Ab Initio theory towards reliable neutrinoless double beta decay NMEs.

Antoine Belley

75th Anniversary of the Shell Model Symposium

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

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THE UNIVERSITY OF BRITISH COLUMBIA

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Arthur B. McDonald Canadian Astroparticle Physics Research Institute

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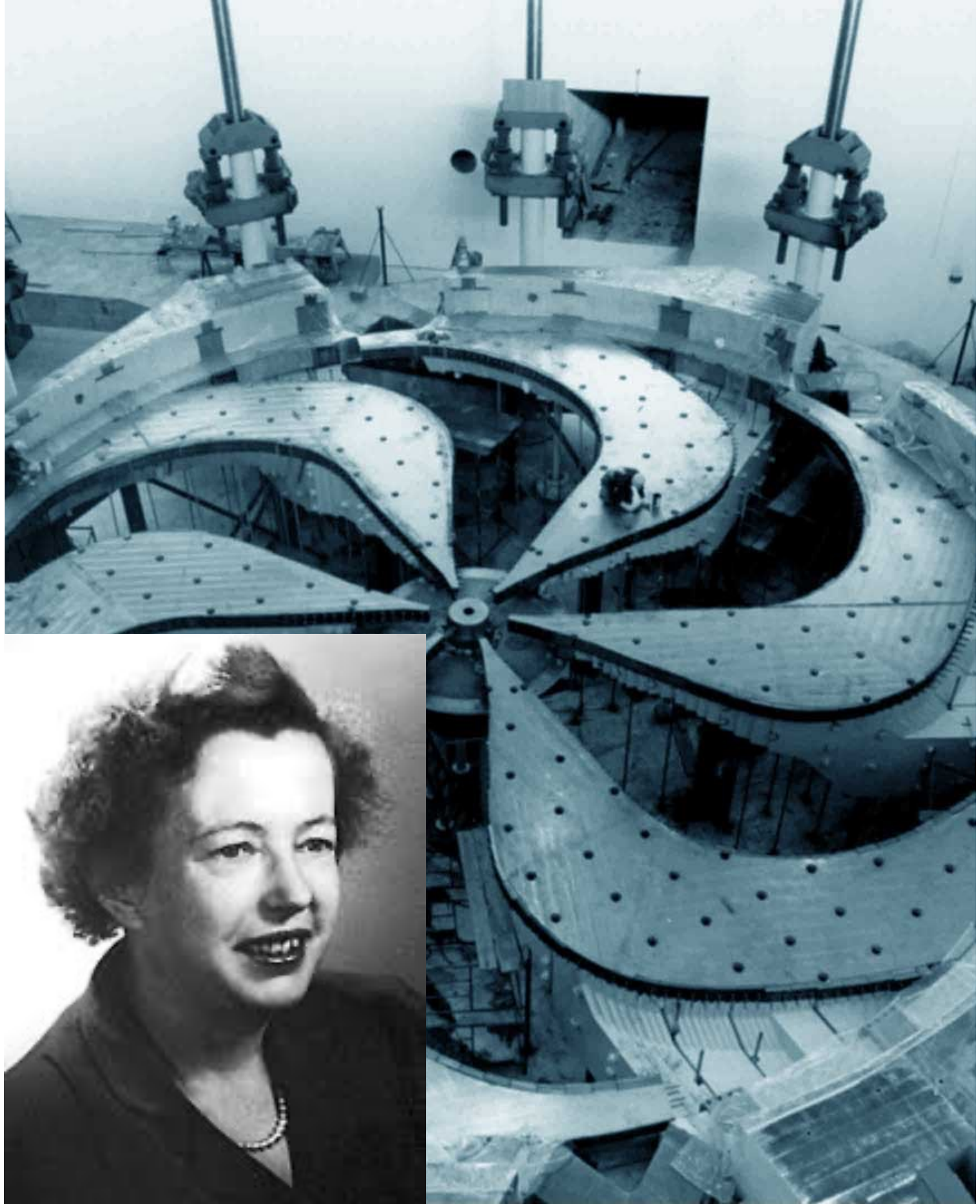
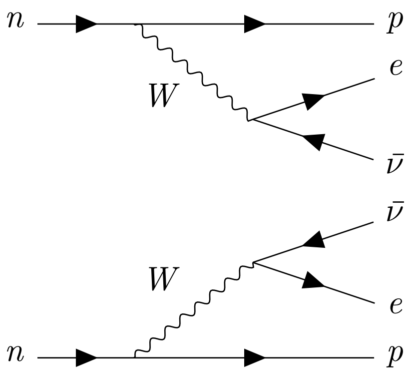
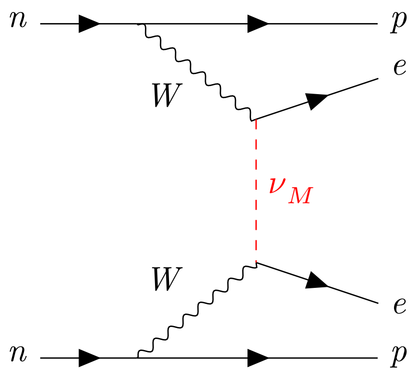


Discovery, accelerated

2νββ vs 0νββ

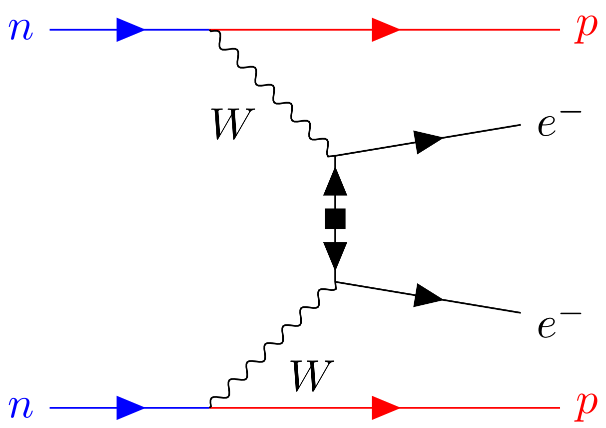
Decay	$2\nu\beta\beta$	$0\nu\beta\beta$
Diagram		
Half-life Formula	$[T^{2\nu}_{1/2}]^{-1} = G^{2\nu}\|M^{2\nu}\|^2$	$[T^{0\nu}_{1/2}]^{-1} = G^{0\nu}\|M^{0\nu}\|^2 \left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2$
NME Formula	$M^{2\nu} \approx M^{2\nu}_{GT}$	$M^{0\nu} = M^{0\nu}_{GT} - (\frac{g_v}{g_a})^2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

*NME : Nuclear matrix elements

**LNV : Lepton number violation

Lepton Number Violation

$$[T^{0\nu}_{1/2}]^{-1} = G^{0\nu}_i |M^{0\nu}|^2 \left(\frac{\langle m_{\beta\beta} \rangle}{m_e} \right)^2$$



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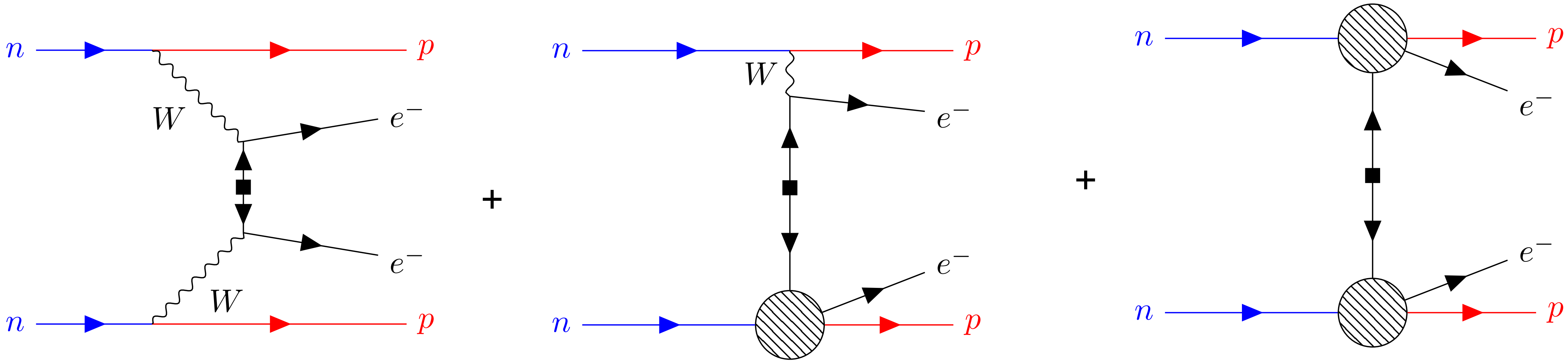
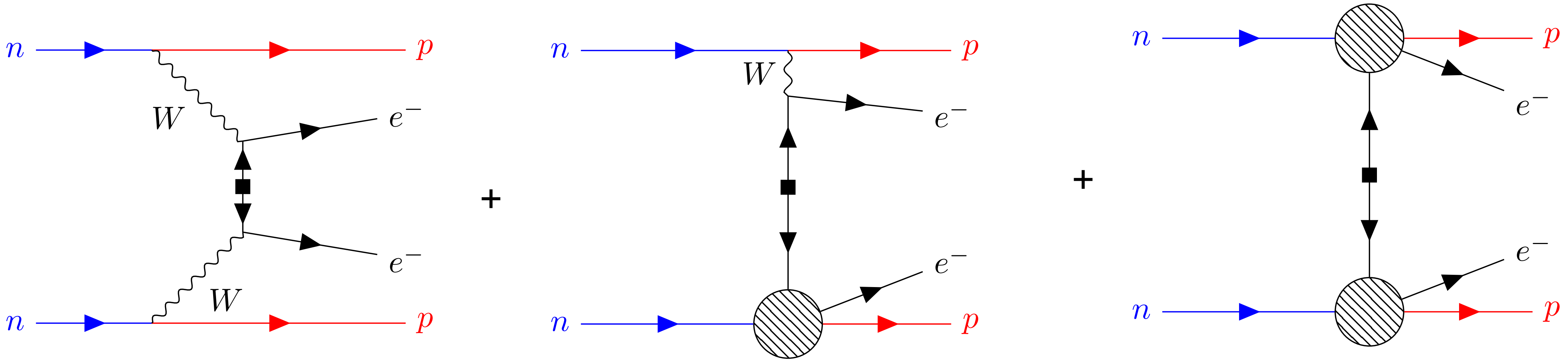


Lepton Number Violation

$$[T^{0\nu}_{1/2}]^{-1} = G^{0\nu}_i |M^{0\nu}|^2 \left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2 \quad \longrightarrow \quad [T^{0\nu}_{1/2}]^{-1} = G^{0\nu} |M^{0\nu}|^2 \left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2 + \sum_i G^{0\nu}_i |M^{0\nu}_i|^2 \eta_i^2$$



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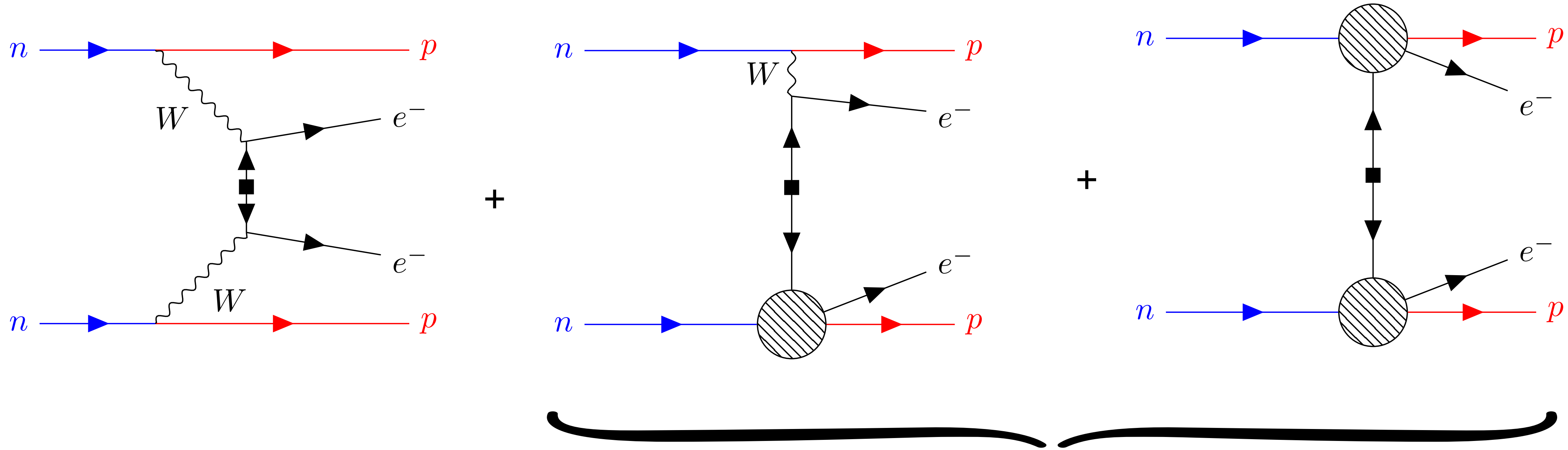
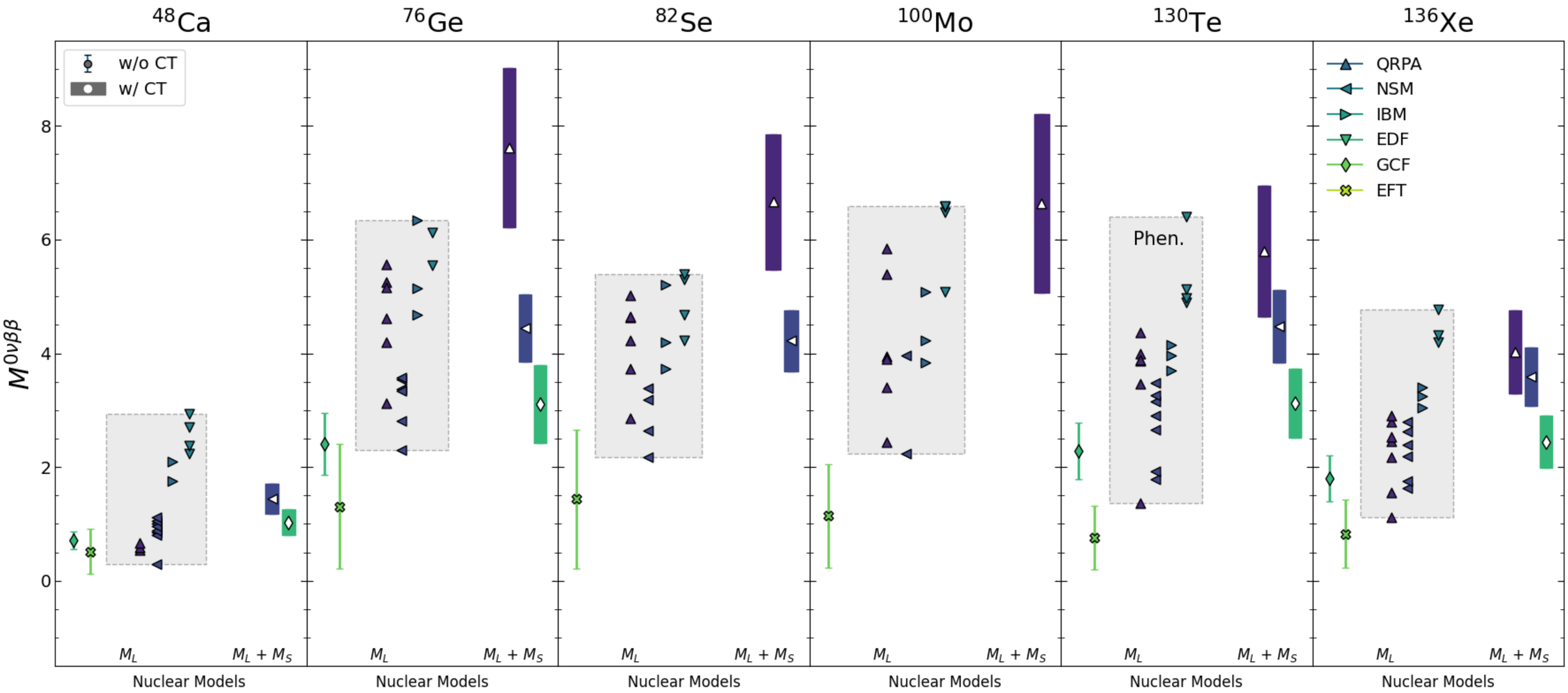


Models can be differentiated but require the uncertainty on the NMEs for each mechanism to be less than 15%, see Gráf et al., Phys. Rev. D **106**, 035022.

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)

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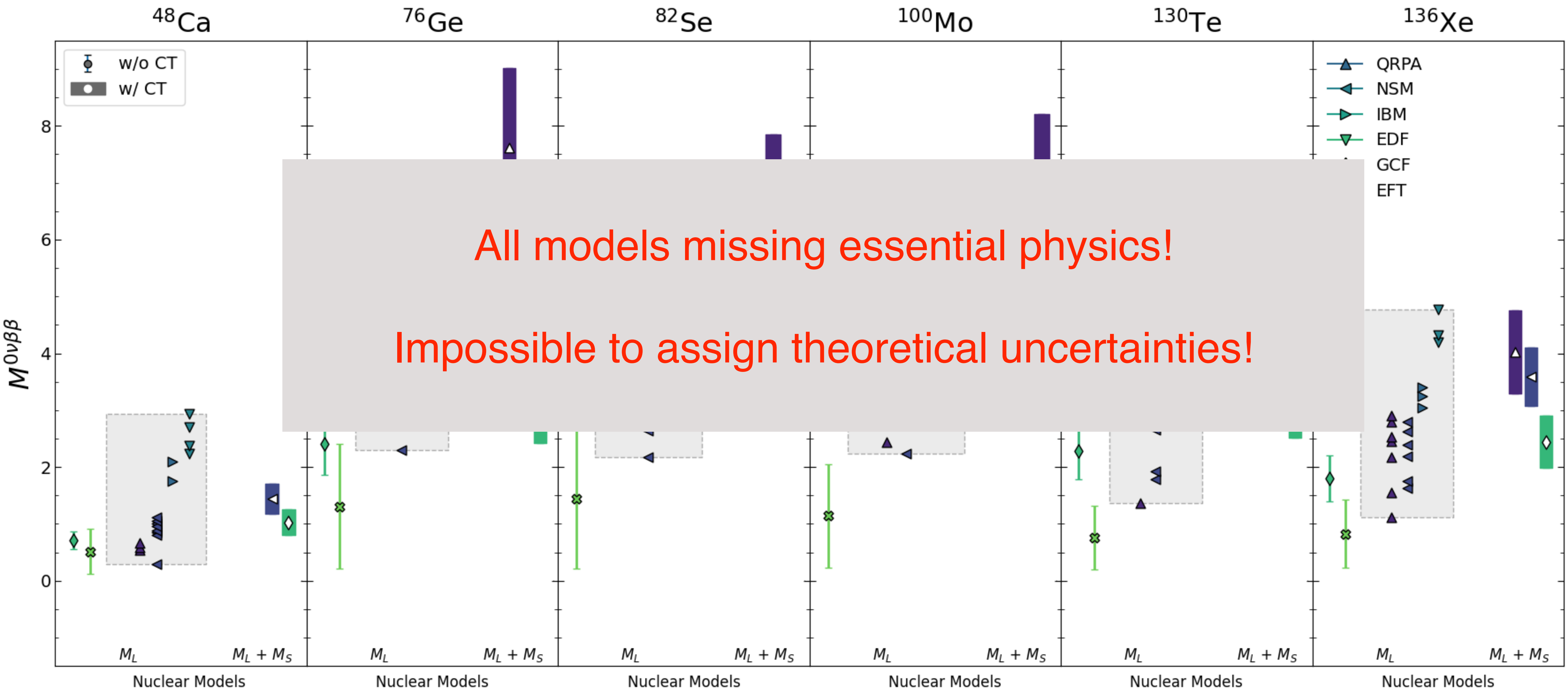

All models missing essential physics!

Impossible to assign theoretical uncertainties!

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 thesis

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

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

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

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- Obtaining a **reliable** result:
  - Uncertainty quantification

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  - 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)
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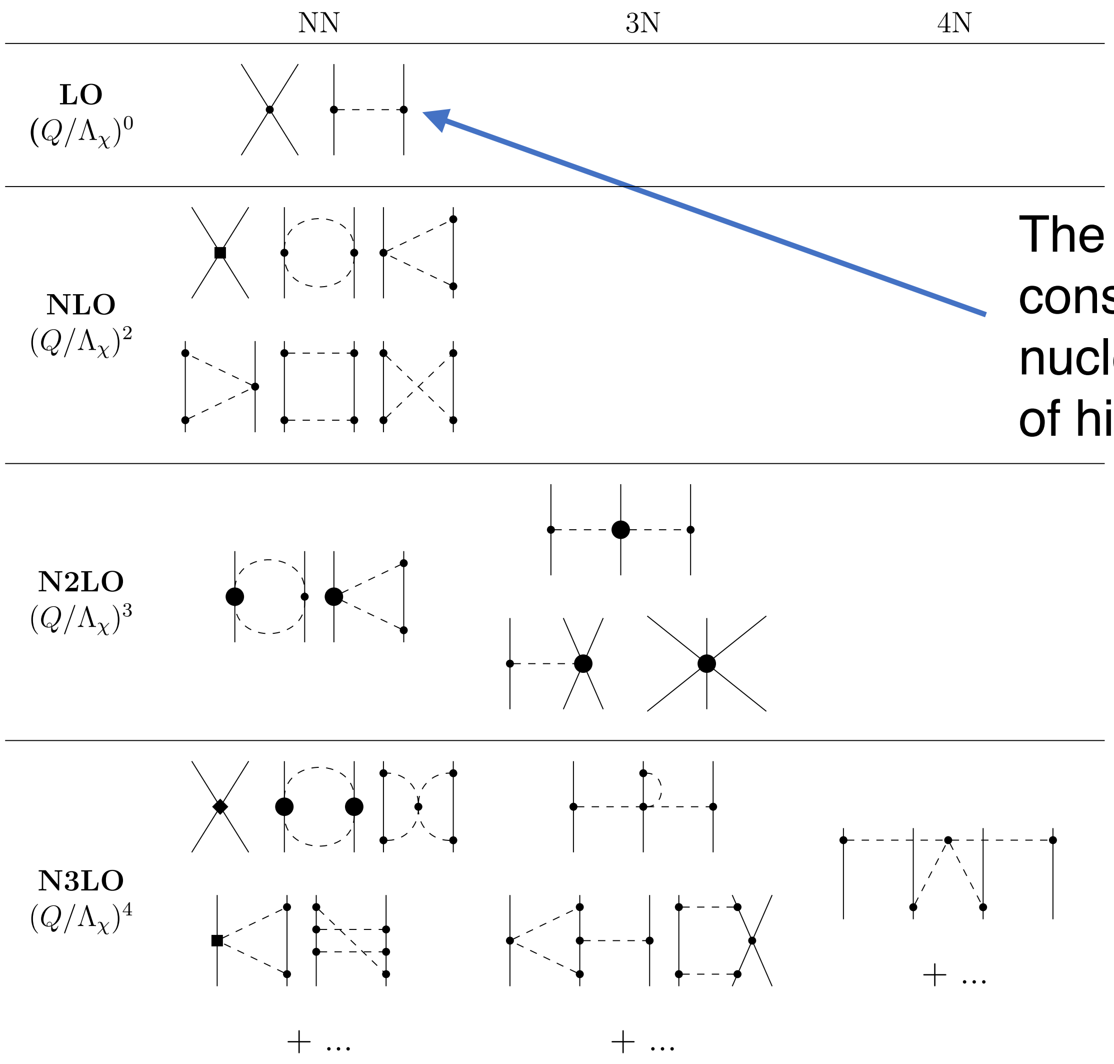
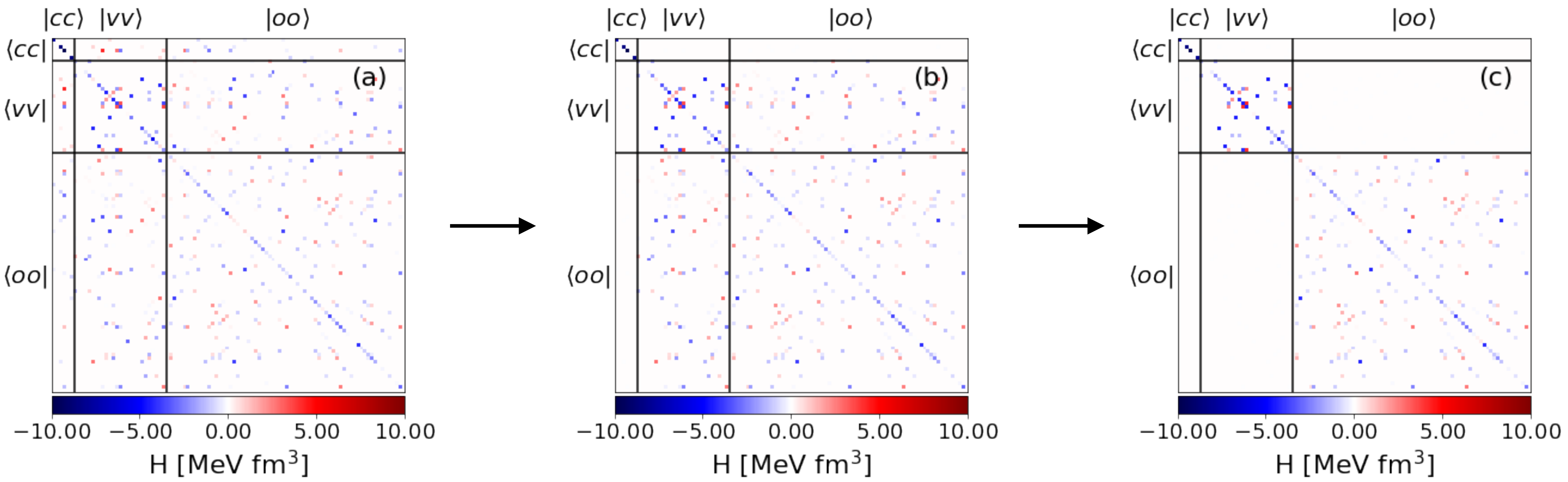
Expansion order by order of the nuclear forces

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-nucleon data to absorb the effect of higher order terms

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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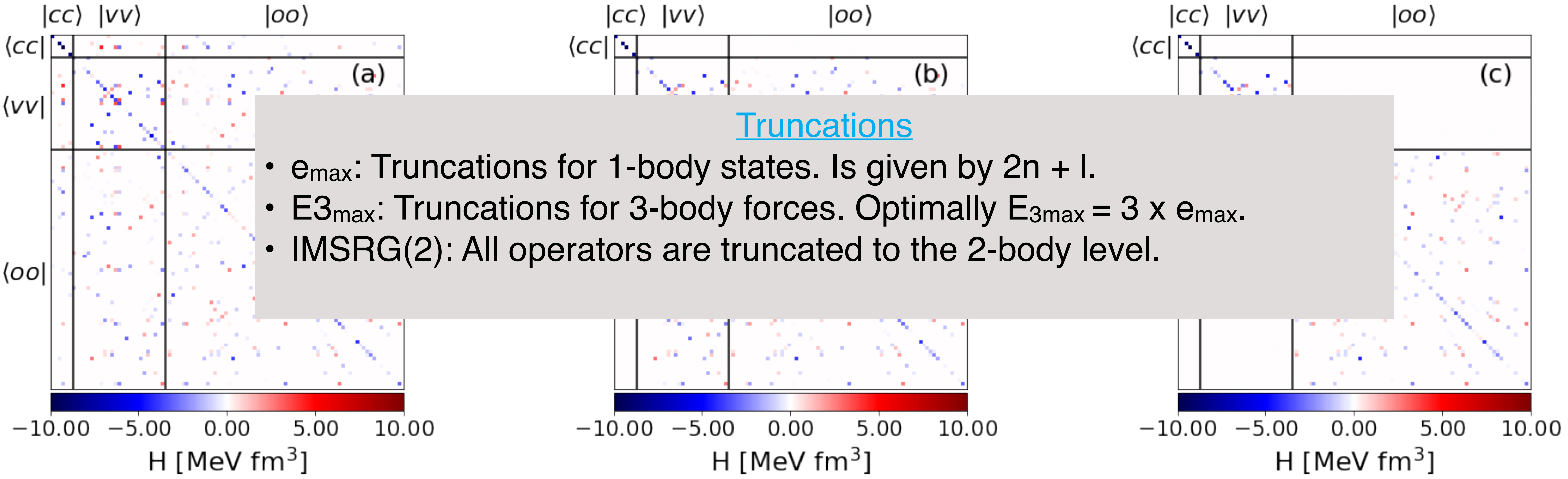

Truncations

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

Bare Hamiltonian

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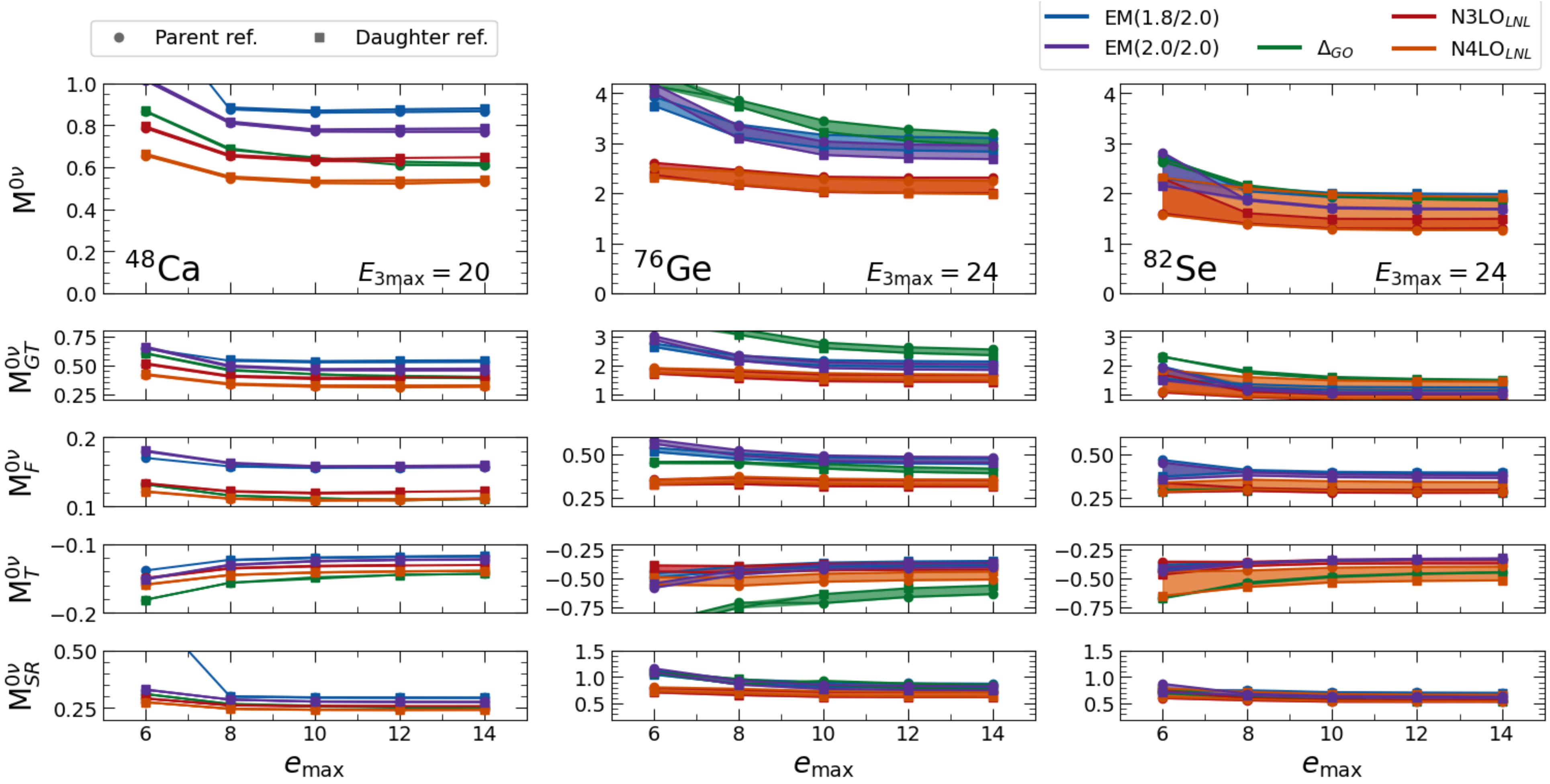
Obtaining a result

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.



Belley, et al., PRL126.042502

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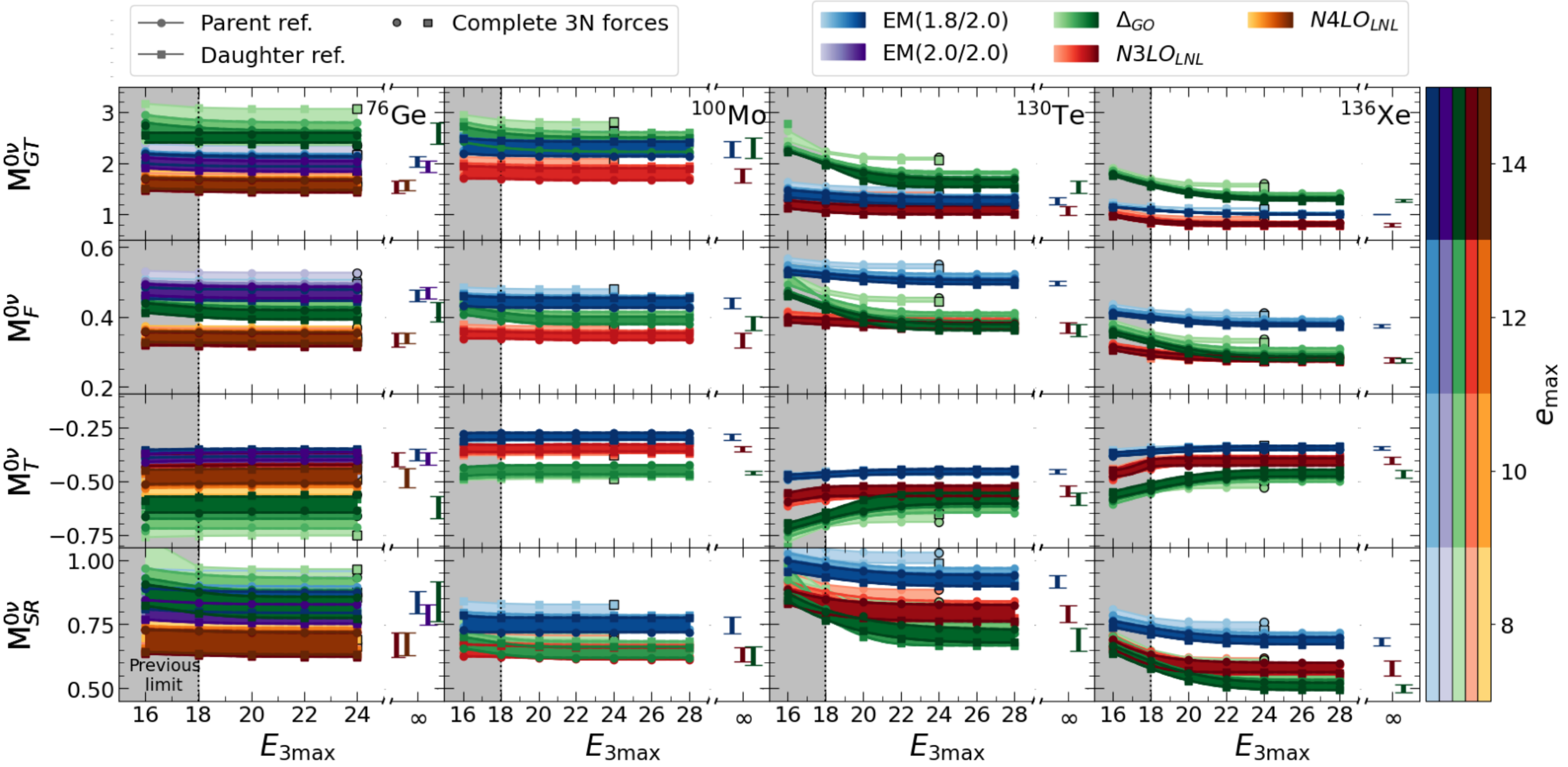
Ab Initio $0\nu\beta\beta$ Decay: ^{100}Mo, ^{130}Te and ^{136}Xe

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

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

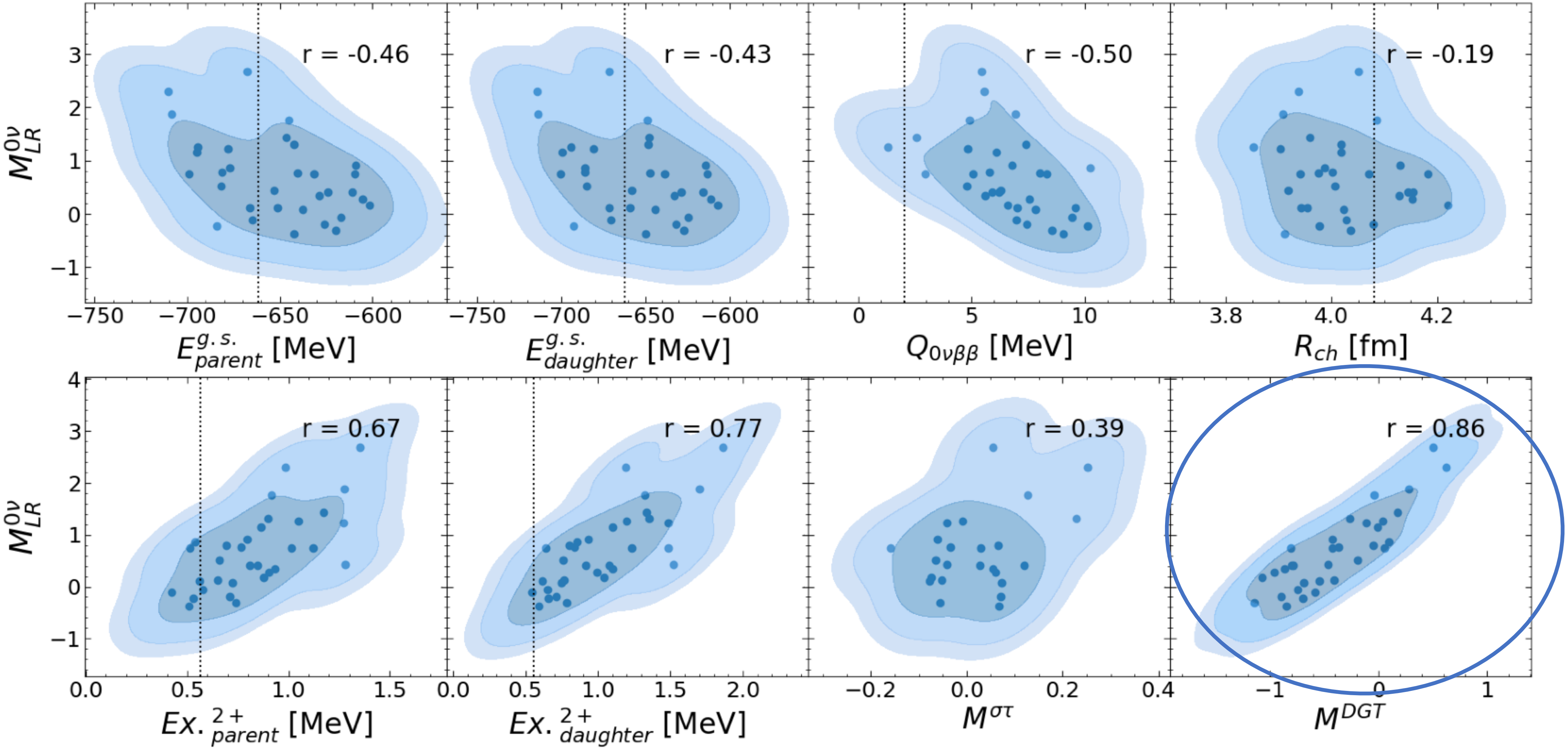


Belley, et al., arXiv:2307.15156

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.

List of challenges

- Obtaining a result:

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

  - Deriving an expression for the nuclear potential (χ-EFT)
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- Obtaining a **reliable** result:
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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-nucleon data, i.e. each LEC has an uncertainty $\delta\alpha$ associated with it.

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

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

Bayesian statistics!

Bayesian Approach

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

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

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

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.

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The catch

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

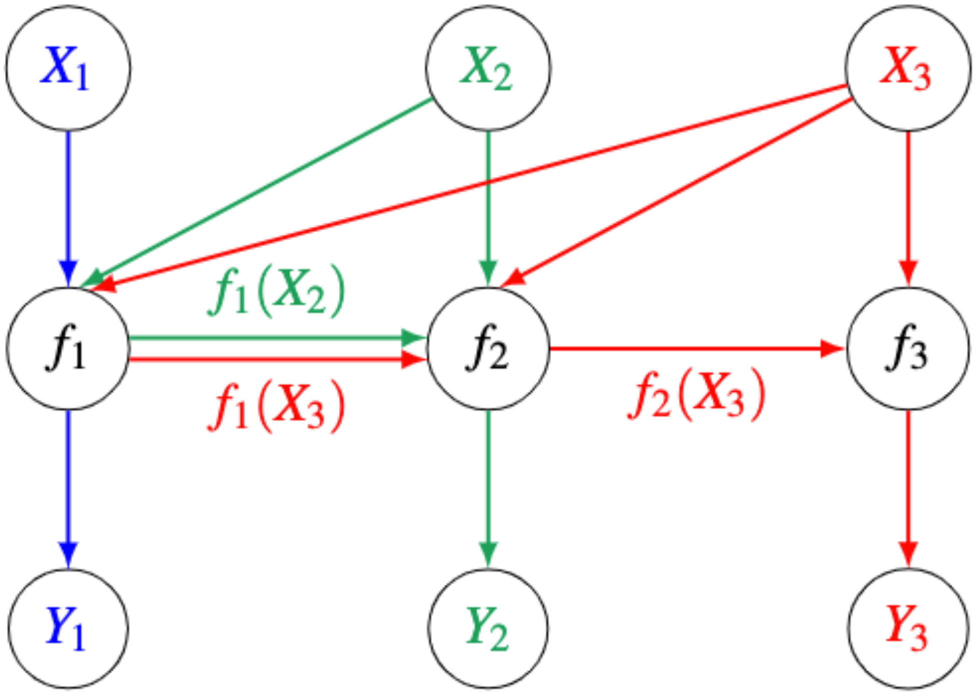
Due to the very large cost of many-body methods, this becomes very quickly non-feasible as the number of samples grows.

The MM-DGP Algorithm

- Deep Gaussian Processes [1] link multiple Gaussian Processes inside an 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.

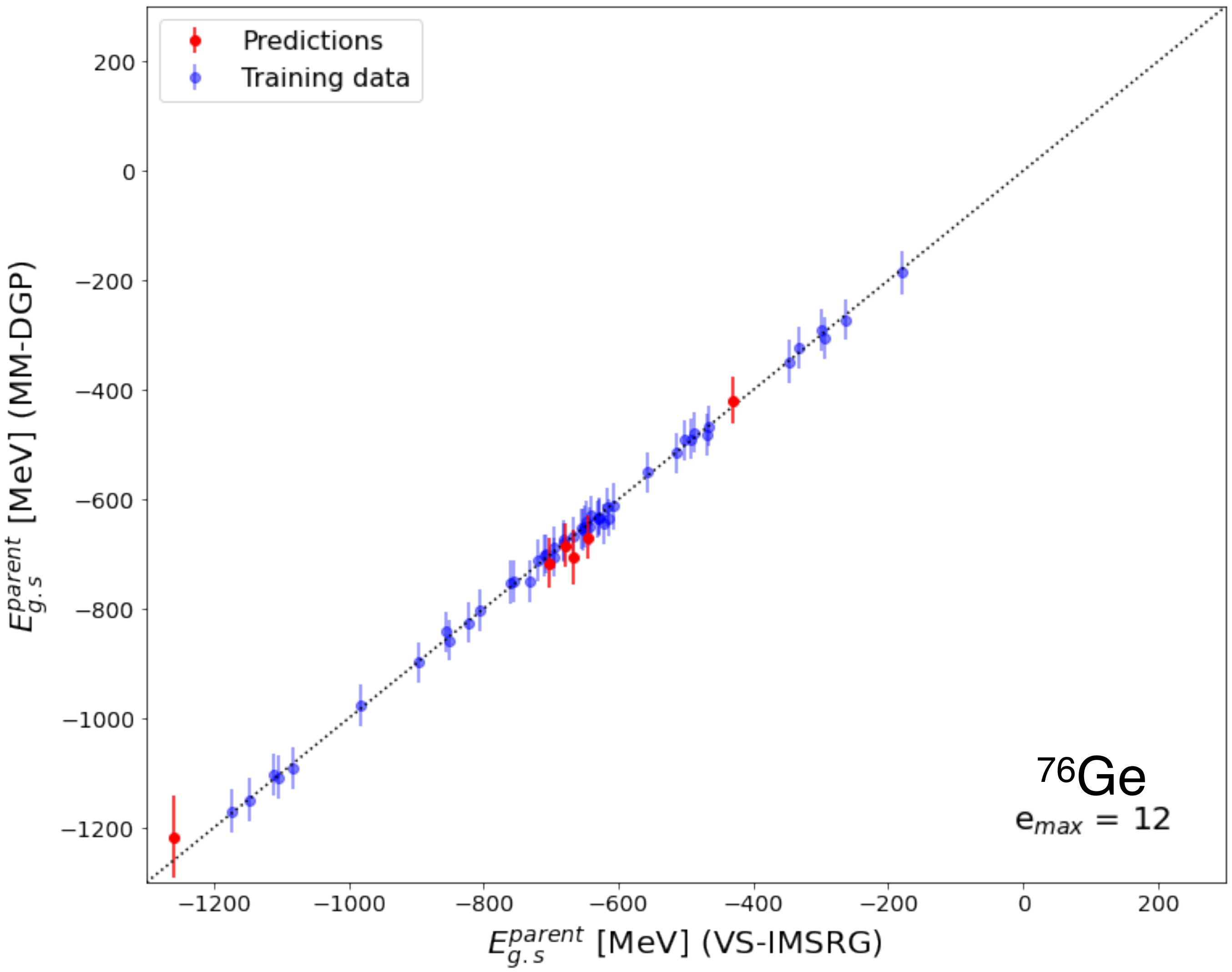


[1] Kurt Cutajar, Mark Pullin, Andreas Damianou, Neil Lawrence, Javier González arXiv:1903.07320 (2021).

The MM-DGP Algorithm: Energies

Using Δ-full chiral EFT interactions at N2LO:

50 training points



Root Mean Square Error = 11 MeV

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

Using Δ-full chiral EFT interactions at N2LO:

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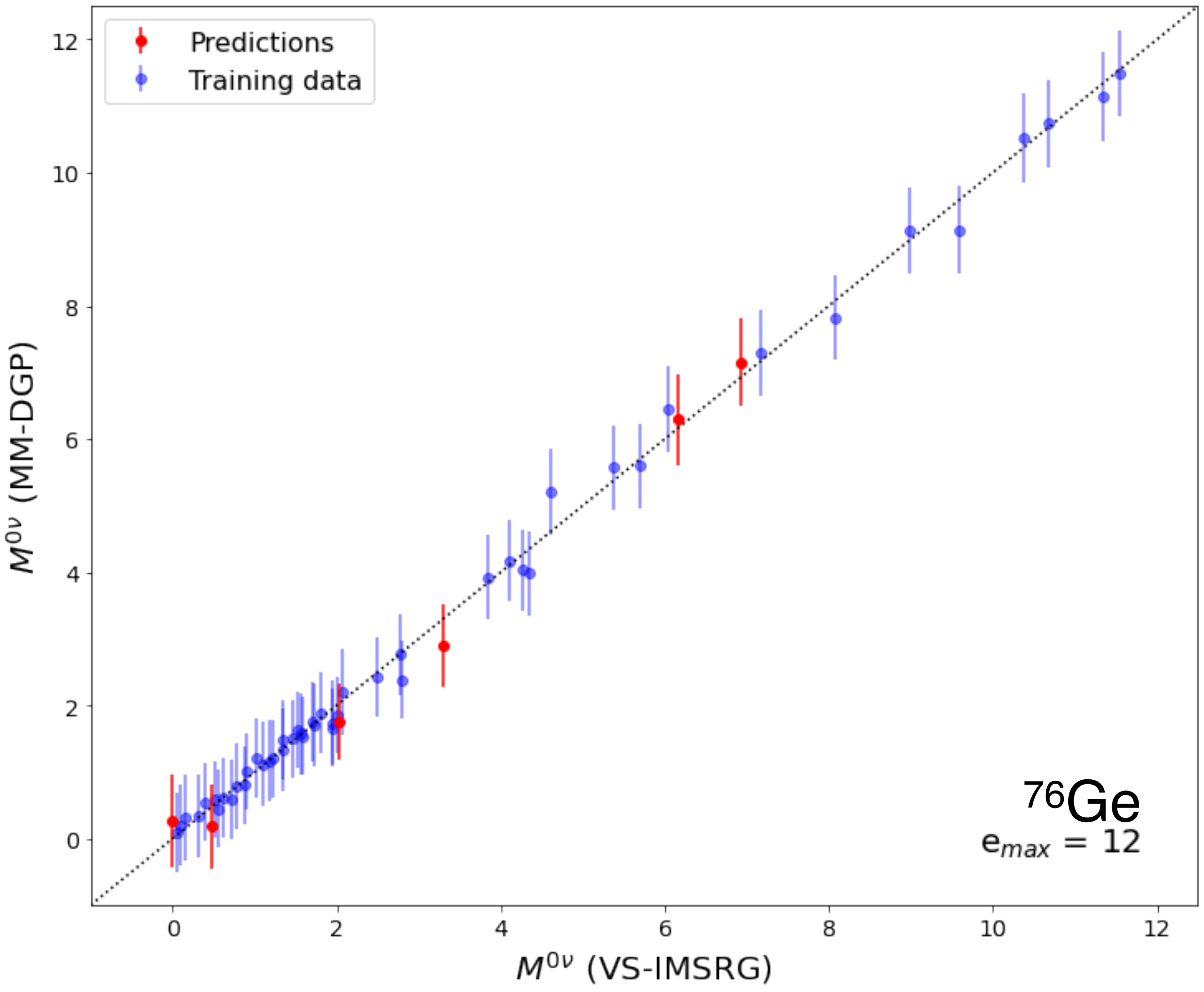
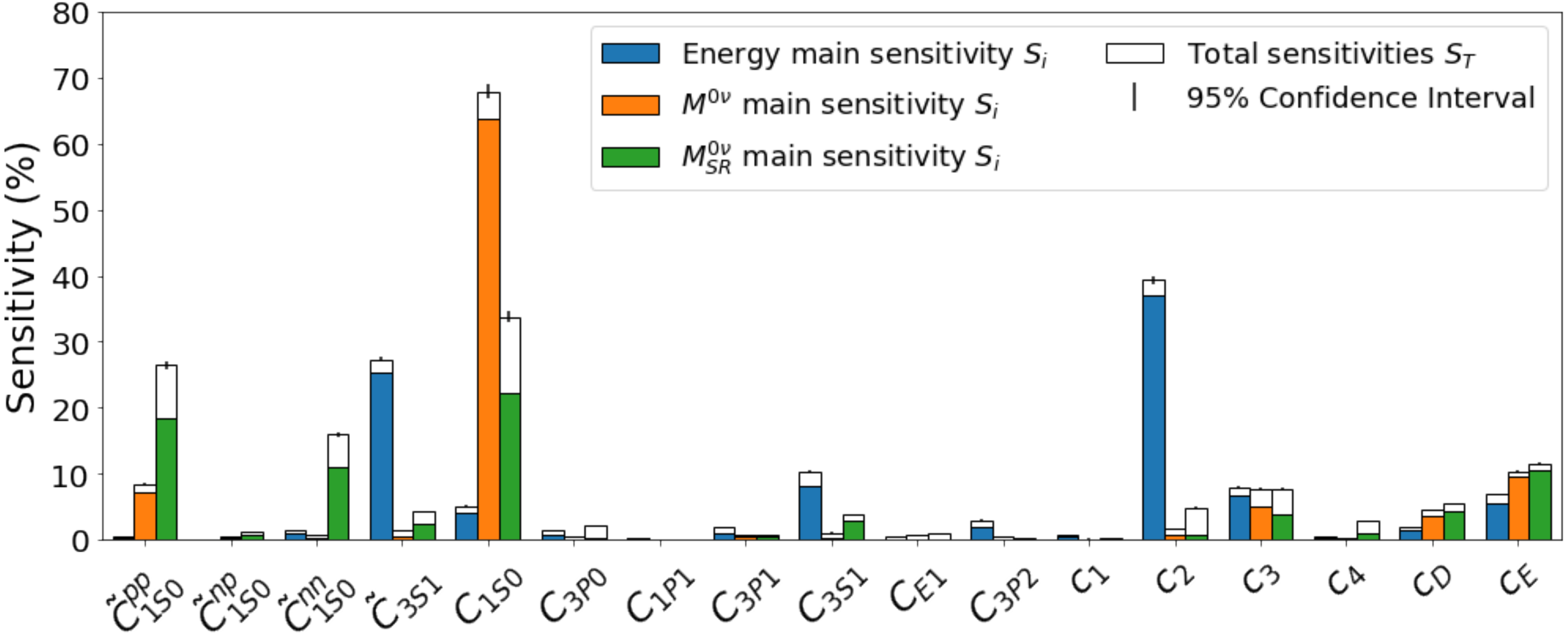


Root Mean Square Error = 0.13

The MM-DGP Algorithm: GSA



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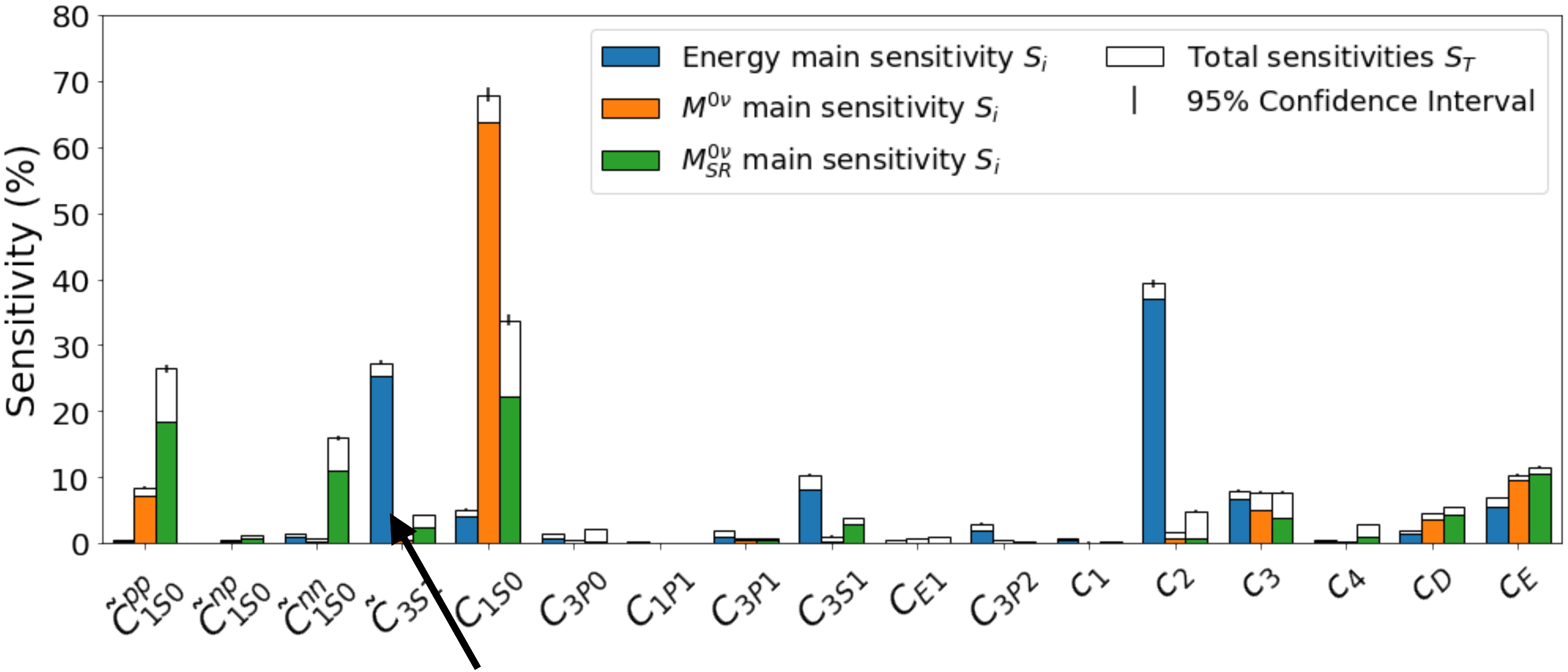
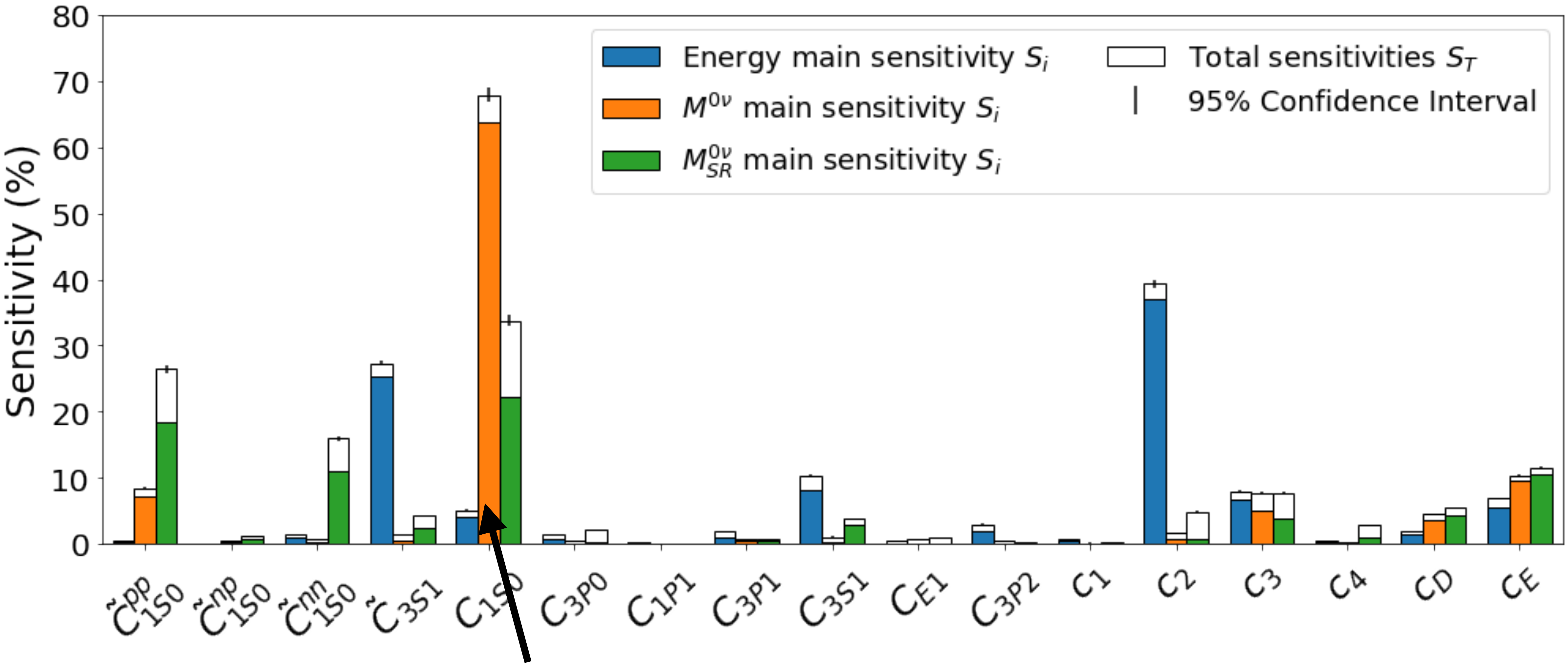


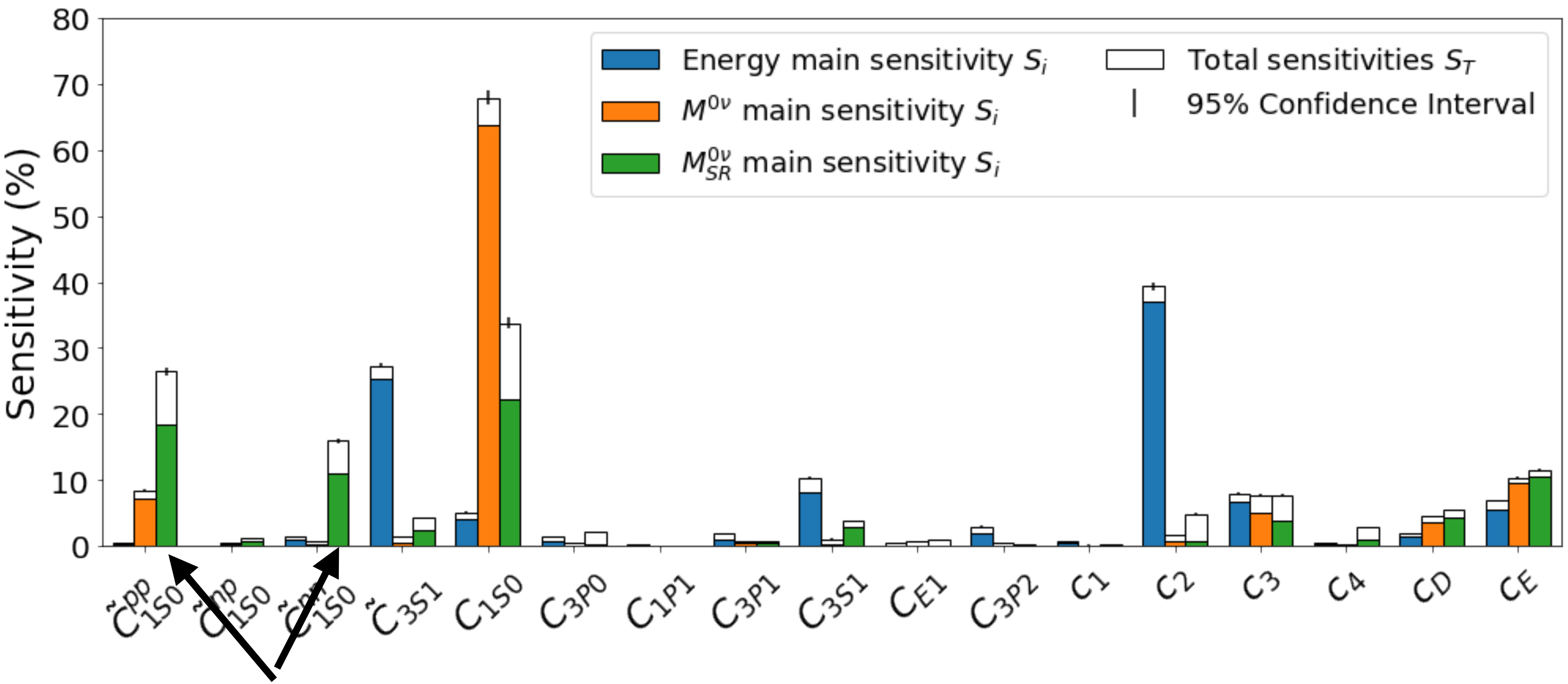
Results for energies are consistent with results of physics-based emulators of the coupled cluster method.

The MM-DGP Algorithm: GSA



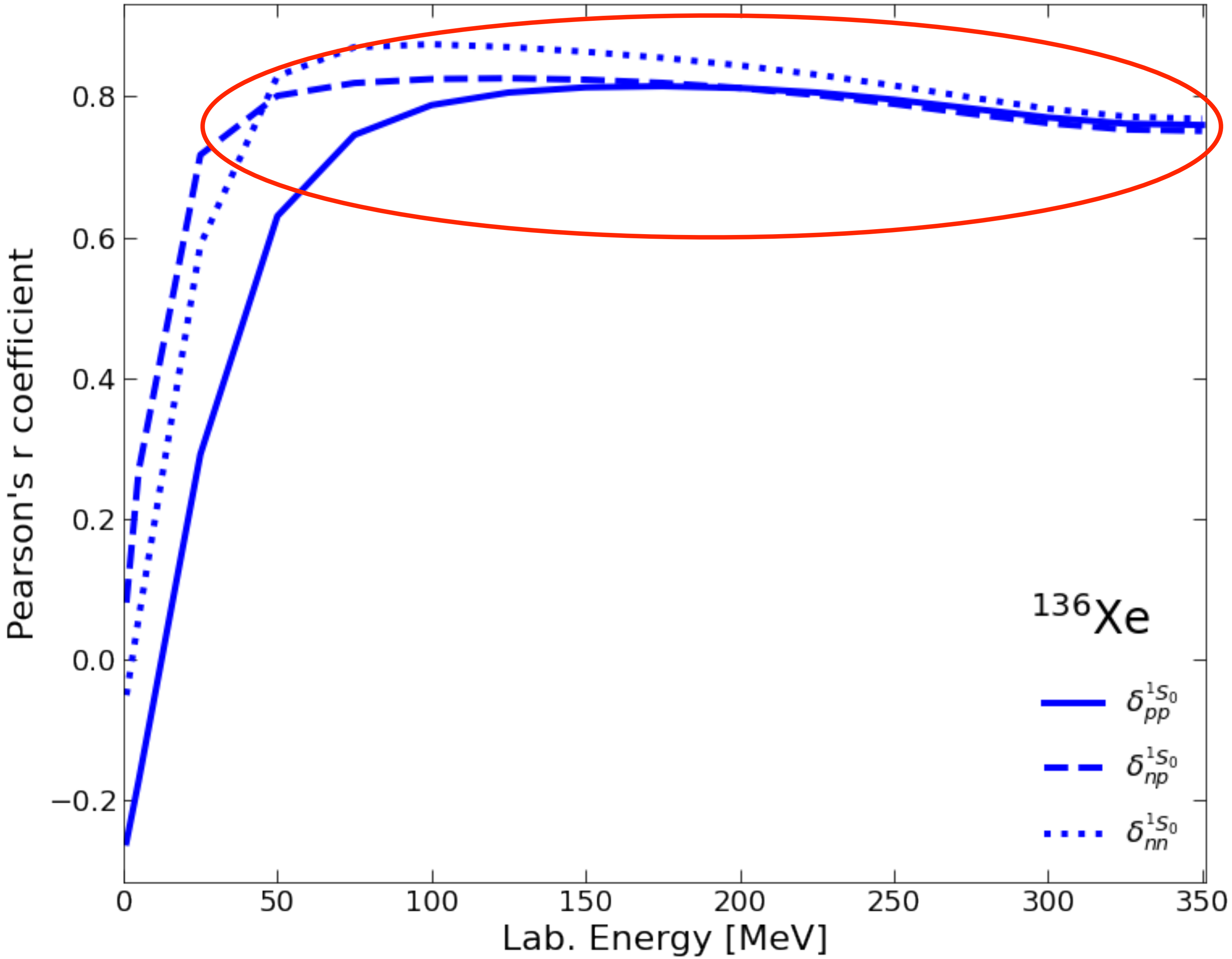
The total matrix element mostly depends on one LEC!

The MM-DGP Algorithm: GSA



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

Correlation with Phase Shifts



Strong correlation for energies > 50 MeV

⇛

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

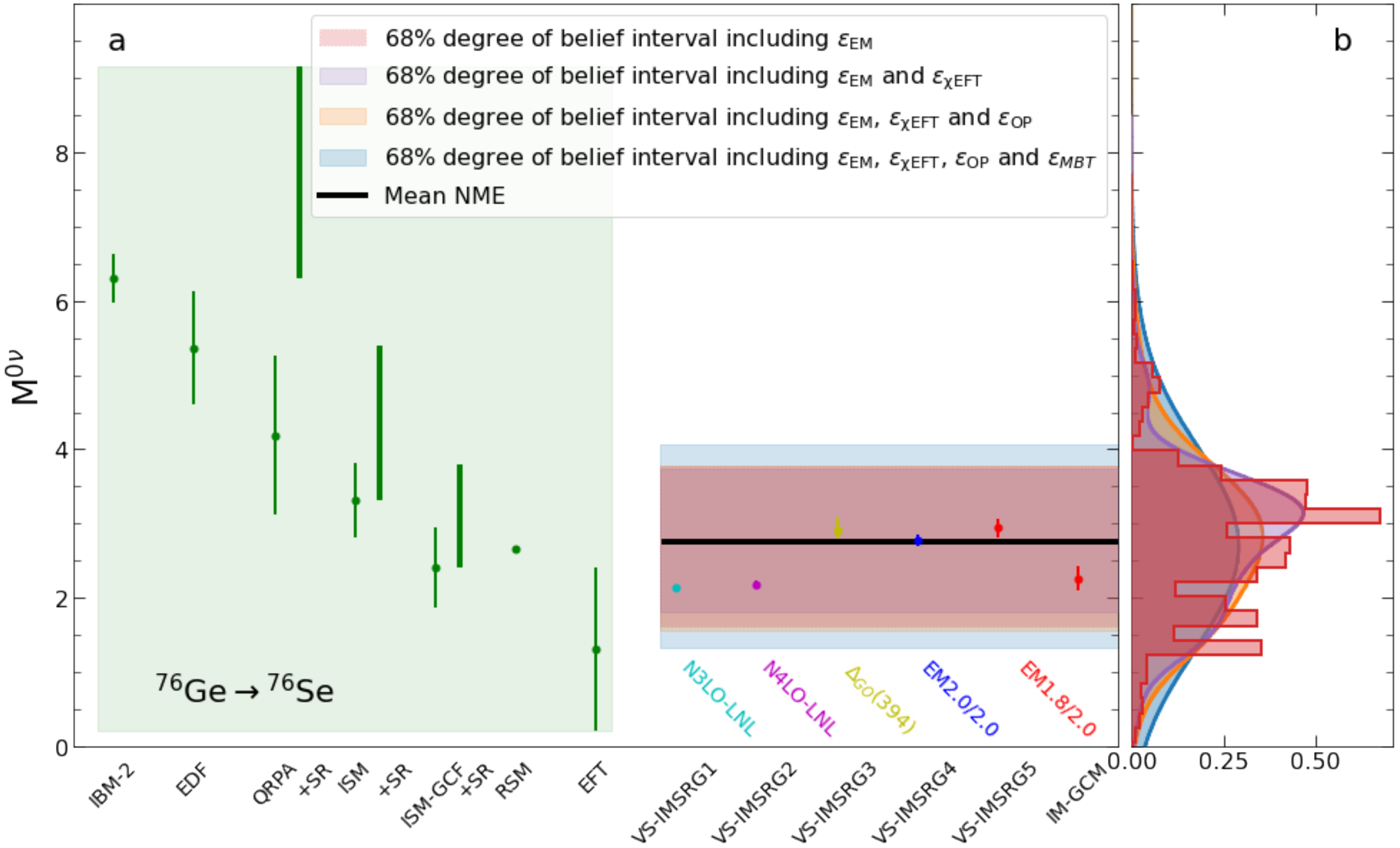
- Use 8188 “non-implausible” samples obtain by Jiang, W. G. et al. (Phys. Rev. C **109**, 064314).
- Many-body problem is “solved” with the MM-DGP.
- Consider all sources of uncertainties by taking:

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

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.

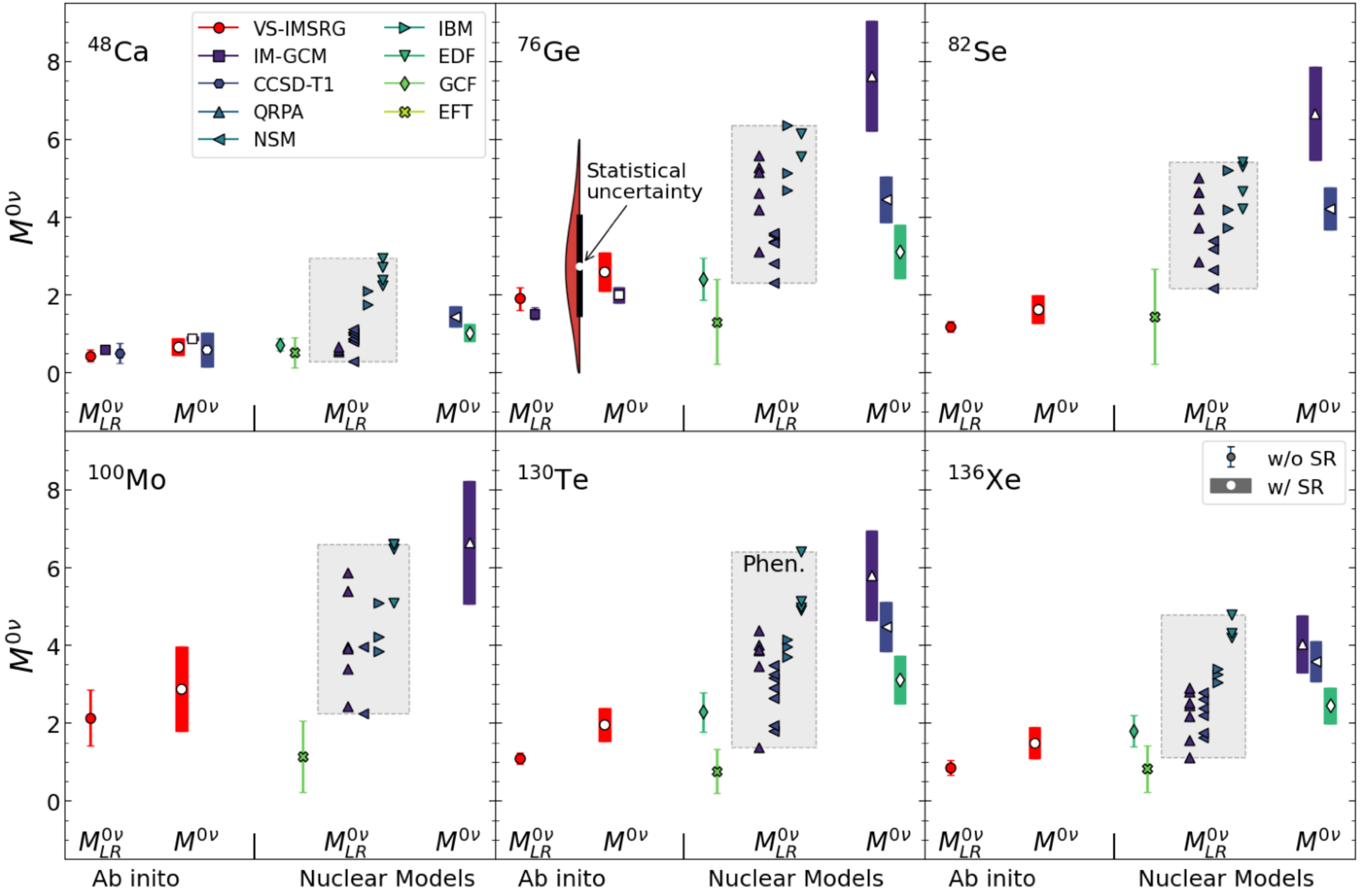
Comparing with Other Interactions



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

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

0νββ-decay Matrix Elements: The Complete Picture



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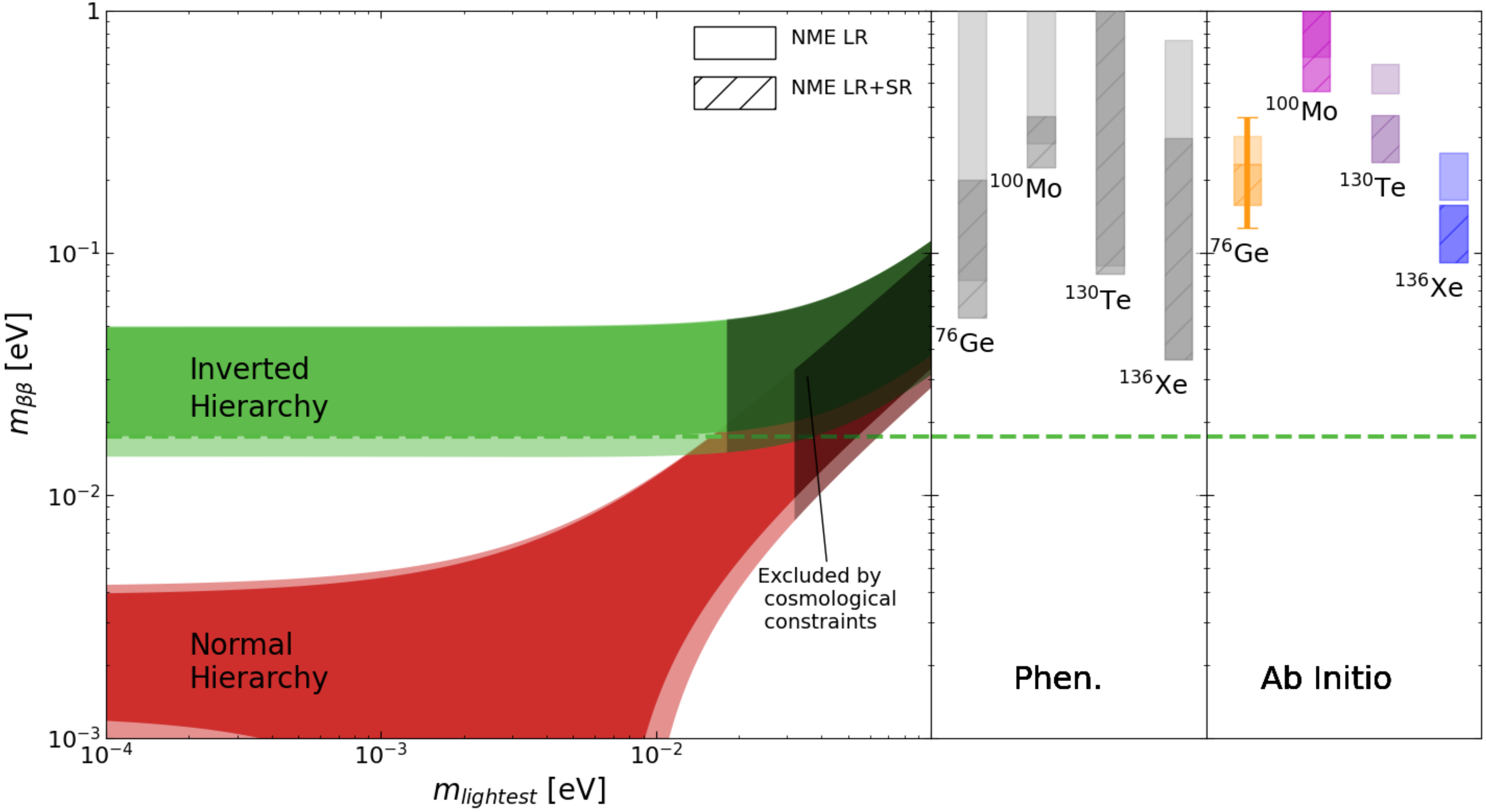
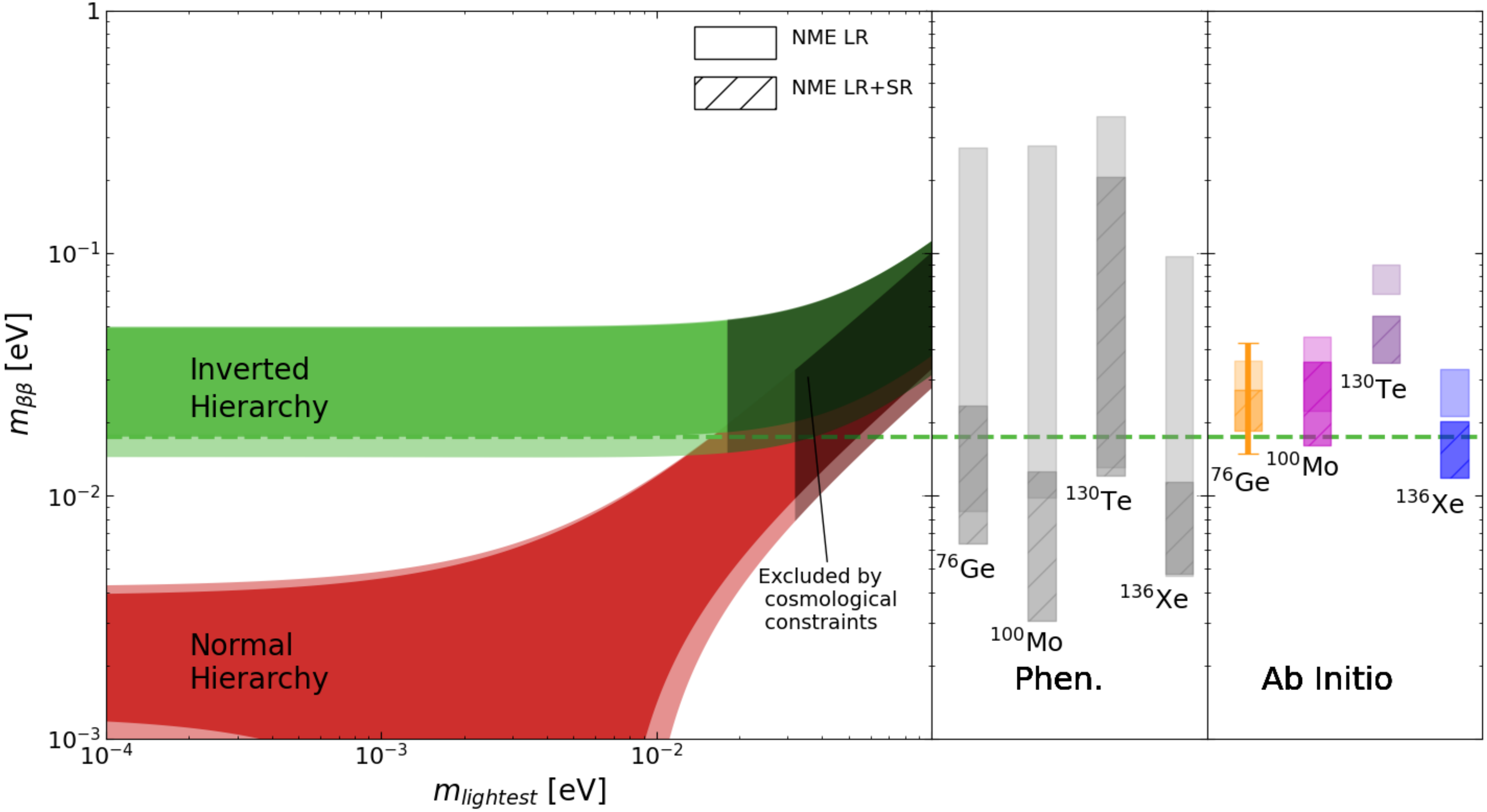
Ab Initio 0νββ Decay: Effect on Experimental Limits



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.

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Summary

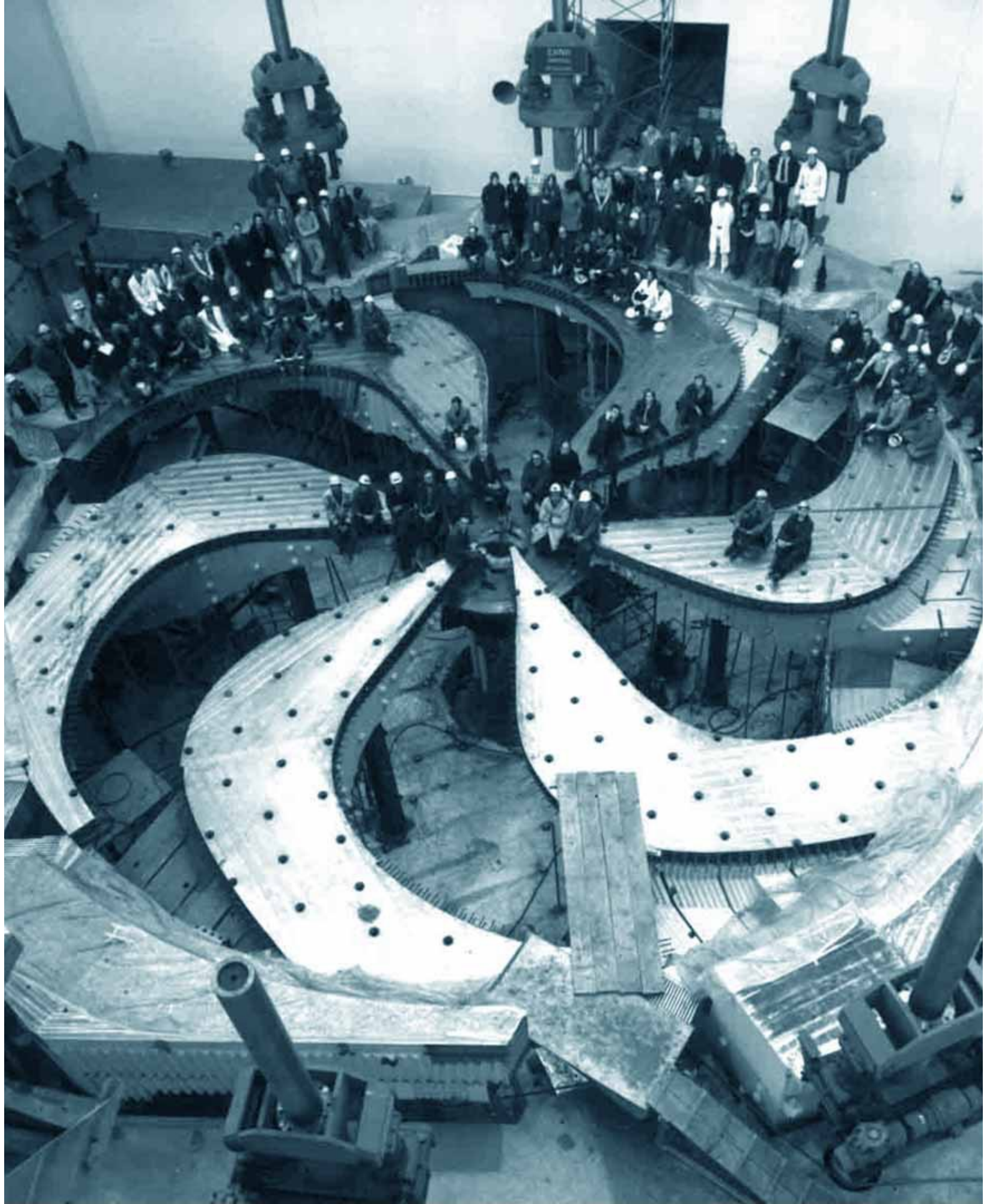
1. Computed first ever ab initio NMEs of isotopes of experimental interest as a first step towards computing NMEs with reliable theoretical uncertainties.

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

3. Studied correlation of the NMEs with multiple other nuclear observables.

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.



Discovery, accelerated

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Questions?

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Discovery, accelerated

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.:

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

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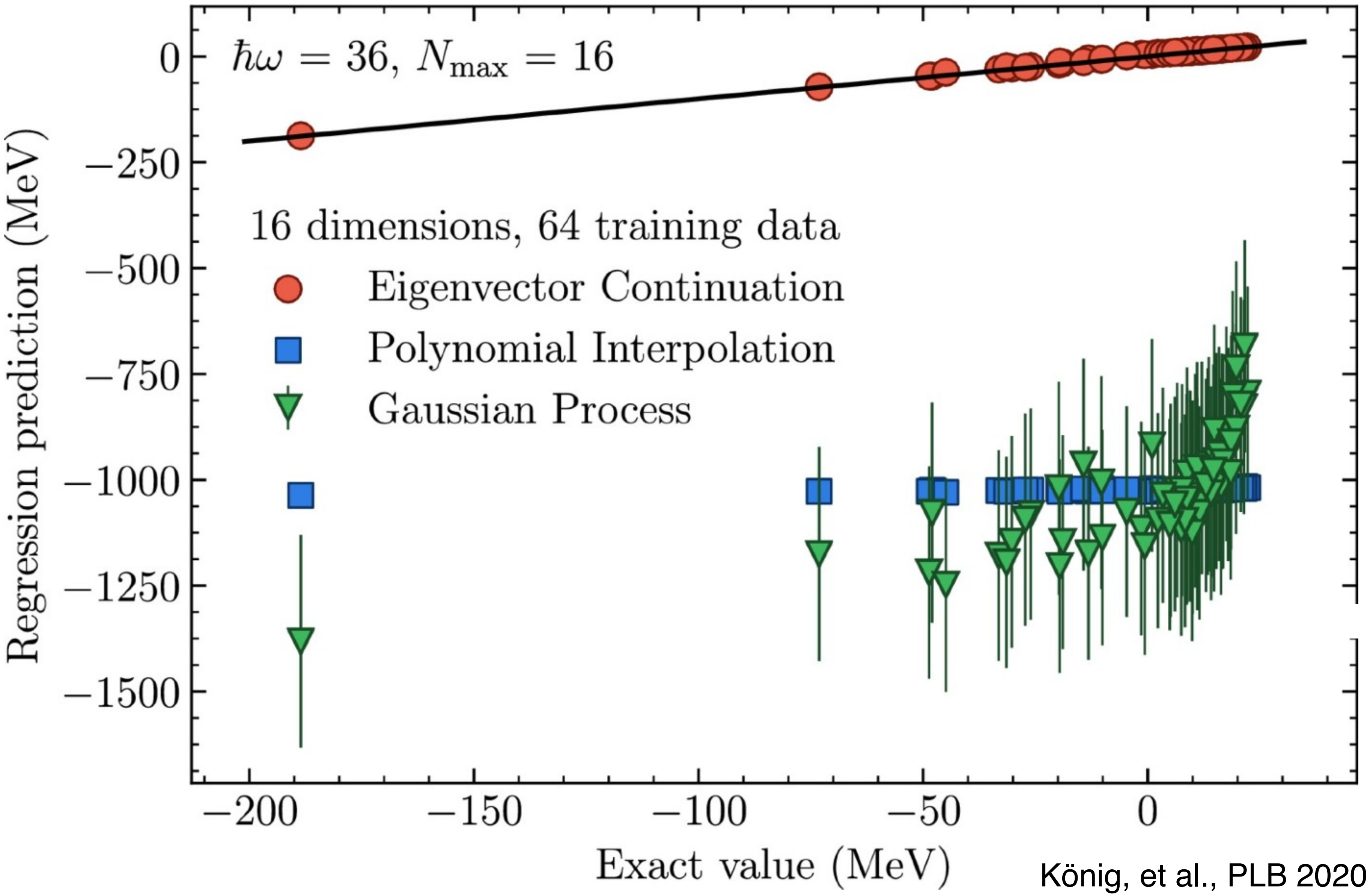
$$P_{Y*|Y} \sim \mathcal{N}\left(0 + \Sigma_{X*X}\Sigma_{XX}^{-1}(Y - 0), \Sigma_{X*X*} - \Sigma_{X*X}\Sigma_{XX}^{-1}\Sigma_{XX*}\right).$$

Normalizing inputs

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

Using Gaussian Process as an Emulator



König, et al., PLB 2020.135814

Using Gaussian Process as an Emulator

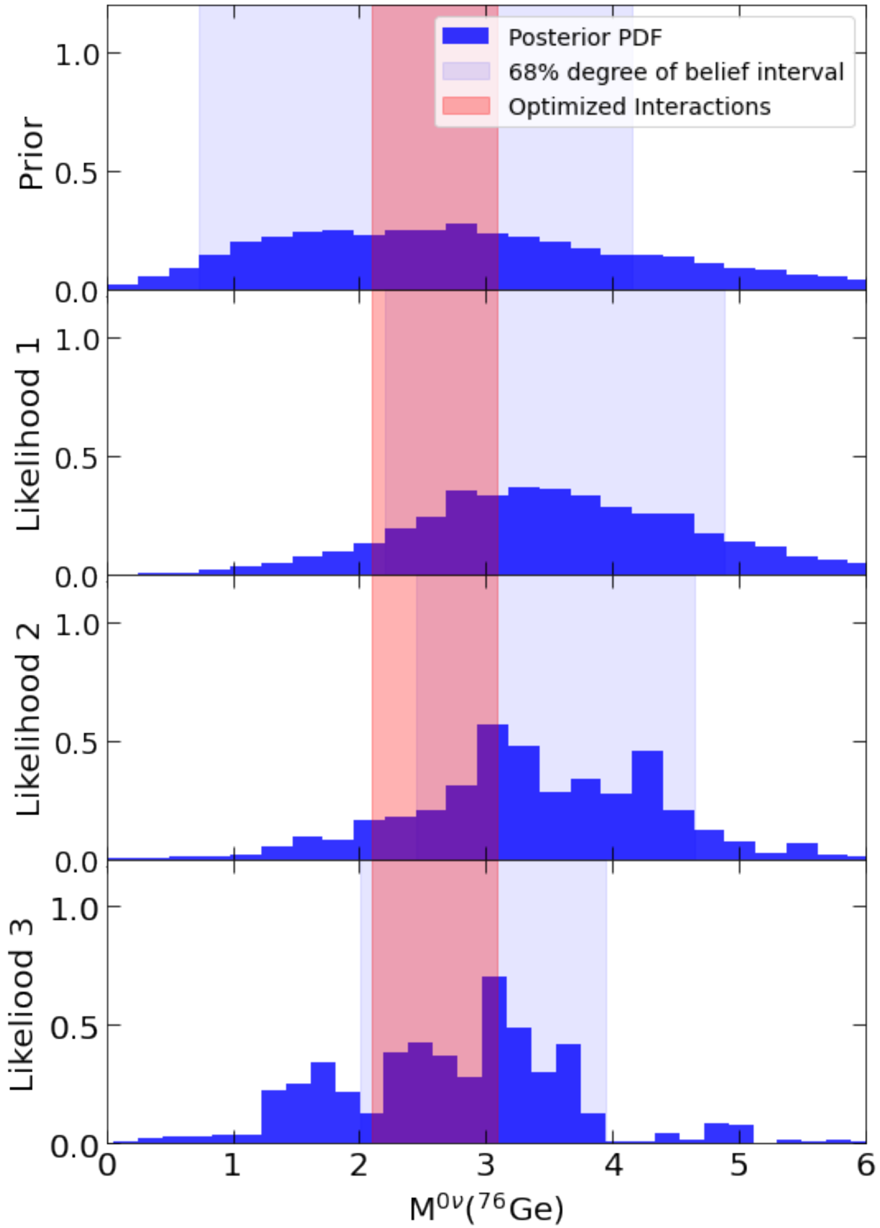
- Multi-Task Gaussian Process: Uses multiple correlated outputs from the same inputs by defining the kernel as $K_{inputs} \otimes K_{outputs}$. This allows us to increase the number of data points without needing to do more expensive calculations.

- 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 between the low- and high-fidelity calculations.

What Next?

1. Further the use of the MM-DGP algorithm to do large search of correlation for multiple nuclear observables in multiple isotopes.
2. $0\nu\beta\beta$:
   - Reduction of theoretical uncertainties.
   - Extension to other $0\nu\beta\beta$ mechanisms.
   - Extension to double neutrinoless electron capture.
3. Symmetry violation:
   - Applying the emulator to sample parameter space of the parity violating (PV) and time violating (TV) nuclear interaction and collaborate closely with experimental efforts to fix these parameters.

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.

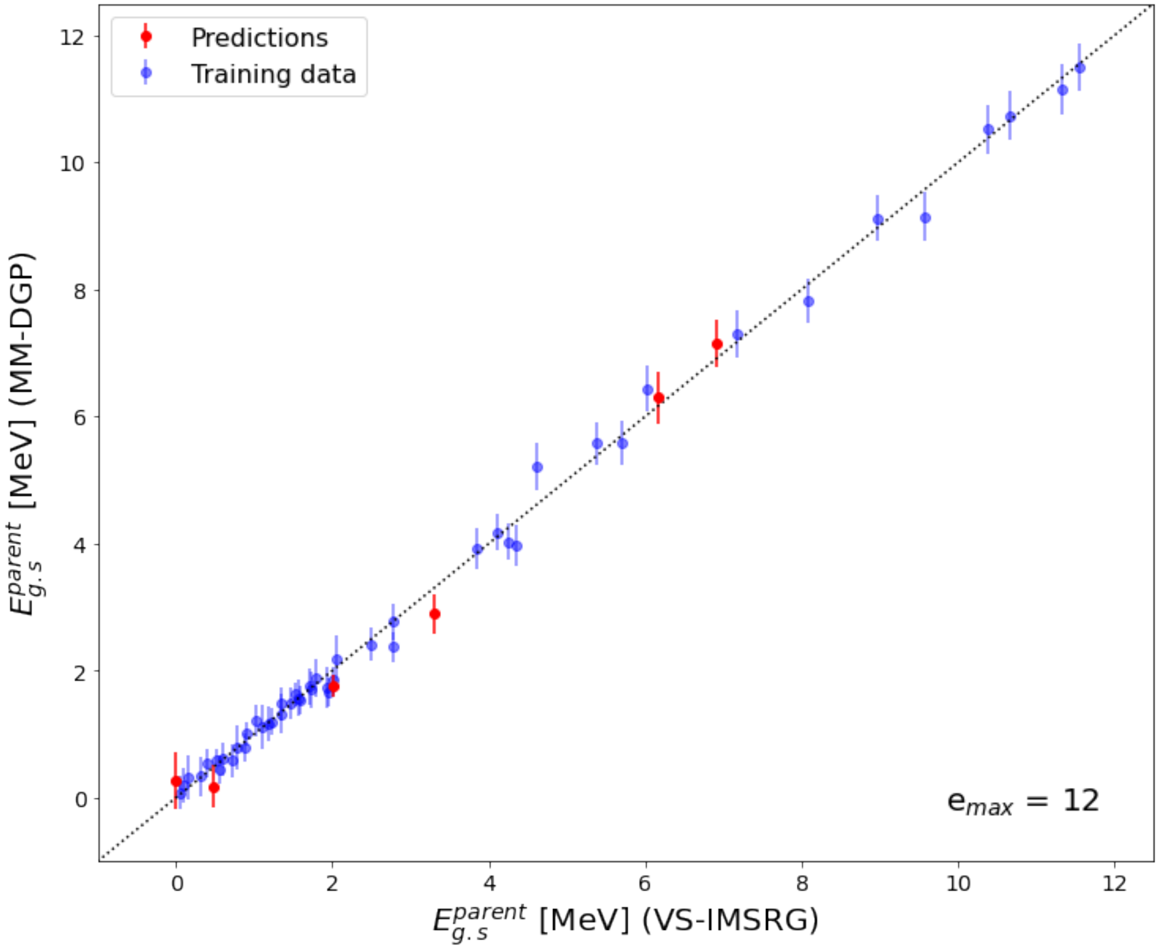
A2-4: $E(^2H)$, $r_p(^2H)$, $Q(^2H)$, $E(^3H)$, $E(^4He)$, $r_p(^4He)$

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).



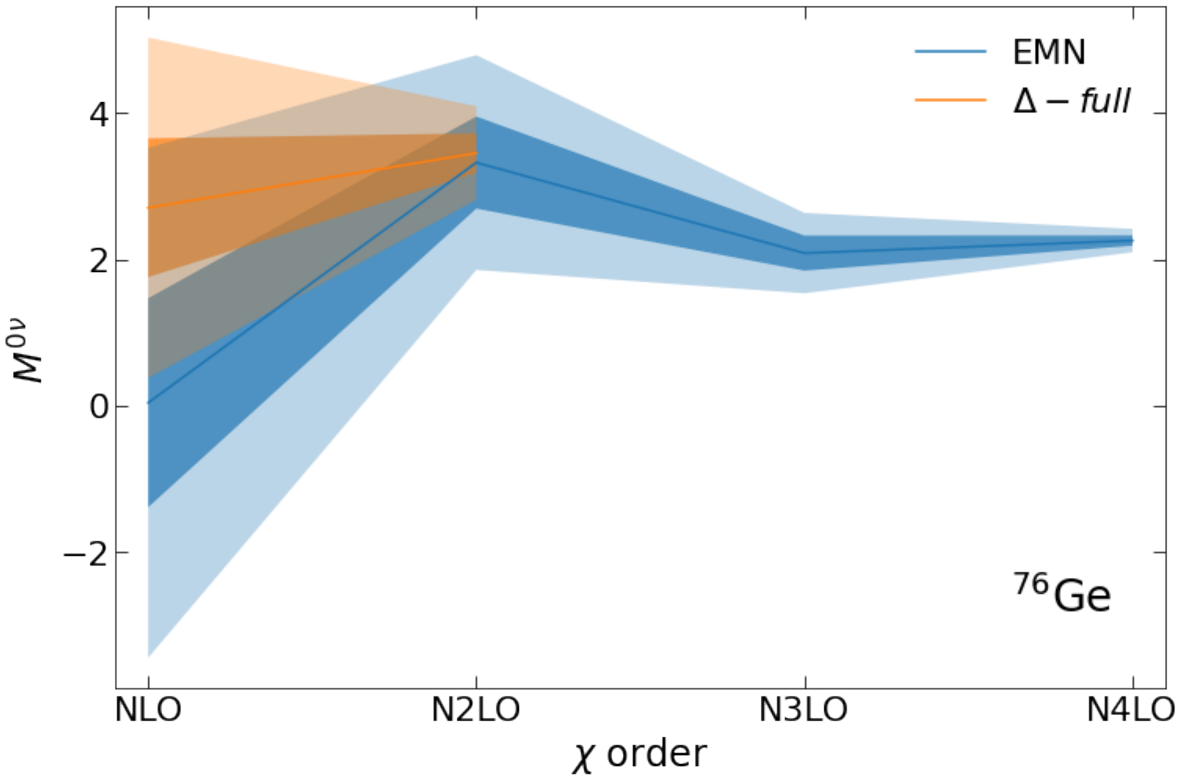
EFT Truncation Error

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

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, without delta excitations, to verify convergence of chiral expansion.

Using the Δ-full interaction of this work, only NLO and N2LO orders are available. Using expansion from BUQEYE collaboration, we get $\epsilon_{EFT} = 0.3$.

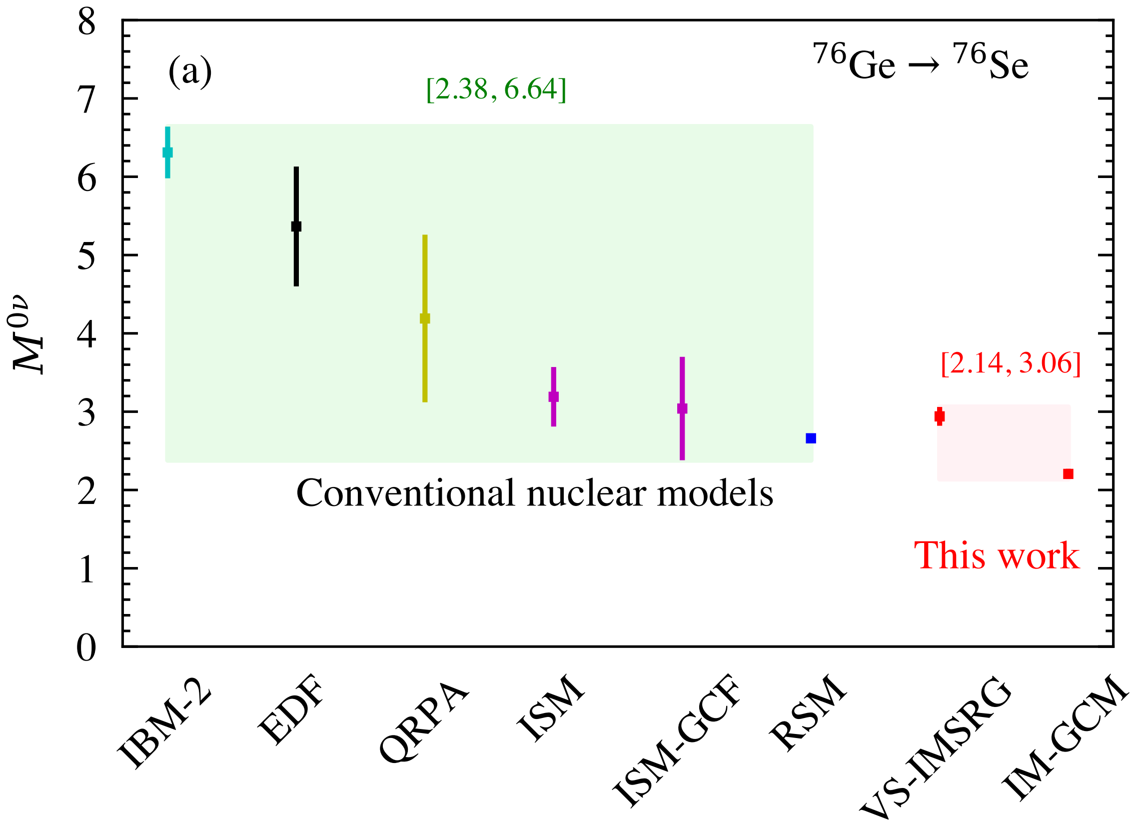


Many-Body Error

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

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.



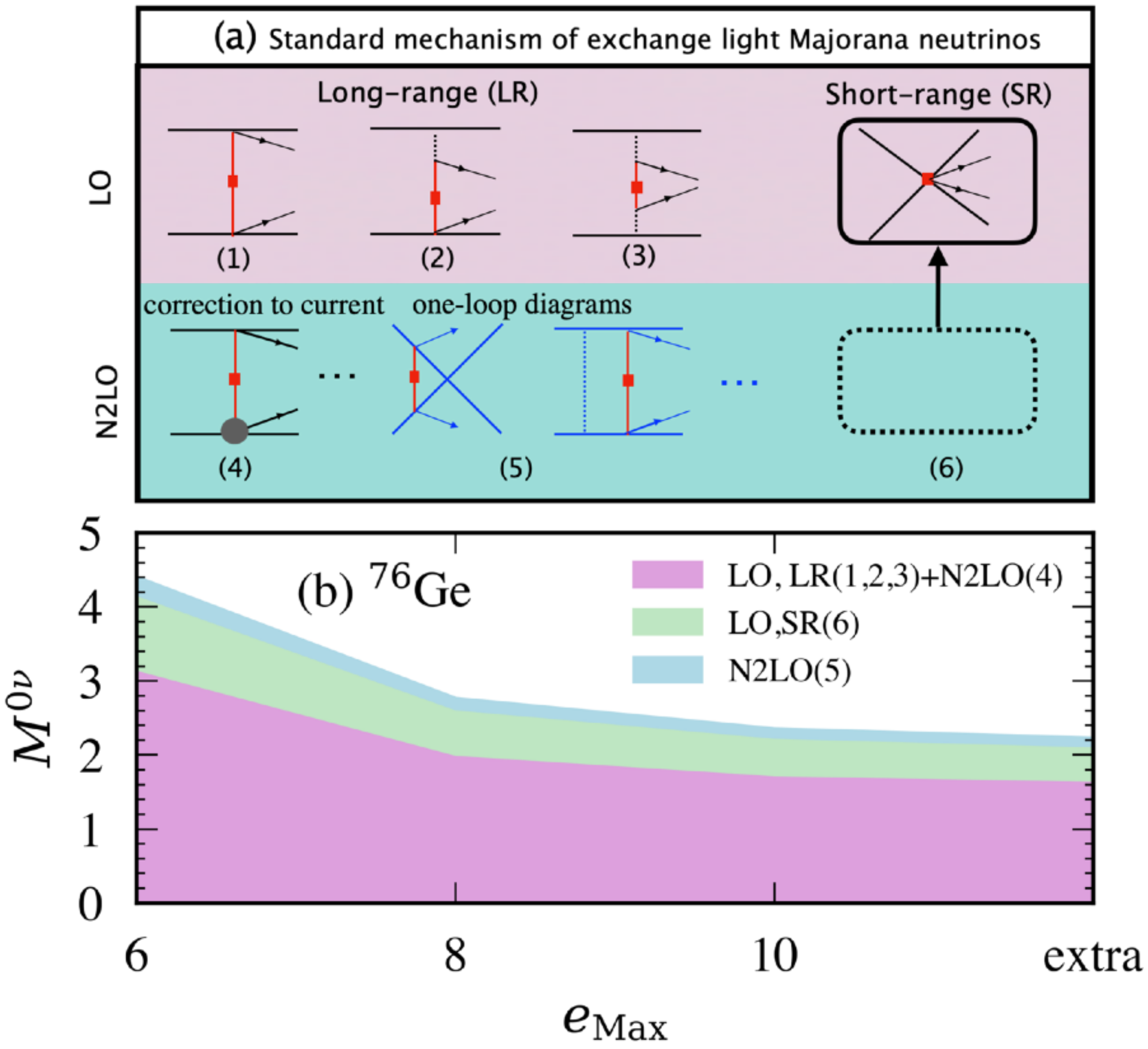
Operator Error

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

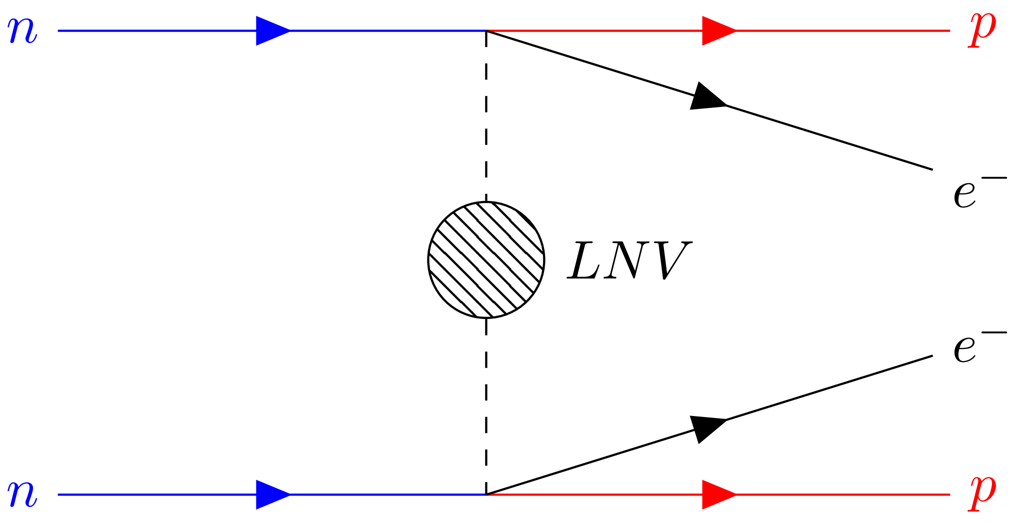
Error due to the truncation of the operator in chiral expansion + closure energy correction + value of the contact LEC.

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

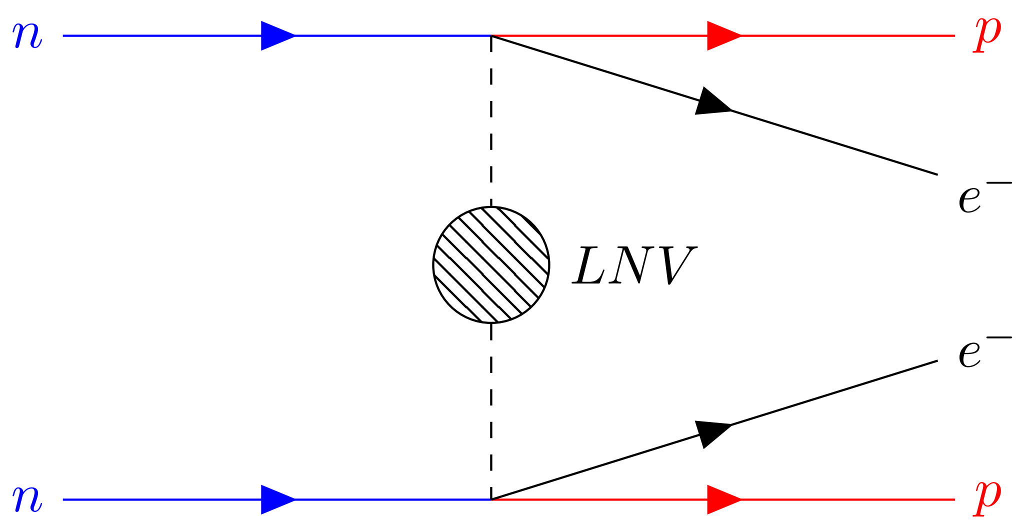
Total error amounts to $\epsilon_{operator}$ = 0.47.



$0\nu\beta\beta$

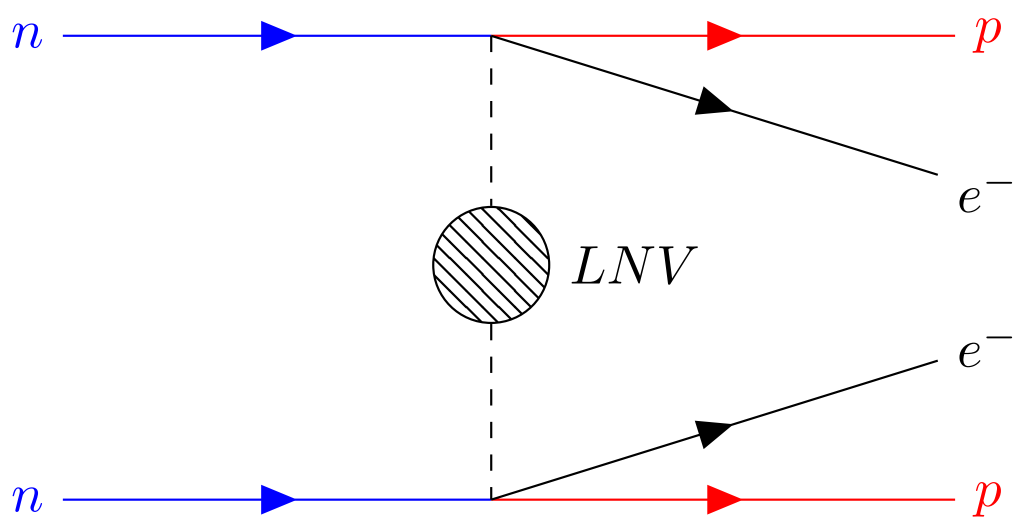


$$[T_{1/2}^{0\nu}]^{-1} = \sum_i G_i^{0\nu}\,|M_i^{0\nu}|^2\eta_i^2$$



$$[T^{0\nu}_{1/2}]^{-1} = \sum_i G^{0\nu}_i |M^{0\nu}_i|^2 \eta_i^2$$

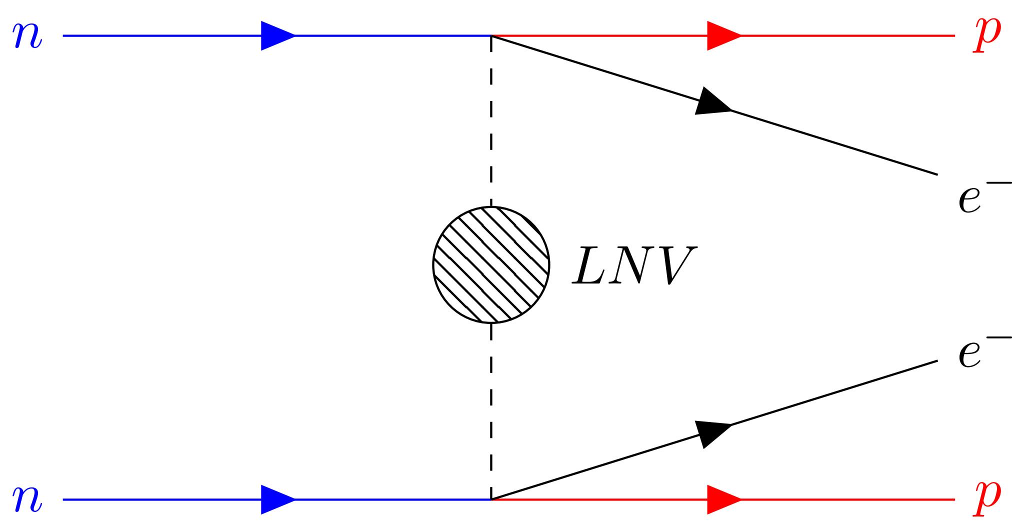
Couplings to new physics: Majorana mass, New Heavy Particles Mass, Couplings to new bosons…



$$[T_{1/2}^{0\nu}]^{-1} = \sum_i G_i^{0\nu} |M_i^{0\nu}|^2 \eta_i^2$$

Couplings to new physics: Majorana mass, New Heavy Particles Mass, Couplings to new bosons…

The nuclear matrix element, dependent on the LNV mechanism and the isotope.



The phase space factor.
Well under control.

$$[T_{1/2}^{0\nu}]^{-1} = \sum_i G_i^{0\nu} |M_i^{0\nu}|^2 \eta_i^2$$

Couplings to new physics:
Majorana mass, New Heavy Particles Mass, Couplings to new bosons…

The nuclear matrix element, dependent of the LNV mechanism and the isotope.

Lepton Number Violation

Most general Lorentz invariant effective Hamiltonian:

$$\mathscr{H}_W = \frac{G_\beta}{\sqrt{2}}\left[j_L^\mu J_{L,\mu}^\dagger + \sum_{\alpha,\beta} \epsilon_\alpha^\beta j_\alpha J_\beta^\dagger\right]$$

Lepton Number Violation

Most general Lorentz invariant effective Hamiltonian:

Lepton currents

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Hadron currents Lepton currents

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Lepton Number Violation

Most general Lorentz invariant effective Hamiltonian:

Hadron currents   Lepton currents

$$\mathscr{H}_W = \frac{G_\beta}{\sqrt{2}}\Big[\underbrace{j_L^{\mu} J^{\dagger}_{L,\mu}} + \underbrace{\sum_{\alpha,\beta} \epsilon_\alpha^\beta j_\alpha J_\beta^\dagger}\Big]$$

Standard V-A weak interaction

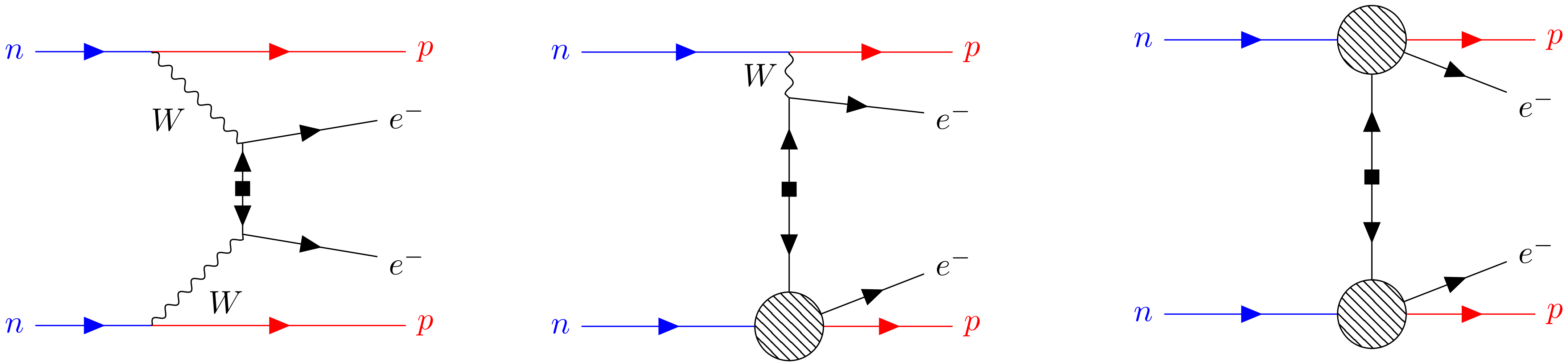
All other exotic mechanisms

Lepton Number Violation

Since $0\nu\beta\beta$ decay is a 2nd order weak process:

$$\mathscr{A}^{0\nu}_{i\to f} \propto \langle f \,|\, T[\mathscr{H}_W(x_1)\mathscr{H}_W(x_2)] \,|\, i \rangle$$

$$\propto \langle f \,|\, T[j^\mu_L J^\dagger_{L,\mu} j^\nu_L J^\dagger_{L,\nu}] + \sum_{\alpha,\beta} \epsilon^\beta_\alpha T[j^\mu_L J^\dagger_{L,\mu} j_\alpha J^\dagger_\beta] + \sum_{\alpha,\beta,\gamma,\sigma} \epsilon^\beta_\alpha \epsilon^\sigma_\gamma T[j_\alpha J^\dagger_\beta j_\gamma J^\dagger_\sigma] \,|\, i \rangle$$



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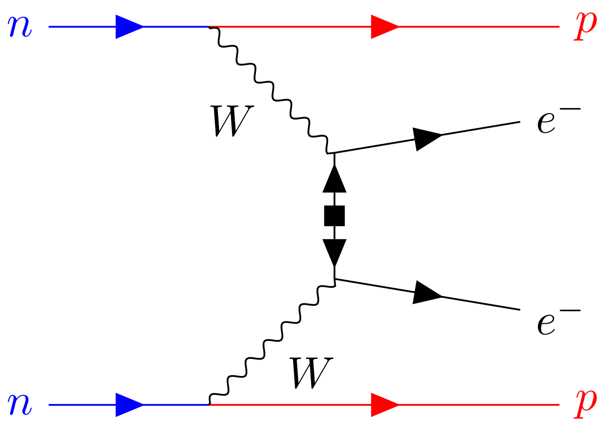
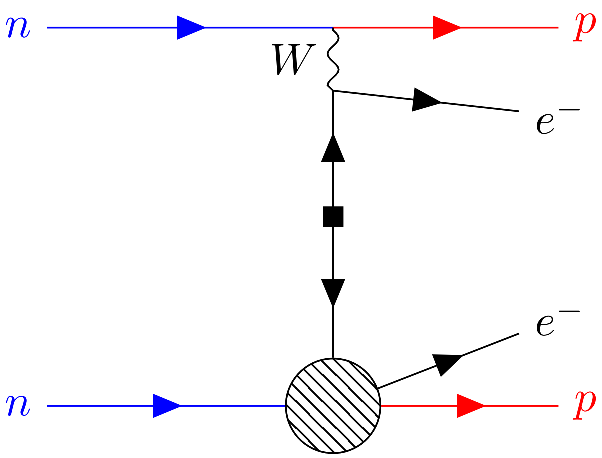
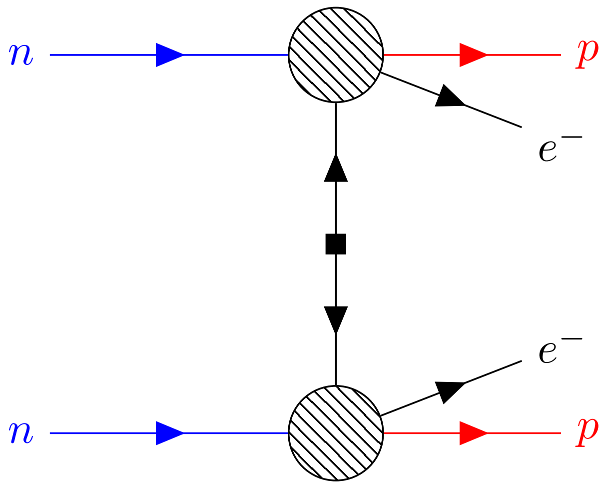
$$\propto \langle f \,|\, T[j^{\mu}_L J^{\dagger}_{L,\mu} j^{\nu}_L J^{\dagger}_{L,\nu}] + \sum_{\alpha,\beta} \epsilon^{\beta}_{\alpha} T[j^{\mu}_L J^{\dagger}_{L,\mu} j_{\alpha} J^{\dagger}_{\beta}] + \sum_{\alpha,\beta,\gamma,\sigma} \epsilon^{\beta}_{\alpha}\epsilon^{\sigma}_{\gamma} T[j_{\alpha} J^{\dagger}_{\beta} j_{\gamma} J^{\dagger}_{\sigma}] \,|\, i\rangle$$







Models can be differentiated but require the uncertainty on the NMEs for each mechanism to be less than 15%, see Gráf et al., Phys. Rev. D **106**, 035022.

Long-Range Matrix Elements

$$M_L^{0\nu} = M_{GT}^{0\nu} - \left(\frac{g_V}{g_A}\right)^2 M_F^{0\nu} + M_T^{0\nu}$$

Long-Range Matrix Elements

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(under closure approximation)

$$M_\alpha^{0\nu} = \langle 0_f^+ \,|\, V_\alpha(\boldsymbol{q}) S_\alpha(\boldsymbol{q}) \tau_1^+ \tau_2^+ \,|\, 0_i^+ \rangle$$

Long-Range Matrix Elements

$$M_L^{0\nu} = M_{GT}^{0\nu} - \left(\frac{g_V}{g_A}\right)^2 M_F^{0\nu} + M_T^{0\nu}$$

$$M_\alpha^{0\nu} = \langle 0_f^+ | V_\alpha(\boldsymbol{q}) S_\alpha(\boldsymbol{q}) \tau_1^+ \tau_2^+ | 0_i^+ \rangle$$

Scalar potential

$$V_\alpha(q) = \frac{R_{Nucl}}{2\pi^2} \frac{h_\alpha(q)}{q(q + E_{cl})}$$

Long-Range Matrix Elements

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$$V_\alpha(q) = \frac{R_{Nucl}}{2\pi^2} \frac{h_\alpha(q)}{q(q + E_{cl})}$$

E_{cl} → Closure energy

Long-Range Matrix Elements

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$$V_\alpha(q) = \frac{R_{Nucl}}{2\pi^2} \frac{h_\alpha(q)}{q(q + E_{cl})}$$

Neutrino Potential

$$h_F(q) = \frac{g_V^2(q)}{g_V^2}$$

$$h_{GT}(q) = \frac{1}{g_A^2}\left[g_A^2(q) - \frac{g_A(q)g_P(q)q^2}{3m_N} + \frac{g_P^2(q)q^4}{12m_N^2} + \frac{g_M^2(q)q^2}{6m_N^2}\right]$$

$$h_T(q) = \frac{1}{g_A^2}\left[\frac{g_A(q)g_P(q)q^2}{3m_N} - \frac{g_P^2(q)q^4}{12m_N^2} + \frac{g_M^2(q)q^2}{12m_N^2}\right].$$

Long-Range Matrix Elements

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$$M_\alpha^{0\nu} = \langle 0_f^+ | V_\alpha(\boldsymbol{q}) S_\alpha(\boldsymbol{q}) \tau_1^+ \tau_2^+ | 0_i^+ \rangle$$

Operator acting on spin

$$V_\alpha(q) = \frac{R_{Nucl}}{2\pi^2} \frac{h_\alpha(q)}{q(q + E_{cl})}$$

$$h_F(q) = \frac{g_V^2(q)}{g_V^2}$$

$$h_{GT}(q) = \frac{1}{g_A^2}\left[g_A^2(q) - \frac{g_A(q)g_P(q)q^2}{3m_N} + \frac{g_P^2(q)q^4}{12m_N^2} + \frac{g_M^2(q)q^2}{6m_N^2}\right]$$

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$$S_F = 1$$

$$S_{GT} = \boldsymbol{\sigma_1} \cdot \boldsymbol{\sigma_2}$$

$$S_T = -3[(\boldsymbol{\sigma_1} \cdot \hat{\boldsymbol{q}})(\boldsymbol{\sigma_2} \cdot \hat{\boldsymbol{q}}) - (\boldsymbol{\sigma_1} \cdot \boldsymbol{\sigma_2})].$$

Long-Range Matrix Elements

$$M_L^{0\nu} = M_{GT}^{0\nu} - \left(\frac{g_V}{g_A}\right)^2 M_F^{0\nu} + M_T^{0\nu}$$

$$M_\alpha^{0\nu} = \langle 0_f^+ | V_\alpha(\boldsymbol{q}) S_\alpha(\boldsymbol{q}) \tau_1^+ \tau_2^+ | 0_i^+ \rangle$$

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$$h_{GT}(q) = \frac{1}{g_A^2}\left[g_A^2(q) - \frac{g_A(q)g_P(q)q^2}{3m_N} + \frac{g_P^2(q)q^4}{12m_N^2} + \frac{g_M^2(q)q^2}{6m_N^2}\right]$$

$$h_T(q) = \frac{1}{g_A^2}\left[\frac{g_A(q)g_P(q)q^2}{3m_N} - \frac{g_P^2(q)q^4}{12m_N^2} + \frac{g_M^2(q)q^2}{12m_N^2}\right].$$

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Short-Range Matrix Elements

$$M_S^{0\nu} = -2g_{\nu\nu}M_{CT}^{0\nu}$$

Short-Range Matrix Elements

$$M_S^{0\nu} = -2g_{\nu\nu}M_{CT}^{0\nu}$$

Unknown coupling constants.

Method by Cirigliano et al. (JHEP05(2021)289) proivdes a way to extract this coupling for ab initio methods with 30% accuracy for each nuclear interaction.

Short-Range Matrix Elements

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Unknown coupling constants.

Method by Cirigliano et al. (JHEP05(2021)289) proivdes a way to extract this coupling for ab initio methods with 30% accuracy for each nuclear interaction.

Contact operator regularized with non-local regulator matching the nuclear interaction used:

$$M_{CT}^{0\nu} = \langle 0_f^+ | \frac{R_{Nucl}}{8\pi^3} \left(\frac{m_N g_A^2}{4 f_\pi^2} \right)^2 \exp(-(\frac{p}{\Lambda_{int}})^{2n_{int}}) \exp(-(\frac{p'}{\Lambda_{int}})^{2n_{int}}) | 0_i^+ \rangle$$

VS-IMSRG

Similarity Renormalization Group

The general idea is to simplify the Hamiltonian by using a continuous unitary transformation:

$$\hat{H}(s) = \hat{U}(s)\hat{H}(0)\hat{U}^{\dagger}(s)$$

where s parameterized the continuous transformation, and $\hat{H}(0)$ is the starting Hamiltonian.

Similarity Renormalization Group: The Flow Equation

Since we are looking for a continuous transformation of $\hat{H}(s)$, we are interested in finding how it changes as we vary the parameter, i.e.

$$\frac{d\hat{H}(s)}{ds} = \frac{d\hat{U}(s)}{ds}\hat{H}(0)\hat{U}^{\dagger}(s) + \hat{U}(s)\hat{H}(0)\frac{d\hat{U}^{\dagger}(s)}{ds}$$

By inserting the identity in the form of $\hat{I} = \hat{U}^{\dagger}(s)\hat{U}(s)$, we get

$$\frac{d\hat{H}(s)}{ds} = \frac{d\hat{U}(s)}{ds}\left(\hat{U}^{\dagger}(s)\hat{U}(s)\right)\hat{H}(0)\hat{U}^{\dagger}(s) + \hat{U}(s)\hat{H}(0)\left(\hat{U}^{\dagger}(s)\hat{U}(s)\right)\frac{d\hat{U}^{\dagger}(s)}{ds}$$

$$= \frac{d\hat{U}(s)}{ds}\hat{U}^{\dagger}(s)\hat{H}(s) + \hat{H}(s)\hat{U}(s)\frac{d\hat{U}^{\dagger}(s)}{ds}$$

Similarity Renormalization Group: The Generator

Note that $\hat{U}(s)$ being unitary implies that

$$\frac{d}{ds}\left(\hat{U}(s)\hat{U}^{\dagger}(s)\right) = \frac{d}{ds}\left(\hat{I}\right) = 0 \Rightarrow \frac{d\hat{U}(s)}{ds}\hat{U}^{\dagger}(s) = -\hat{U}(s)\frac{d\hat{U}^{\dagger}(s)}{ds}$$

We now define

$$\hat{\eta}(s) \equiv \frac{d\hat{U}(s)}{ds}\hat{U}^{\dagger}(s) = -\hat{\eta}^{\dagger}(s)$$

where we call $\hat{\eta}(s)$ the generator of the flow. We also note by the equation above that the generator is an anti-Hermitian operator.

Similarity Renormalization Group: Final Form of the Flow Equation

We found the flow in the s parameter for our Hamiltonian to be

$$\frac{d\hat{H}(s)}{ds} = \frac{d\hat{U}(s)}{ds}\hat{U}^\dagger(s)\hat{H}(s) + \hat{H}(s)\hat{U}(s)\frac{d\hat{U}^\dagger(s)}{ds}$$

Writing the expression above in terms of the generator we have defined, we get

$$\begin{aligned}\frac{d\hat{H}(s)}{ds} &= \frac{d\hat{U}(s)}{ds}\hat{U}^\dagger(s)\hat{H}(s) + \hat{H}(s)\hat{U}(s)\frac{d\hat{U}^\dagger(s)}{ds} \\ &= \hat{\eta}(s)\hat{H}(s) + \hat{H}(s)\hat{\eta}^\dagger(s) \\ &= \hat{\eta}(s)\hat{H}(s) - \hat{H}(s)\hat{\eta}(s)\end{aligned}$$

We see that the last line is simply the commutator of the generator and the Hamiltonian. Thus, we get for the flow equation:

$$\boxed{\frac{d\hat{H}(s)}{ds} = \left[\hat{\eta}(s), \hat{H}(s)\right]}$$

The IMSRG: Normal Ordering

Going to second quantization, we define Fermionic creation and annihilation operators $a_i^\dagger$ and a_i acting on a reference state $|\Phi\rangle$. The idea in the IMSRG is to use a reasonable approximation of the ground state as the reference state rather than the vacuum.

Contraction with reference state

$$\{a_i^\dagger a_j\} = a_i^\dagger a_j - \overbrace{\langle\Phi|a_i^\dagger a_j|\Phi\rangle}$$

Normal ordered operator

Reference state

The IMSRG: NO2B Hamiltonian

Considering the nuclear Hamiltonian:

$$\hat{H} = \left(1 - \frac{1}{\hat{A}}\right) \sum_i \frac{\hat{\boldsymbol{p}}_i^2}{2m} + \frac{1}{\hat{A}} \left(- \frac{1}{m} \sum_{i<j} \hat{\boldsymbol{p}}_i \hat{\boldsymbol{p}}_j \right) + \hat{V}^{[2]} + \hat{V}^{[3]}$$

The IMSRG: NO2B Hamiltonian

Considering the nuclear Hamiltonian:

$$\hat{H} = \left(1 - \frac{1}{\hat{A}}\right) \boxed{\sum_i \frac{\hat{\boldsymbol{p}}_i^2}{2m}} + \frac{1}{\hat{A}}\left(- \frac{1}{m} \sum_{i<j} \hat{\boldsymbol{p}}_i \hat{\boldsymbol{p}}_j \right) + \hat{V}^{[2]} + \hat{V}^{[3]}$$

One-body kinetic energy $\hat{T}^{[1]}$

The IMSRG: NO2B Hamiltonian

Considering the nuclear Hamiltonian:

Two-body kinetic energy $\hat{T}^{[2]}$

$$\hat{H} = \left(1 - \frac{1}{\hat{A}}\right)\sum_i \frac{\hat{\boldsymbol{p}}_i^2}{2m} + \frac{1}{\hat{A}}\left(-\frac{1}{m}\sum_{i<j}\hat{\boldsymbol{p}}_i\hat{\boldsymbol{p}}_j\right) + \hat{V}^{[2]} + \hat{V}^{[3]}$$

The IMSRG: NO2B Hamiltonian

Considering the nuclear Hamiltonian:

NN forces

$$\hat{H} = \left(1 - \frac{1}{\hat{A}}\right) \sum_i \frac{\hat{\boldsymbol{p}}_i^2}{2m} + \frac{1}{\hat{A}}\left(- \frac{1}{m} \sum_{i<j} \hat{\boldsymbol{p}}_i \hat{\boldsymbol{p}}_j \right) + \hat{V}^{[2]} + \hat{V}^{[3]}$$

The IMSRG: NO2B Approximation

Considering the nuclear Hamiltonian:

3N forces

$$\hat{H} = \left(1 - \frac{1}{\hat{A}}\right) \sum_i \frac{\hat{\boldsymbol{p}}_i^2}{2m} + \frac{1}{\hat{A}}\left(- \frac{1}{m} \sum_{i<j} \hat{\boldsymbol{p}}_i \hat{\boldsymbol{p}}_j \right) + \hat{V}^{[2]} + \boxed{\hat{V}^{[3]}}$$

The IMSRG: NO2B Approximation

Considering the nuclear Hamiltonian:

$$\hat{H} = \left(1 - \frac{1}{\hat{A}}\right) \sum_i \frac{\hat{\boldsymbol{p}}_i^2}{2m} + \frac{1}{\hat{A}} \left(- \frac{1}{m} \sum_{i<j} \hat{\boldsymbol{p}}_i \hat{\boldsymbol{p}}_j \right) + \hat{V}^{[2]} + \hat{V}^{[3]}$$

We can rewrite the Hamiltonian in terms of normal ordered operators as:

$$\hat{H} = E + \sum_{ij} f_{ij} \{a_i^\dagger a_j\} + \frac{1}{4} \sum_{ijkl} \Gamma_{ijkl} \{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{36} \sum_{ijklmn} W_{ijklmn} \{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}$$

The IMSRG: NO2B Approximation

$$\hat{H} = E + \sum_{ij} f_{ij}\{a_i^\dagger a_j\} + \frac{1}{4}\sum_{ijkl}\Gamma_{ijkl}\{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{36}\sum_{ijklmn} W_{ijklmn}\{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}$$

$$E = \left(1 - \frac{1}{A}\right)\sum_a \langle a|\hat{T}^{[1]}|a\rangle n_a + \frac{1}{2}\sum_{ab}\langle ab|\frac{1}{A}\hat{T}^{[2]} + \hat{V}^{[2]}|ab\rangle n_a n_b + \frac{1}{6}\sum_{abc}\langle abc|\hat{V}^{[3]}|abc\rangle n_a n_b n_c$$

The IMSRG: NO2B Approximation

$$\hat{H} = E + \sum_{ij} f_{ij}\{a_i^\dagger a_j\} + \frac{1}{4}\sum_{ijkl}\Gamma_{ijkl}\{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{36}\sum_{ijklmn} W_{ijklmn}\{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}$$

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$$f_{ij} = \left(1 - \frac{1}{A}\right)\langle i|\hat{T}^{[1]}|j\rangle + \sum_a \langle ia|\frac{1}{A}\hat{T}^{[2]} + \hat{V}^{[2]}|ja\rangle n_a + \frac{1}{2}\sum_{abc}\langle iab|\hat{V}^{[3]}|jab\rangle n_a n_b$$

The IMSRG: NO2B Approximation

$$\hat{H} = E + \sum_{ij} f_{ij}\{a_i^\dagger a_j\} + \frac{1}{4}\sum_{ijkl}\Gamma_{ijkl}\{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{36}\sum_{ijklmn} W_{ijklmn}\{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}$$

$$E = \left(1 - \frac{1}{A}\right)\sum_a \langle a|\hat{T}^{[1]}|a\rangle n_a + \frac{1}{2}\sum_{ab}\langle ab|\frac{1}{A}\hat{T}^{[2]} + \hat{V}^{[2]}|ab\rangle n_a n_b + \frac{1}{6}\sum_{abc}\langle abc|\hat{V}^{[3]}|abc\rangle n_a n_b n_c$$

$$f_{ij} = \left(1 - \frac{1}{A}\right)\langle i|\hat{T}^{[1]}|j\rangle + \sum_a \langle ia|\frac{1}{A}\hat{T}^{[2]} + \hat{V}^{[2]}|ja\rangle n_a + \frac{1}{2}\sum_{abc}\langle iab|\hat{V}^{[3]}|jab\rangle n_a n_b$$

$$\Gamma_{ijkl} = \langle ij|\frac{1}{A}\hat{T}^{[2]} + \hat{V}^{[2]}|kl\rangle + \sum_a \langle ija|\hat{V}^{[3]}|kla\rangle n_a$$

The IMSRG: NO2B Approximation

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$$E = \left(1 - \frac{1}{A}\right)\sum_a \langle a|\hat{T}^{[1]}|a\rangle n_a + \frac{1}{2}\sum_{ab}\langle ab|\frac{1}{A}\hat{T}^{[2]} + \hat{V}^{[2]}|ab\rangle n_a n_b + \frac{1}{6}\sum_{abc}\langle abc|\hat{V}^{[3]}|abc\rangle n_a n_b n_c$$

$$f_{ij} = \left(1 - \frac{1}{A}\right)\langle i|\hat{T}^{[1]}|j\rangle + \sum_a \langle ia|\frac{1}{A}\hat{T}^{[2]} + \hat{V}^{[2]}|ja\rangle n_a + \frac{1}{2}\sum_{abc}\langle iab|\hat{V}^{[3]}|jab\rangle n_a n_b$$

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$$W_{ijklmn} = \langle ijk|\hat{V}^{[3]}|lmn\rangle$$

The VS-IMSRG

Choose the generator in order to decouple the valence-space from the excluded space:

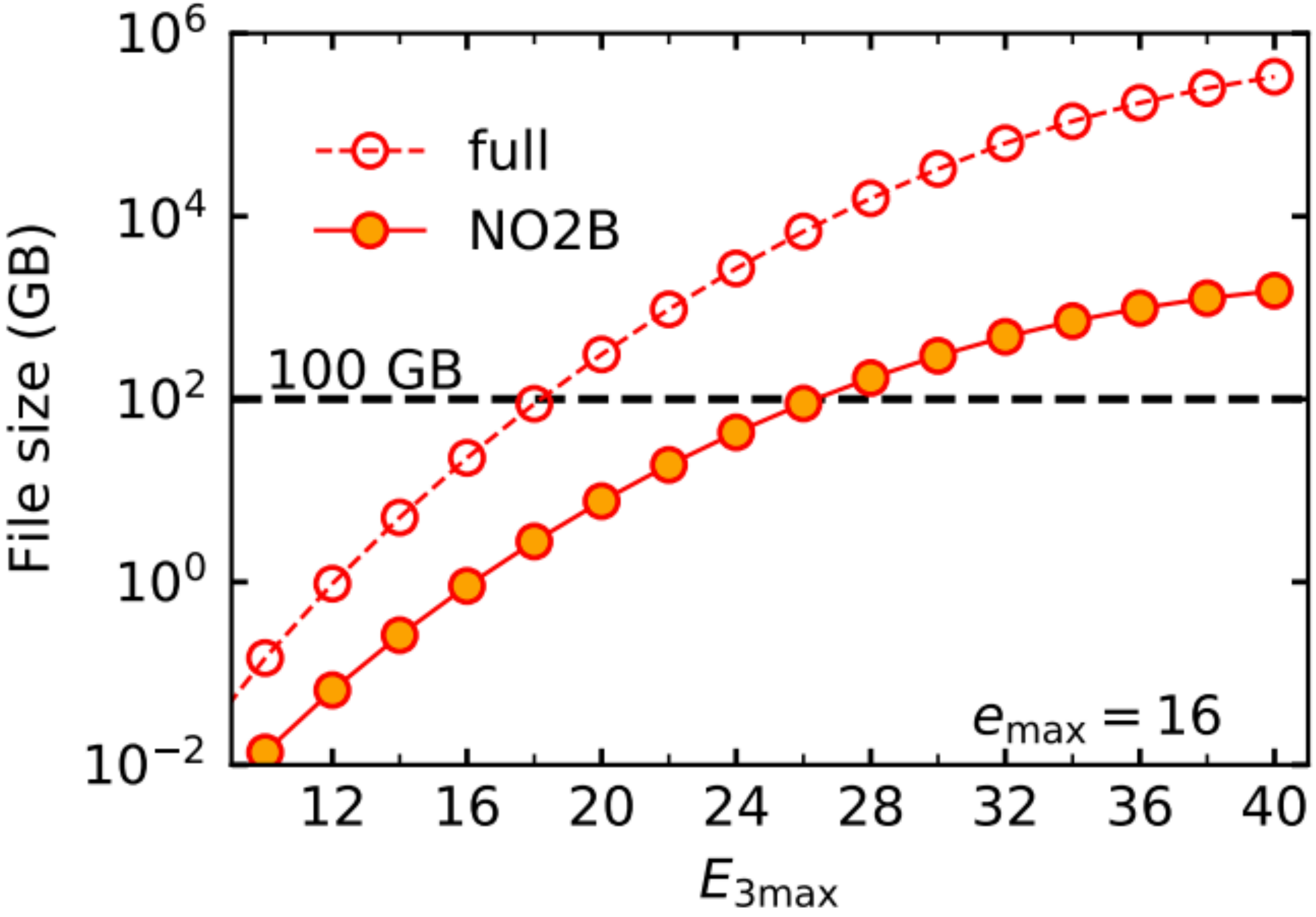
$$\eta = \sum_{ij} \eta_{ij}\{a_i^\dagger a_j\} + \sum_{ijkl} \eta_{ijkl}\{a_i^\dagger a_j^\dagger a_l a_k\}$$

for $ij \in [pc, ov]$ and $ijkl \in [pp'cc', pp'vc, opvv']$ for c in the core, v in the valence-space, o outside the valence-space and p not in the core.

$$\eta_{ij} = \frac{1}{2}\arctan\left(\frac{2f_{ij}}{f_{ii} - f_{jj} + \Gamma_{ijij}}\right)$$

$$\eta_{ijkl} = \frac{1}{2}\arctan\left(\frac{2\Gamma_{ijkl}}{f_{ii} + f_{jj} - f_{kk} - f_{ll} + \Gamma_{ijij} + \Gamma_{klkl} - \Gamma_{ikik} - \Gamma_{ilil} - \Gamma_{jkjk} - \Gamma_{jljl}}\right)$$

3N Forces Storage



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