



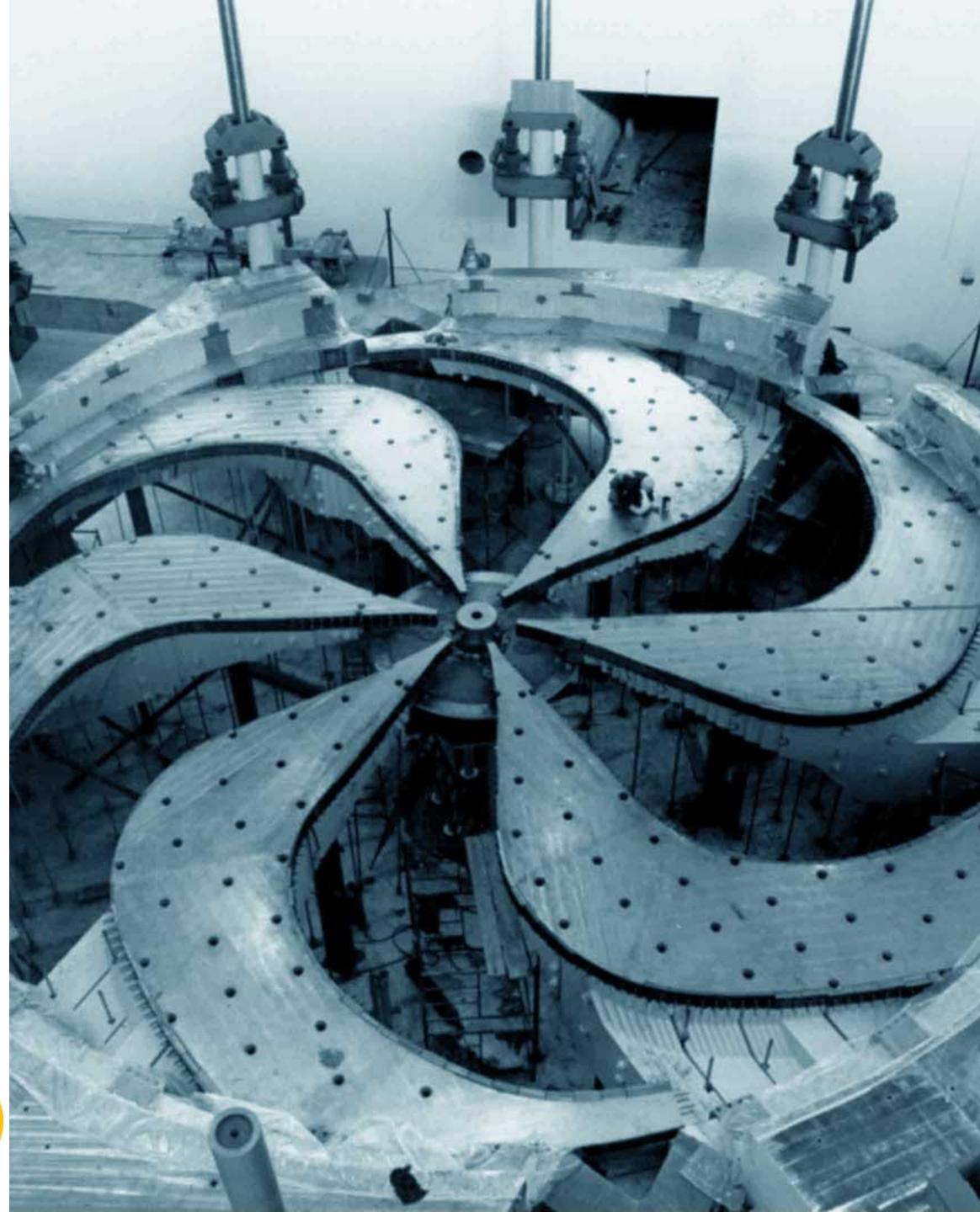
Towards reliable nuclear matrix elements for neutrinoless double beta decay

Antoine Belley
PAINT Workshop 2023

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



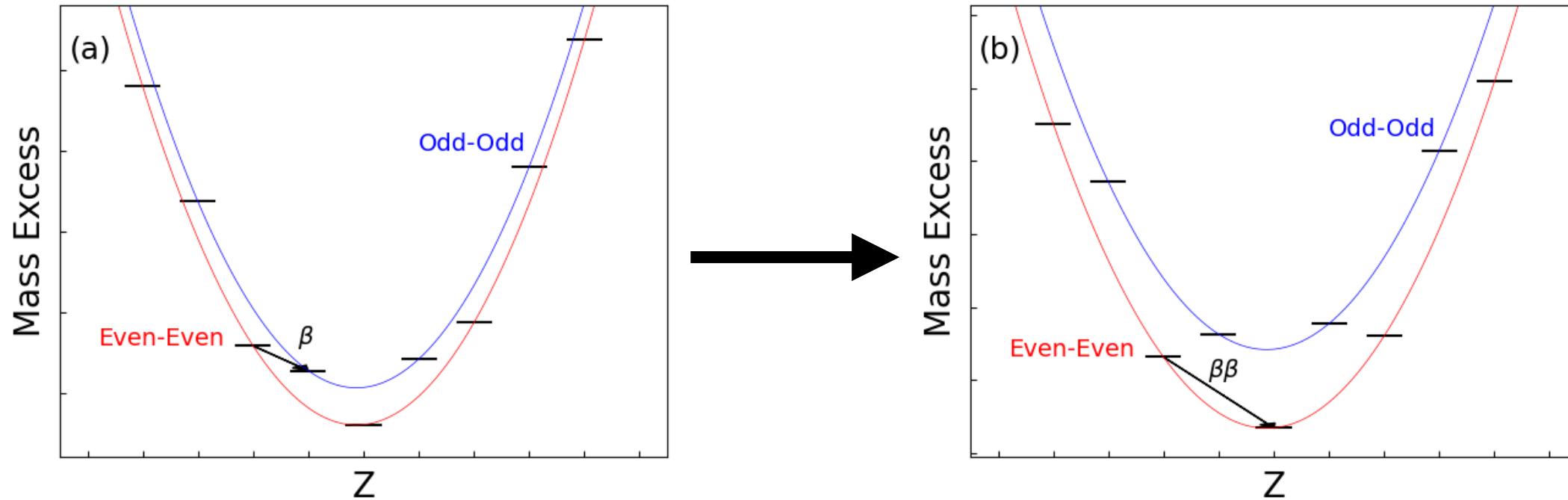
Arthur B. McDonald
Canadian Astroparticle Physics Research Institute



Double beta decays

Second order order weak process

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



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

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

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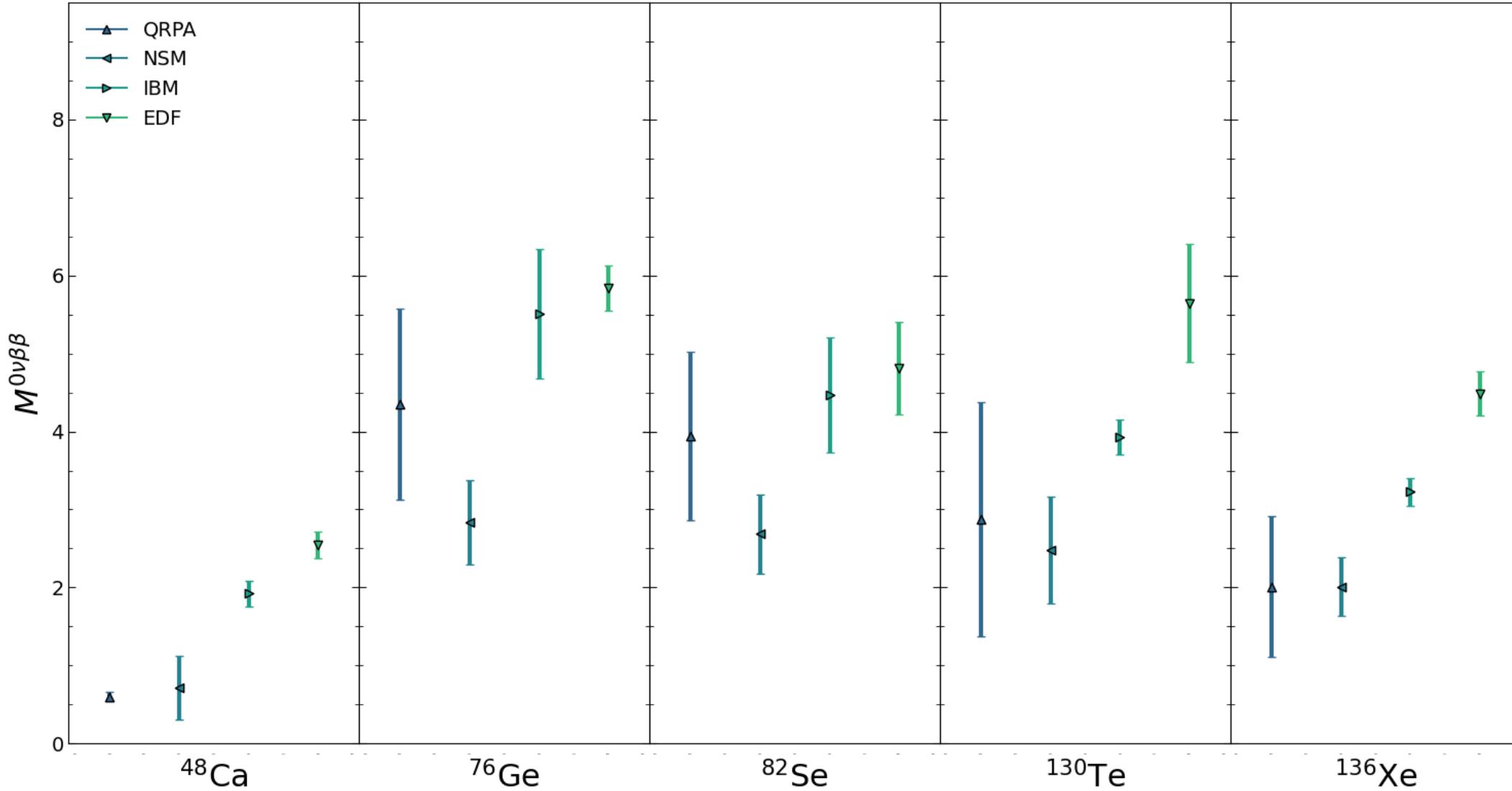
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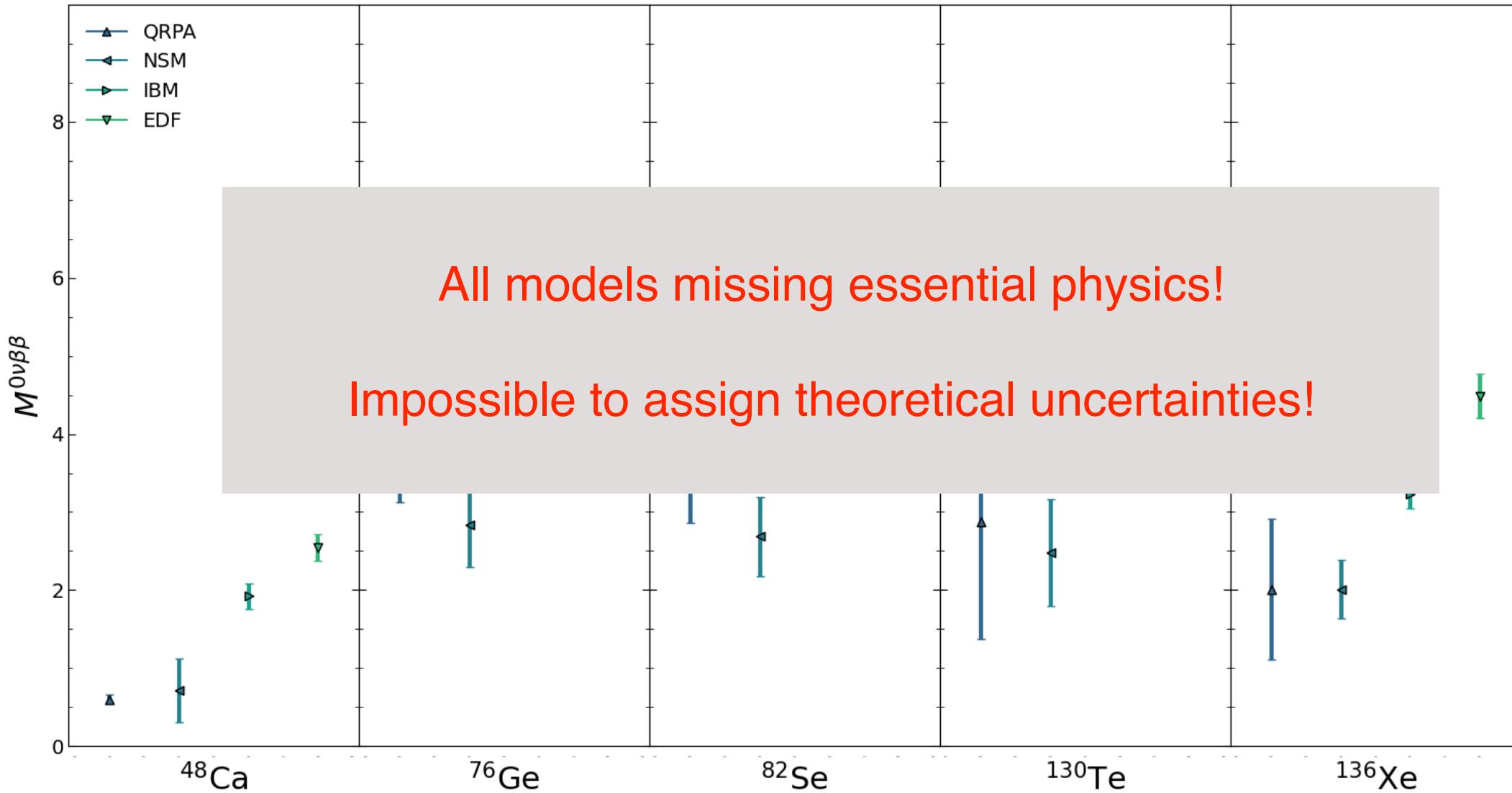
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Current calculations from phenomenological models have large spread in results.

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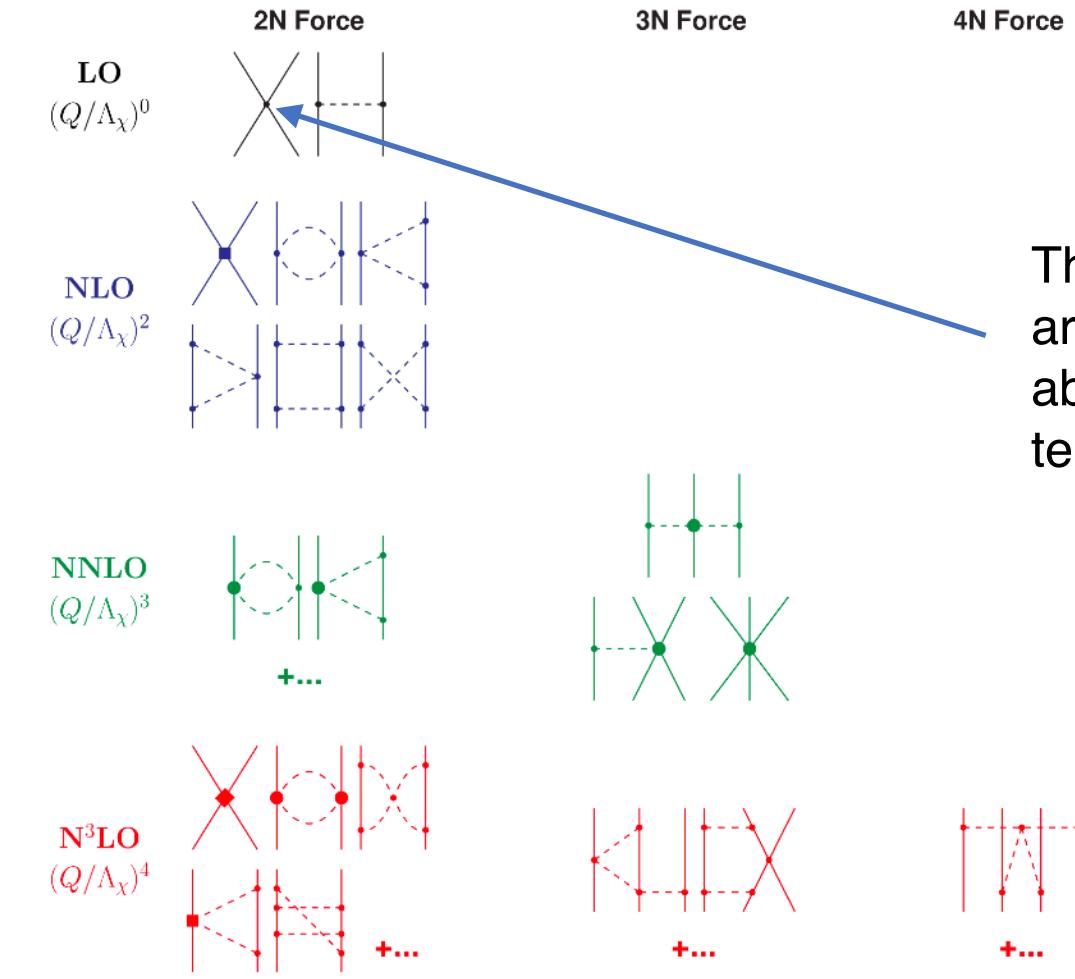


Ab initio nuclear theory

Expansion order by order of the nuclear forces

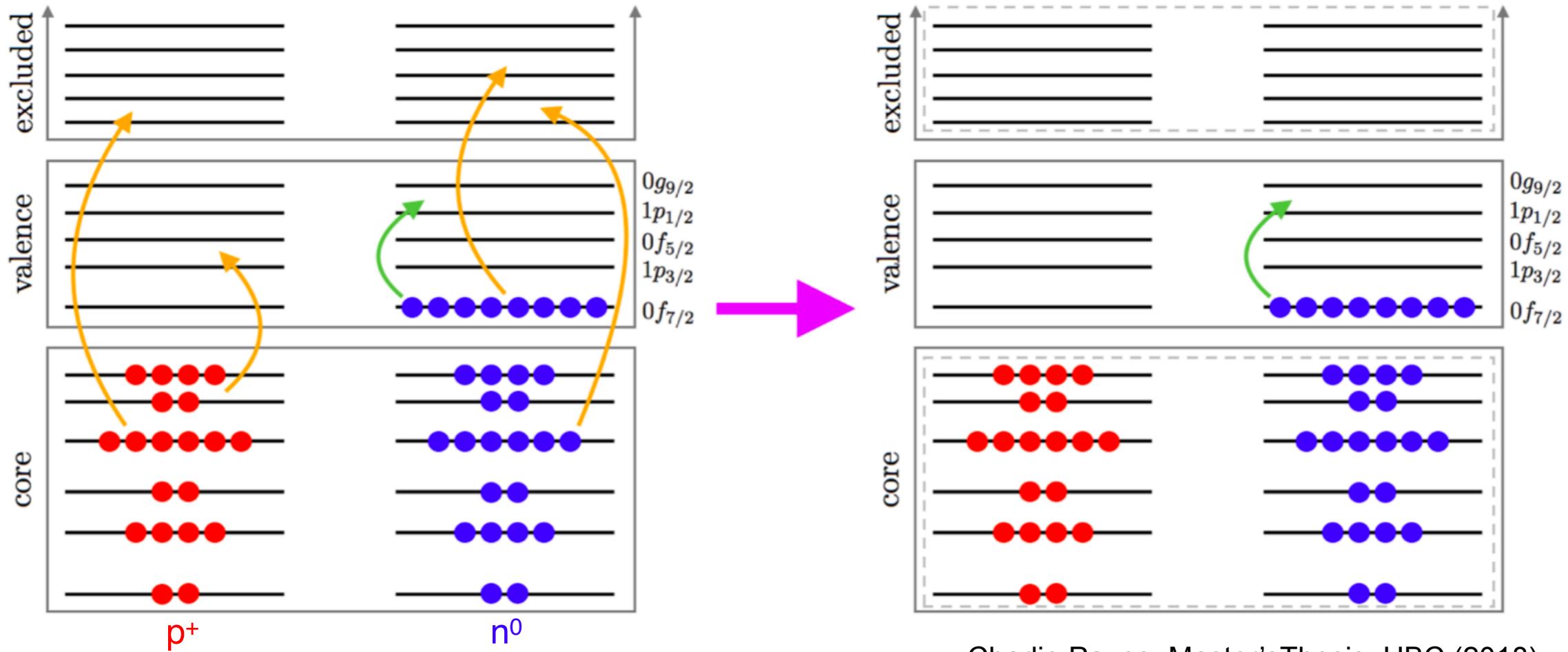
Reproduces symmetries of low-energy QCD using nucleons as fields and pions as force carriers.

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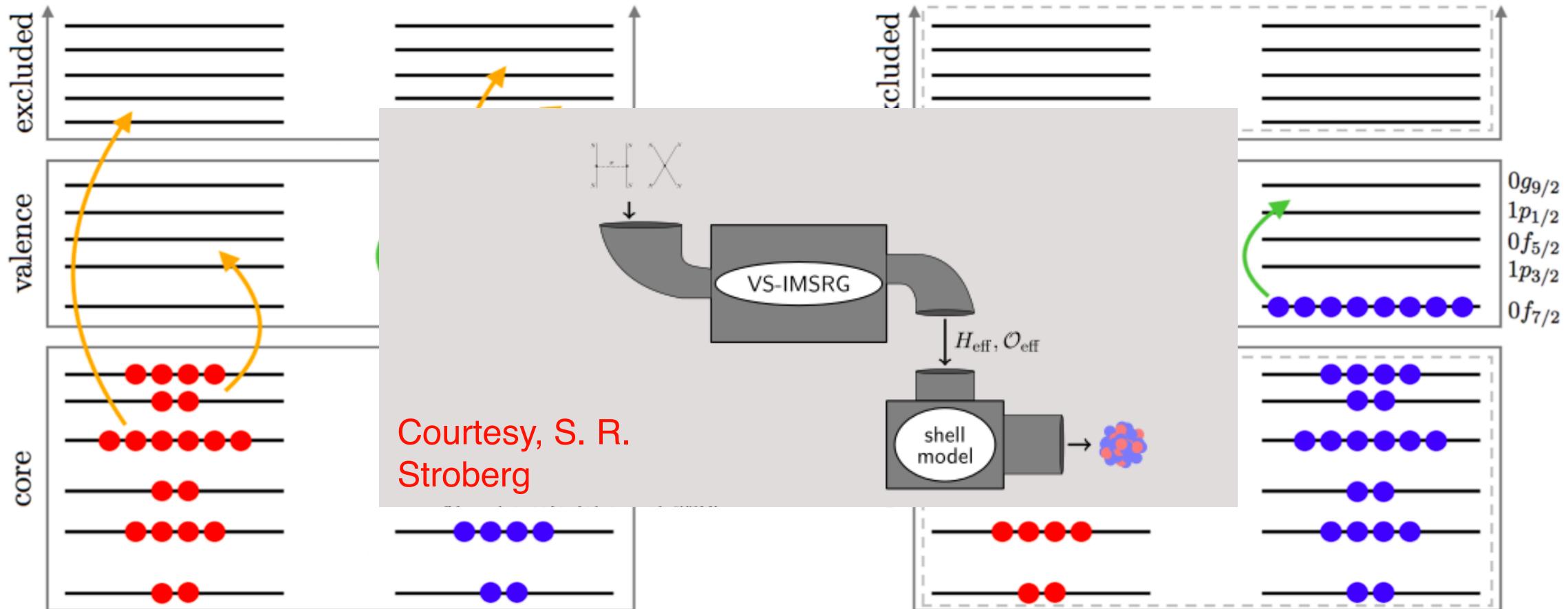
The different coupling constants are fitted to few nucleons data to absorb effect of higher order terms

Valence-Space In Medium Similarity Renormalization Group

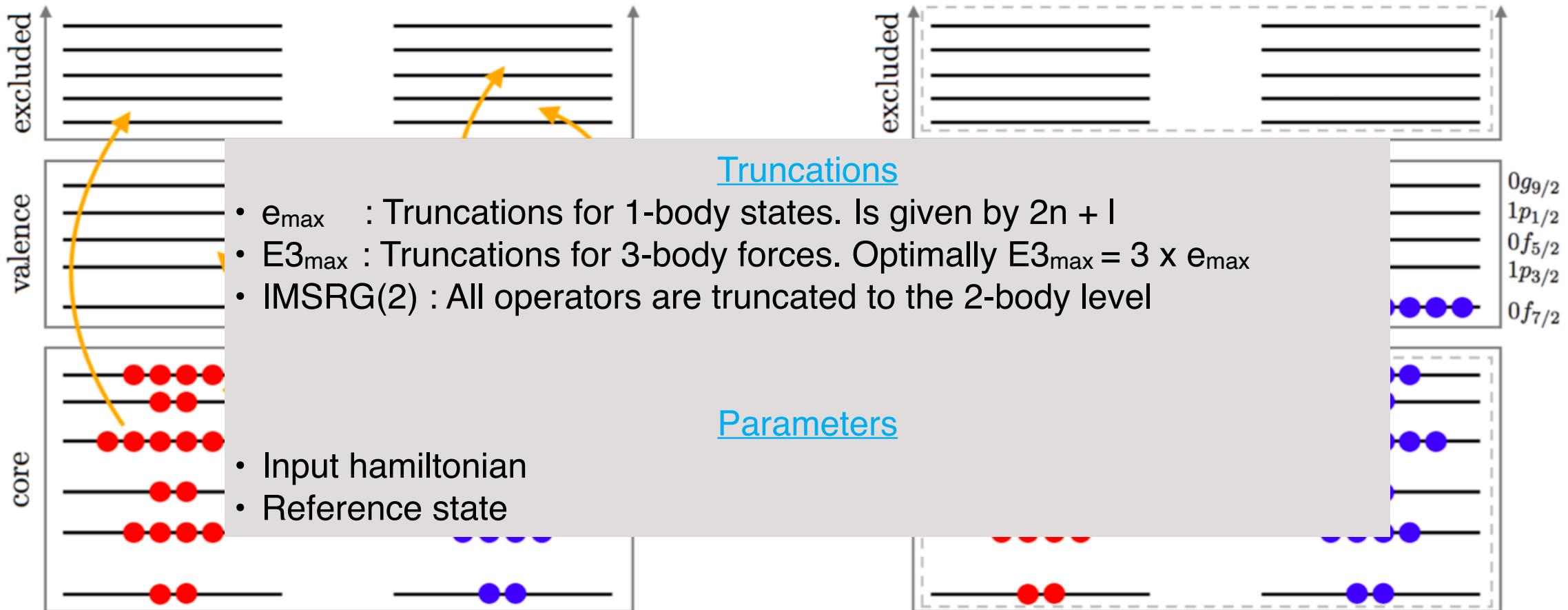


Charlie Payne, Master's Thesis, UBC (2018)

Valence-Space In Medium Similarity Renormalization Group

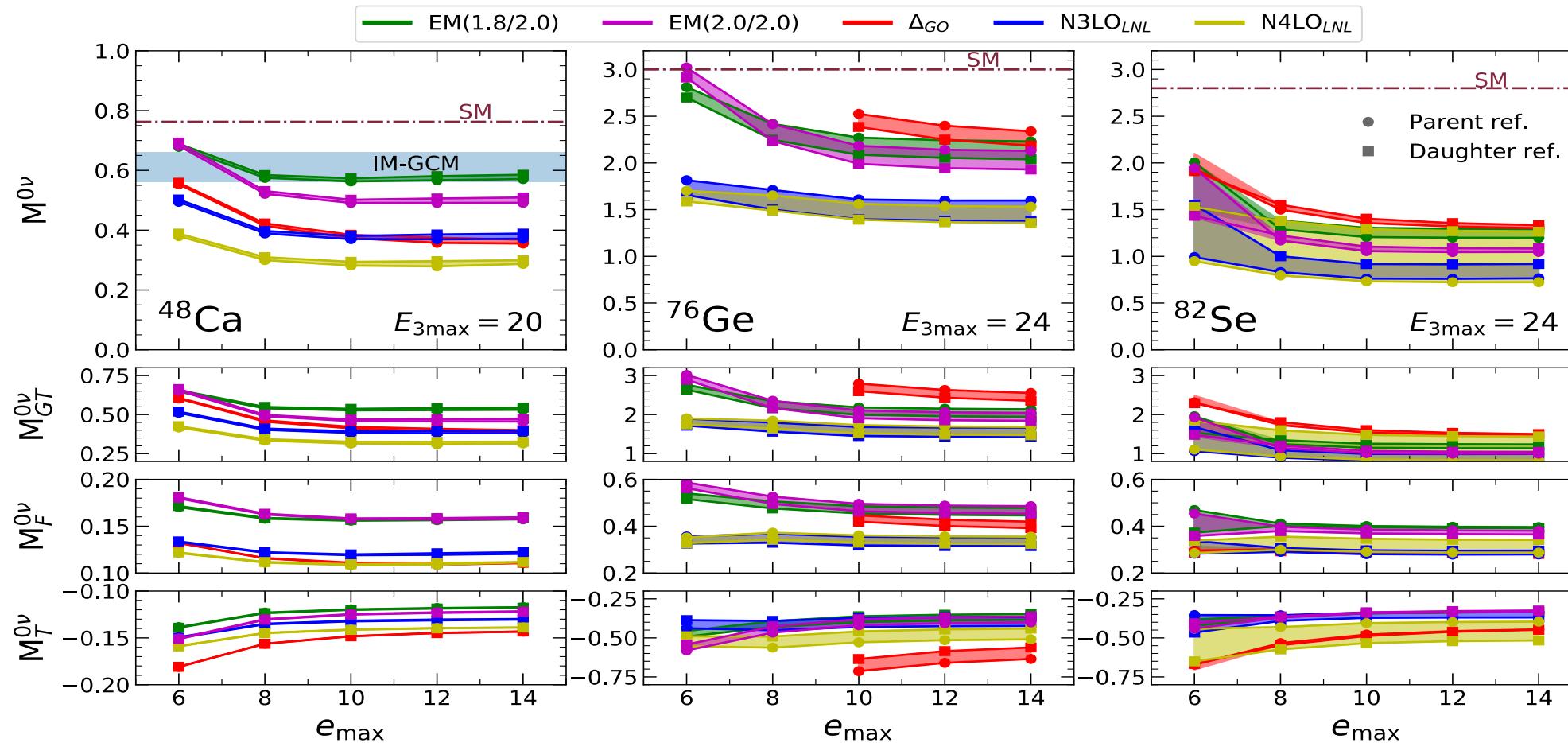


Valence-Space In Medium Similarity Renormalization Group



Results

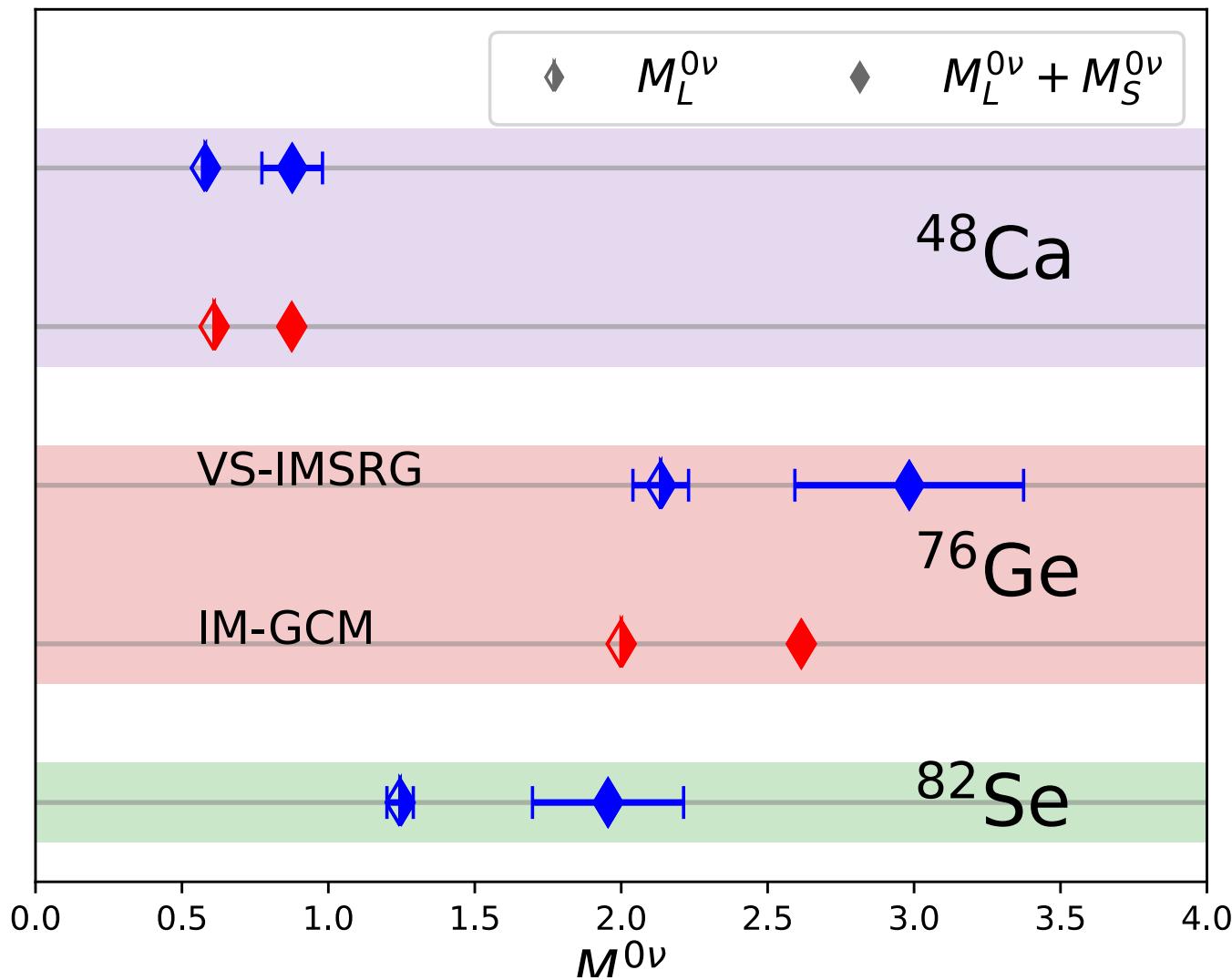
Results with 5 different input hamiltonians to study uncertainty from interaction choice.



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

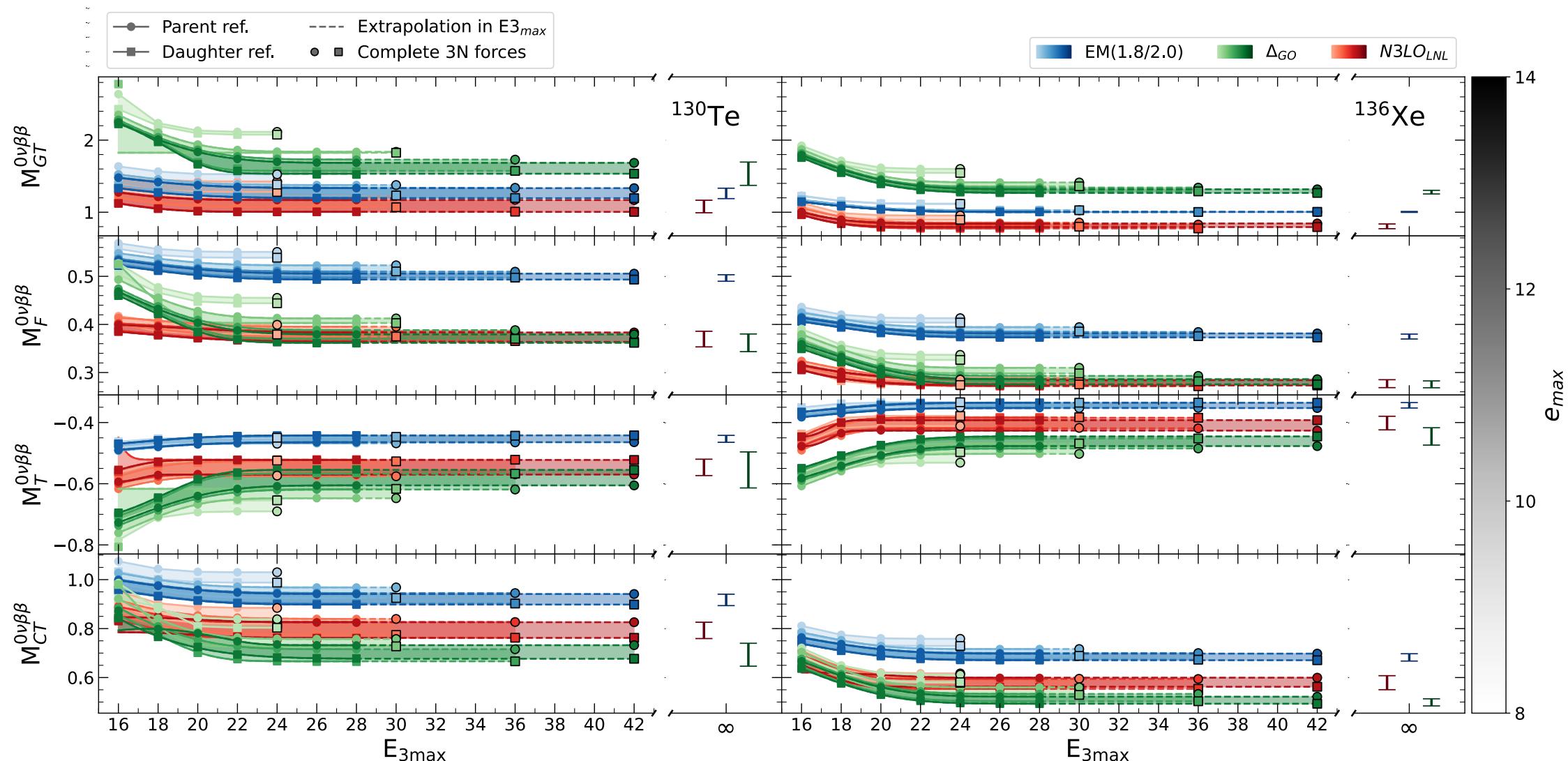
Belle, et al., PRL126.042502

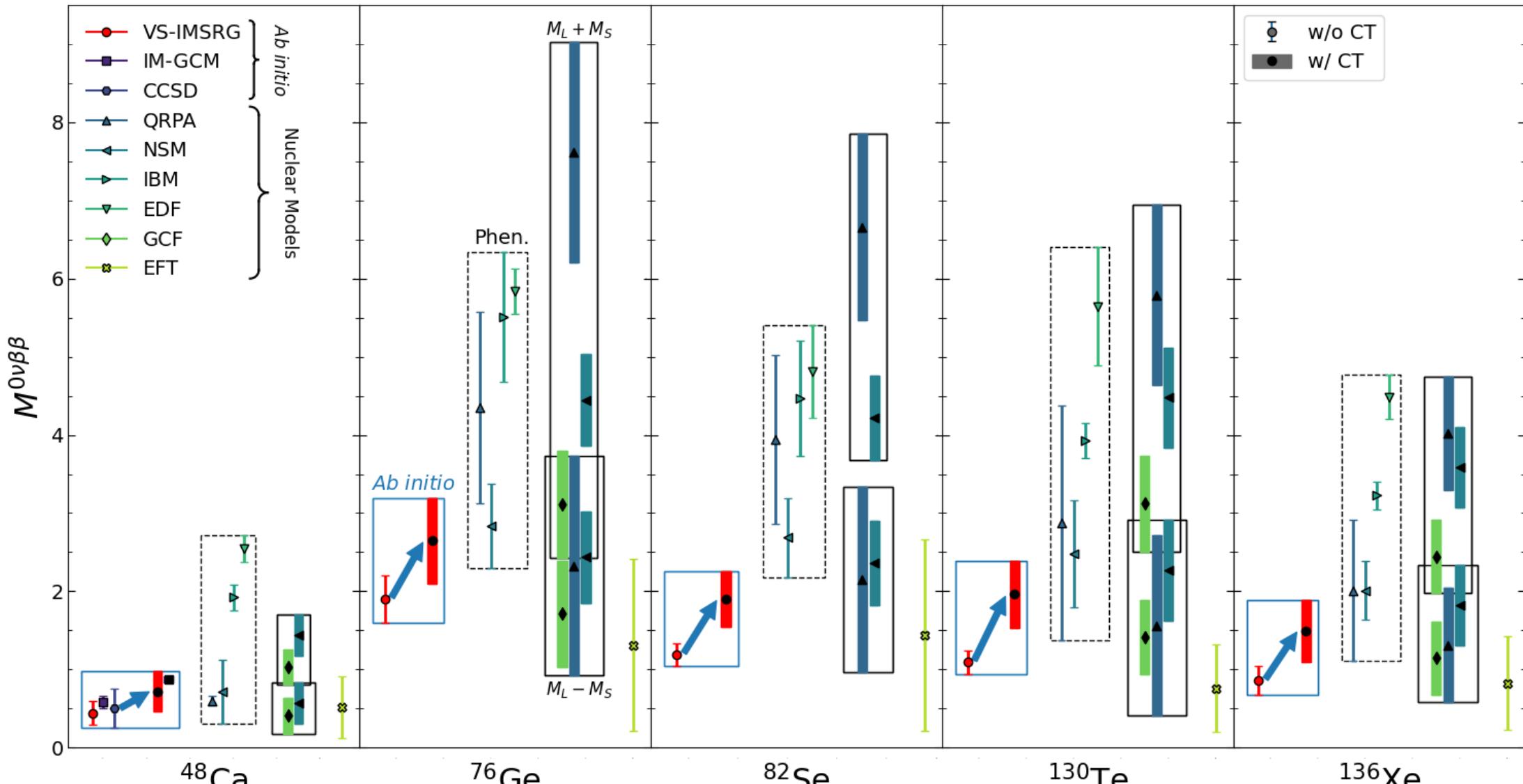
Belle, et al., in prep

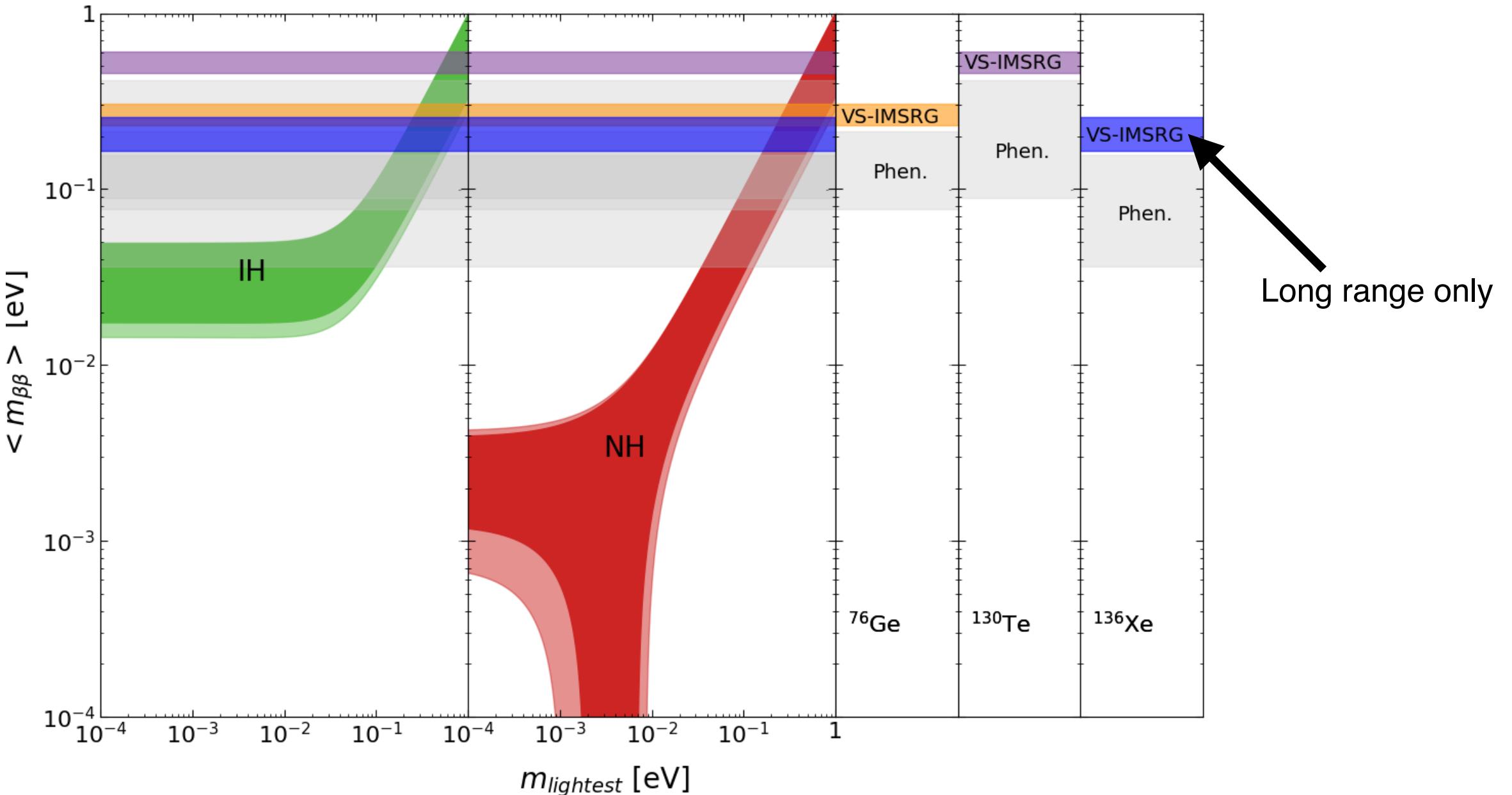


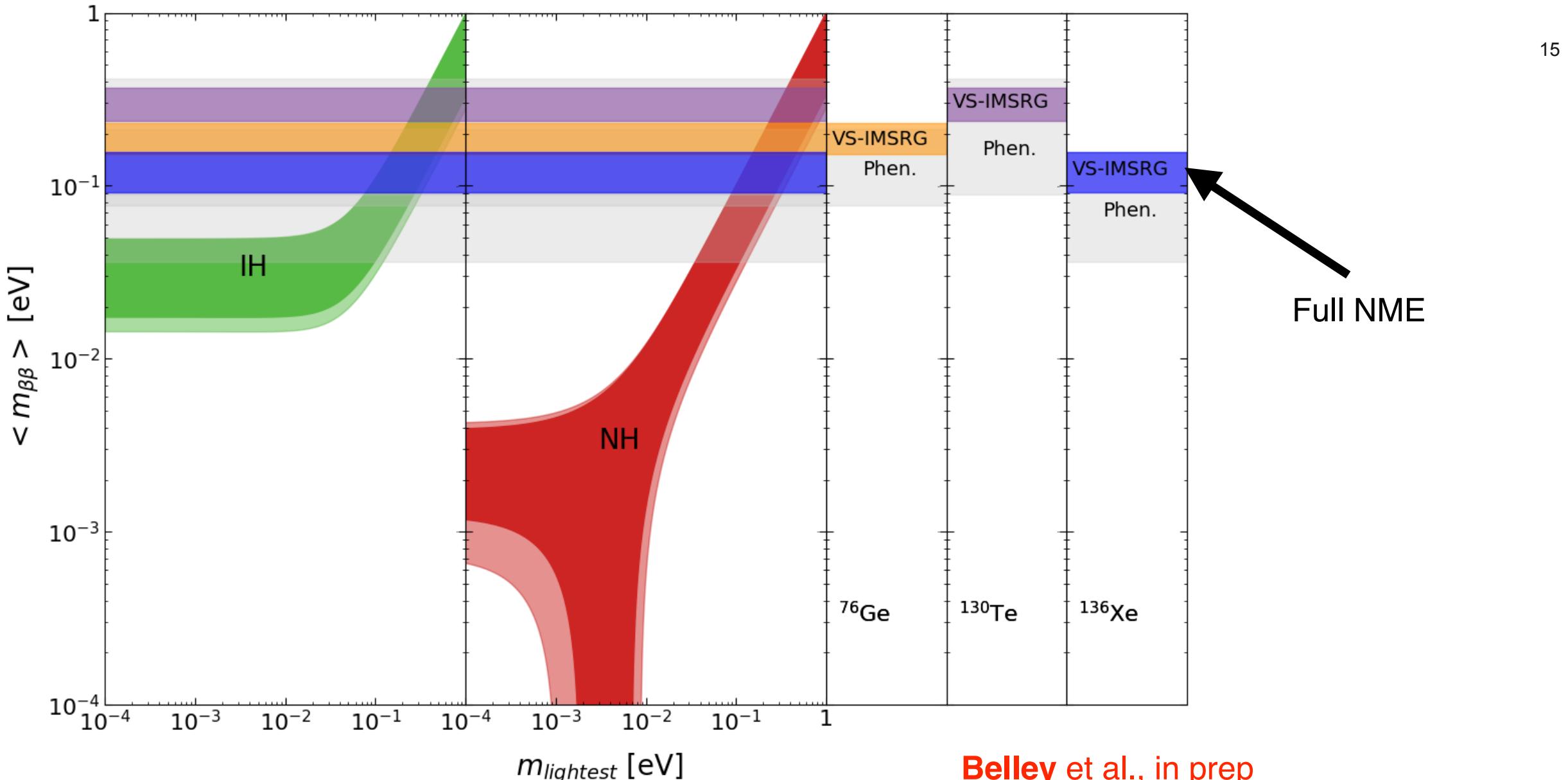
^{130}Te , ^{136}Xe major players in global searches with SNO+, CUORE and nEXO

Increased $E_{3\max}$ capabilities allow first converged ab initio calculations [EM1.8/2.0, Δ_{GO} , N3LO_{LNL}] ¹²

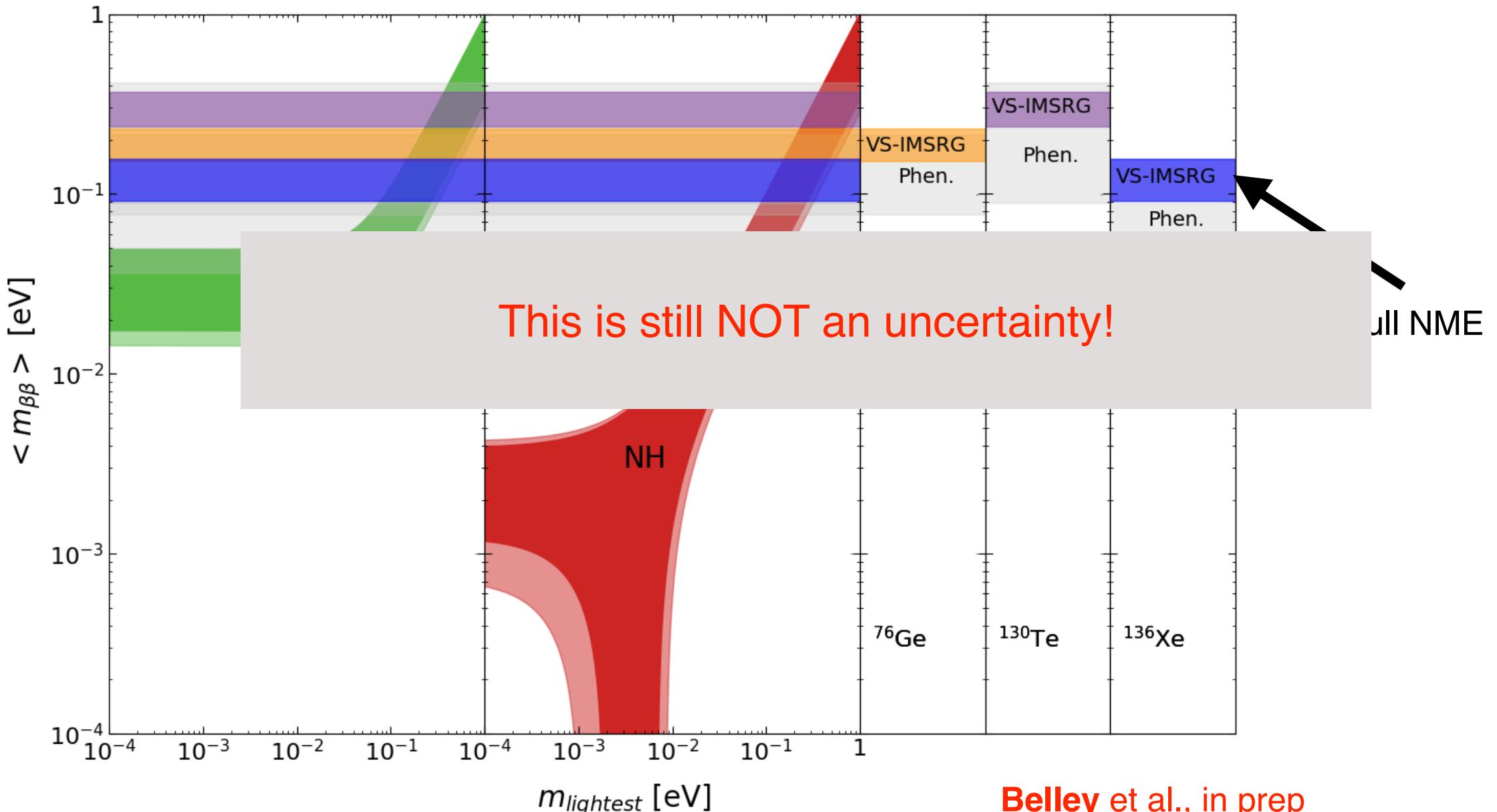




Ab Initio $0\nu\beta\beta$ Decay: Effect on experimental limits

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Belley et al., in prep



Assessing the uncertainty

Uncertainty can be split into 3 sources:

- The many-body method (VS-IMSRG)
- The χ -EFT interaction
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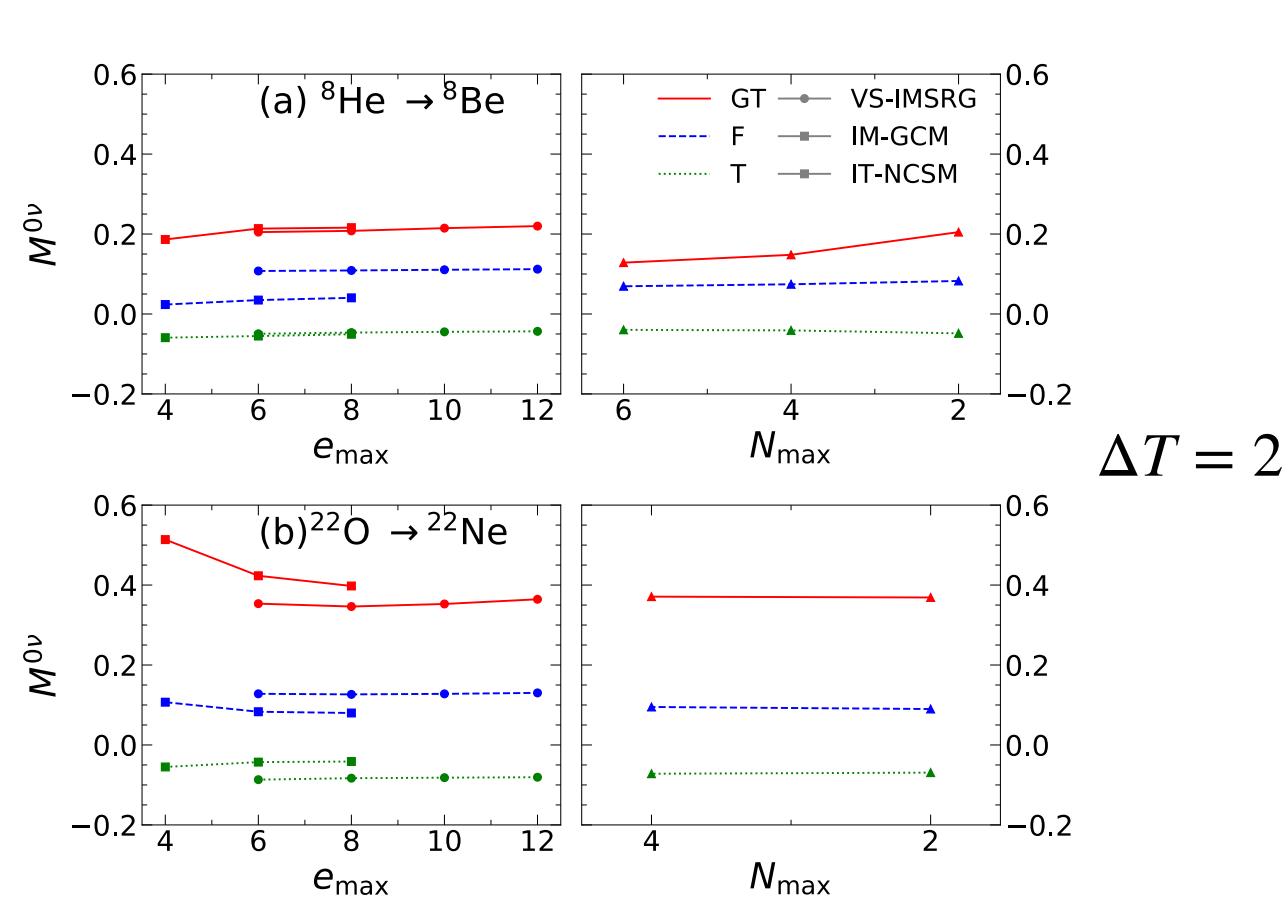
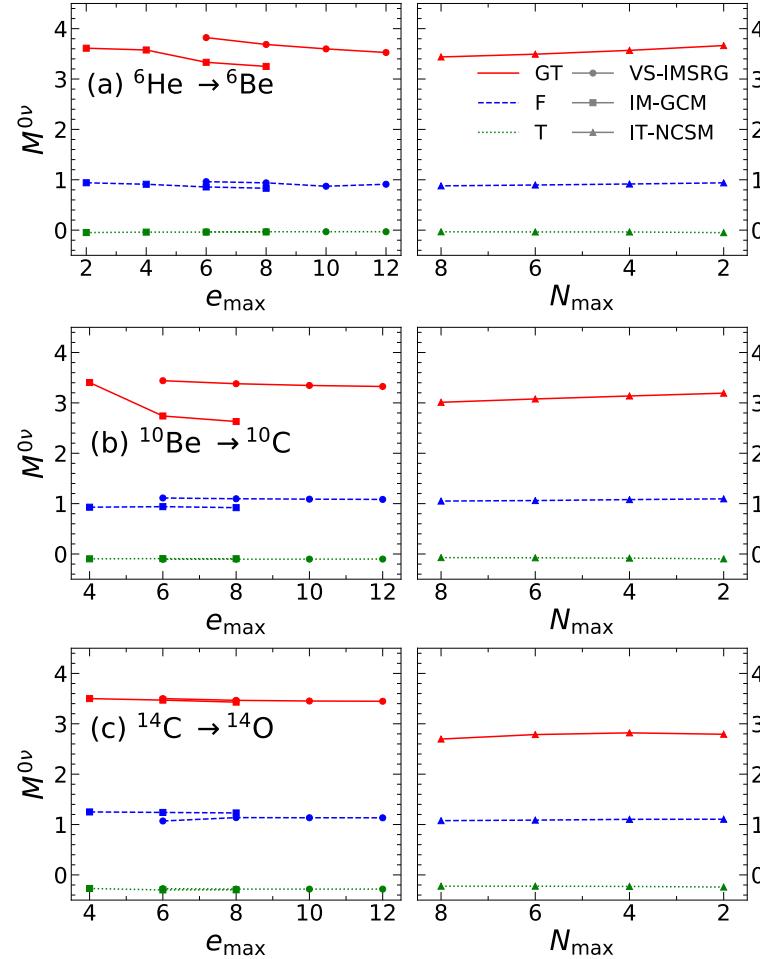
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Benchmark with other ab initio method for fictitious decays in light nuclei

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 $\Delta T = 0$ 

Yao, Belley, et al., PhysRevC.103.014315

Reasonable to good agreement in all cases

Assessing the uncertainty

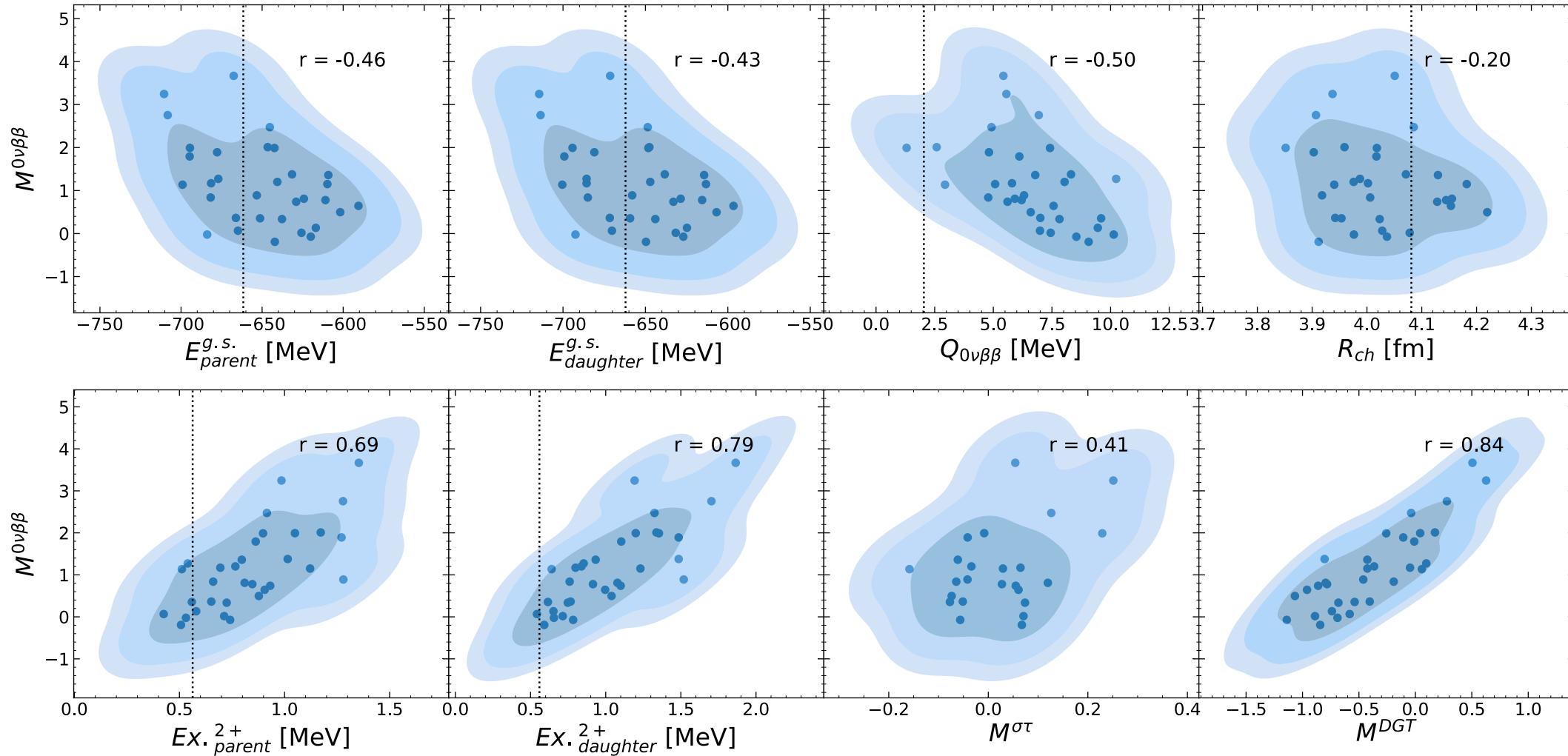
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$\ln^{76}\text{Ge}$:

Belley et al., arXiv:2210.05809

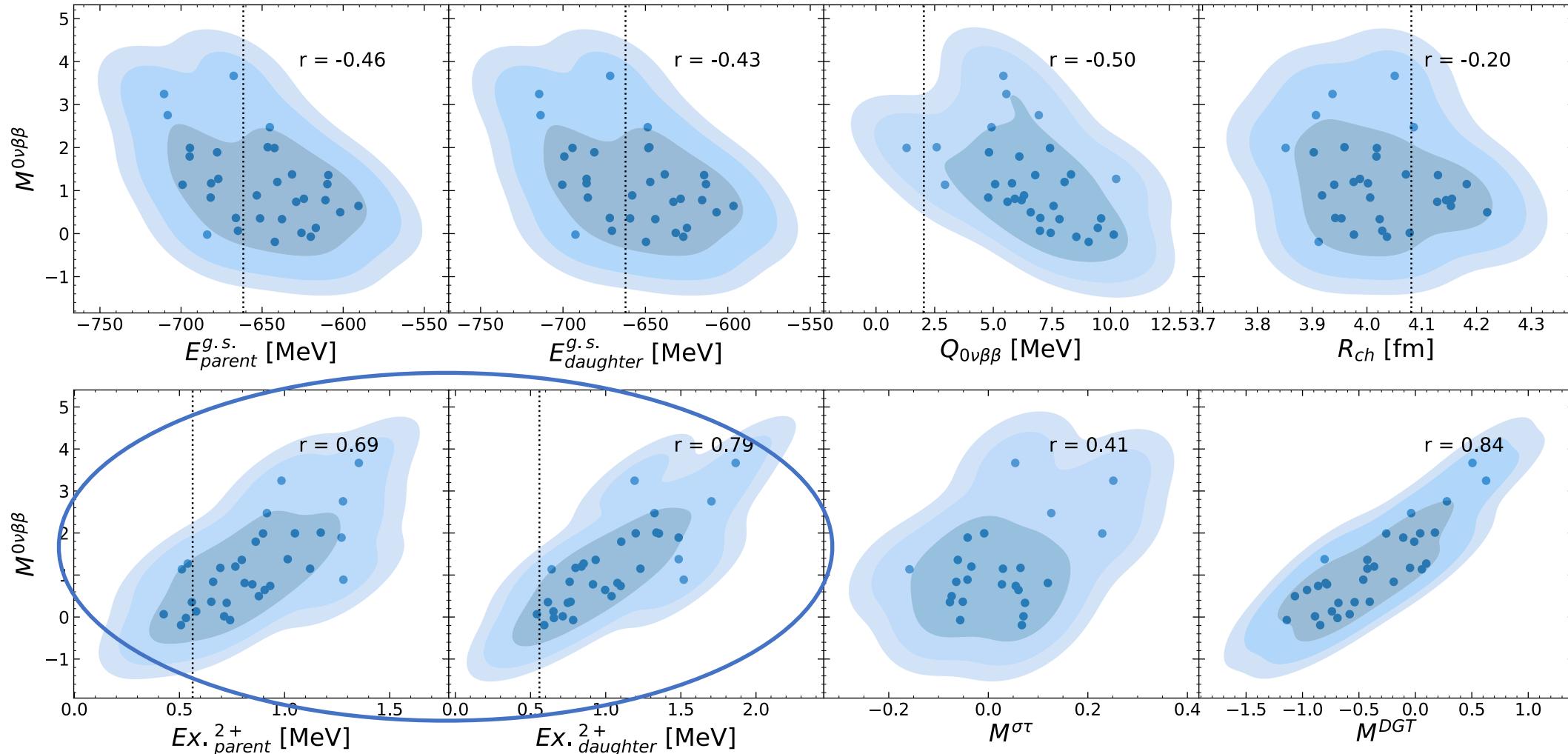
19



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19

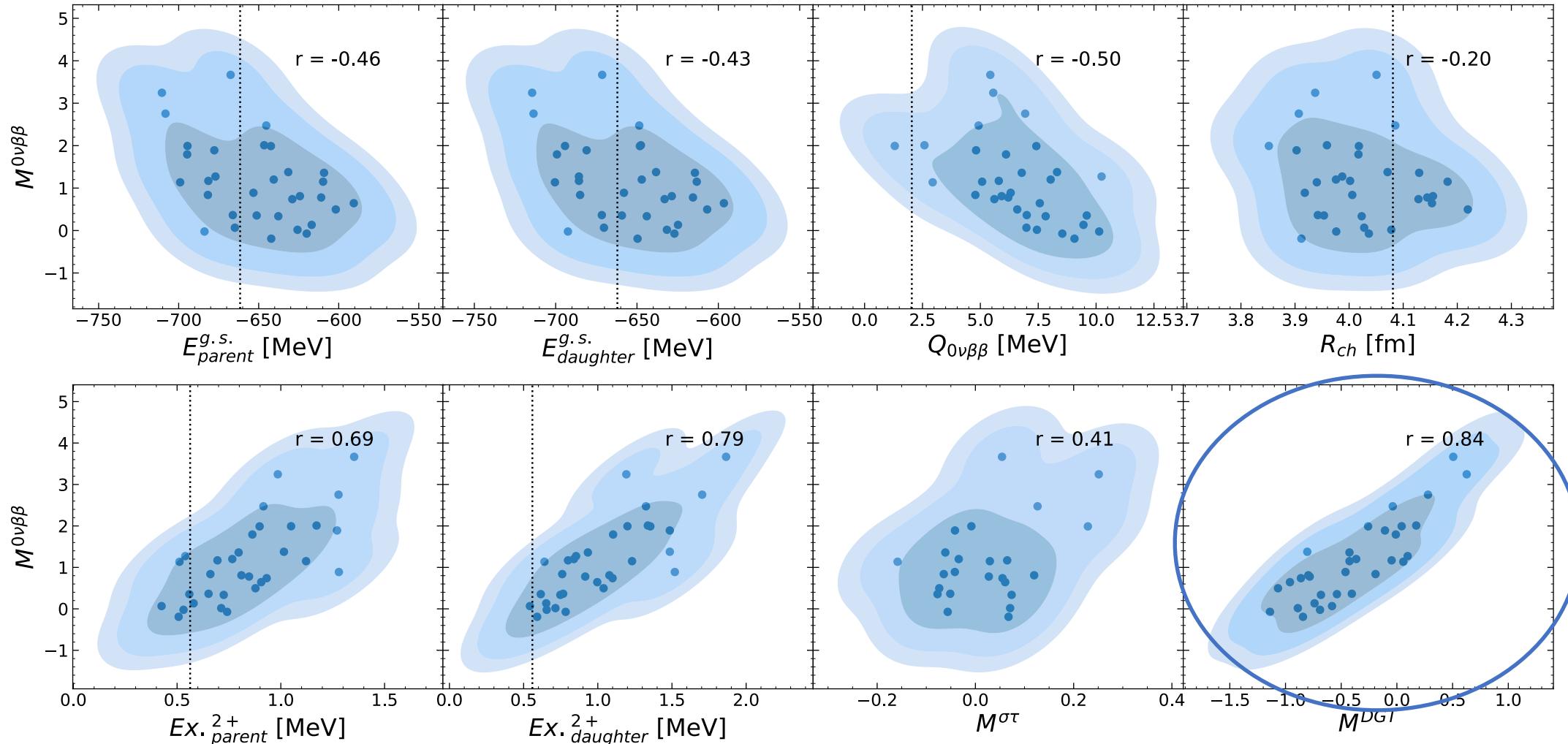


Only seen for ^{76}Ge , probably due to deformed nuclei involved.

$\ln^{76}\text{Ge}$:

Belley et al., arXiv:2210.05809

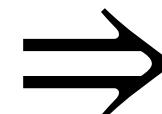
19



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

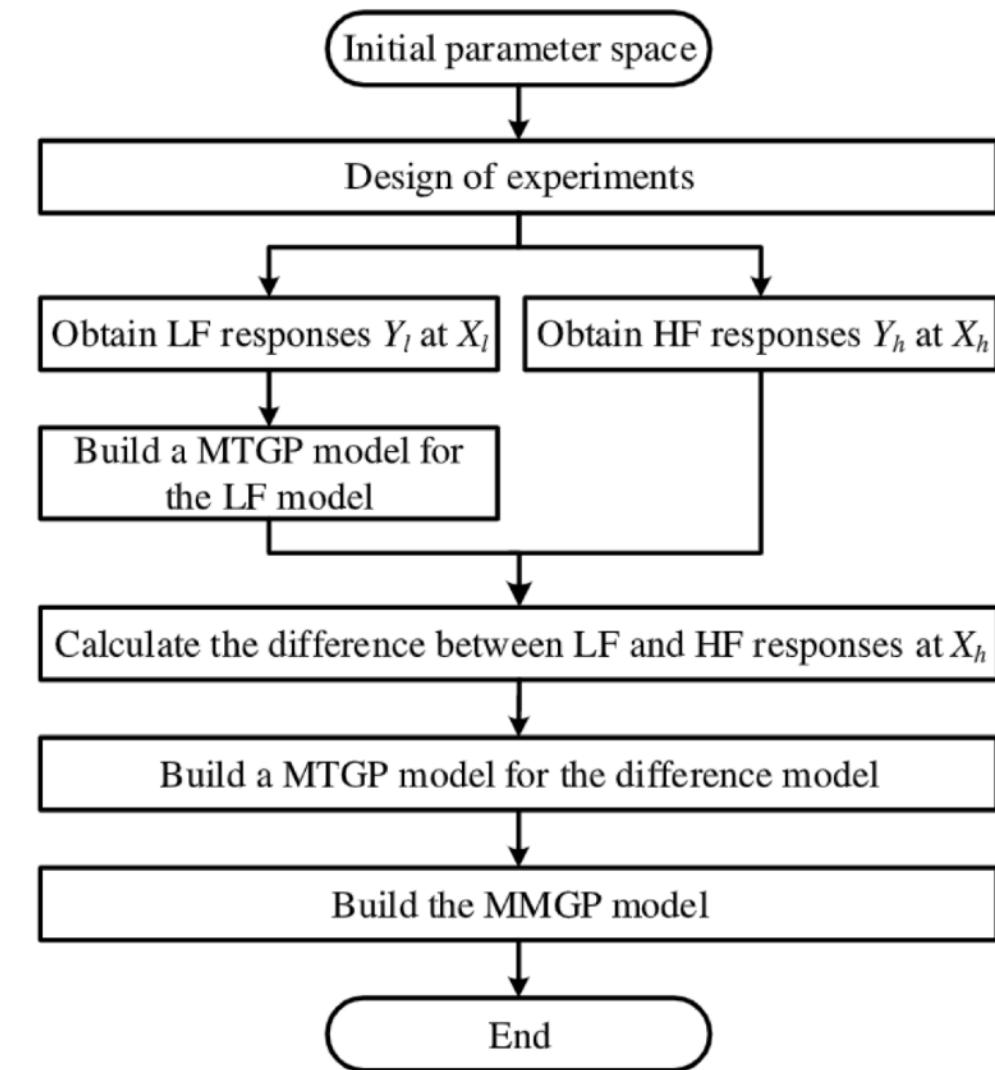
Global sensitivity analysis can probe how dependent the final result is to each input but require thousands of samples in order to do so.

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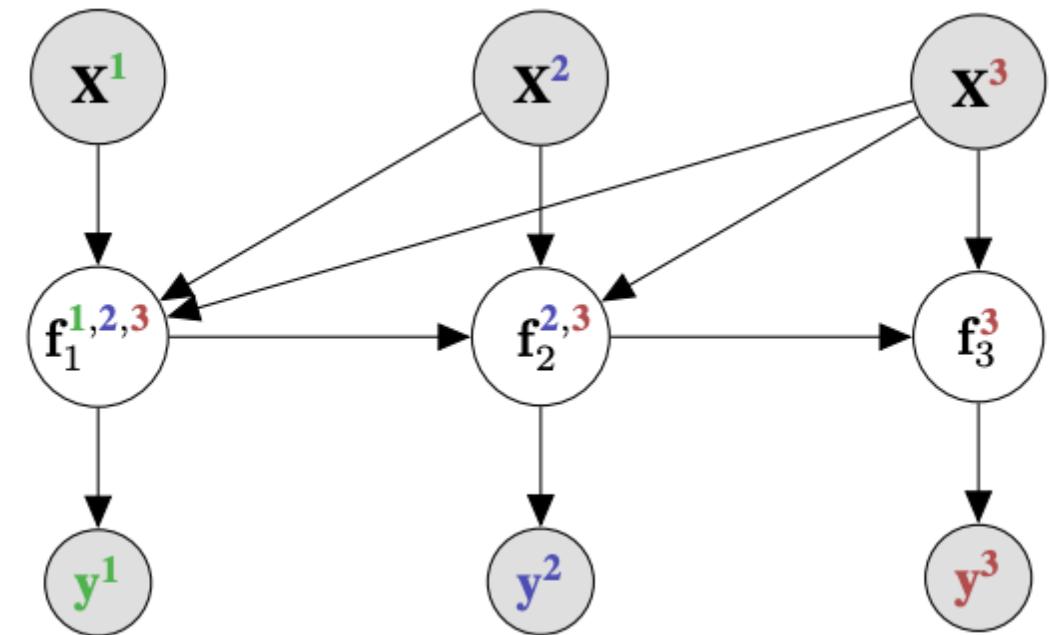
Need emulators to speed up calculations.

- Multi-output Multi-Fidelity Gaussian Process (MMGP) can be used to probe LEC space.
- Multi-Tasks Gaussian Process: Uses multiple correlated outputs from 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 expansive 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.



Taken from [1].

- When the relation between low-fidelity and high-fidelity data is complicated, the simple multi-fidelity approach does not produce good results.
- Deep gaussian process [1] link multiple gaussian processes inside a neural network to improve results.
- This can be used to model the difference function between the low-fidelity and high-fidelity by including outputs of the previous fidelity as an input of higher fidelity.
- 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](#).
- Even if we use the same number of low- and high-fidelity data, using multiple-fidelities still improves the fit!



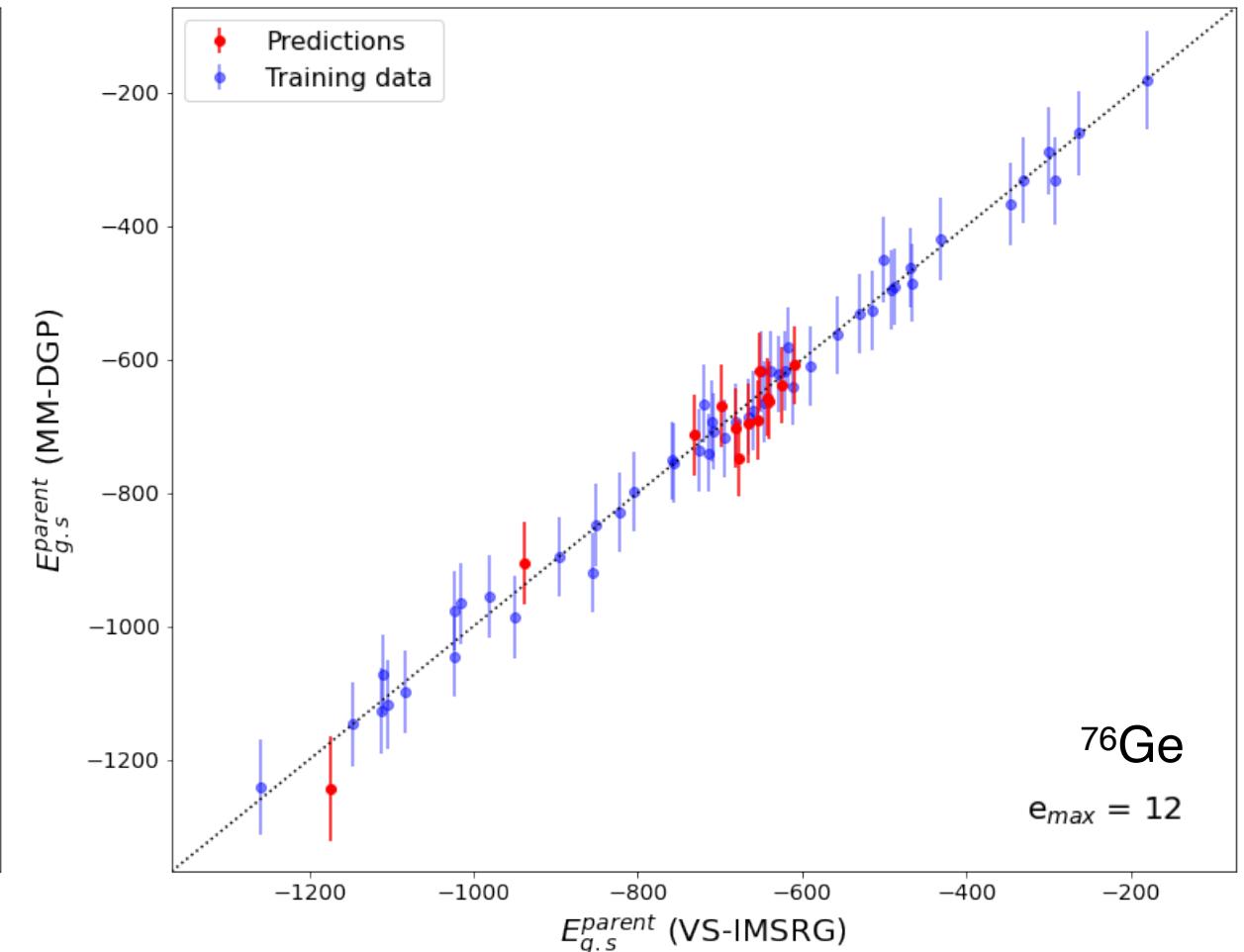
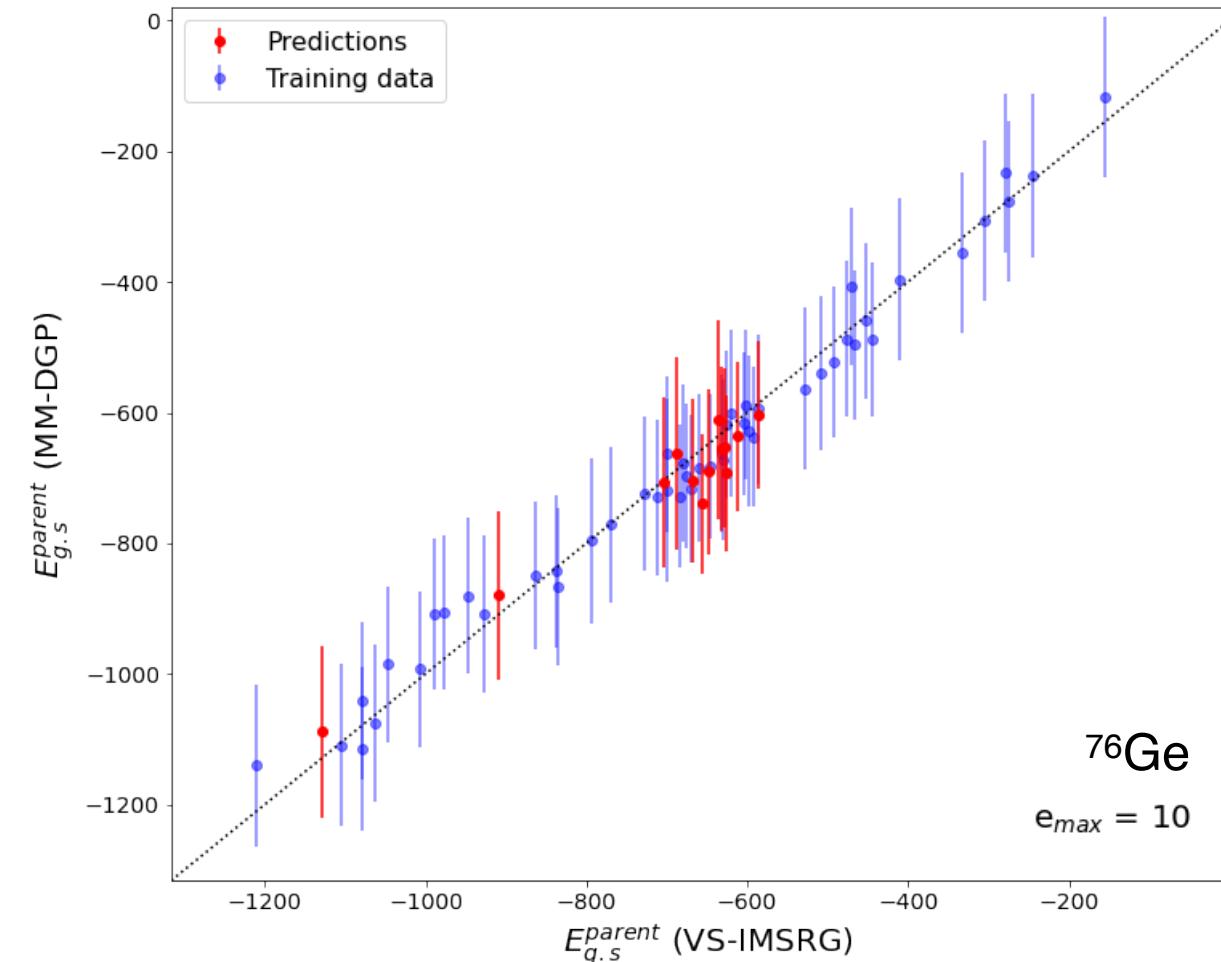
Taken from [1].

Using Δ -full chiral EFT interactions at N2LO:

Low-Fidelity



High-Fidelity

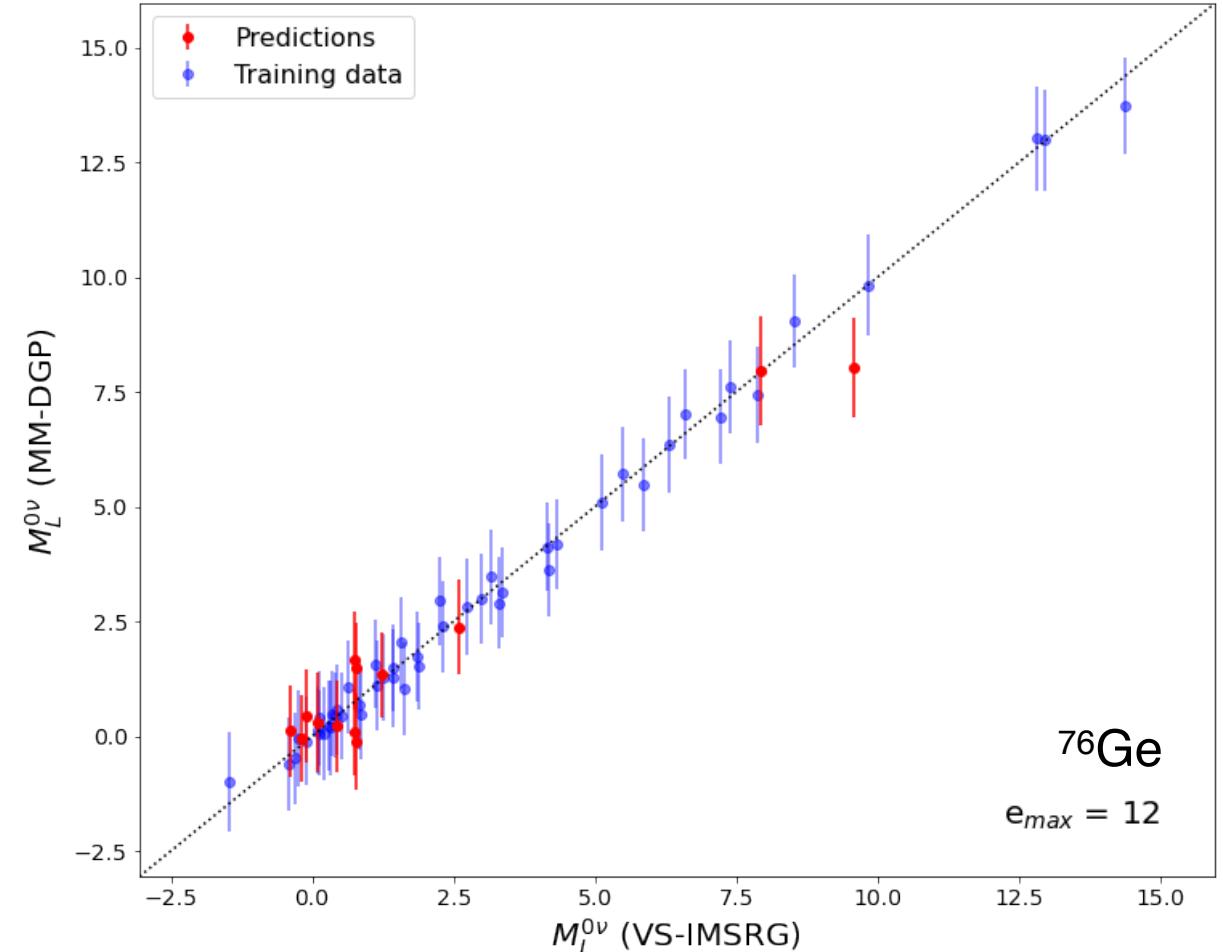
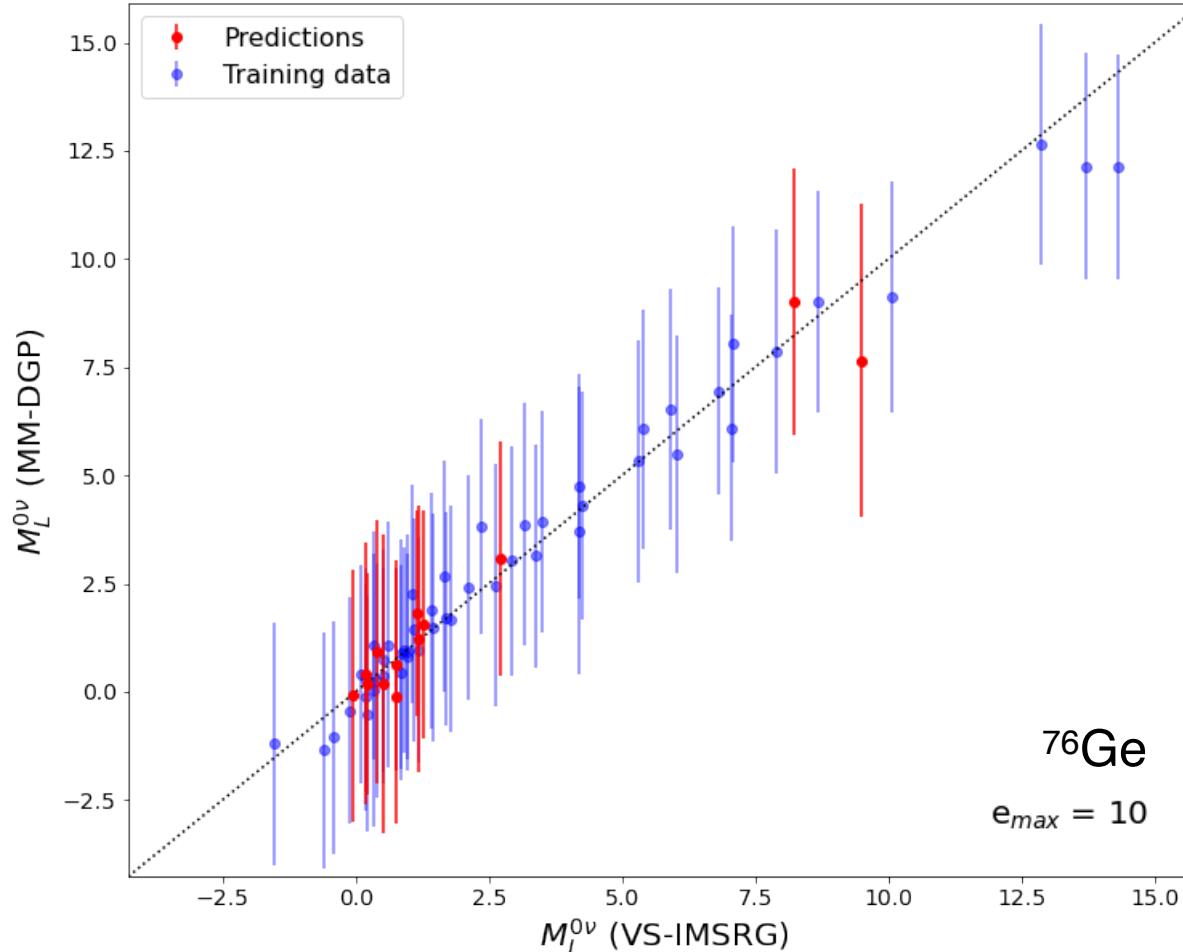


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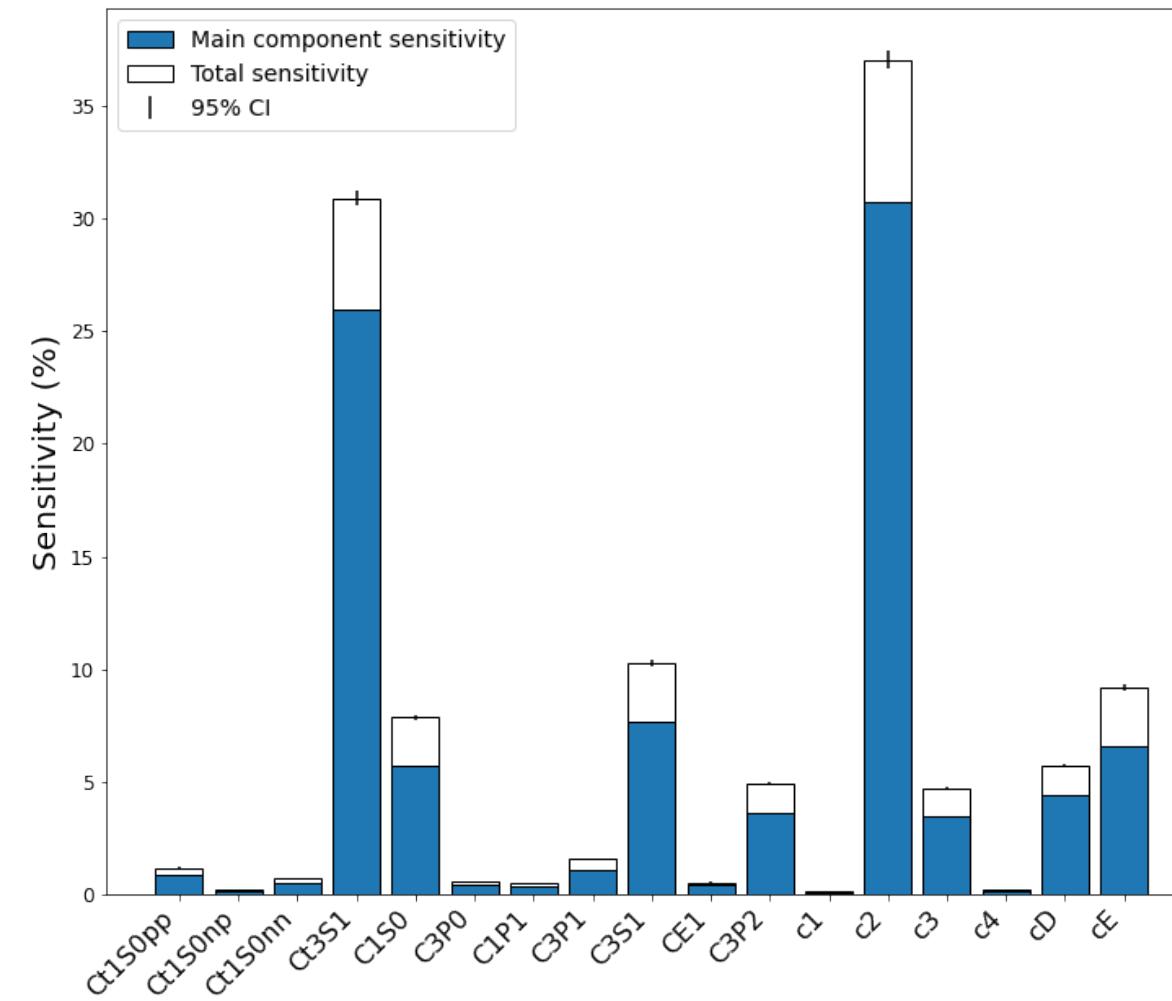
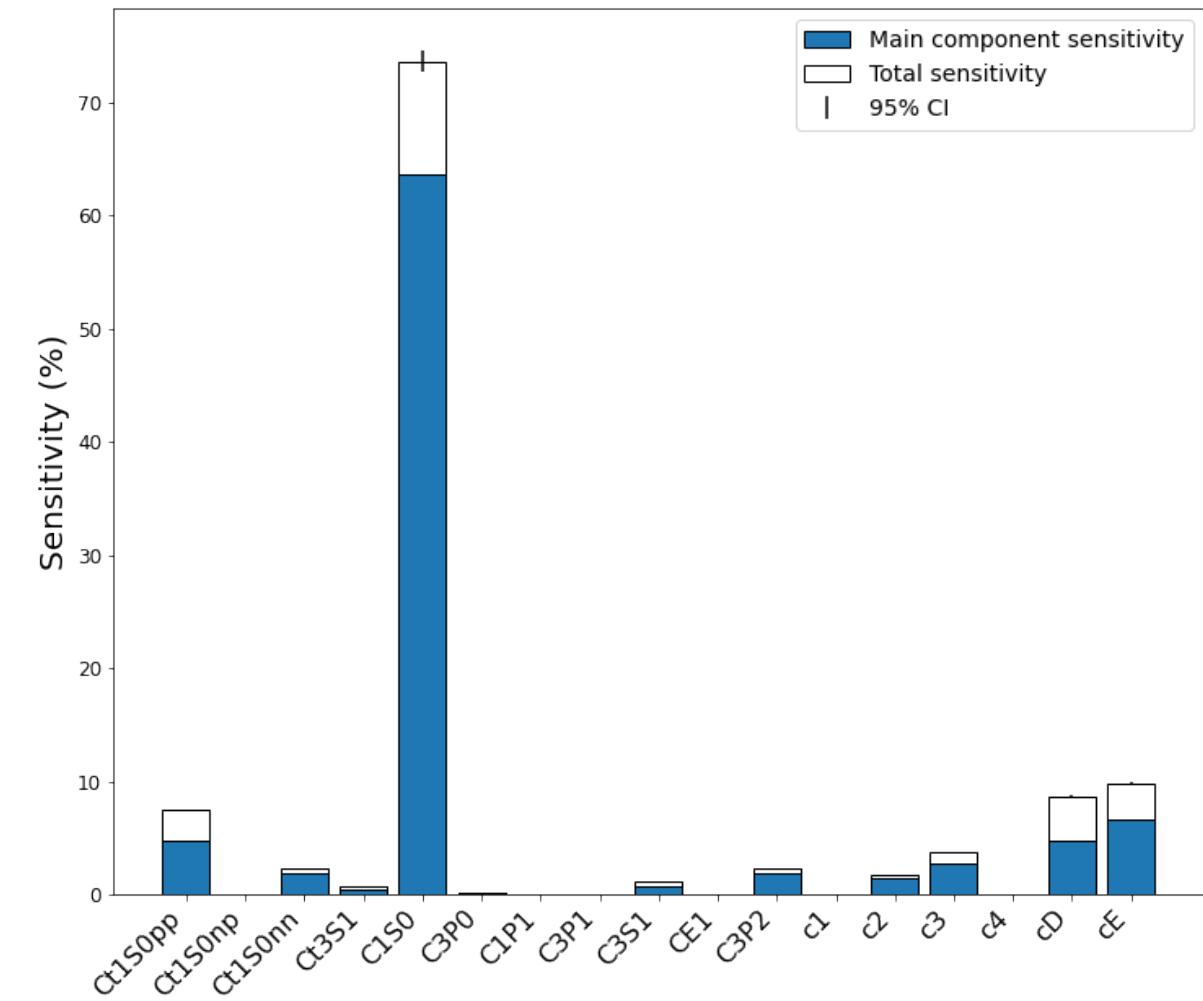
Low-Fidelity



High-Fidelity



Ground state energies

 $M_L^{0\nu}$ 

Summary...

- 1) Computed first ever ab initio NMEs of isotopes of experimental interest, which is a first step towards computing NME with reliable theoretical uncertainties.
- 2) Computed NME with multiple interactions for ^{48}Ca , ^{76}Ge , ^{82}Se , ^{130}Te and ^{136}Xe .
- 3) Study of effect of the contact term on the NMEs.
- 4) Studied correlations between multiple operators using a wide range of interactions.
- 5) Developed an emulator for the VS-IMSRG based on Gaussian processes.

... and outlook

- 1) Include finite momentum 2-body currents and other higher order effects.
- 2) Large scale ab initio uncertainty analysis with other methods for “final” NMEs.
- 3) Study other exotic mechanism proposed for $0\nu\beta\beta$.



Questions?

abelley@triumf.ca

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

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

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

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Scalar potential

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

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Neutrino Potential

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

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

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

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Operator acting on spin

$$S_F = 1$$

$$S_{GT} = \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

$$S_T = -3[(\boldsymbol{\sigma}_1 \cdot \hat{\mathbf{q}})(\boldsymbol{\sigma}_2 \cdot \hat{\mathbf{q}}) - (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)].$$

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Unknown coupling constants.

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

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Unknown coupling constants.

Method by Cirigliano et al. (JHEP05(2021)289) allows to extract this coupling for ab initio method with 30% uncertainty for each nuclear interaction

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

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

Considering the nuclear Hamiltonian:

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

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

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NN forces

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3N forces

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Choose 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.

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

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