TRIUMF

THE UNIVERSITY OF BRITISH COLUMBIA

Constraining neutrinoless double beta decay nuclear matrix elements with *ab initio* theory

Antoine Belley

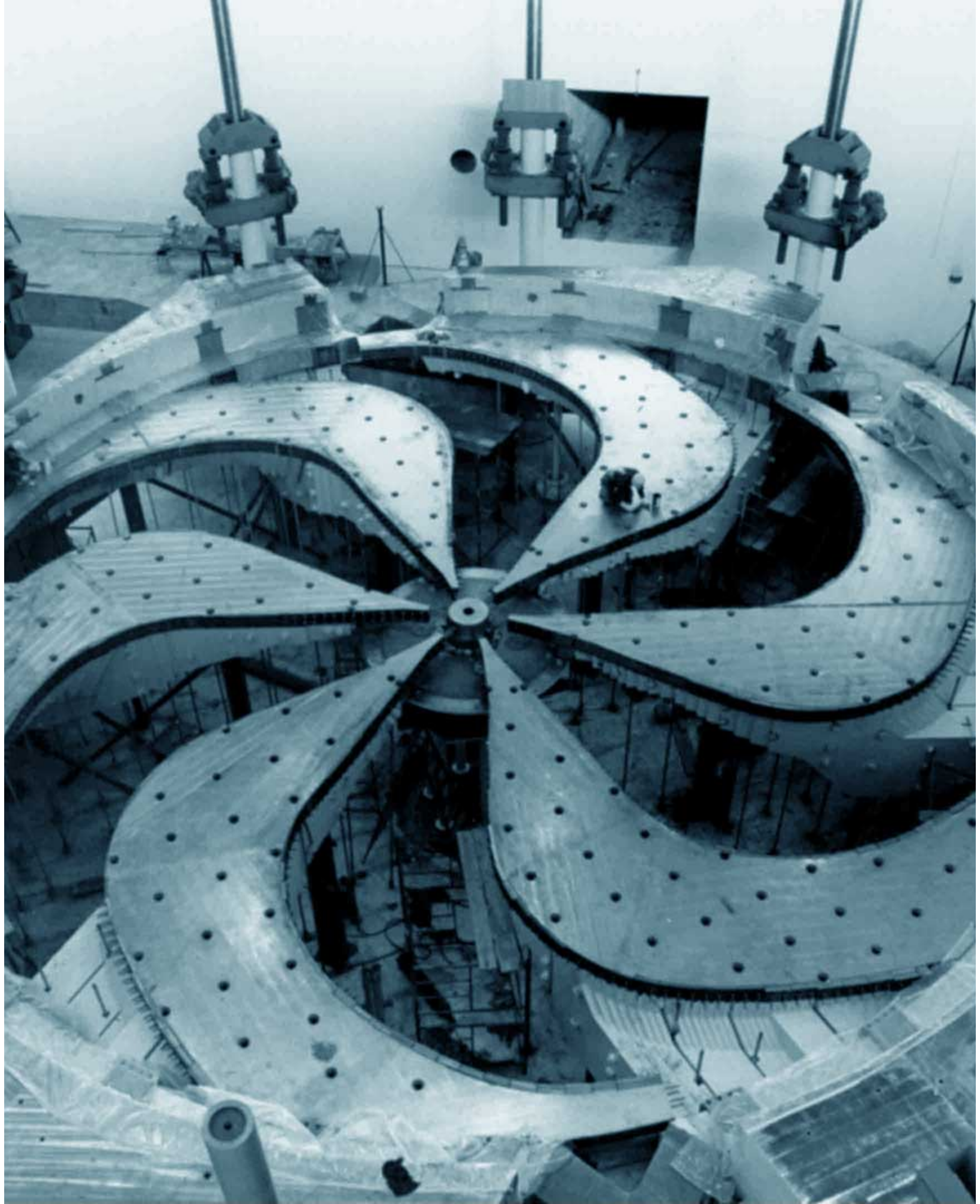
APCTP 2022

CINP ICPN

NSERC CRSNG

Arthur B. McDonald Canadian Astroparticle Physics Research Institute

NRC·CNRC

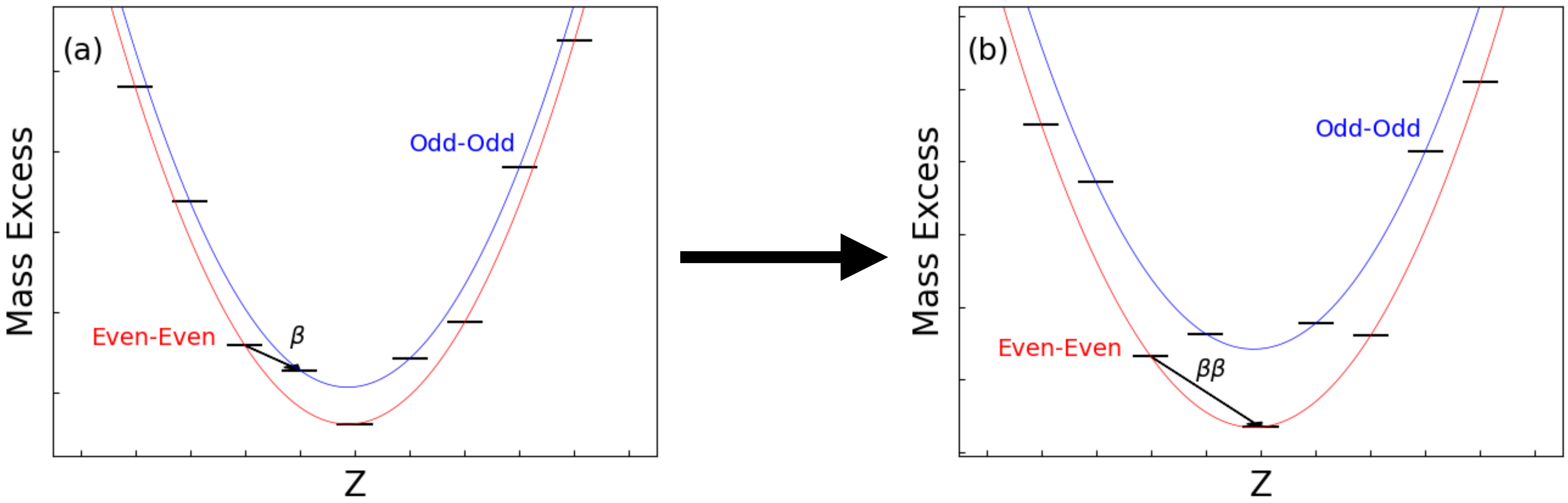


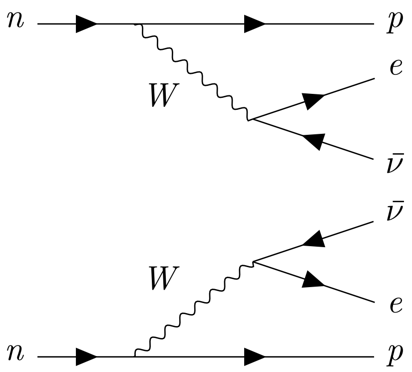
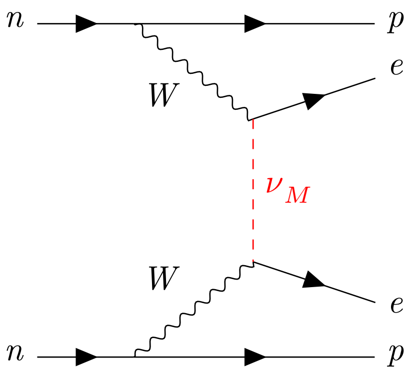
Discovery, accelerated

Double beta decays

Second order order weak process

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

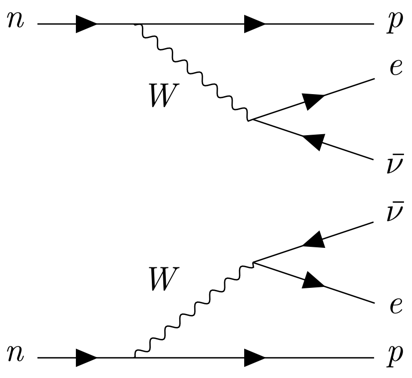
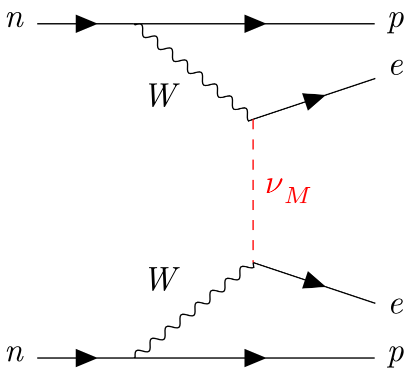


Decay	$2\nu\beta\beta$	$0\nu\beta\beta$
Diagram		
Half-life Formula	$[T^{2\nu}_{1/2}]^{-1} = G^{2\nu}\|M^{2\nu}\|^2$	$[T^{0\nu}_{1/2}]^{-1} = G^{0\nu}\|M^{0\nu}\|^2 \left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2$
NME Formula	$M^{2\nu} \approx M^{2\nu}_{GT}$	$M^{0\nu} = M^{0\nu}_{GT} - (\frac{g_v}{g_a})^2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

*NME : Nuclear matrix elements

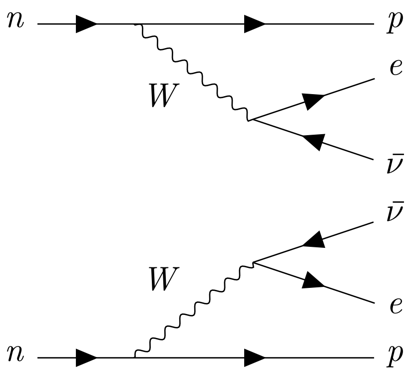
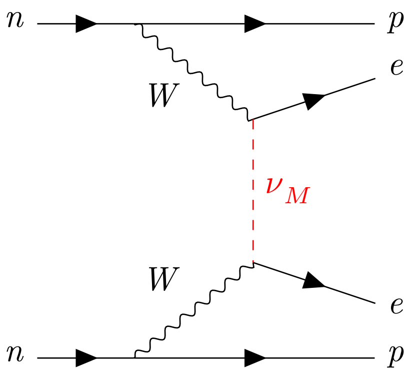
**LNV : Lepton number violation

2νββ vs 0νββ

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

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

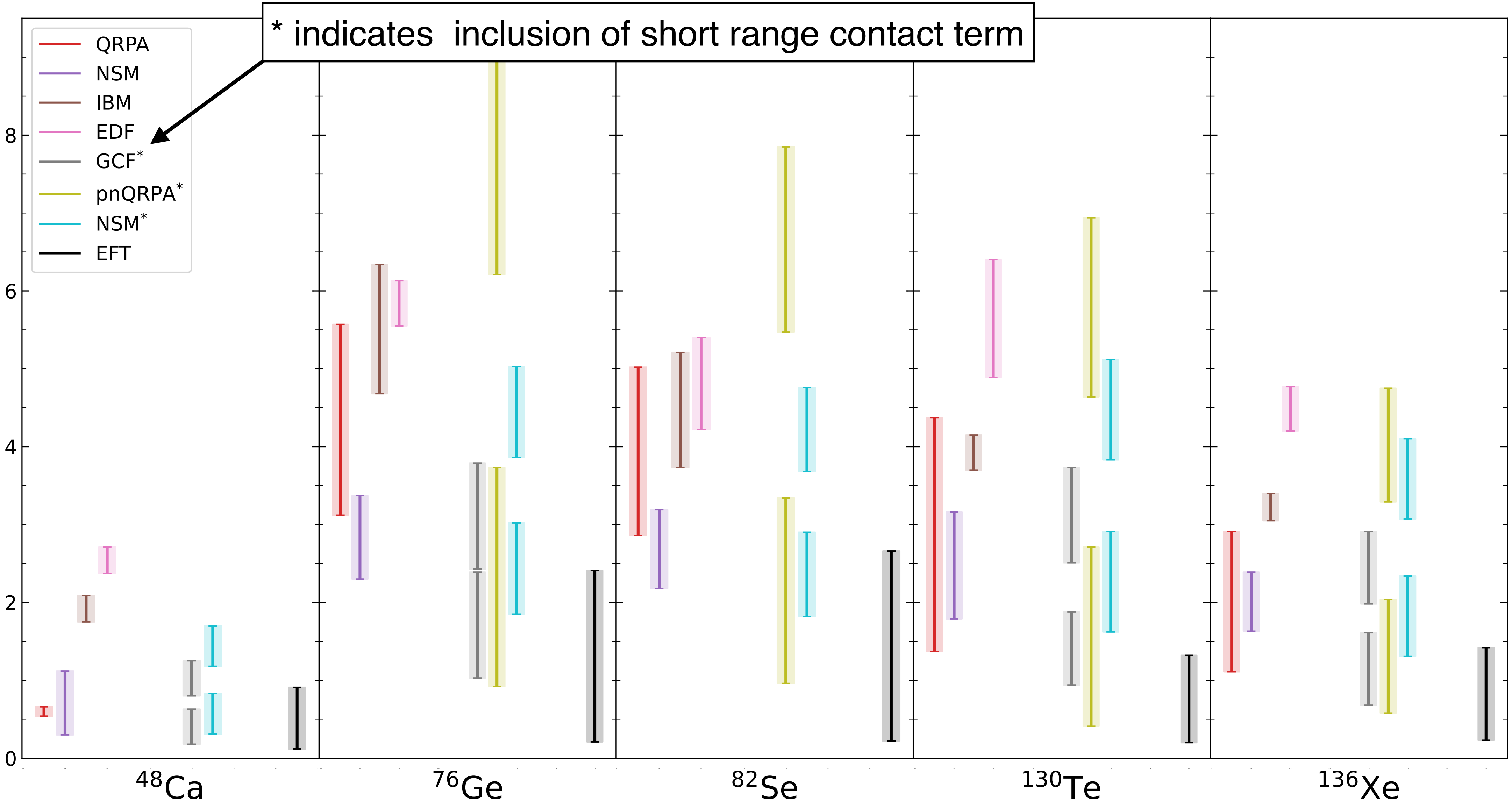
Decay	$2\nu\beta\beta$	$0\nu\beta\beta$
Diagram		
Half-life Formula	$[T^{2\nu}_{1/2}]^{-1} = G^{2\nu}\|M^{2\nu}\|^2$	$[T^{0\nu}_{1/2}]^{-1} = G^{0\nu}\|M^{0\nu}\|^2 \left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2$
NME Formula	$M^{2\nu} \approx M^{2\nu}_{GT}$	$M^{0\nu} = M^{0\nu}_{GT} - (\frac{g_v}{g_a})^2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

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

TRIUMF

Status of 0νββ-decay Matrix Elements

Current calculations from phenomenological models have large spread in results.

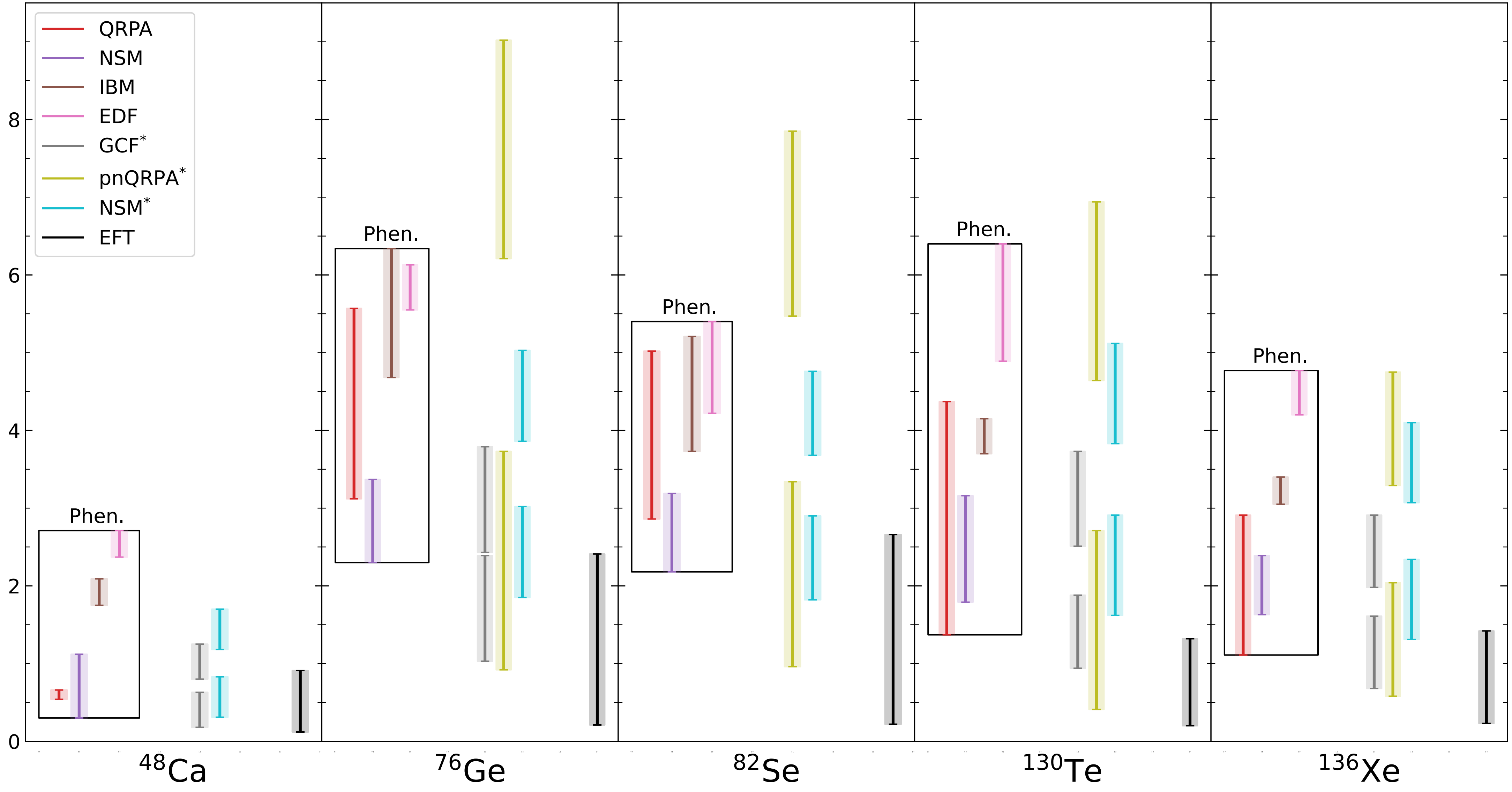


Compiled values from Engel and Menéndez, Rep. Prog. Phys. **80** 046301 (2017); Yao, arXiv:2008.13249 (2020); Brase et al, arXiv:2108.11805 (2021)

TRIUMF

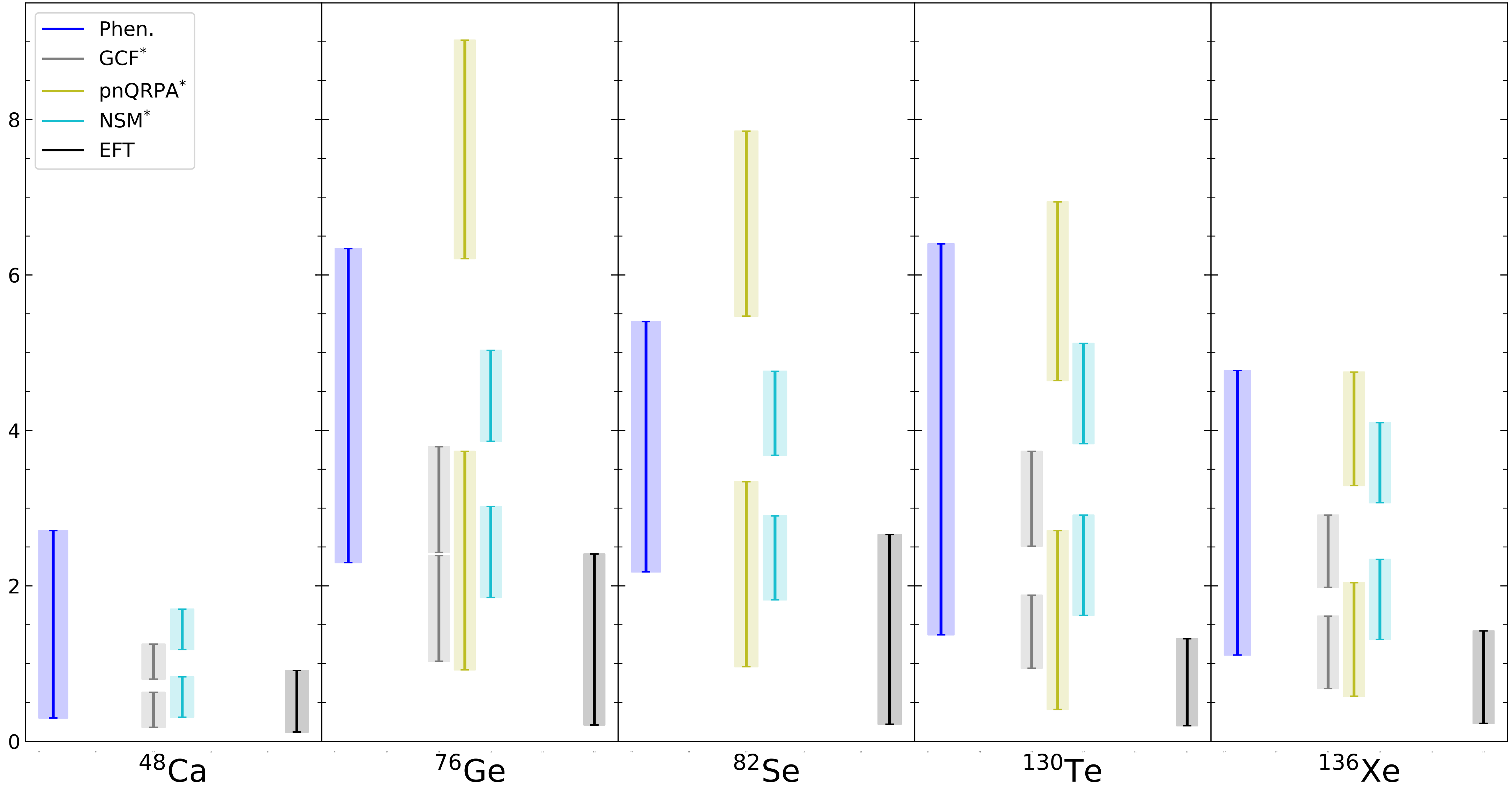
Status of 0νββ-decay Matrix Elements

Current calculations from phenomenological models have large spread in results.



Status of 0νββ-decay Matrix Elements

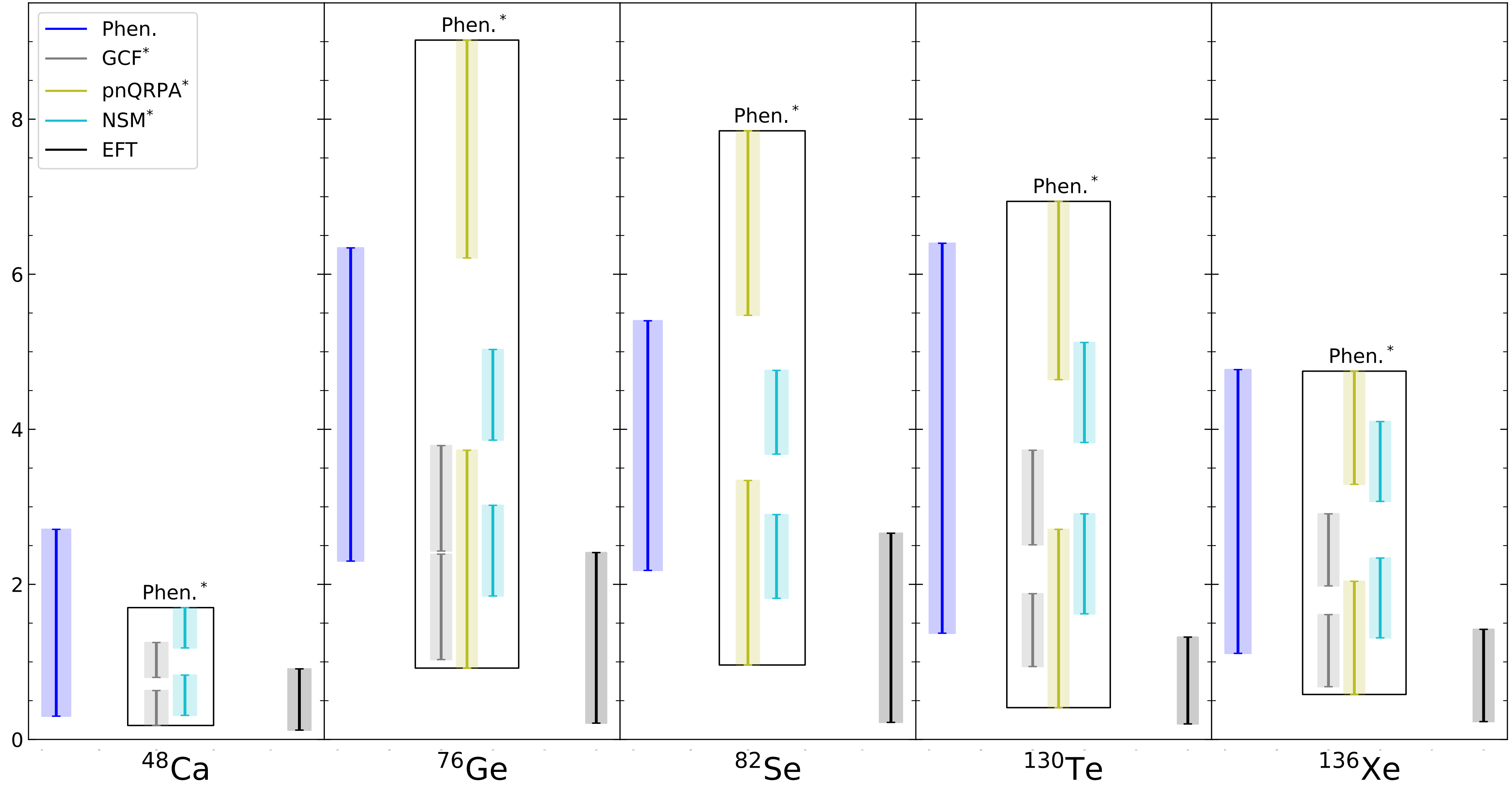
Current calculations from phenomenological models have large spread in results.



TRIUMF

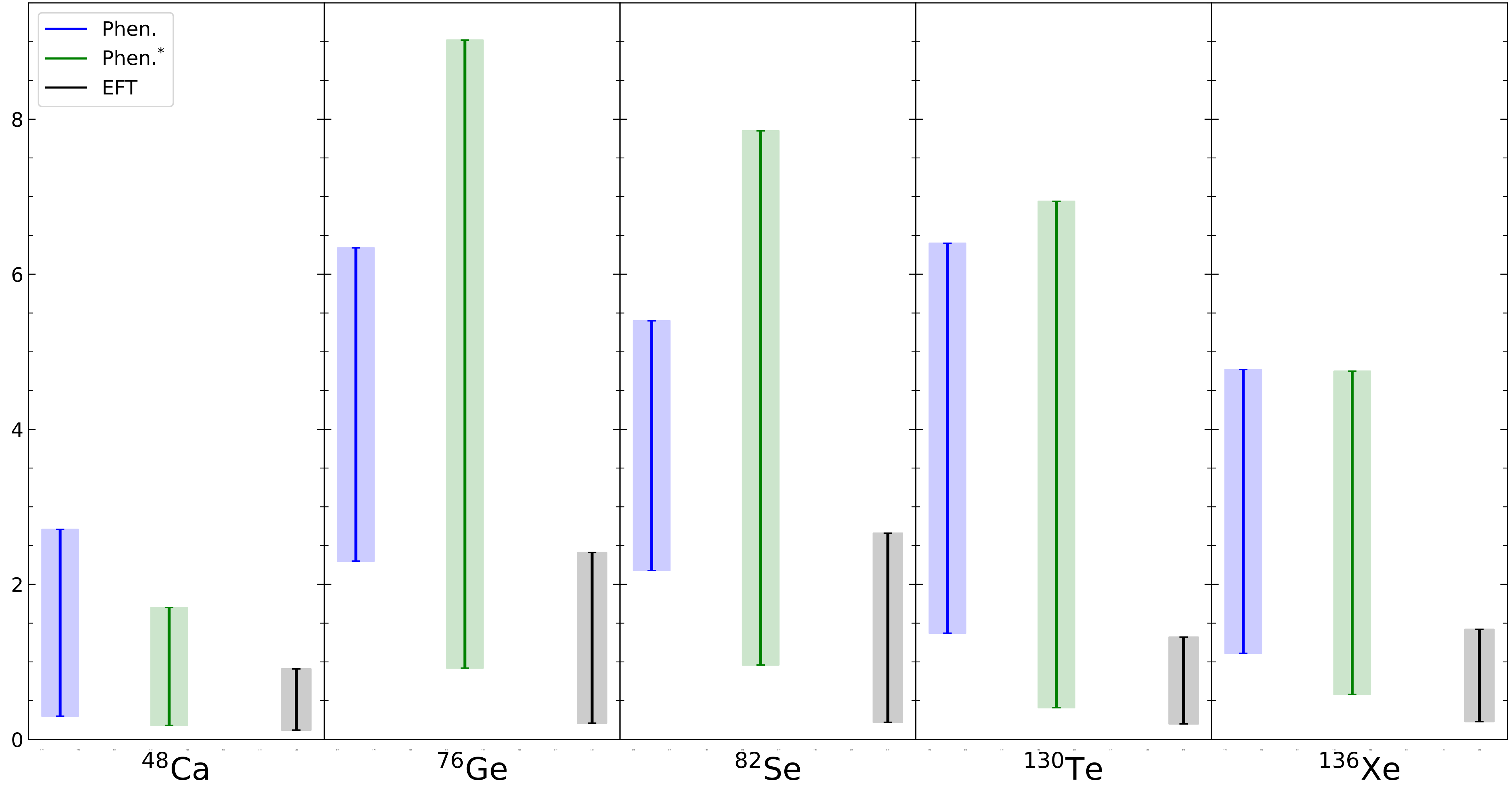
Status of 0νββ-decay Matrix Elements

Current calculations from phenomenological models have large spread in results.



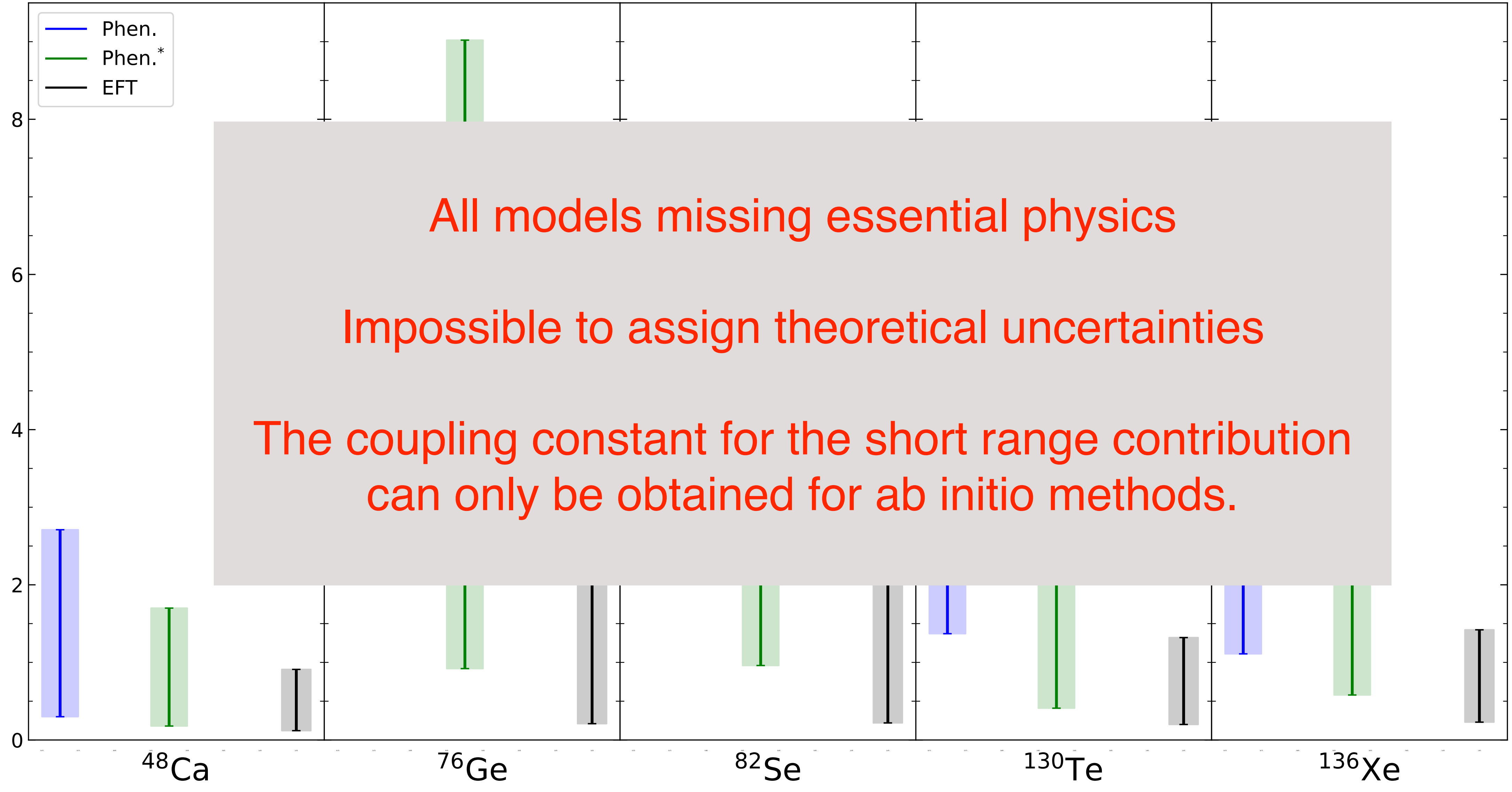
Status of 0νββ-decay Matrix Elements

Current calculations from phenomenological models have large spread in results.



Status of 0νββ-decay Matrix Elements

Current calculations from phenomenological models have large spread in results.



All models missing essential physics

Impossible to assign theoretical uncertainties

The coupling constant for the short range contribution can only be obtained for ab initio methods.

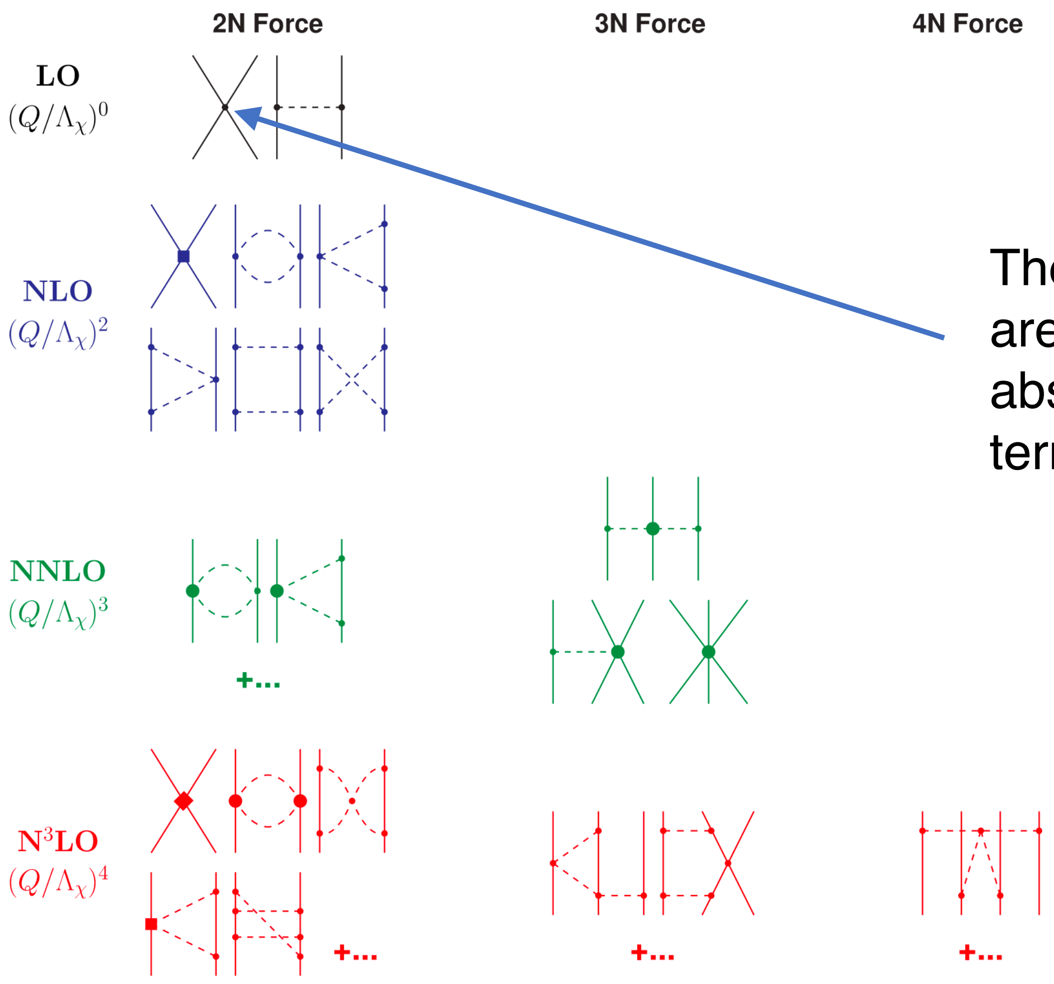
Ab initio nuclear theory

Ab initio nuclear theory: The recipe

1. Construct nuclear interaction from principle (using chiral effective field theory (χ-EFT))
2. Solve the many-body Schrödinger equation for the nucleus with this interaction

Expansion order by order of the nuclear forces

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



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

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

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 in the s parameter for our Hamiltonian to be

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

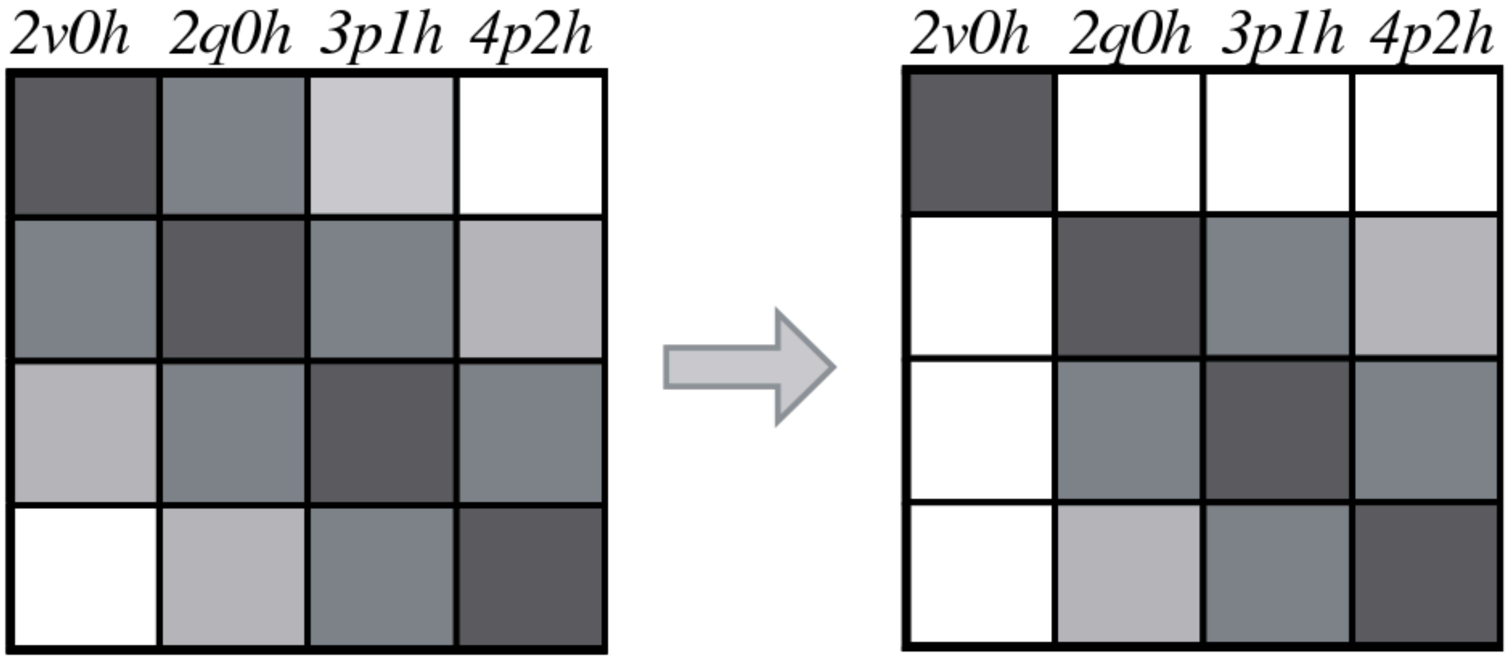
Writing the expression above in term of the generator we have defined, we get

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

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

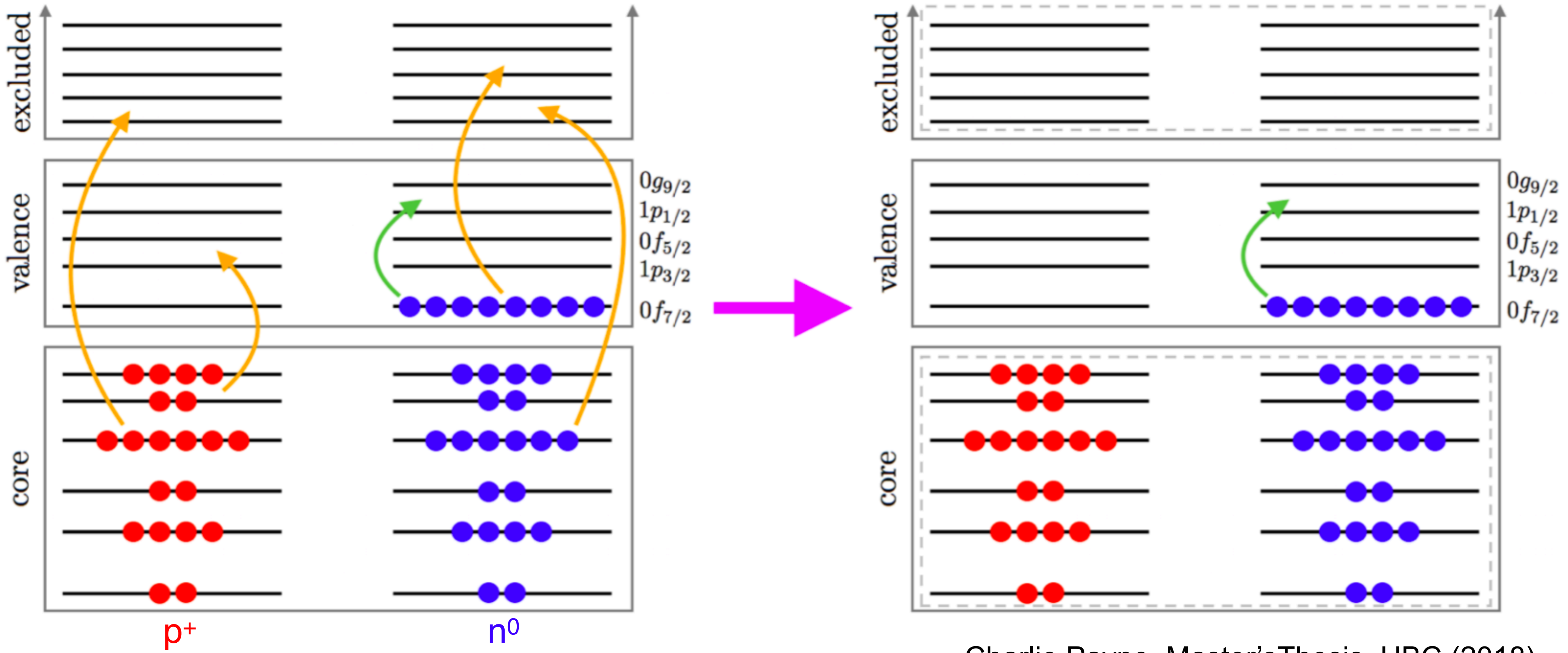
$$\boxed{\frac{d\hat{H}(s)}{ds} = \left[\hat{\eta}(s), \hat{H}(s)\right]}$$

Valence-Space In Medium Similarity Renormalization Group



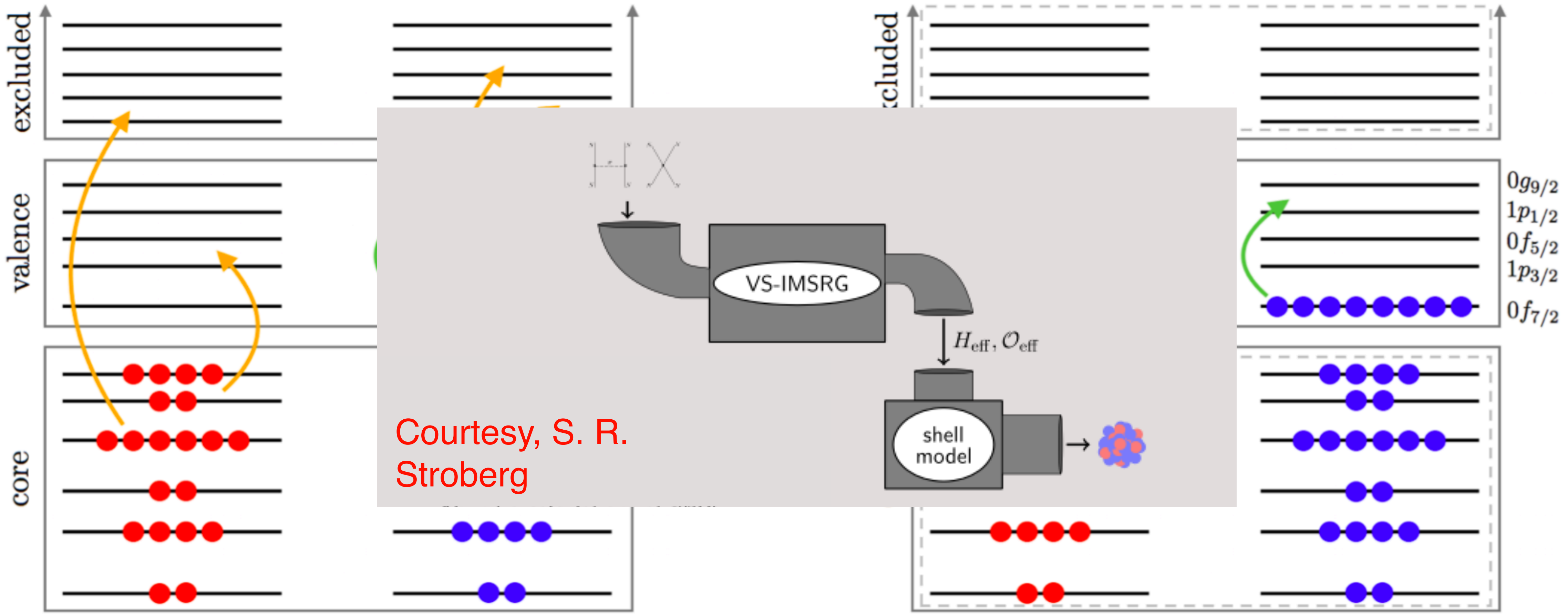
$$\hat{H}(0) \longrightarrow \hat{H}(s) = e^{\Omega(s)}\hat{H}(0)e^{-\Omega(s)}$$

Valence-Space In Medium Similarity Renormalization Group

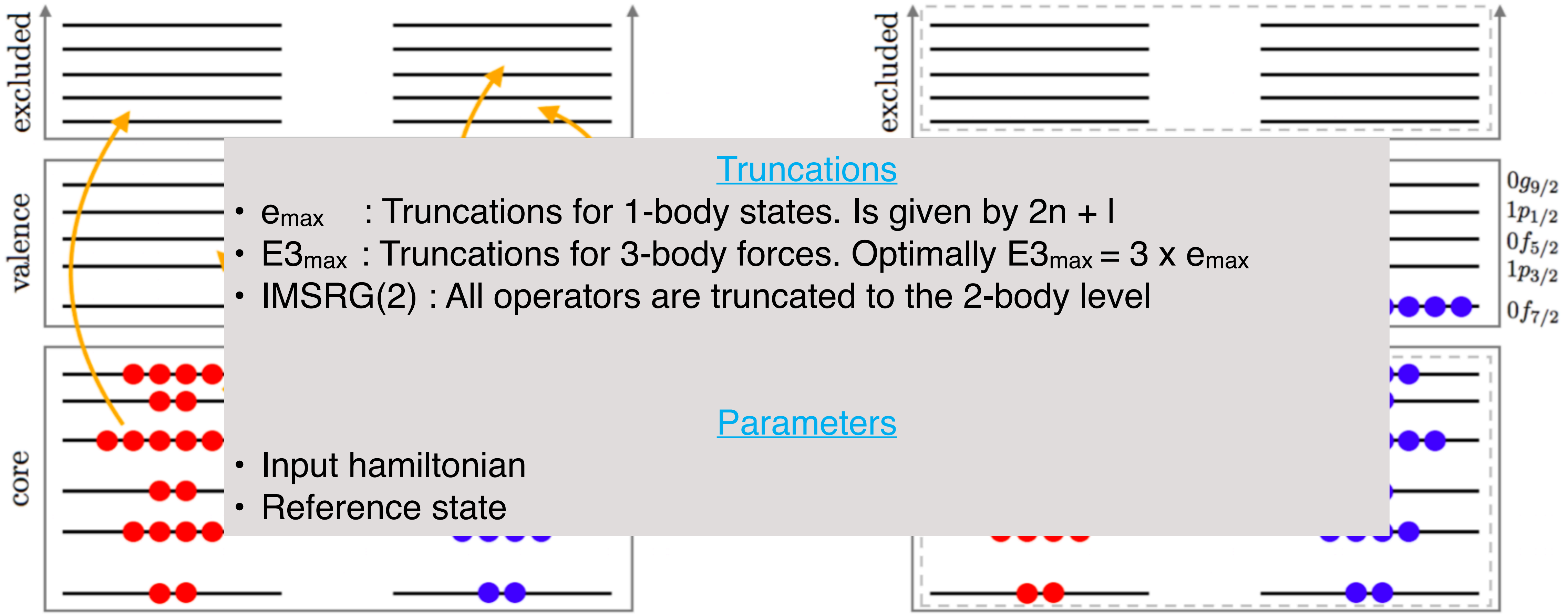


Charlie Payne, Master'sThesis, UBC (2018)

Valence-Space In Medium Similarity Renormalization Group



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

Parameters

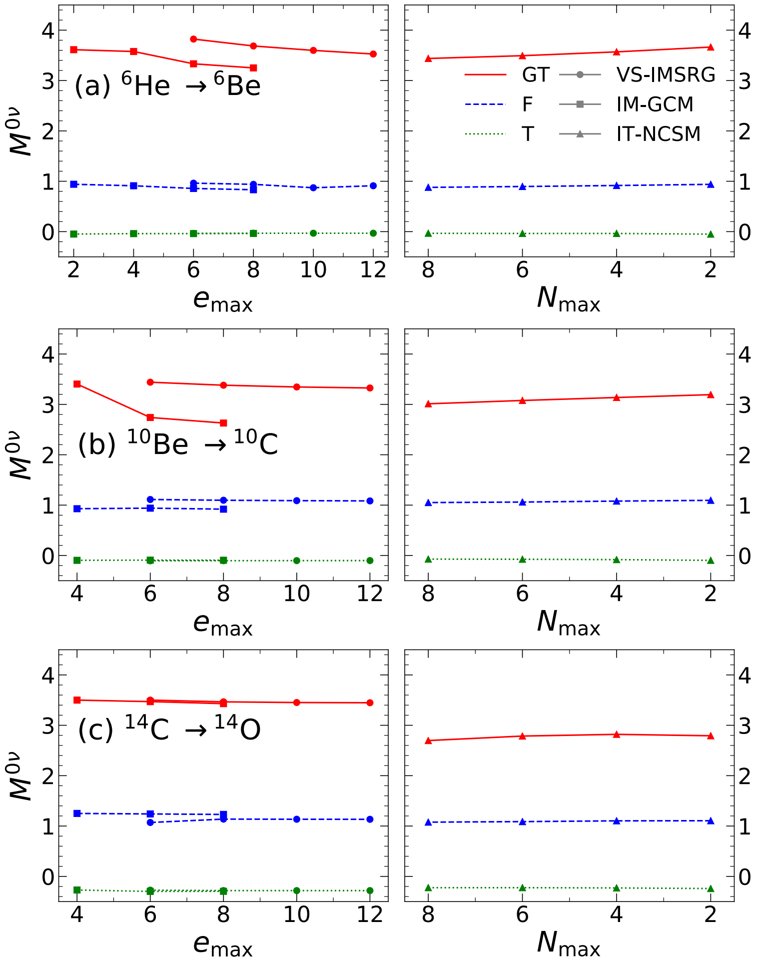
- Input hamiltonian
- Reference state

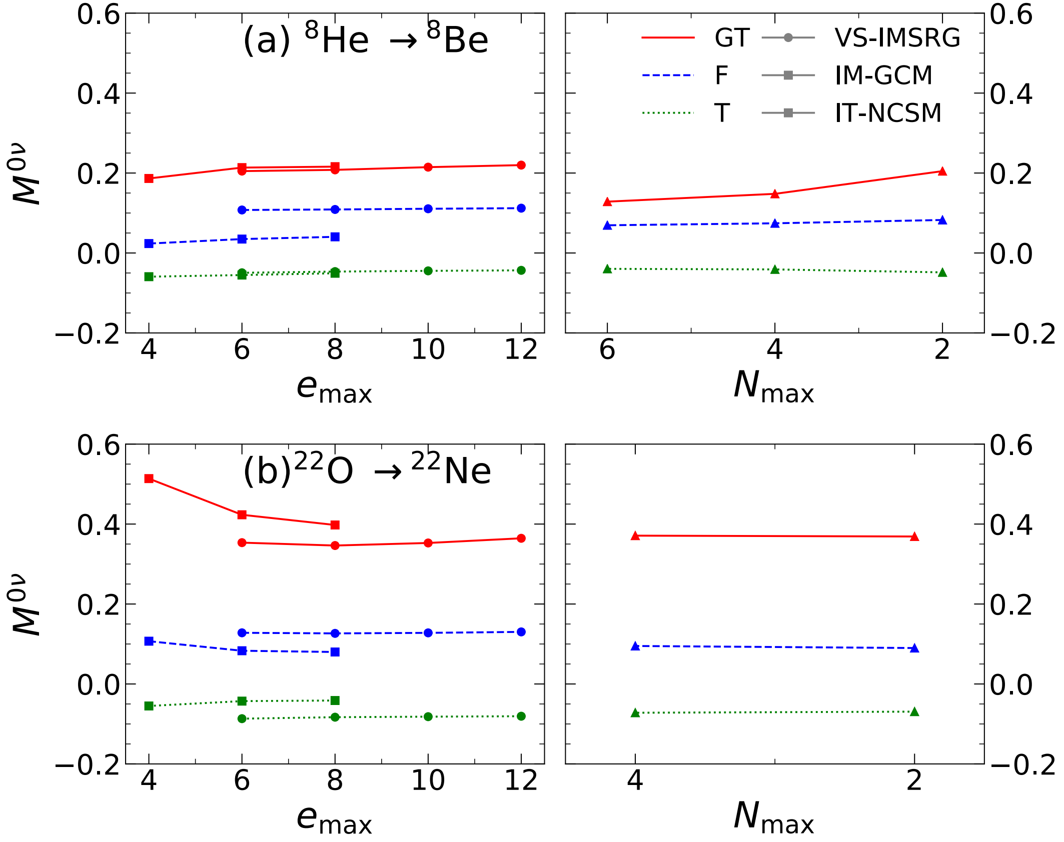
Results

Benchmarking 0νββ Decay in Light Nuclei: Summary

Benchmark with other ab initio method for fictitious decays in light nuclei

$\Delta T = 0$





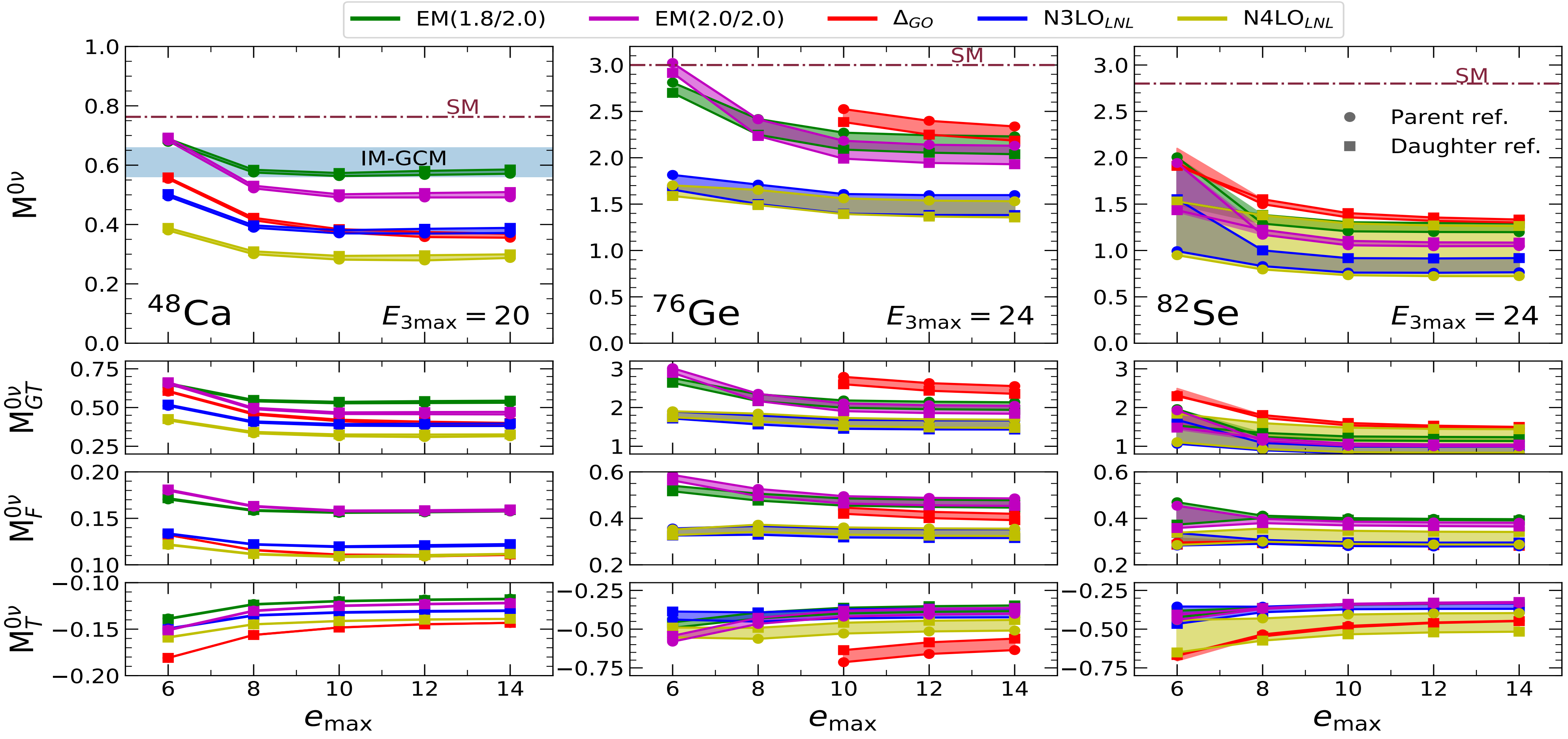
$\Delta T = 2$

Yao, **Belley**, et al., PhysRevC.103.014315

Reasonable to good agreement in all cases

Ab Initio 0νββ Decay: ^{48}Ca, ^{76}Ge and ^{82}Se

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

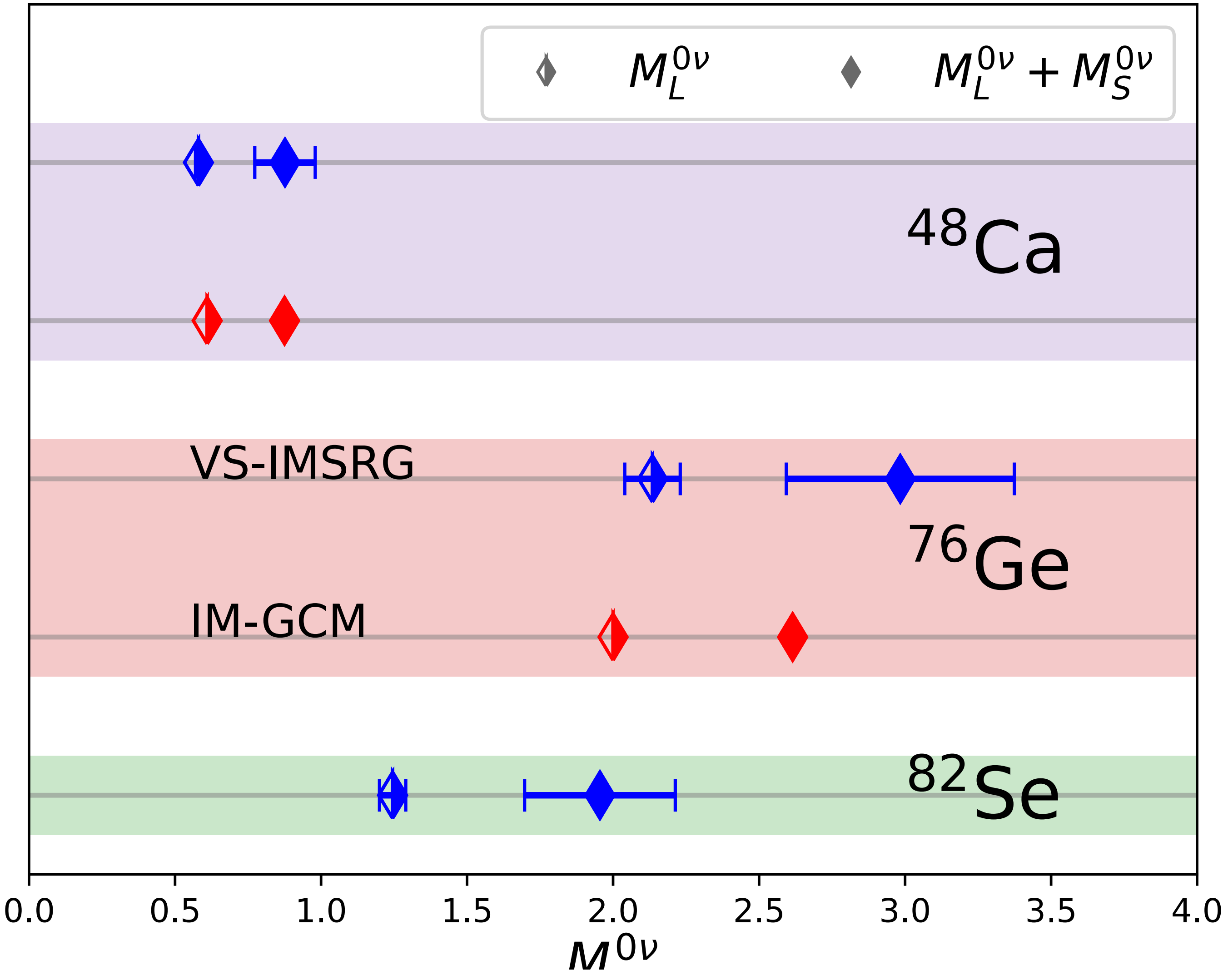


Things to add: valence space variation, two-body currents, IMSRG(3), …

Belley, et al., in prep

TRIUMF

Ab Initio 0νββ Decay: The contact term

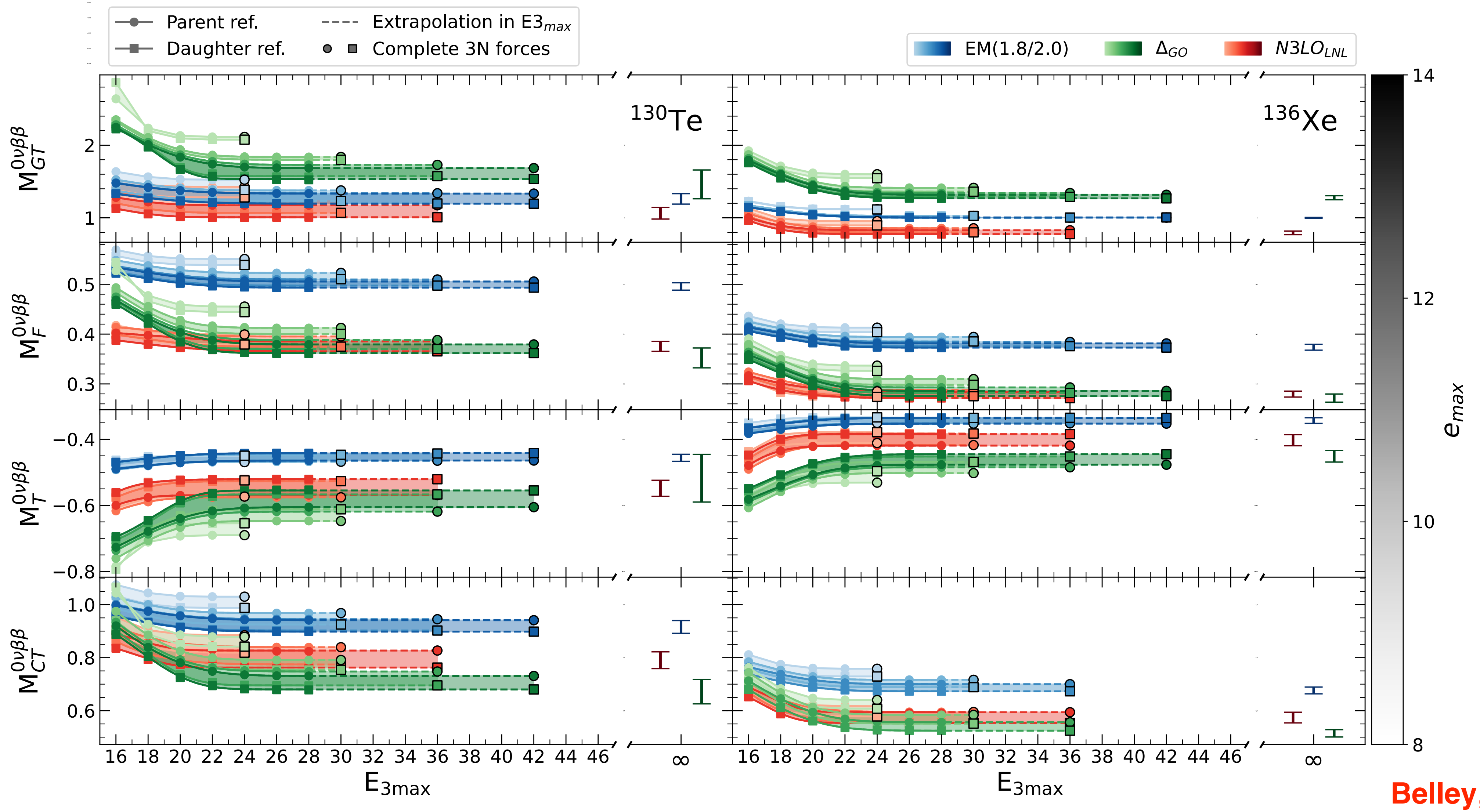


Belley, et al., in prep

Ab Initio 0νββ Decay: ^{130}Te, ^{136}Xe

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

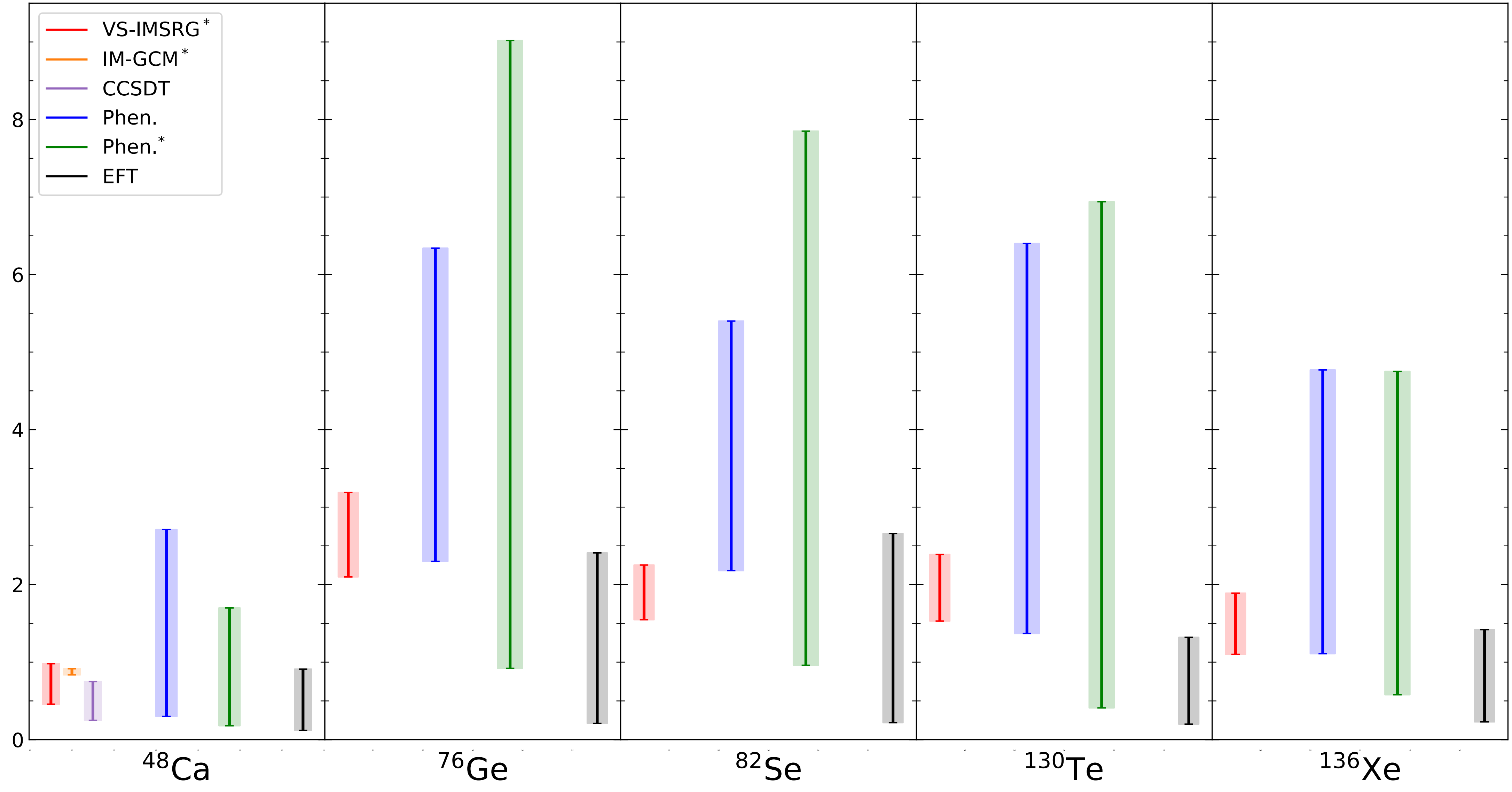
Increased E_{3max} capabilities allow first converged ab initio calculations [EM1.8/2.0, Δ_{GO}, $N3LO_{LNL}$]



Belley, et al., in prep

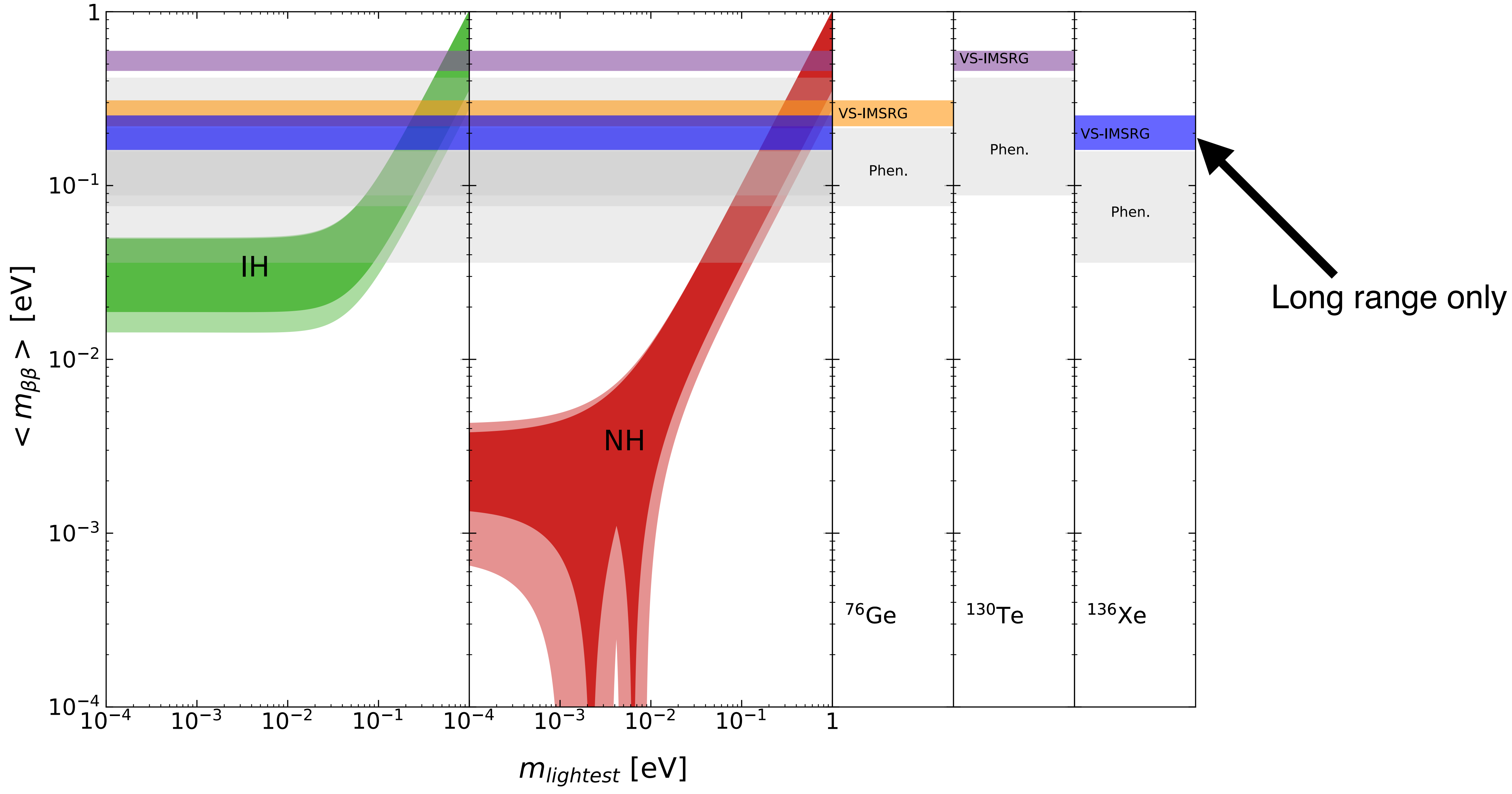
TRIUMF

0νββ-decay Matrix Elements: The new picture



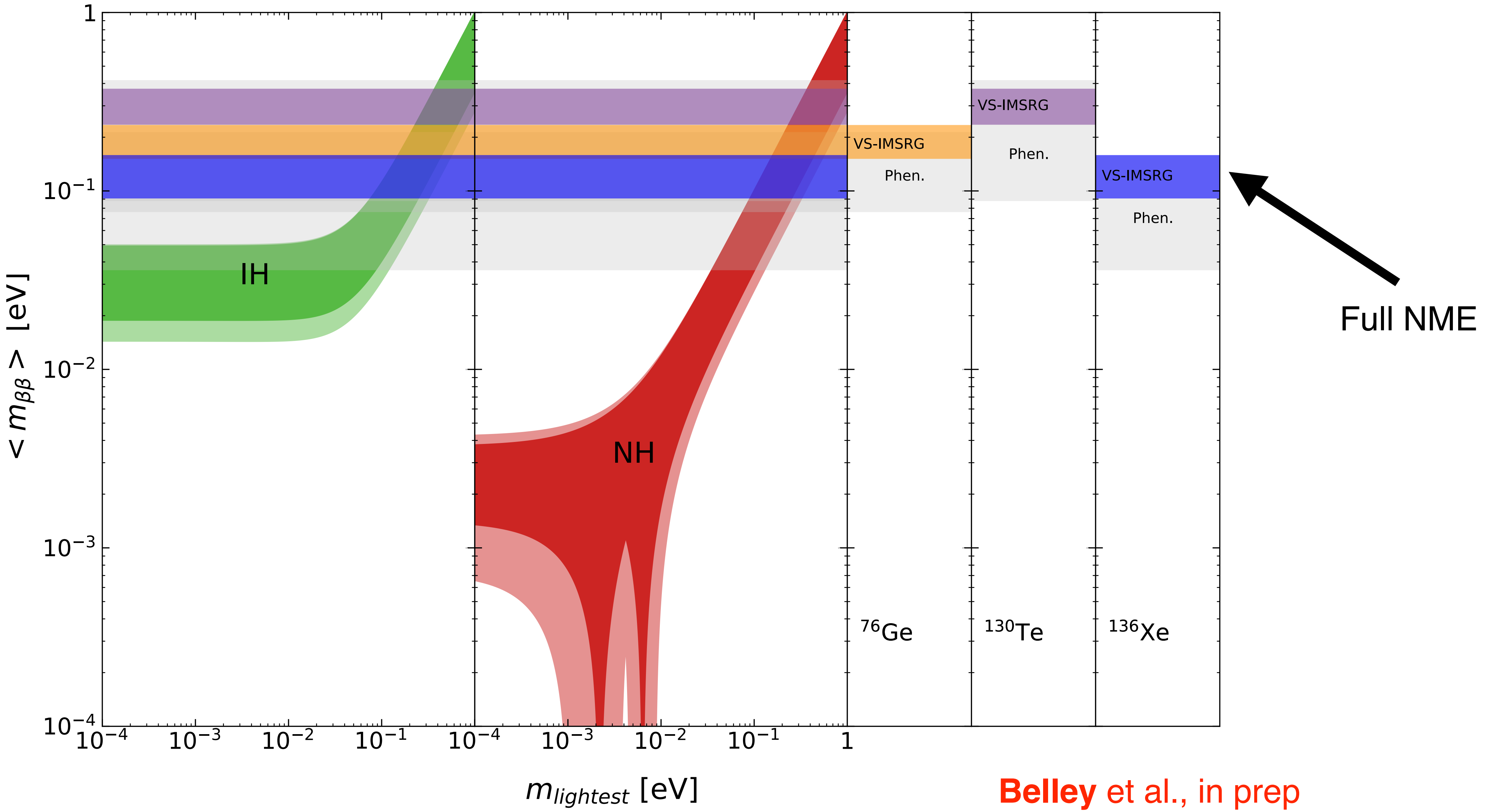
Belley, et al., in prep

Ab Initio 0νββ Decay: Effect on experimental limits



TRIUMF

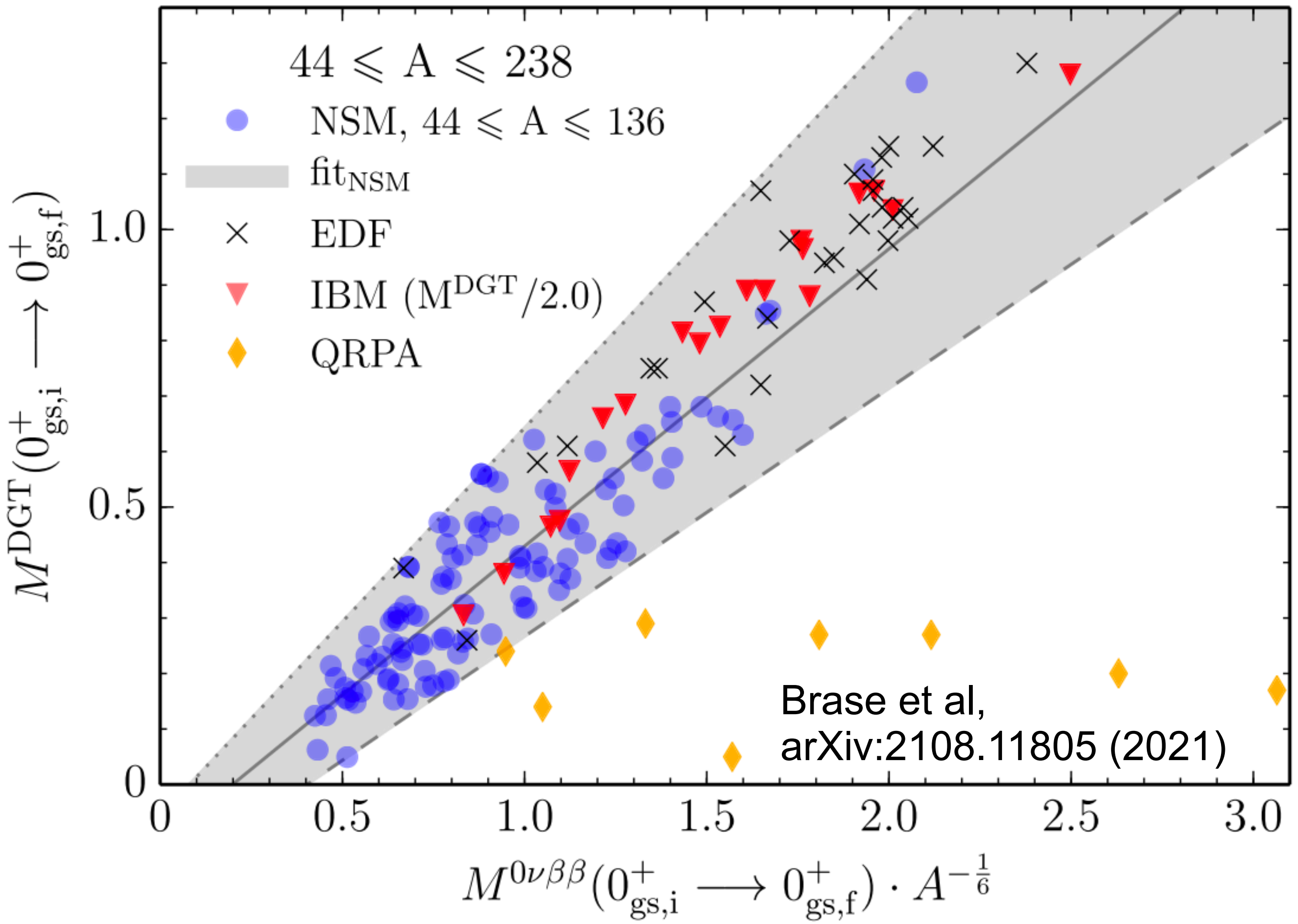
Ab Initio 0νββ Decay: Effect on experimental limits



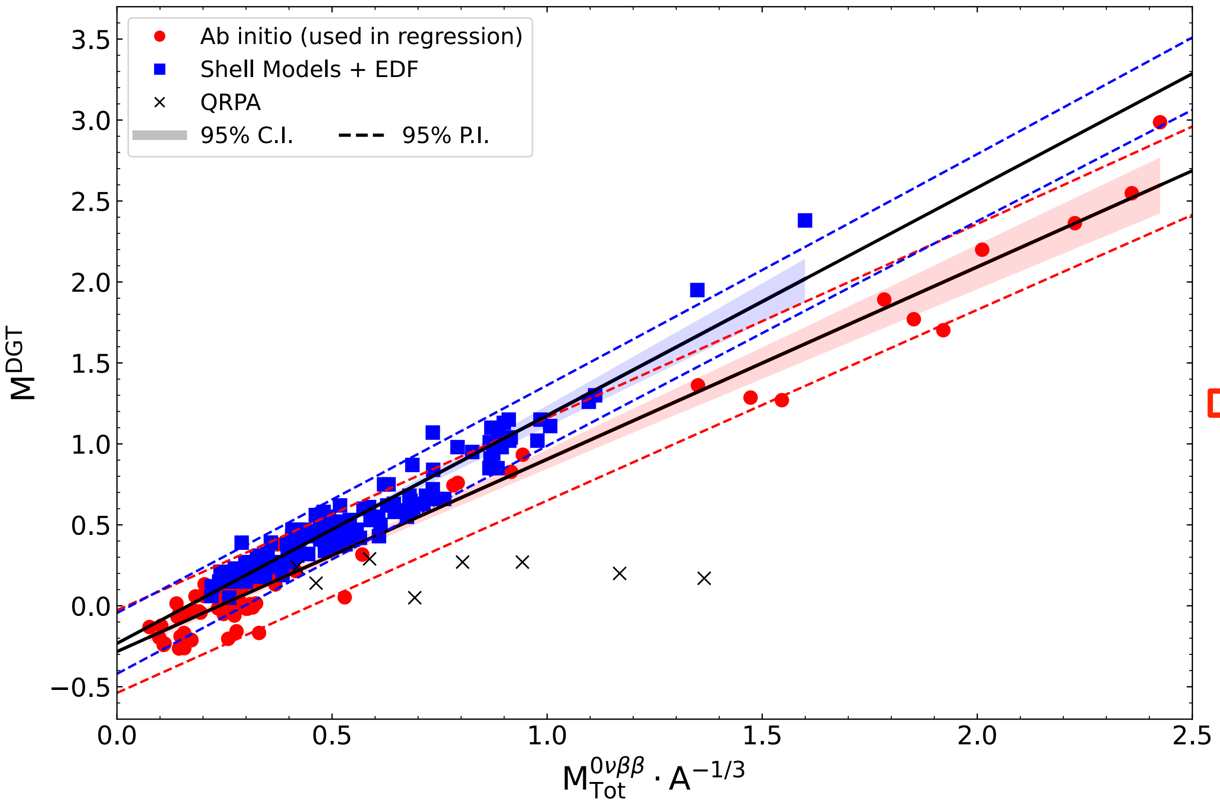
Belley et al., in prep

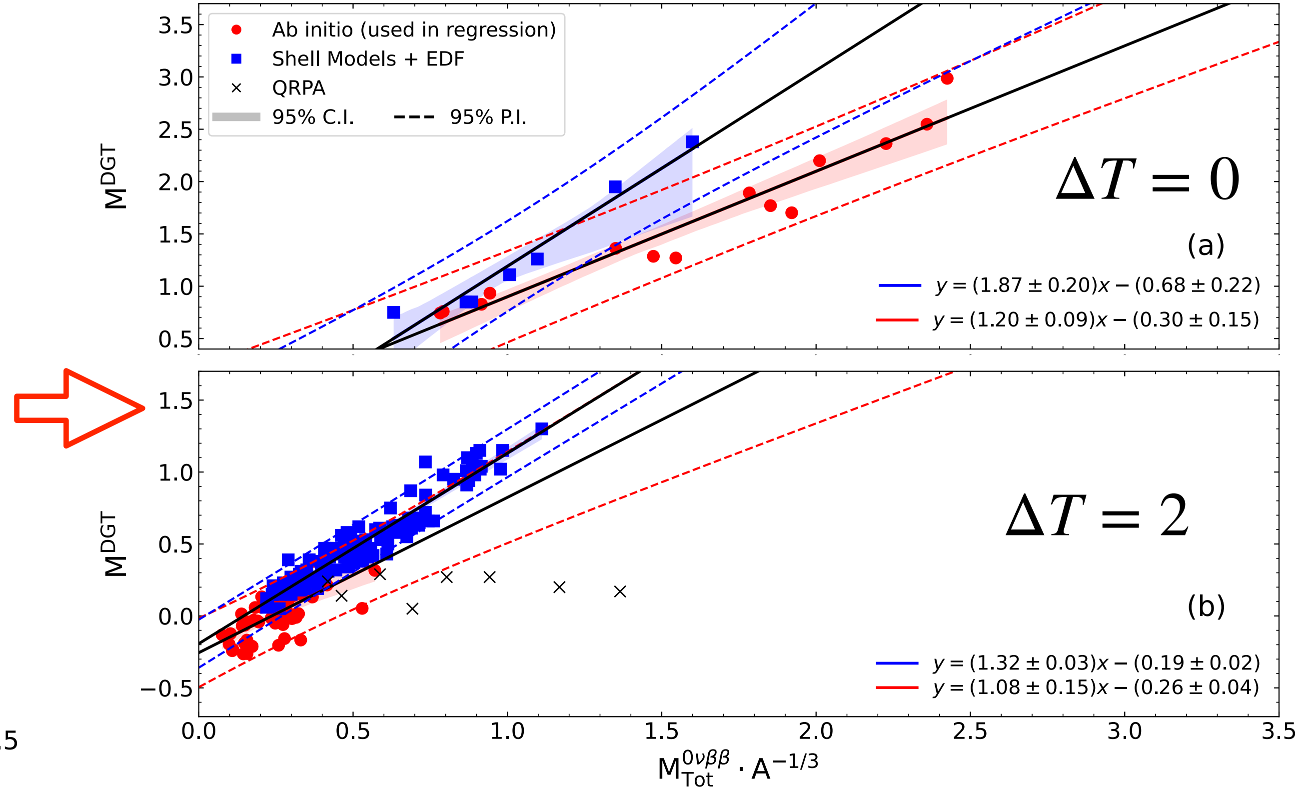
Constraining uncertainty:correlation with DGT

Double Gamow-Teller giant resonance is a charge exchange process whose NMEs have been found to be correlated to 0νββ NMEs in nuclear shell models, EDF and IBM.



Constraining uncertainty:correlation with DGT from ab initio

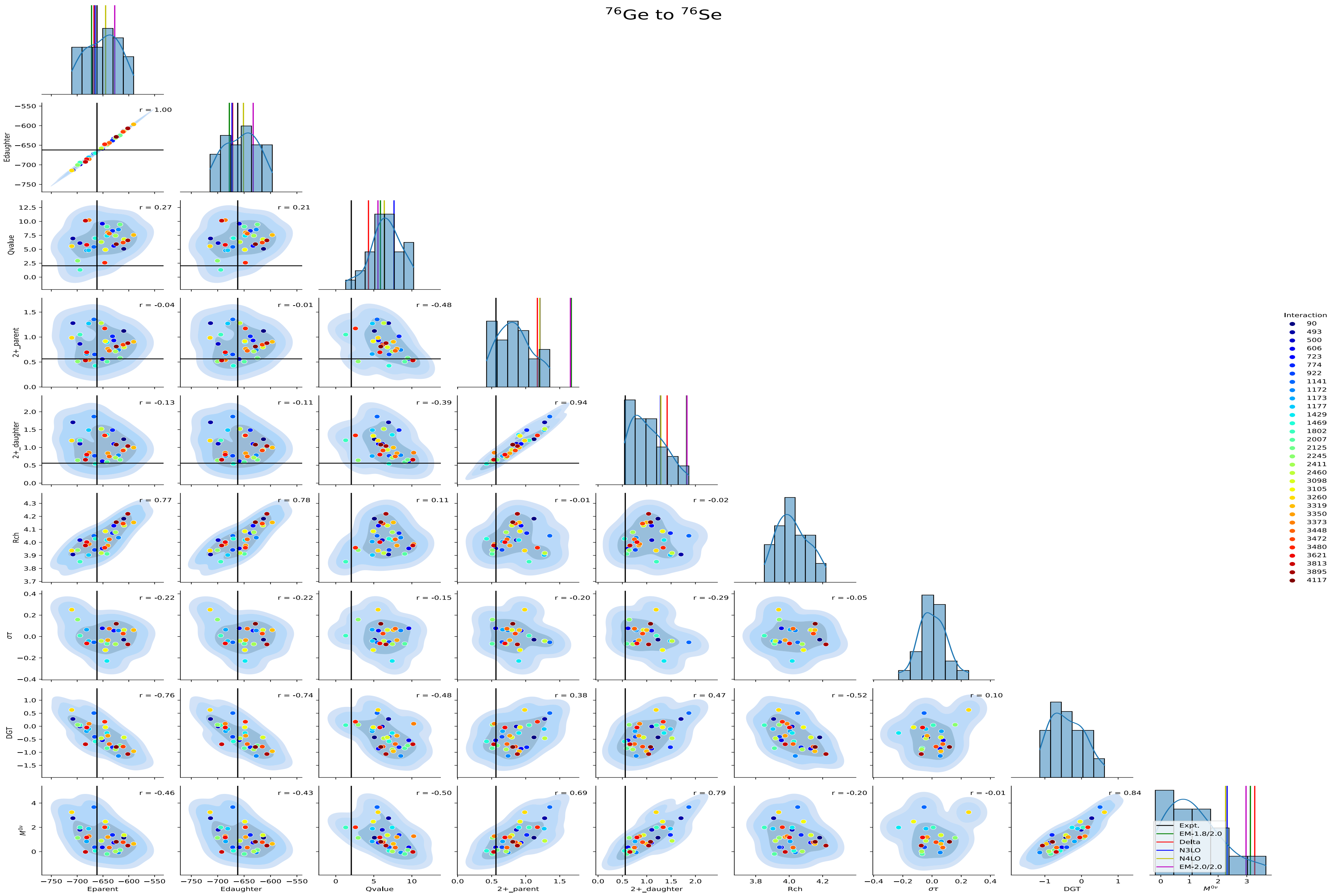




Yao, **Ginnett**, **Belley** et al., arXiv:2204.12971 (2022)

TRIUMF

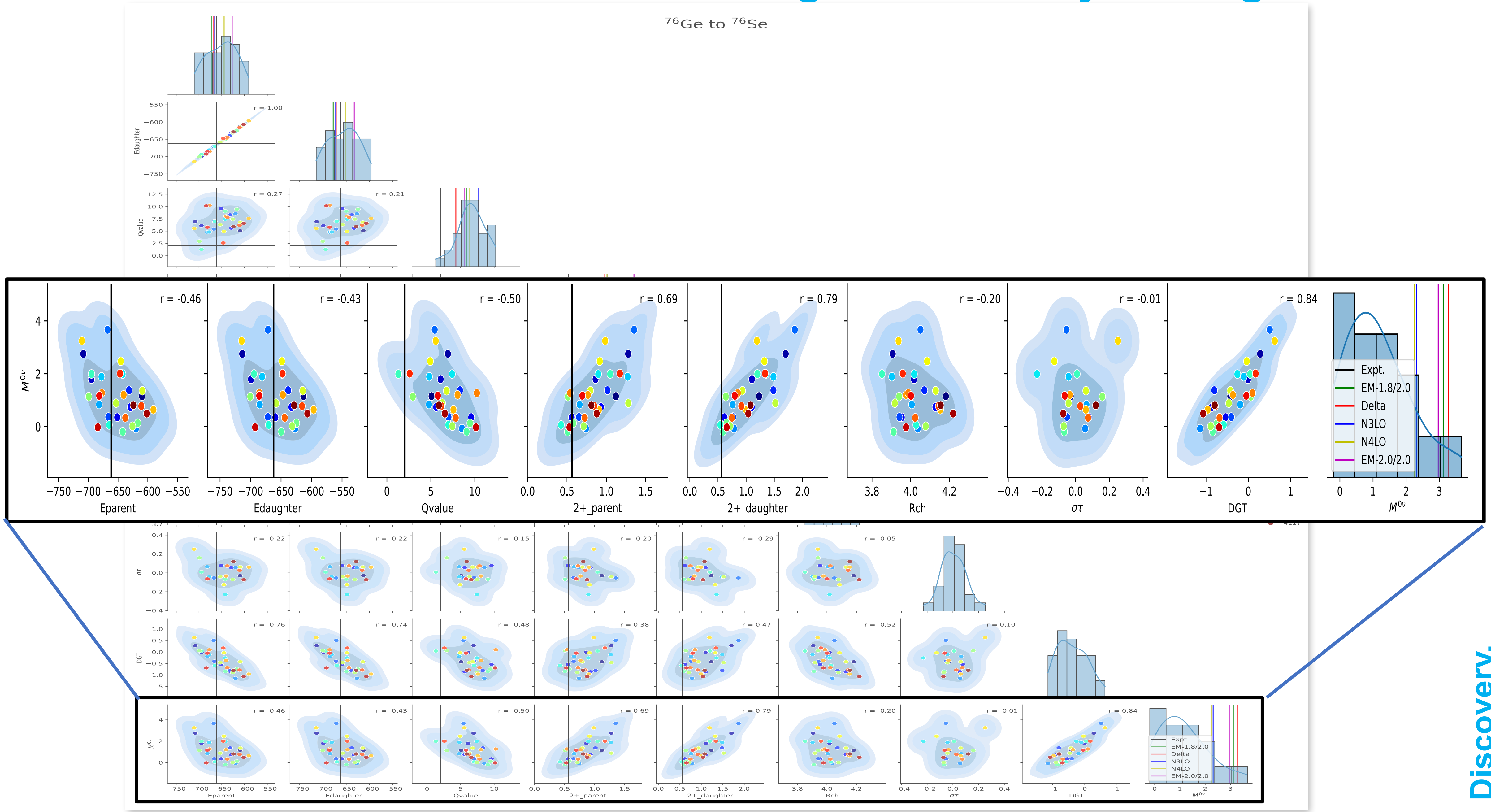
Constraining uncertainty: using emulators



Discovery, accelerated

TRIUMF

Constraining uncertainty: using emulators



Discovery, accelerated

TRIUMF

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 correlation between DGT and $0\nu\beta\beta$ for a wide range of isotopes.

5) Studied correlations between multiple operators using a wide range of interactions based on emulators.

… and outlook

1) Include finite momentum 2-body currents.

2) Large scale ab initio uncertainty analysis with other methods for “final” NMEs.

3) Study other exotic mechanism proposed for $0\nu\beta\beta$.

4) Compute the NME for $0\nu EC$

Discovery, accelerated

TRIUMF

Questions?

abelley@triumf.ca

Discovery, accelerated

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

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

(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

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

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

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

E_{cl} → Closure energy

Long-Range Matrix Elements

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

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

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

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

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

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

Operator acting on spin

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

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

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

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

$$S_F = 1$$

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

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

Long-Range Matrix Elements

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

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

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

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

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

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

$$S_F = 1$$

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

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

Short-Range Matrix Elements

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

Short-Range Matrix Elements

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

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

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) 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:

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

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:

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

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

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

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

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

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

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

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

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

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

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

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

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

The IMSRG:NO2B Approximation

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

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

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

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

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

The VS-IMSRG

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.

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

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

Exotic Mechanisms

Exotic Mechanisms

Most general Lorentz invariant effective Hamiltonian:

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

Exotic Mechanisms

Most general Lorentz invariant effective Hamiltonian:

Lepton currents

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

Exotic Mechanisms

Most general Lorentz invariant effective Hamiltonian:

Hadron currents   Lepton currents

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

Exotic Mechanisms

Most general Lorentz invariant effective Hamiltonian:

Hadron currents   Lepton currents

$$\mathscr{H}_W = \frac{G_\beta}{\sqrt{2}}\Big[\underbrace{j_L^\mu J_{L,\mu}^\dagger}_{\text{Standard V-A weak interaction}} + \underbrace{\sum_{\alpha,\beta} \epsilon_\alpha^\beta j_\alpha J_\beta^\dagger}_{\text{All other exotic mechanisms}}\Big]$$

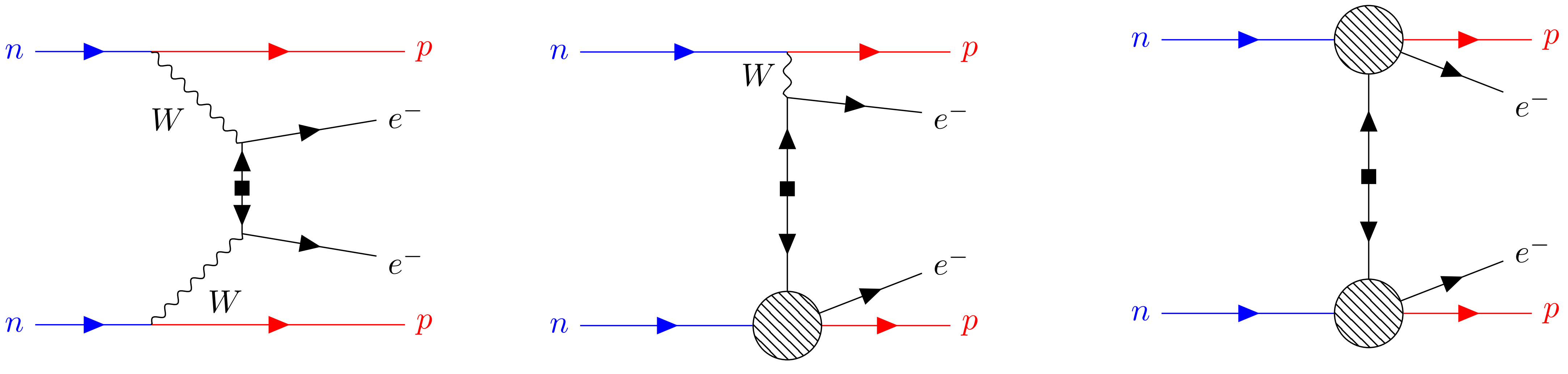
Standard V-A weak interaction

All other exotic mechanisms

Exotic Mechanisms

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

$$\mathscr{A}^{0\nu}_{i\to f} \propto \langle f \,|\, T[\mathscr{H}_W(x_1)\mathscr{H}_W(x_2)] \,|\, i\rangle$$
$$\propto \langle f \,|\, T[j^\mu_L J^\dagger_{L,\mu} j^\nu_L J^\dagger_{L,\nu}] + \sum_{\alpha,\beta} \epsilon^\beta_\alpha T[j^\mu_L J^\dagger_{L,\mu} j_\alpha J^\dagger_\beta] + \sum_{\alpha,\beta,\gamma,\sigma} \epsilon^\beta_\alpha \epsilon^\sigma_\gamma T[j_\alpha J^\dagger_\beta j_\gamma J^\dagger_\sigma] \,|\, i\rangle$$



Non-Closure NME

Non-Closure NME

Assuming that both electron carry the same energy:

$$O(\boldsymbol{q}) = \frac{R_{Nucl}}{2\pi^2 g_a^2} \sum_N \frac{J^\mu(\boldsymbol{q})\,|\,N\rangle\langle N\,|\,J_\mu(-\boldsymbol{q})}{q\left(q + E_N - \frac{E_i + E_f}{2}\right)}$$

where, under the impulse approximation, the currents are given by

$$J^0(\boldsymbol{q}) = \tau^+\left[g_V(q^2) - \frac{g_M(q^2) - g_V(q^2)}{4m_N^2}q^2\right]$$

$$J^k(\boldsymbol{q}) = -\,\tau^+\left[g_A(q^2)\boldsymbol{\sigma} + i g_M(q^2)\frac{\boldsymbol{\sigma}\times\boldsymbol{q}}{2m_N} - g_P(q^2)\frac{\boldsymbol{\sigma}\cdot\boldsymbol{q}}{2m_N}\boldsymbol{q}\right]$$

Closure approximation

The closure approximation consist in taking $E_N - \frac{E_i + E_f}{2} \approx E_C$ for every intermediate state, allowing to factor out the energy denominator:

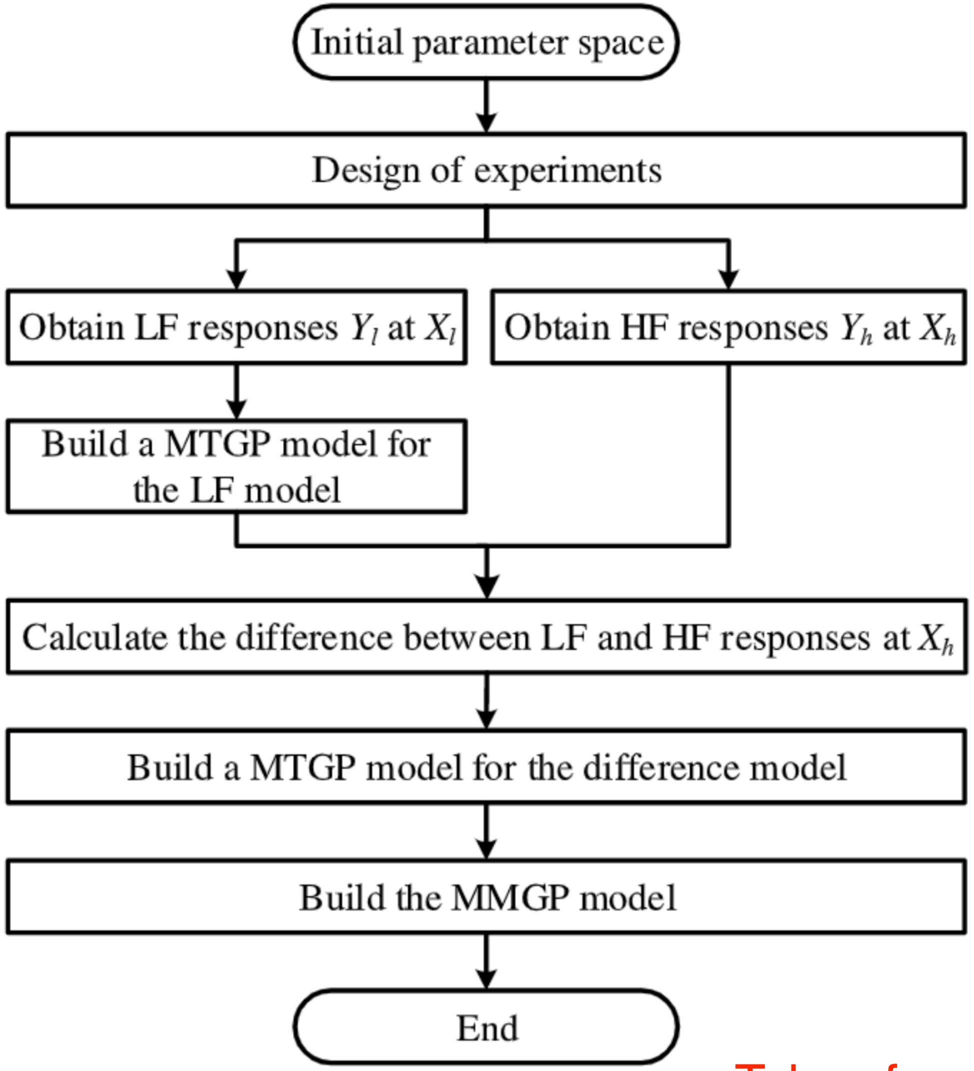
$$O(\boldsymbol{q}) = \frac{R_{Nucl}}{2\pi^2 g_a^2} \sum_N \frac{J^\mu(\boldsymbol{q})\,|N\rangle\langle N|\,J_\mu(-\boldsymbol{q})}{q\left(q + E_N - \frac{E_i + E_f}{2}\right)} \rightarrow \frac{R_{Nucl}}{2\pi^2 g_a^2} \frac{1}{q\left(q + E_C\right)} J^\mu(\boldsymbol{q}) J_\mu(-\boldsymbol{q})$$

Taking the product of the currents then allows to obtain the usual GT, F and T part.

Usual test of the closure approximation, reintroduce the dependance in the denominator and do the summation over the intermediate states but still consider a two-body scalar operator rather than the product of 2 vector currents.

Using Gaussian Process as an emulator

- Multi-tasks Multi-Fidelity Gaussian Process (MMGP) proposed in [1] 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 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). 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].

[1] Q. Lin, J. Hu, Q. Zhou, Y. Cheng, Z. Hu, I. Couckuyt, and T. Dhaene, Knowledge-Based Systems 227, 107151 (2021).