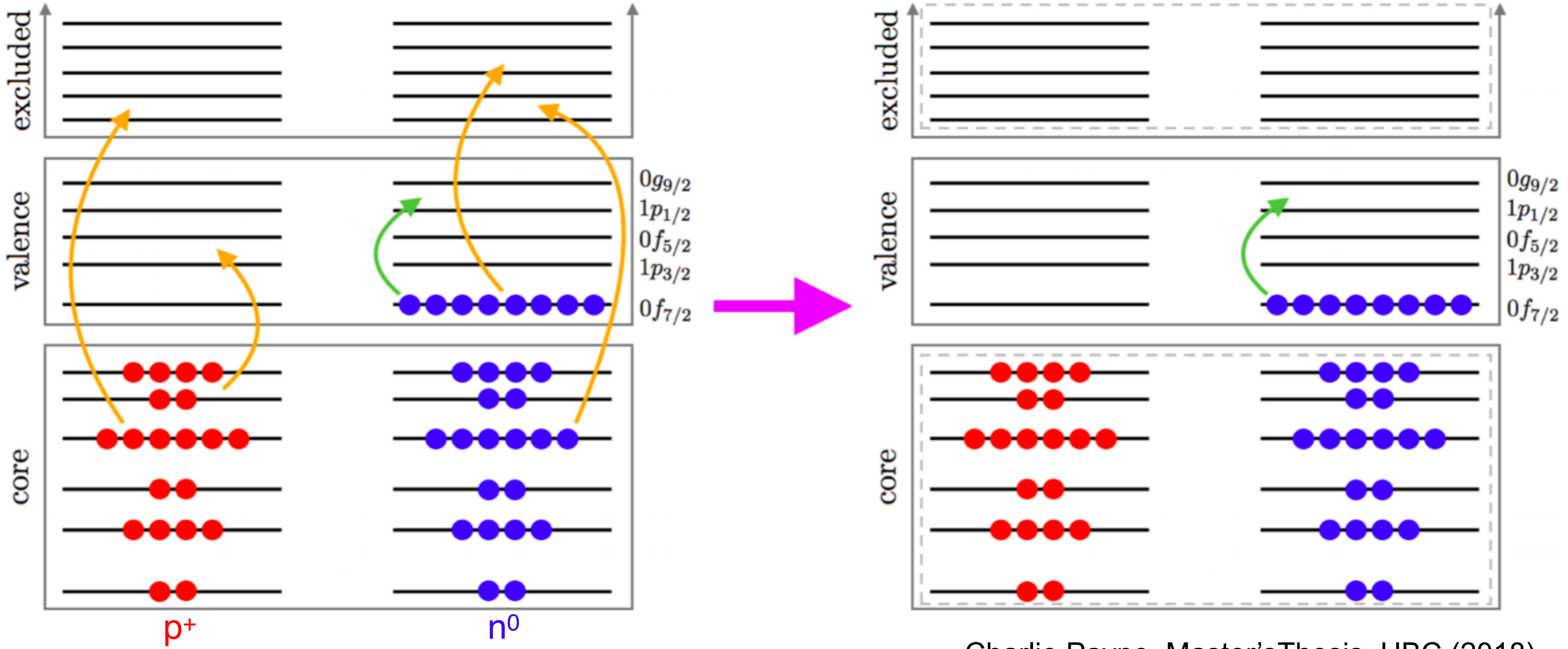
Valence-Space In Medium Similarity Renormalization Group



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

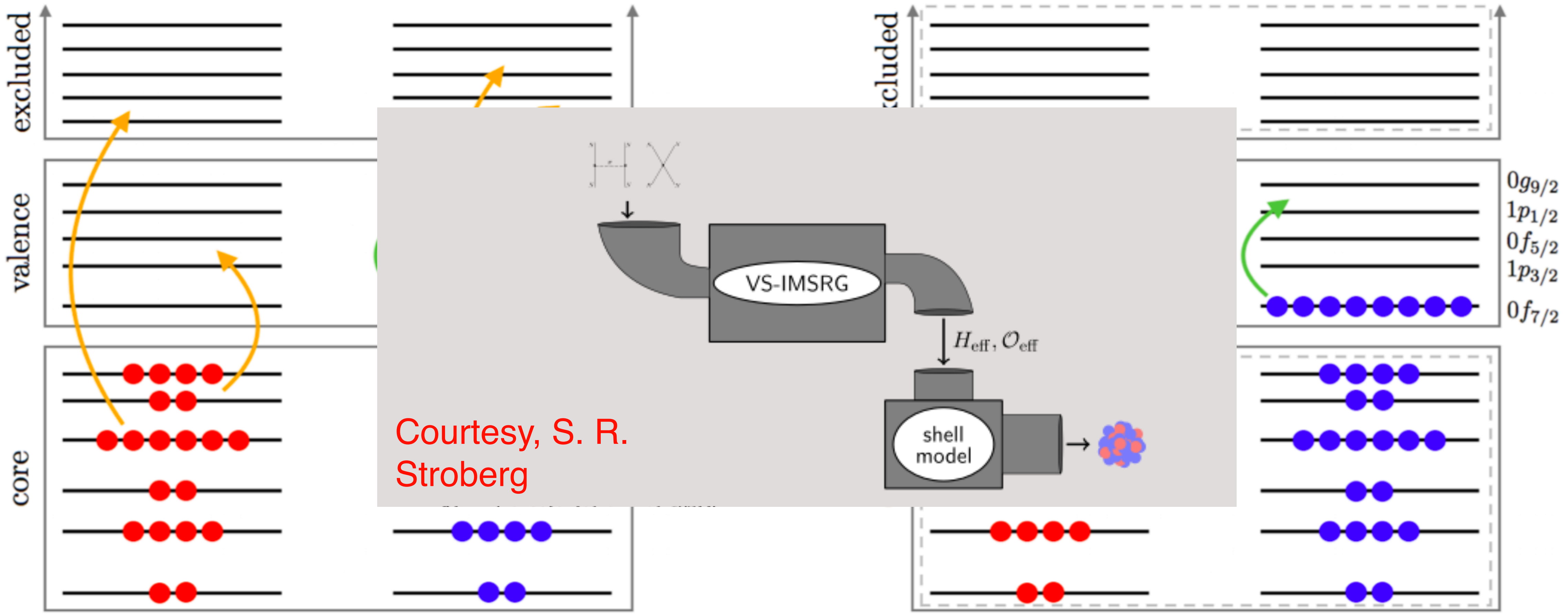
Tsukiyama et al., Phys. Rev. C **85**, 061304(R) (2012)

Valence-Space In Medium Similarity Renormalization Group



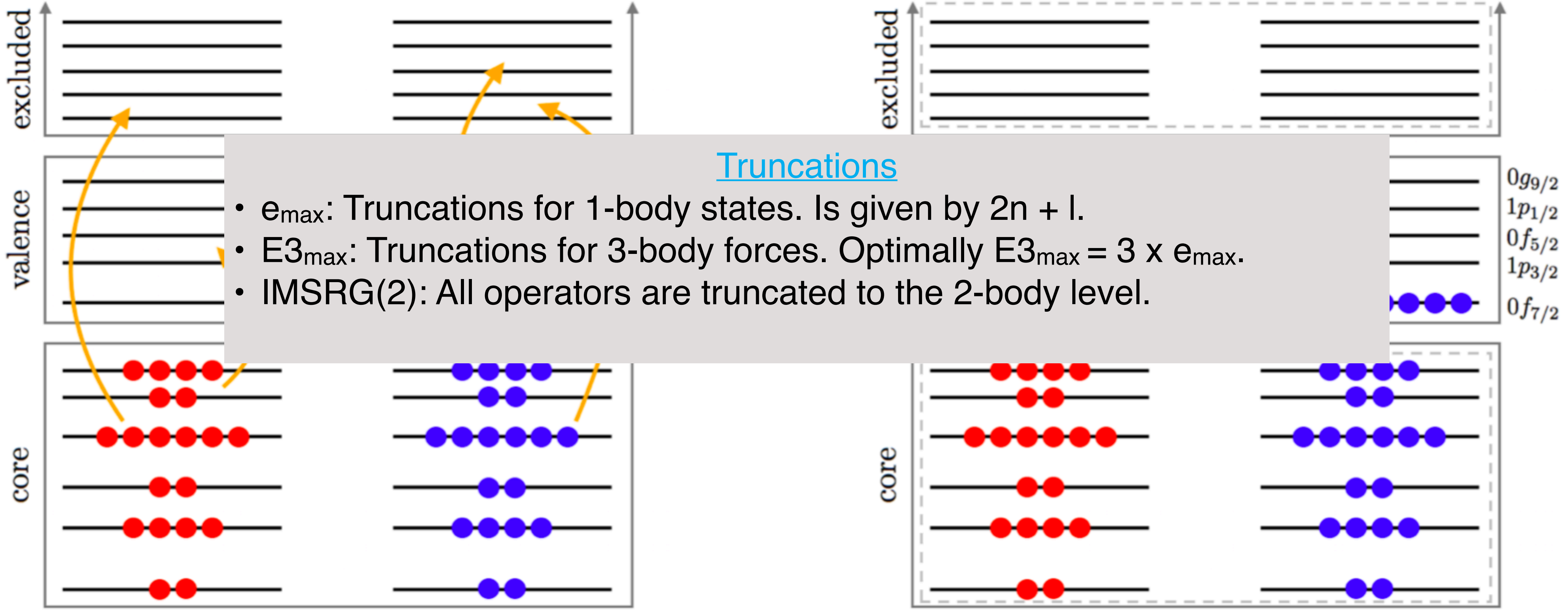
Charlie Payne, Master'sThesis, UBC (2018)

Valence-Space In Medium Similarity Renormalization Group



Courtesy, S. R. Stroberg

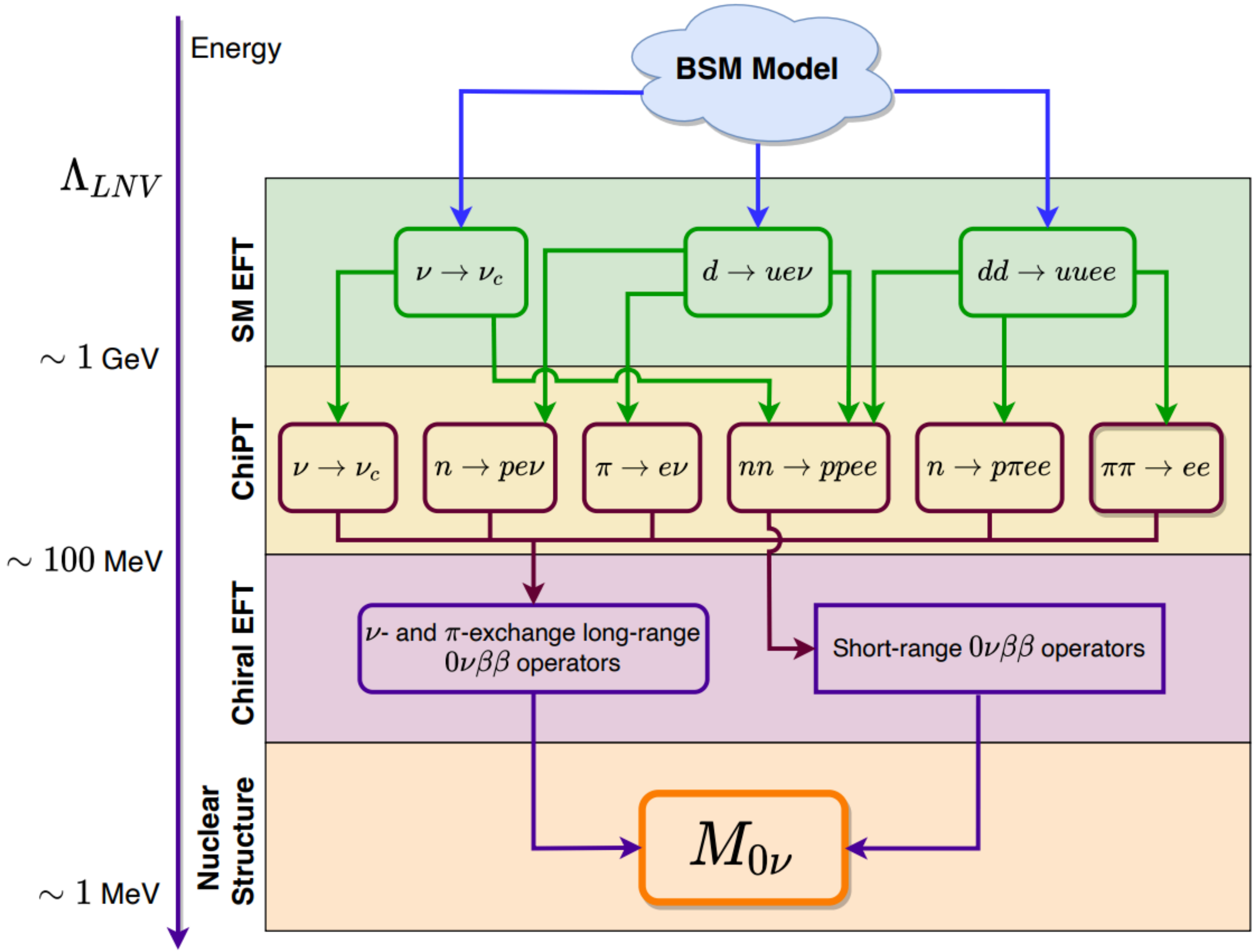
Valence-Space In Medium Similarity Renormalization Group



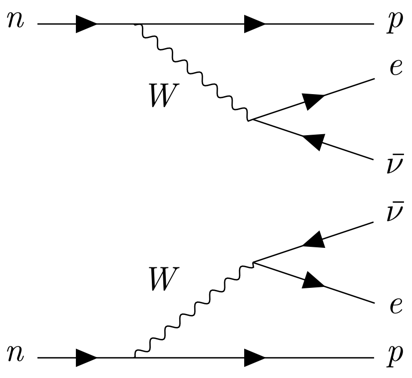
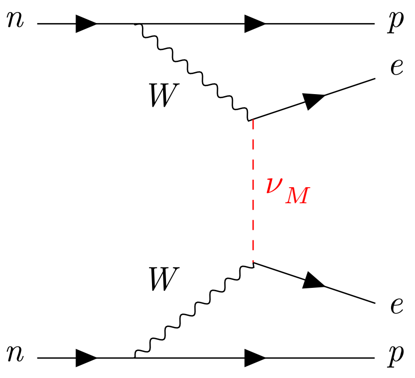
Truncations

- e_{max}: Truncations for 1-body states. Is given by 2n + l.
- $E3_{max}$: Truncations for 3-body forces. Optimally $E3_{max} = 3 \times e_{max}$.
- IMSRG(2): All operators are truncated to the 2-body level.

The EFT ladder for the operators



Cirigliano et al. J. Phys. G: Nucl. Part. Phys. **49** 120502 (2022)

Decay	$2\nu\beta\beta$	$0\nu\beta\beta$
Diagram		
Half-life Formula	$[T^{2\nu}_{1/2}]^{-1} = G^{2\nu}\lvert M^{2\nu}\rvert^2$	$[T^{0\nu}_{1/2}]^{-1} = G^{0\nu}\lvert M^{0\nu}\rvert^2 \left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2$
NME Formula	$M^{2\nu} \approx M^{2\nu}_{GT}$	$M^{0\nu} = M^{0\nu}_{GT} - (\frac{g_v}{g_a})^2 M^{0\nu}_F + M^{0\nu}_T - 2g_{\nu\nu}M^{0\nu}_{CT}$
LNV	No	Yes!
Observed	Yes	No

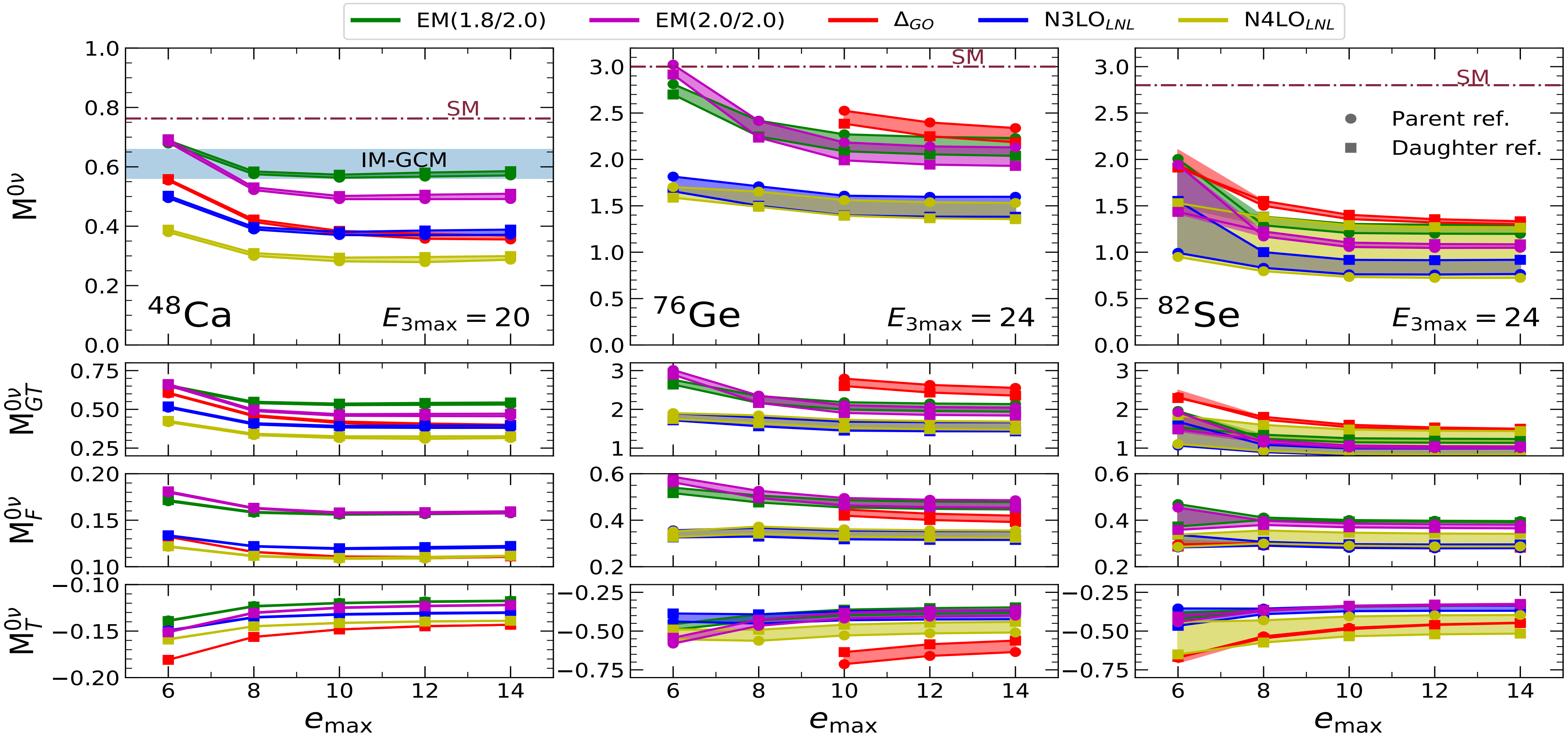
*NME : Nuclear matrix elements
**LNV : Lepton number violation

Obtaining a result

TRIUMF

Ab Initio $0\nu\beta\beta$ Decay: ^{48}Ca, ^{76}Ge and ^{82}Se

Results with 5 different input Hamiltonians to study uncertainty from interaction choice.



Things to add: valence-space variation, two-body currents, IMSRG(3), …

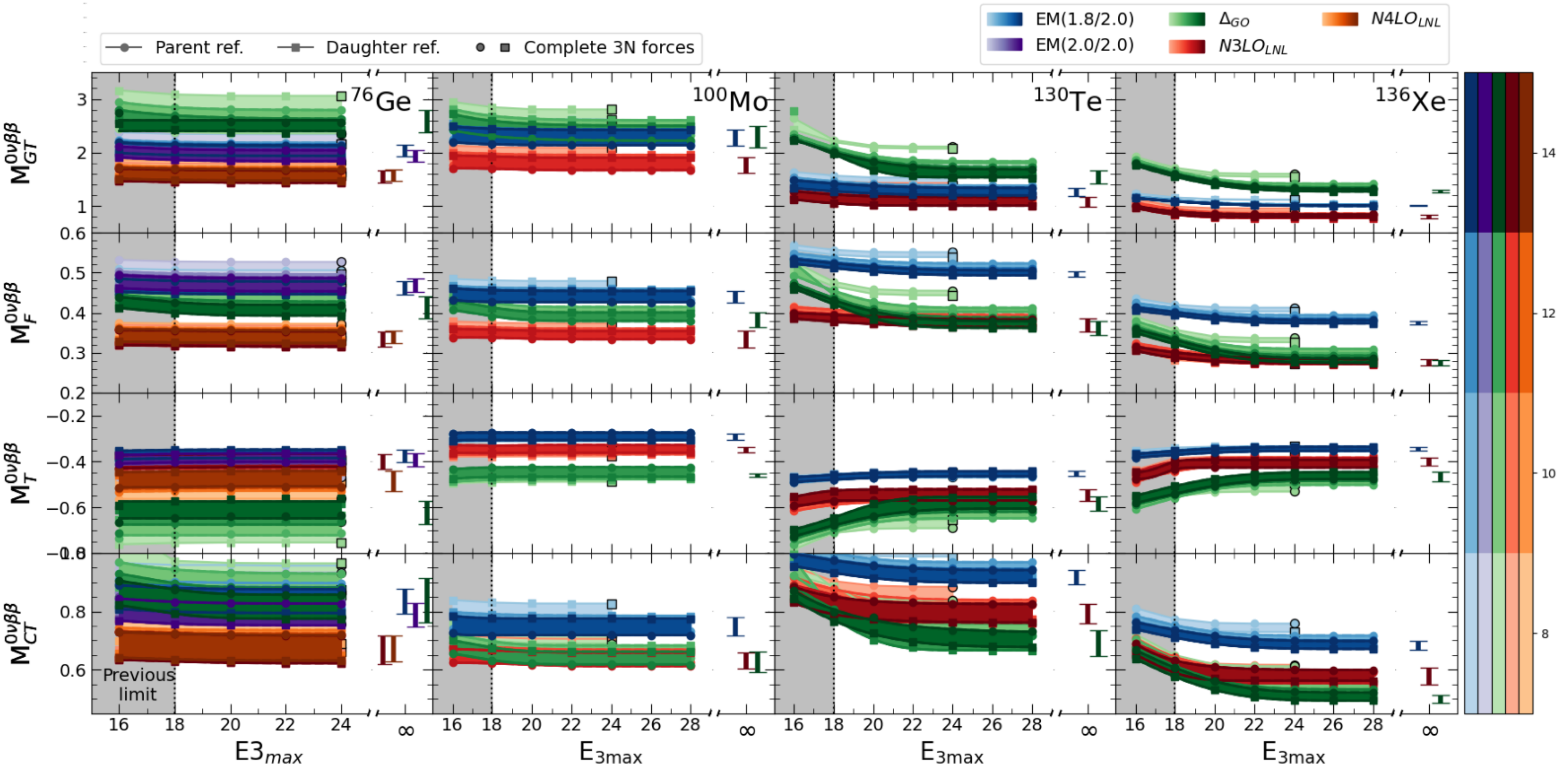
Belley, et al., PRL126.042502

Ab Initio $0\nu\beta\beta$ Decay: ^{130}Te, ^{136}Xe

TRIUMF

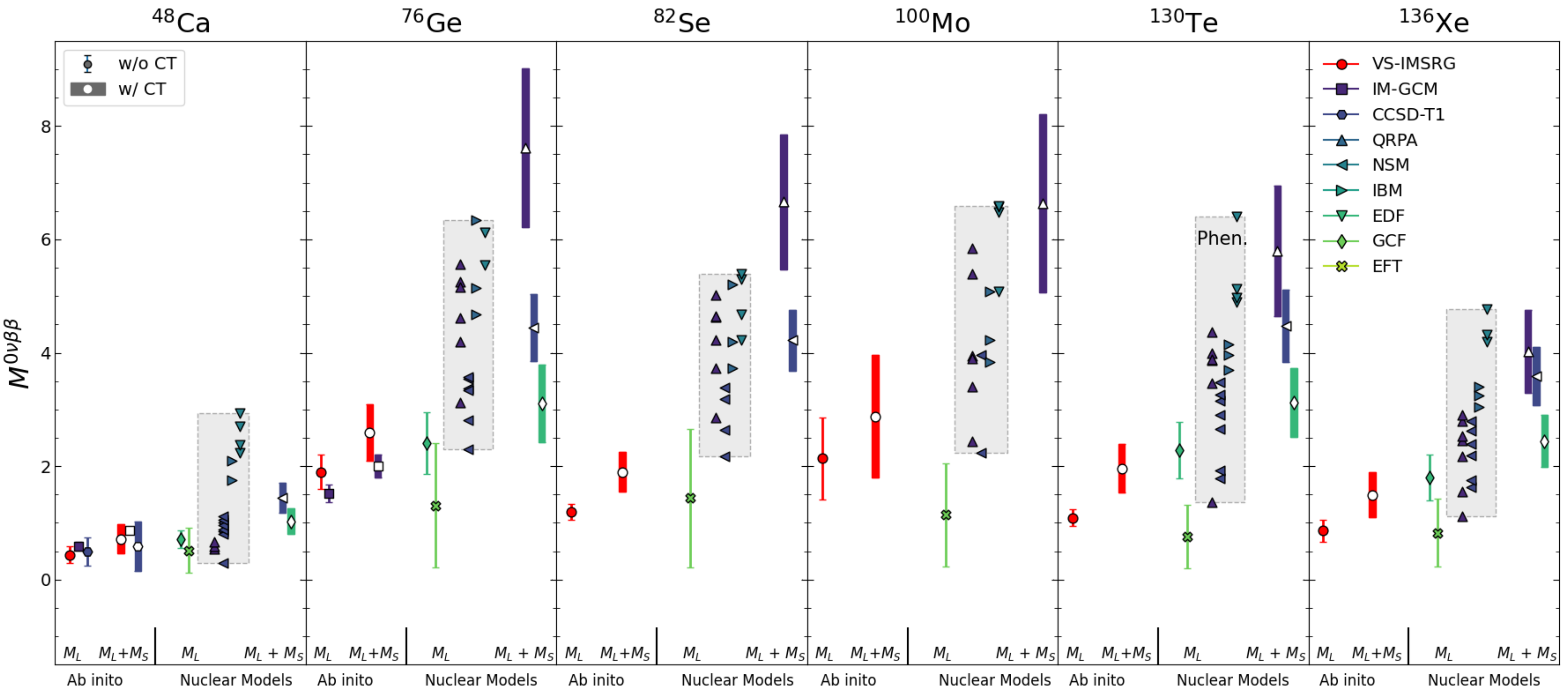
^{100}Mo, ^{130}Te, ^{136}Xe: major players in global searches with Cupid, SNO+, CUORE and nEXO.

Increased E_{3max} capabilities allow first converged ab initio calculations [EM1.8/2.0, Δ_{GO}, N3LO$_{LNL}$]. 24



Belley, et al., arXiv:2307.15156

0νββ-decay Matrix Elements: The new picture



List of challenges

- Obtaining a result:

$$NME = \langle \psi_f | O | \psi_i \rangle$$

  - Deriving an expression for the nuclear potential (χ-EFT)
  - Solving the nuclear many-body problem (VS-IMSRG)
  - Deriving operators consistently with the nuclear interactions (EFTs)
- Obtaining a **reliable** result:
  - Uncertainty quantification

Uncertainty Quantification

Propagating the LECs error

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

$$M^{0\nu\beta\beta}(\alpha) = \langle \psi_f(\alpha) \,|\, O \,|\, \psi_i(\alpha) \rangle$$

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

Propagating the LECs error

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

$$M^{0\nu\beta\beta}(\alpha) = \langle \psi_f(\alpha) \,|\, O \,|\, \psi_i(\alpha) \rangle$$

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

How to propagate $\delta\alpha$ to $\delta M^{0\nu\beta\beta}$?

Propagating the LECs error

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

$$M^{0\nu\beta\beta}(\alpha) = \langle \psi_f(\alpha) \,|\, O \,|\, \psi_i(\alpha) \rangle$$

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

How to propagate $\delta\alpha$ to $\delta M^{0\nu\beta\beta}$?

Bayesian statistics!

Bayesian approach

Value of the nuclear matrix elements (what we are interested in)

Different values obtained with different interactions/ methods

Any other relevant information we have beforehand

$$\underbrace{prob(y \mid y_k, I)} \propto \underbrace{prob(y_k \mid y, I)} \times \underbrace{prob(y \mid I)}$$

We read $prob(A \mid B)$ as probability of A given B

Posterior distribution
Probability distribution for the final value given the data and our previous knowledge (what we want to obtain).

For finite samples, we use sampling/importance resampling to obtain the final PDF.

Likelihood
Probability that this sample gives a result that is representative of experimental values.

Chosen to be a multivariate normal centred at the experimental value for few observables we have data on (calibrating observables).

Prior
Assume a uniform prior for low energy constants of natural size. Then use history matching to remove implausible samples from the set. Assume each of the remaining samples to be as likely as the others.

Procedure for UQ in the bayesian approach

1. Generate a set of LECs samples equally distributed in a reasonable range.

2. Using History Matching, reduce the number of samples in the set to “non-implausible” samples.

3. These “non-implausible” samples are now your prior and are taken to be equally probable.

4. Assign a likelihood to each sample by comparing their performance for certain calibrating observables. To give sensible estimate of the target observable, the calibrating observables should correlate with the target observable.

5. Resample the LECs a large number of times ($>10^6$) with probability of being sampled given by the likelihood of the sample (Sampling/Importance Resampling).

6. Evaluate the target observables with the resampled set to obtain a posterior predictive distribution.

7. Other sources of error can be sampled and added independently in the previous step. Those are taken to be normally distributed.

Procedure for UQ in the bayesian approach.

1. Generate a set of LECs samples equally distributed in a reasonable range.

2. Using History Matching, reduce the number of samples in the set to "non-implausible" samples.

3. These "non-imp

4. Assign a likeliho ... observables. To give sensible ... elate with the target observab

5. Resample the l ... given by the likelihood of the

6. Evaluate the tar ... bution.

7. Other sources of error can be sampled and added independently in the previous step. Those are taken to be normally distributed.

The catch

Need to be able to compute the observables for all the non-implausible samples.

Due to the very large cost of many-body methods this becomes very quickly non-feasible as the number of samples grows.

Using Gaussian Process as an emulator

- Idea behind Gaussian Process regressions is to assume that the distribution of the observable we want to fit is Gaussian:

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

  where μ is a mean function and $K(\mathbf{x}, \mathbf{x})$ is the covariance matrix between the inputs.

- Want to infer the joint distribution of potentially unobserved Y* points and the observed points Y. This can be done via a property of Gaussian distribution called Conditioning, i.e.:

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

Using Gaussian Process as an emulator

- Idea behind Gaussian Process regressions is to assume that the distribution of the observable we want to fit is Gaussian:

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

where μ is a mean function and $K(\mathbf{x}, \mathbf{x})$ is the covariance matrix between the inputs.

- Want to infer the distribution of potentially unobserved Y* points from the observed points Y. This can be done via a property of Gaussian distribution called Conditioning, i.e.:

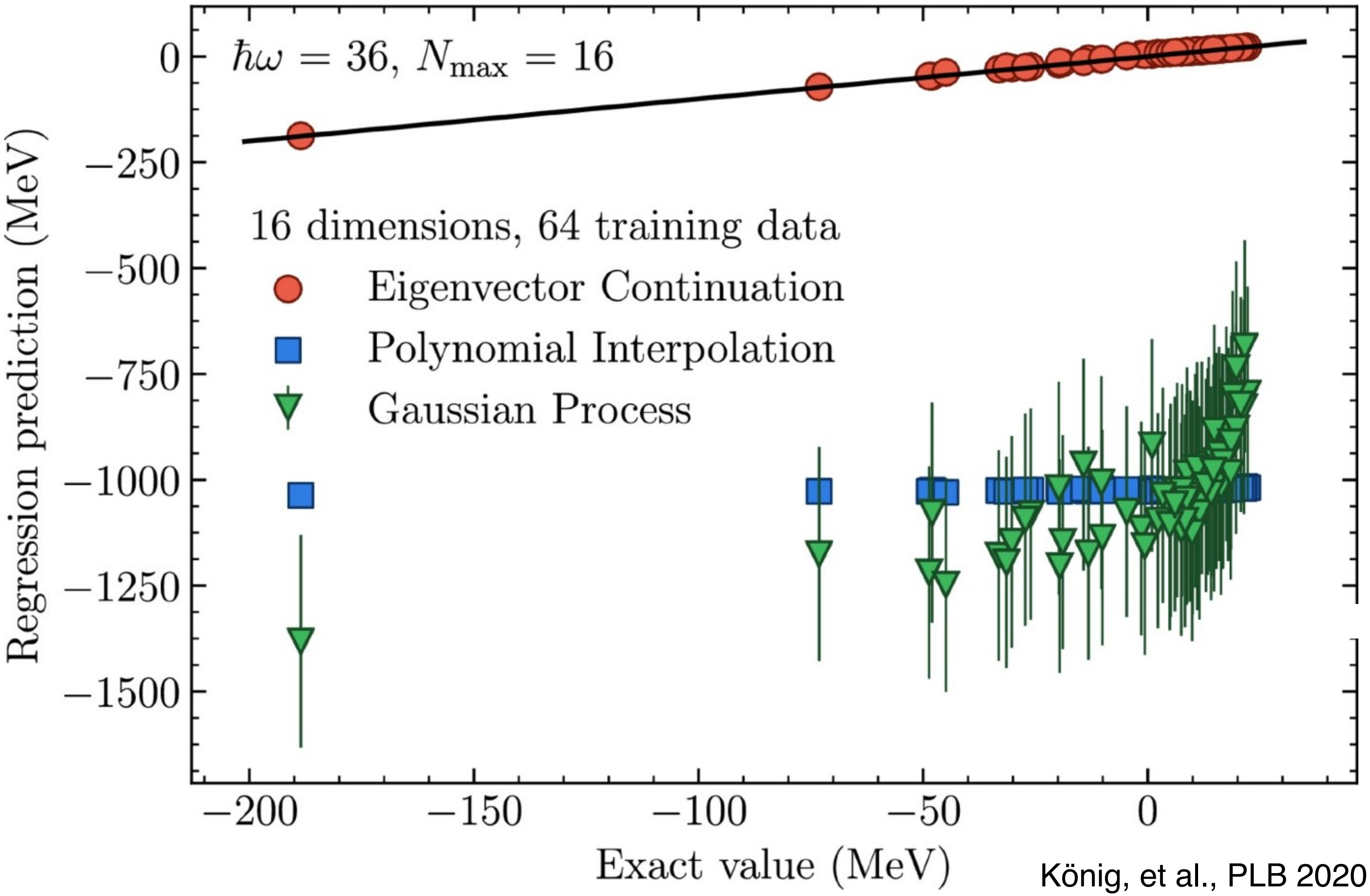
$$P_{Y*|Y} \sim \mathcal{N}\left(0 + \Sigma_{X*X}\Sigma_{XX}^{-1}(Y - 0), \Sigma_{X*X*} - \Sigma_{X*X}\Sigma_{XX}^{-1}\Sigma_{XX*}\right).$$

Normalizing inputs

Only need to optimize hyperparameters of $K(\mathbf{x}, \mathbf{x})$!

TRIUMF

Using Gaussian Process as an emulator



König, et al., PLB 2020.135814

Using Gaussian Process as an emulator

- Multi-Tasks Gaussian Process: Uses multiple correlated outputs from the same inputs by defining the kernel as $K_{inputs} \otimes K_{outputs}$. This allows us to increase the number of data points without needing to do more expensive calculations.

- Multi-Fidelity Gaussian Process: Uses few data points of high fidelity (full IMSRG calculations) and many data points of low fidelity (e.g. Hartree-Fock results, lower e_{max}). The difference function is fitted by a Gaussian Process in order to predict the value of full calculations using the low fidelity data points. This assumes a linear scaling for between the low- and high-fidelity calculations.

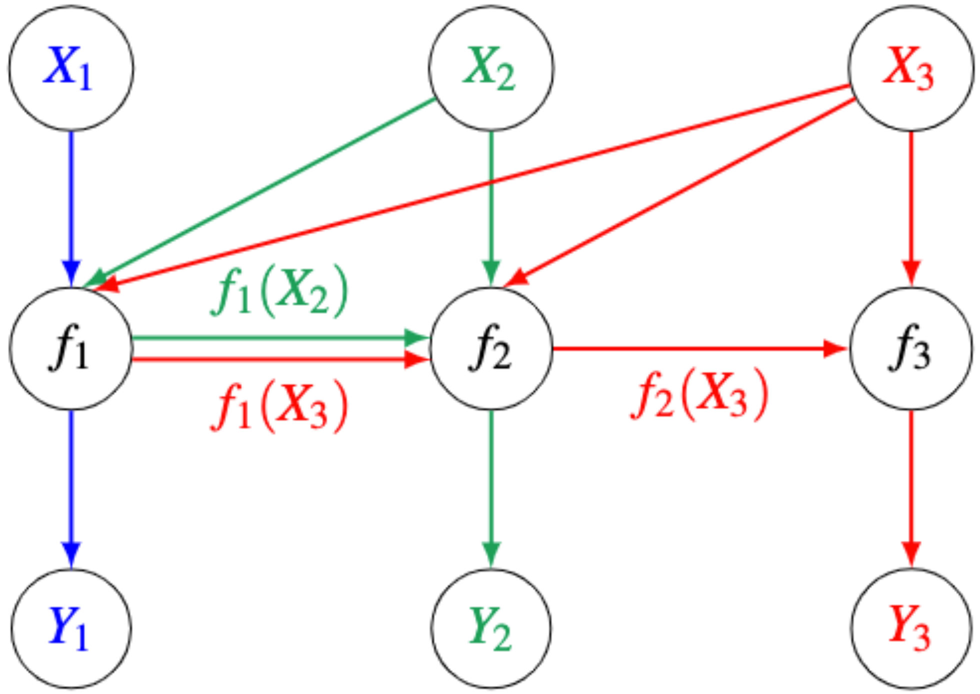
The MM-DGP algorithm

- When the relation between low-fidelity and high-fidelity data is complicated, the simple multi-fidelity approach does not produce good results.

- Deep Gaussian Processes [1] link multiple Gaussian Processes inside a architecture similar to neural network to improve results.

- This can be used to model the difference function between the low- and high-fidelity by including outputs of the previous fidelity as an input of higher fidelity by taking a kernel of the form:
$K(\mathbf{x}, \mathbf{x}) = k(\mathbf{x}, \mathbf{x}) \cdot k(f_{prev}(\mathbf{x}), f_{prev}(\mathbf{x})) + k_{bias}(\mathbf{x}, \mathbf{x})$

- This was developed for single-output Gaussian Processes and we have adapted it for multi-output case, creating the MM-DGP: Multi-output Multi-fidelity Deep Gaussian Process.

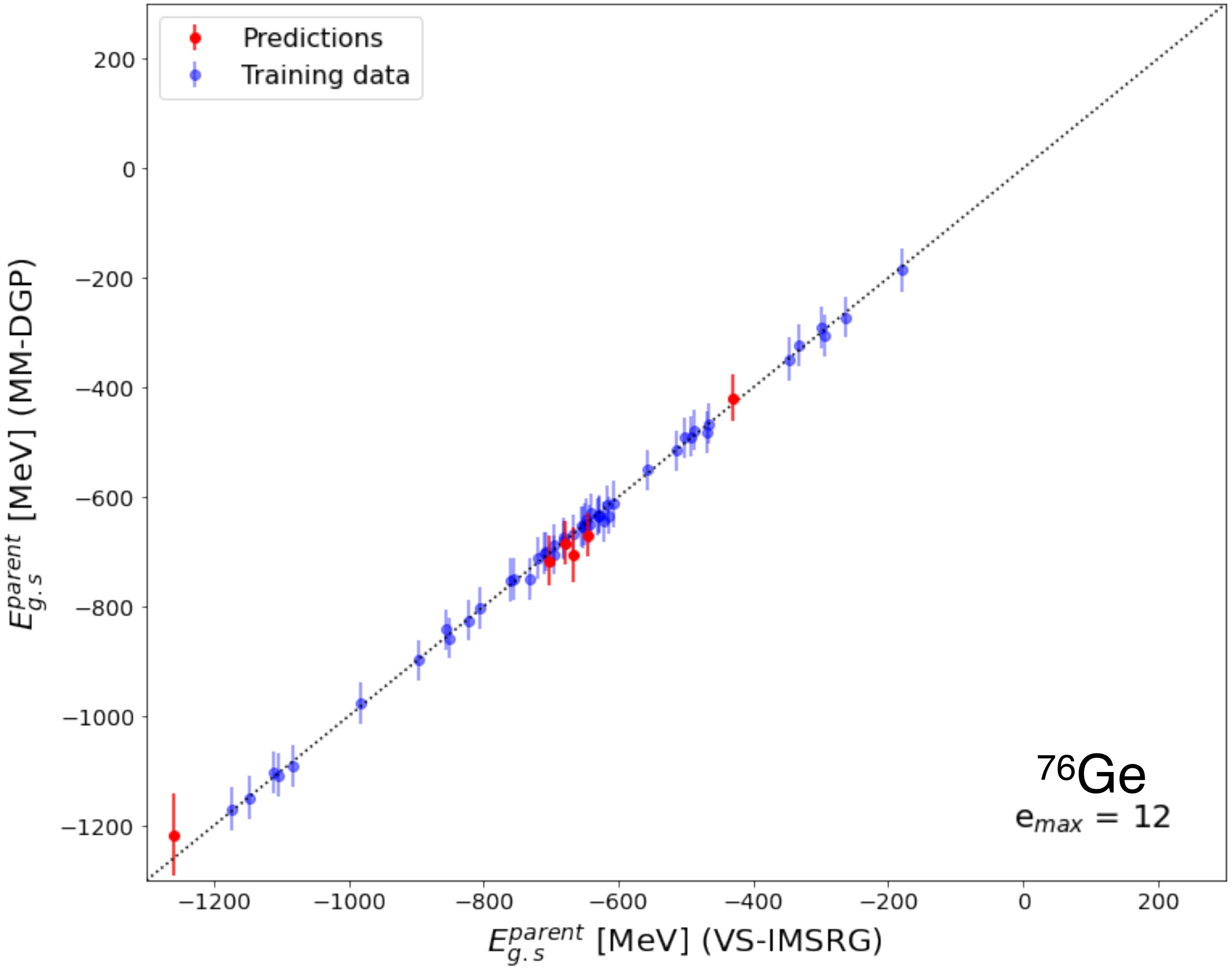


[1] Kurt Cutajar, Mark Pullin, Andreas Damianou, Neil Lawrence, Javier González arXiv:1903.07320 (2021).

The MM-DGP algorithm: Energies

Using Δ-full chiral EFT interactions at N2LO:

50 training points



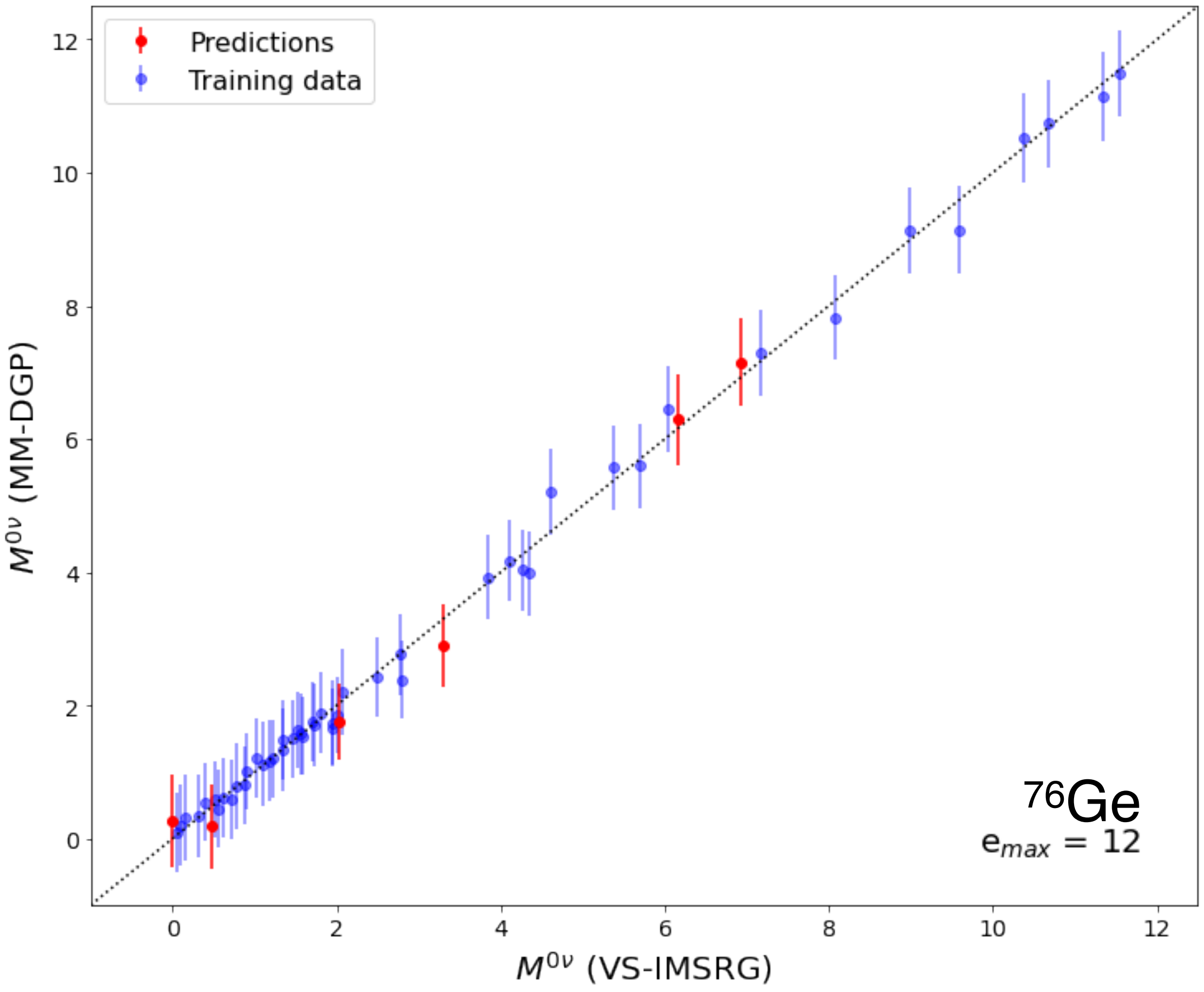
Root Mean Square Error = 11 MeV

Belley, Pitcher et al. in prep.

The MM-DGP algorithm: $0\nu\beta\beta$ NMEs

Using Δ-full chiral EFT interactions at N2LO:

50 training points



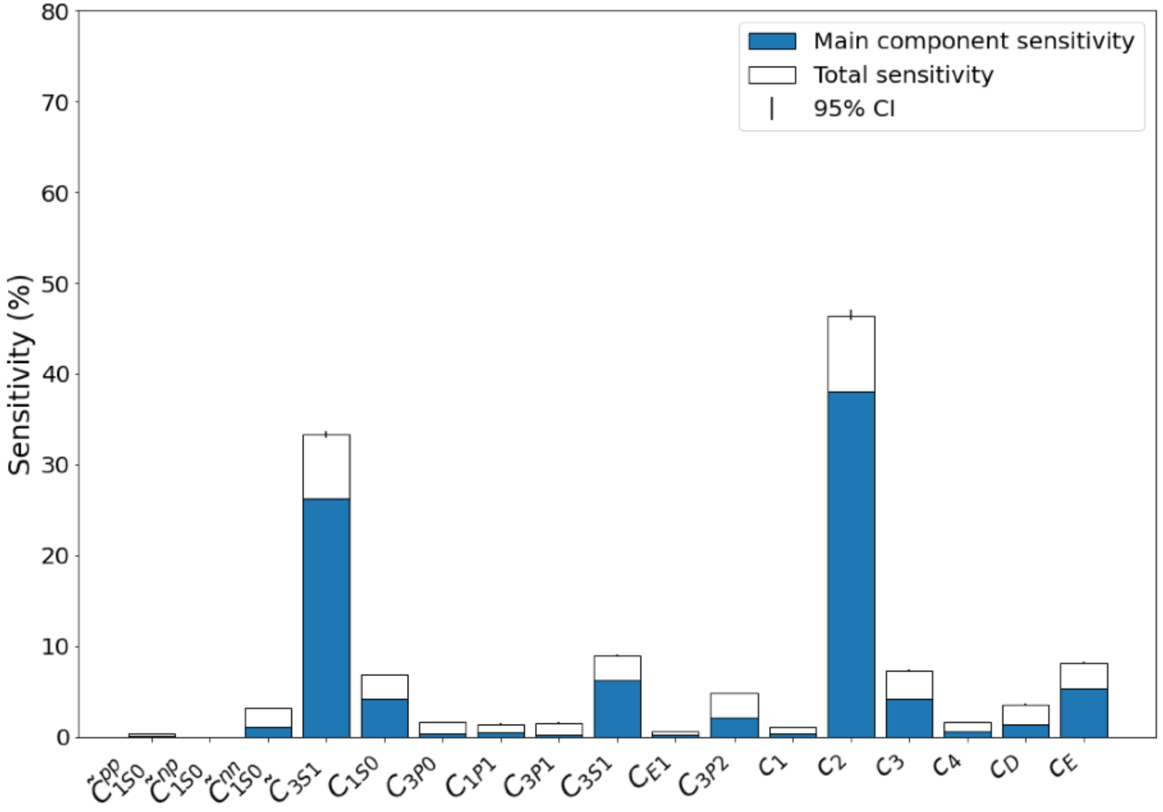
Root Mean Square Error = 0.13

Belley, Pitcher et al. in prep.

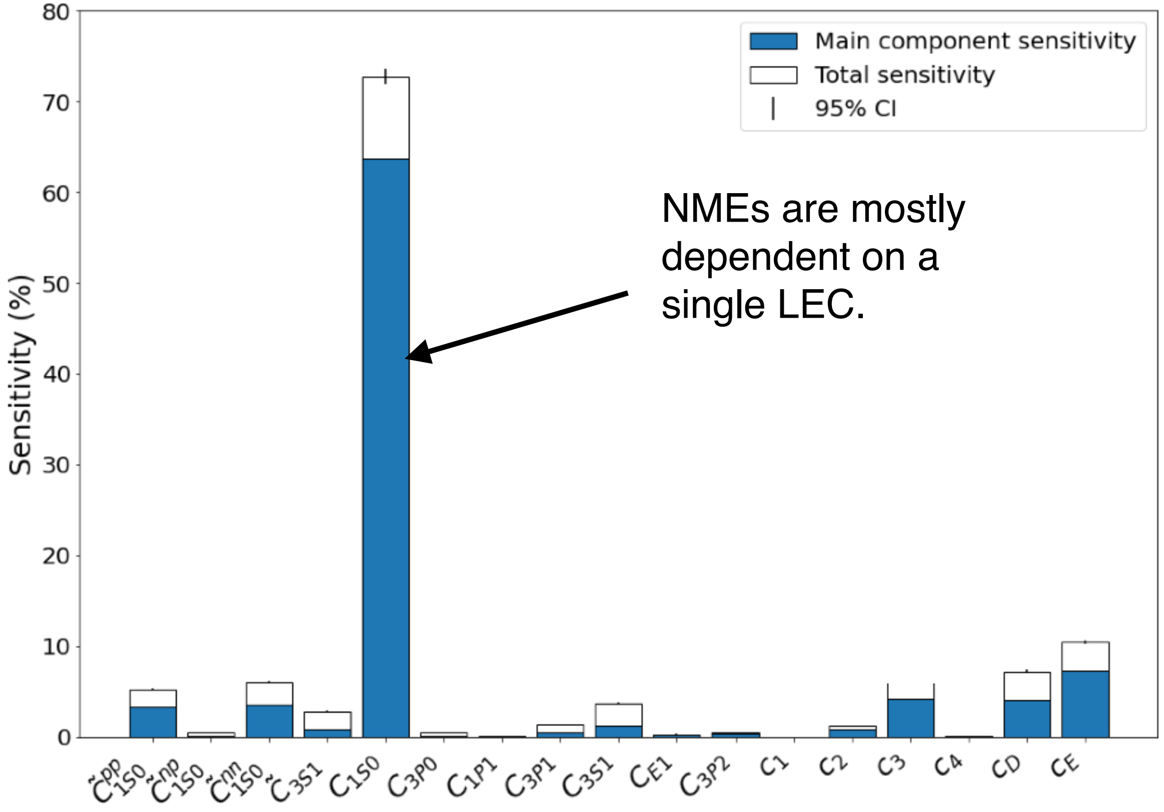
TRIUMF

The MM-DGP algorithm: GSA

Ground state energies



$M_L^{0\nu}$



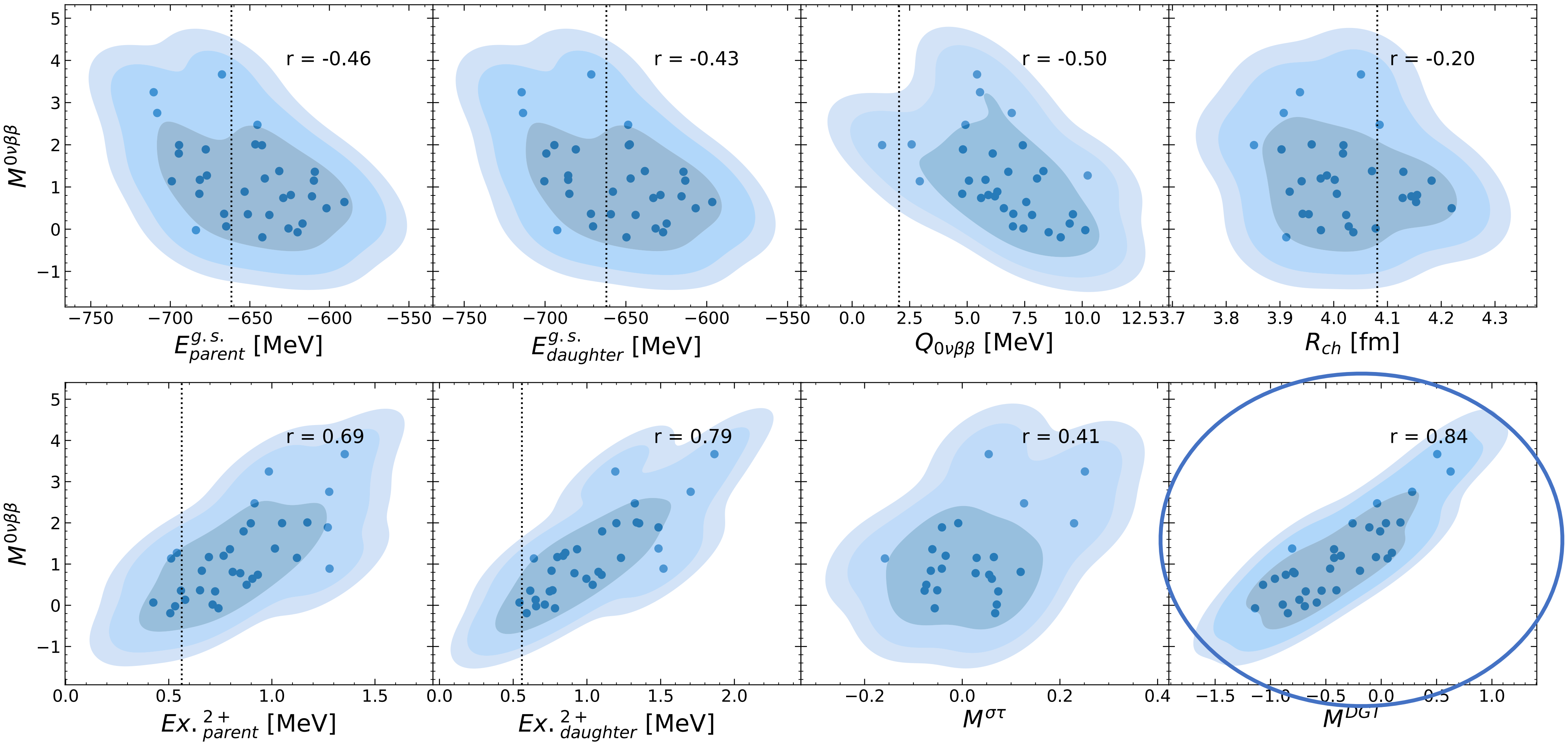
Consistent with results of Coupled Cluster and physics based emulator

Belley, Pitcher et al. in prep.

Correlation between observables

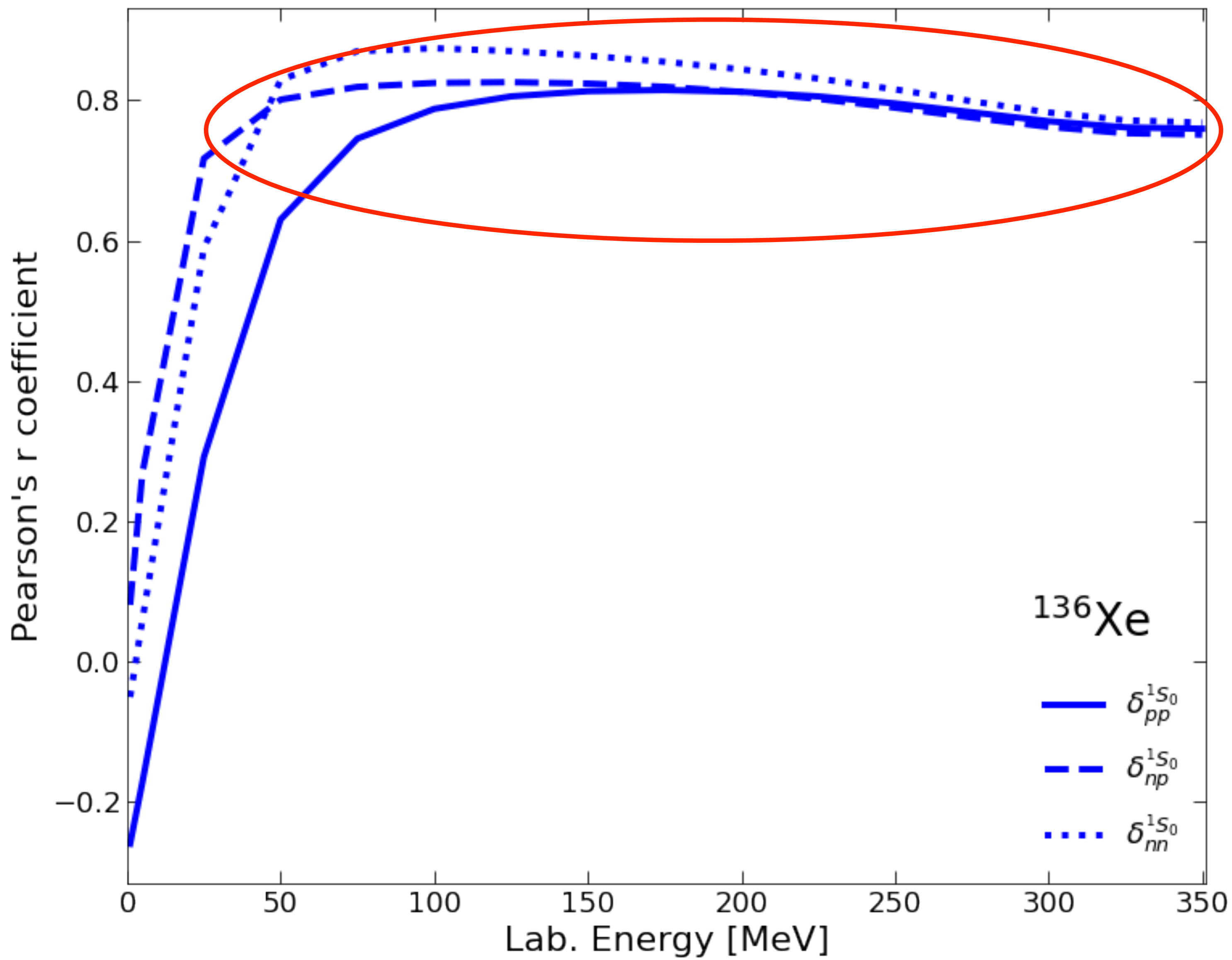
In ^{76}Ge:

Belley et al., arXiv:2210.05809



Only correlation seen in multiple nuclei is with the unobserved double Gamow-Teller transition NME.

Correlation with phase shifts



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.

Belley, Pitcher, et al. in prep.

Posterior distribution of the NMEs

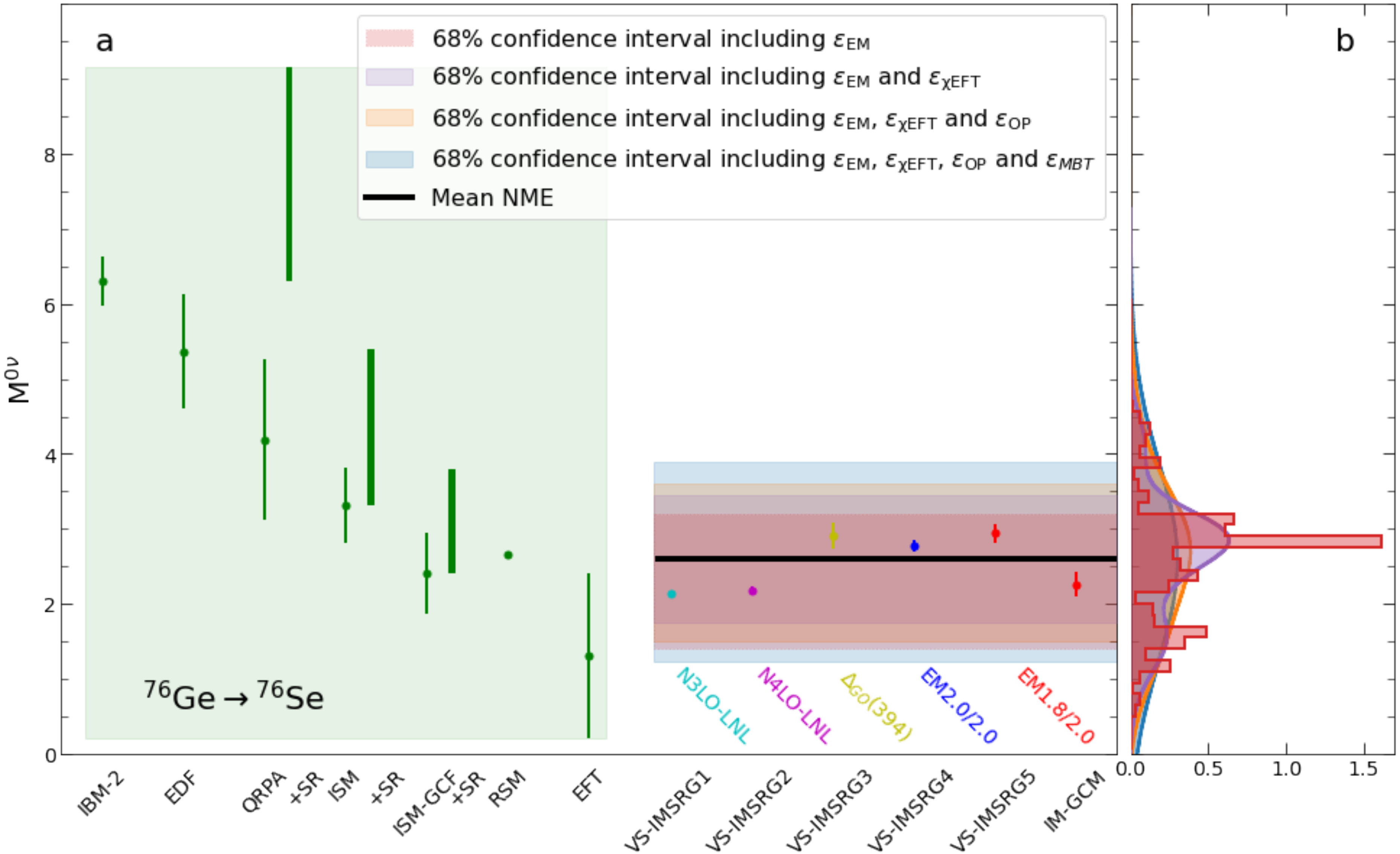
- Use 8188 “non-implausible” samples obtain by Jiang, W. G. et al. (arXiv:2212.13216).
- Many-body problem is “solved” with the MM-DGP.
- Consider all sources of uncertainties by taking:

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

where the ϵ’s are the errors coming from different sources and are assumed to be normally distributed and independent.

- Interactions are weighted by the $^1S_0$ neutron-proton phase shifts at 50 MeV and observables for mass A=2-4,16.

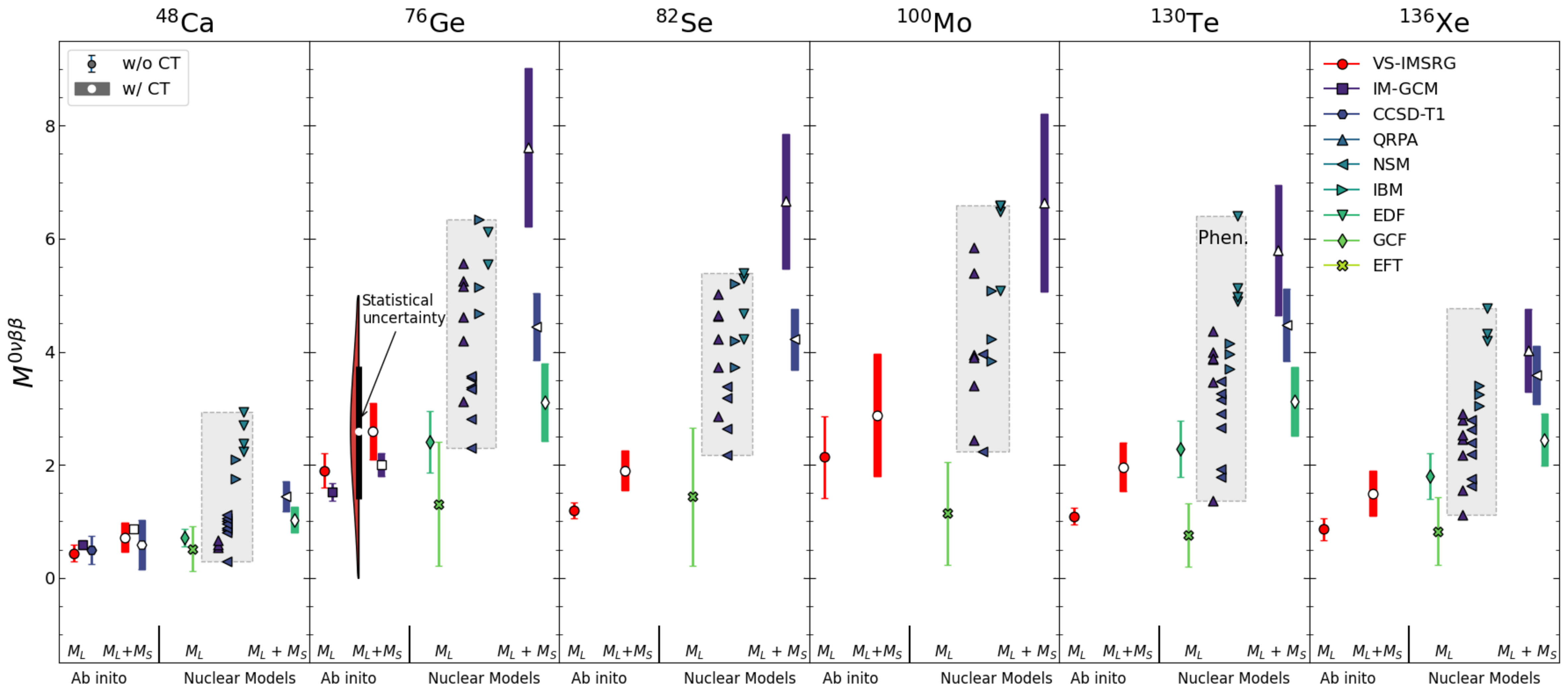
Comparing with other interactions



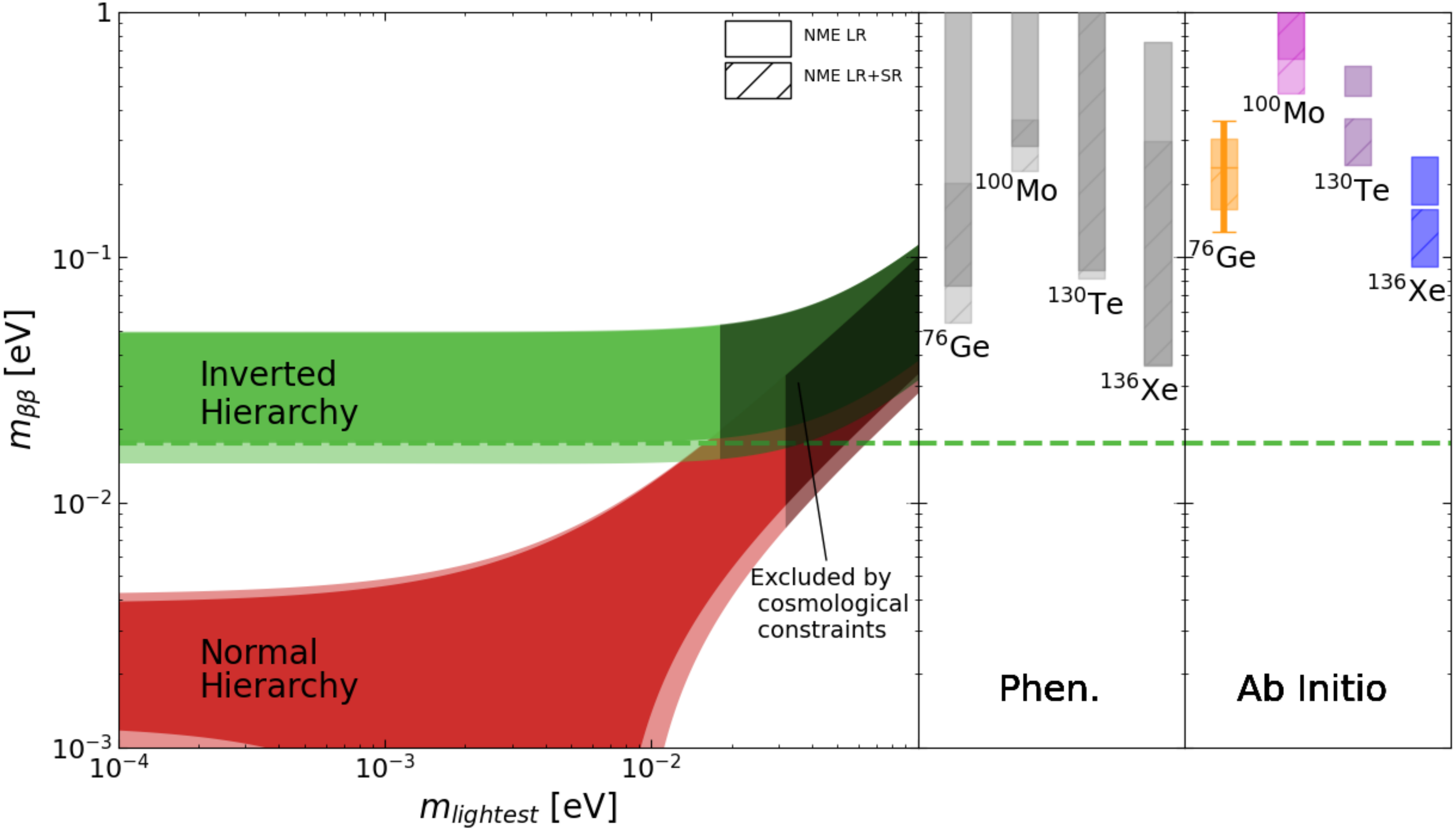
$$M^{0\nu\beta\beta} = 2.60^{+1.28}_{-1.36}$$

Belley, et al., arXiv:2308.15634

0νββ-decay Matrix Elements: The complete picture

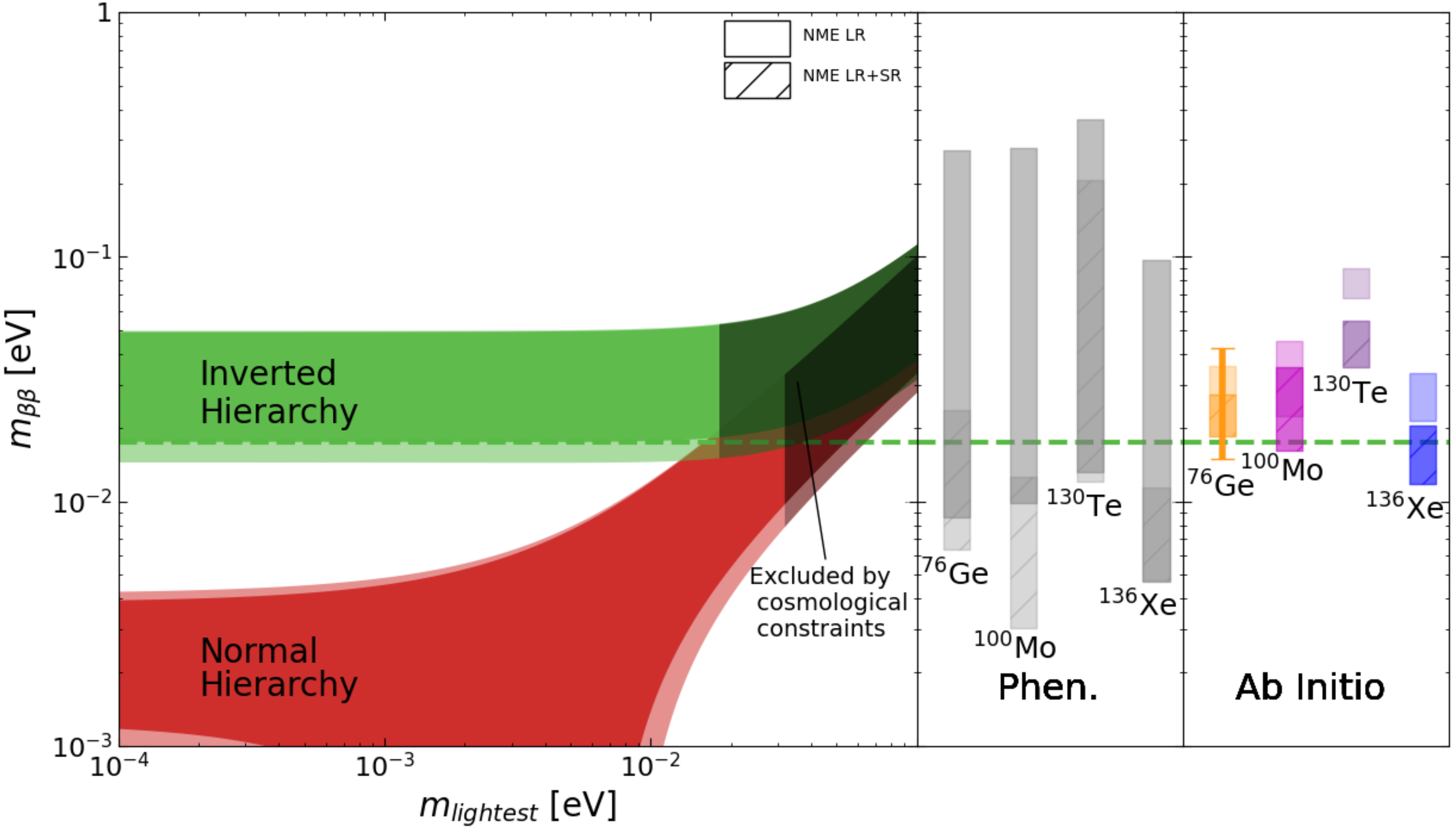


Ab Initio 0νββ Decay: Effect on experimental limits



Experimental limits: **GERDA (^{76}Ge)** Phys. Rev. Lett. 125, 252502, **CUPID-Mo (^{100}100)** Eur. Phys. J. C 82 11, 1033, **CUORE(^{130}Te)** Nature 604, 53–58 and **Kamland Zen (^{136}Xe)** Phys. Rev. Lett. 130, 051801.

Ab Initio 0νββ Decay: Effect on future reach



Expected limits: **LEGEND (^{76}Ge)** arXiv:2107.11462, **CUPID (^{100}100)** arXiv:1907.09376, **SNO+(^{130}Te)** arXiv:2104.11687and **nEXO (^{136}Xe)** J. Phys .G 49 1, 015104.

Summary

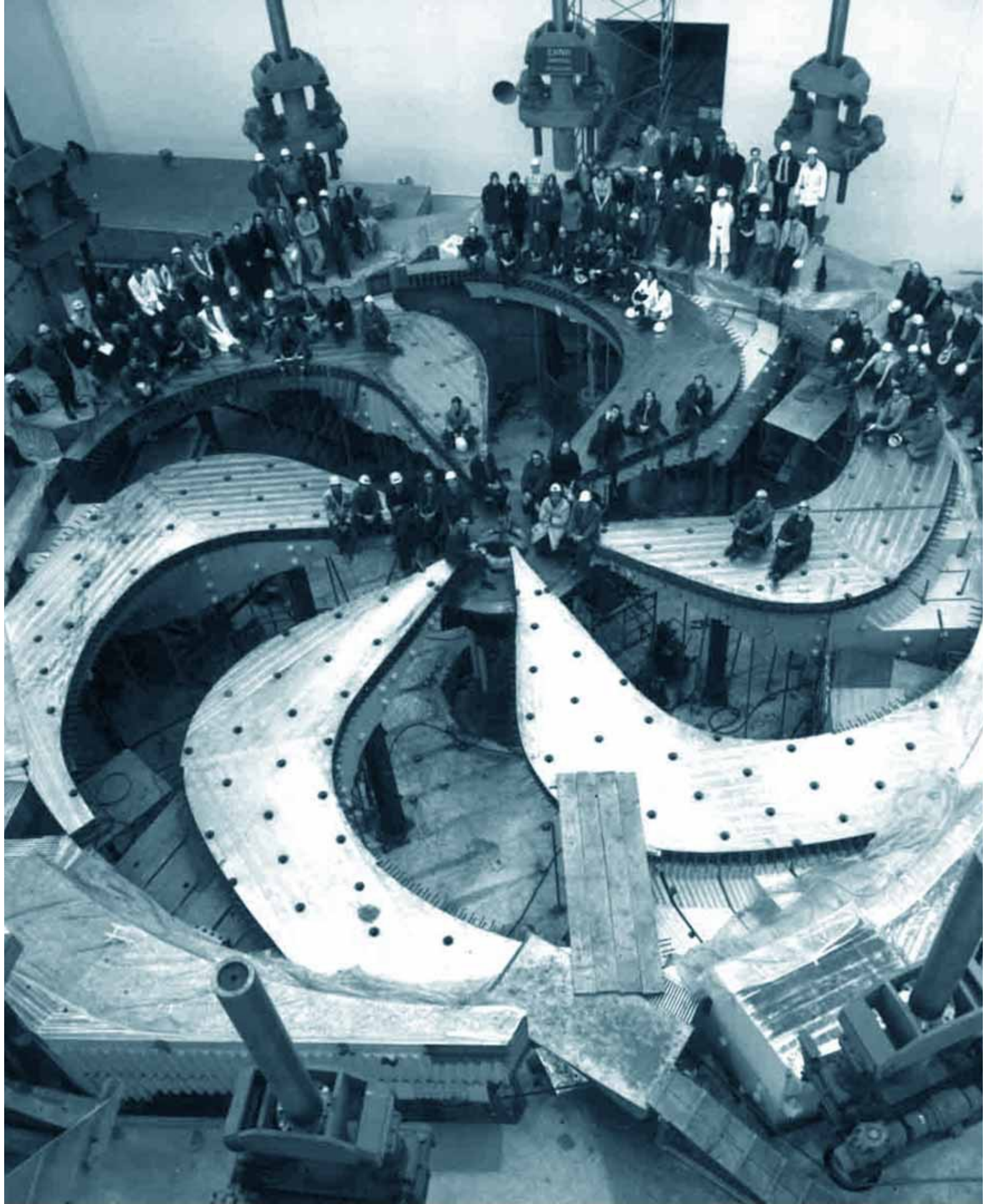
1. Computed first ever ab initio NMEs of isotopes of experimental interest as a first step towards computing NMEs with reliable theoretical uncertainties.

2. Computed NMEs with multiple interactions for ^{48}Ca, ^{76}Ge, ^{82}Se, ^{100}Mo, ^{130}Te and ^{136}Xe.

3. Studied effects of the contact term on the NMEs.

4. Developed an emulator for the VS-IMSRG based on Gaussian Processes.

5. Obtained the first statistical uncertainty for the NMEs which includes all sources of errors in the calculation.



TRIUMF

Questions?

abelley@triumf.ca

Discovery,
accelerated