Neutrinoless double-beta decay matrix elements (NME) with *ab initio* interaction in large shell-model spaces

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Super-Kamiokande had proved that Neutrinos have masses

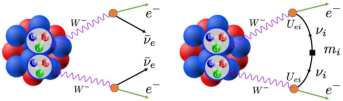
Undetected heavy mass right-hand neutrinos

Dirac fermion

Or

Majorana fermion

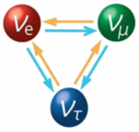
$$\nu_e = \bar{\nu}_e$$



$2\nu\beta\beta$: observed **$0\nu\beta\beta$: not yet**

The importance of NME in $0\nu\beta\beta$ decay

Neutrino oscillation experiments

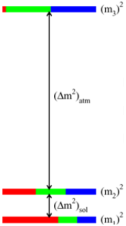


$$\triangle m^2_{sol} \simeq 75 meV^2$$

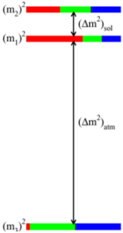
$$\triangle m^2_{atm} \simeq 2400 meV^2$$

$0\nu\beta\beta$ can help us since

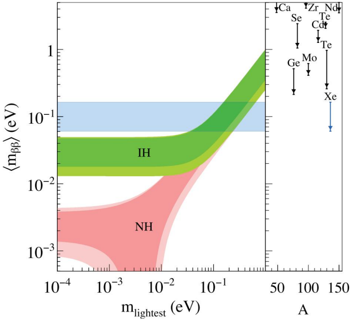
$$[T^{0\nu}_{1/2}]^{-1} = G_{0\nu}(Q, Z)|M_{0\nu}|^2\langle m_{\beta\beta}\rangle^2$$



normal

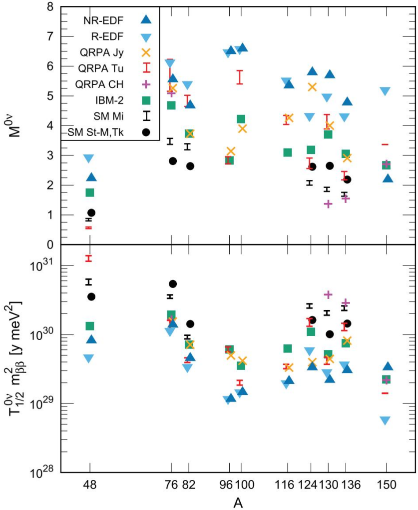


inverted



J. Engel et. al., Rep. Prog. Phys. 80 046301 (2017)

Uncertainty of NME

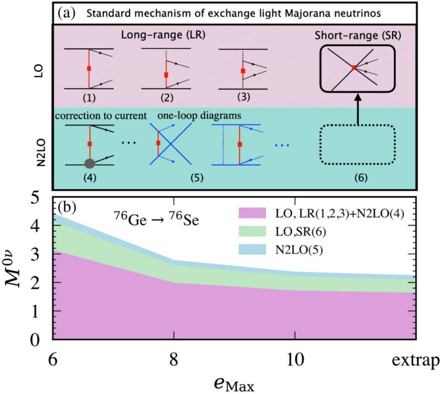


J. Engel et. al., Rep. Prog. Phys. 80 046301 (2017)

$$M^{0\nu} = M^{0\nu}_{GT} - \frac{g_V^2}{g_A^2} M^{0\nu}_F + M^{0\nu}_T + M^{0\nu}_{CT}$$

- ⋆ NME values vary significantly across different nuclear models.
- ⋆ Most of these calculations are phenomenological and have limited predictive power.

Uncertainty of NME



J. M. Yao, A. Belley et. al., PRL. 132, 182502 (2024)

⋆ Nuclear forces have a significant impact on NME results, while phenomenological approaches do not provide reliable uncertainty estimates.

To overcome these limitations, we aim to calculate the NME from first principles, without fitting on nuclear scattering data.

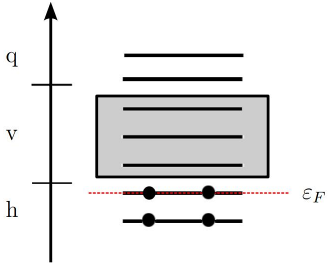
⋆ Effective interactions are derived from chiral effective field theory (χEFT) using a non-perturbative *ab initio* approach, without fitting to finite-nucleus properties.

⋆ Several approximate many-body methods have been developed, such as CC, SCGF, and the in-medium similarity renormalization group (IMSRG).

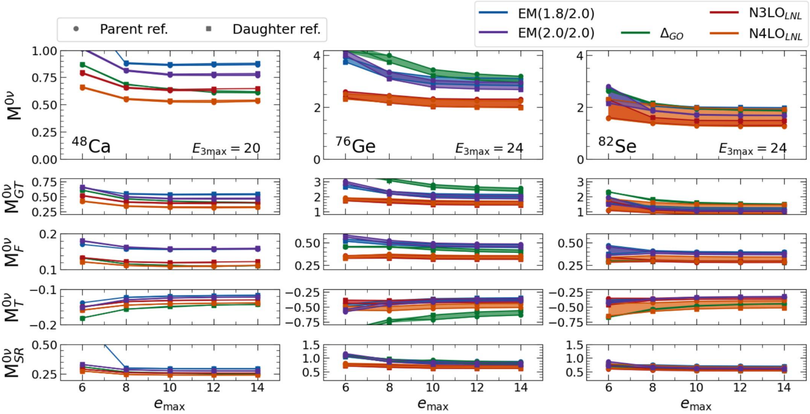
IMSRG

↓ reduce computational cost

valence-space (VS) IMSRG



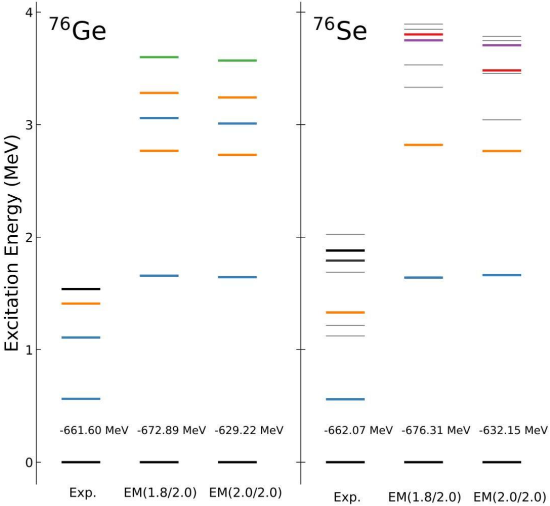
limitation of VS-IMSRG



Antoine Belley, PhD thesis, University of British Columbia, 2024

Standard VS-IMSRG always limits in a major shell, it could not calculate NMEs of ^{96}Zr, ^{100}Mo and ^{150}Nd.

limitation of VS-IMSRG



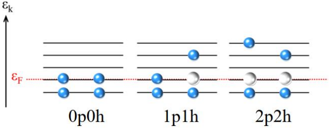
A single major shell unable to capture the cross-shell excitation, fail to reproduce the energy spectra.

J. M. Yao, A. Belley et. al., PRL. 132, 182502 (2024)

Combined with Projected generator coordinate method (PGCM)

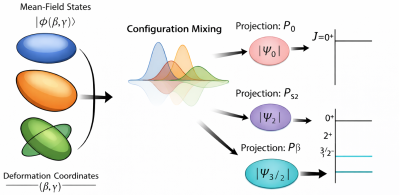
Standard VS-IMSRG

- ⋆ Decoupled to a single major shell, fail to capture quadrupole collectivity driven by cross-shell particle–hole excitations.
- ⋆ Exact diagonalization in the multishell via interacting shell model is computationally prohibitive.

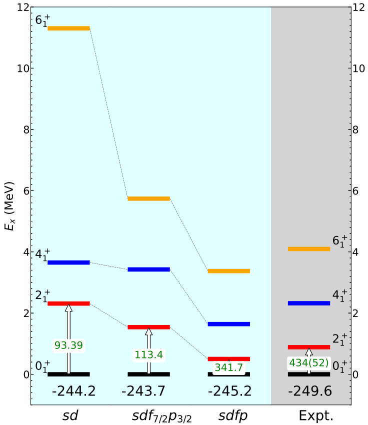


VS-IMSRG + PGCM (VS-IM-GCM)

- ⋆ PGCM makes calculations in large model spaces computationally feasible.
- ⋆ VS-IM-GCM provides us with an opportunity for *ab initio* studies on the heavier open-shell nuclei.



Example of ^{32}Mg



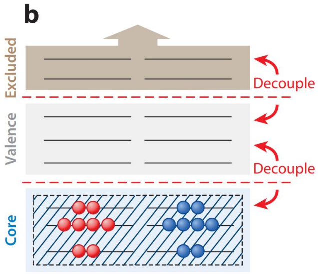
^{32}Mg low-lying spectra in *sd*, $sdf_{7/2}p_{3/2}$, *sdfp* spaces vs. experiment; arrows show reduced electric quadrupole transition probability ($B(E2; 0_1^+ \to 2_1^+)$) ($e^2\text{fm}^4$)

X.C. Cao, C. F. Jiao PLB 871, 140034 (2025)

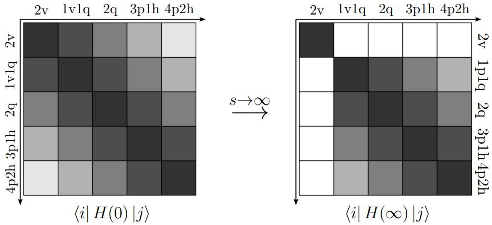
- ⋆ The excitation energy of the first 2^+ state in ^{32}Mg is significantly lowered when expanding the model space from *sd* to $sdf_{7/2}p_{3/2}$ and *sdfp*, indicating the importance of cross-shell excitations.
- ⋆ Calculated $B(E2)$ values are improved as the model space expands.

Starting from the chiral NN+3N forces, we evolve the Hamiltonian using the flow equation:

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



S.R. Stroberg et. al., Annu. Rev. Nucl. Part. Sci. 69, 307 (2019)



H Hergert et. al., Phys. Scr. 92, 023002 (2017)

Hamiltonian, which depends on the flow parameter s, is expressed in normal ordering (NO) form:

$$H(s) = E_0 + \sum_{ab} f_{ab}(s)\{a_a^\dagger a_b\} + \frac{1}{4}\sum_{abcd}\Gamma_{abcd}(s)\{a_a^\dagger a_b^\dagger a_d a_c\}$$

The anti-Hermitian operator $\eta(s)$ is the so-called generator written as

$$\eta = \sum_{ai}\eta_{ai}\{a_a^\dagger a_i\} + \sum_{abij}\eta_{abij}\{a_a^\dagger a_b^\dagger a_j a_i\} - H.c.$$

the generator is defined as:

$$\begin{aligned}
\eta_{ai} &= \frac{1}{2}\arctan\left(\frac{2f_{ai}}{f_{aa} - f_{ii} + \Gamma_{aiai} + \Delta}\right), \\
\eta_{abij} &= \frac{1}{2}\arctan\left(\frac{2\Gamma_{abij}}{f_{aa} + f_{bb} - f_{ii} - f_{jj} + G_{abij} + \Delta}\right), \\
G_{abij} &= \Gamma_{abab} + \Gamma_{ijij} - \left(\Gamma_{aiai} + \Gamma_{bjbj} + [a \leftrightarrow b]\right).
\end{aligned}$$

Magnus expansion

$$\hat{H}_{eff} = e^{\Omega}\hat{H}_0 e^{-\Omega} = \sum_{k=0}^{\infty} \frac{1}{k!} ad_{\Omega}^{k}(\hat{H}_0) \tag{1}$$

$$ad_{\Omega}^{k}(\hat{H}_0) = [\underbrace{\Omega, [\Omega, [\cdots [\Omega}_{k \text{ times}}, \hat{H}_0]] \cdots]] \tag{2}$$

$$\frac{d\Omega}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!} ad_{\Omega}^{k}(\eta(s)) \tag{3}$$

Starting from an initial generator $\eta(0)$, we choose a small flow parameter s and obtain $\Omega(0)$ using Eq. 3. The effective Hamiltonian $\hat{H}_{\mathrm{eff}}(s)$ is then constructed using Eqs. 2 and 1. This procedure is repeated iteratively until the Hamiltonian is fully decoupled.

VS-IMSRG operator transformation

An arbitrary spherical tensor operator can be written as

$$\hat{\mathcal{O}}^{\lambda}_{\mu} = O^{\lambda}_{0b} + \sum_{pq} O^{\lambda}_{pq} \frac{[a^{\dagger}_{p}\tilde{a}_{q}]^{\lambda}_{\mu}}{\sqrt{2\lambda+1}} + \frac{1}{4}\sum_{pqrs} O^{(J_1 J_2)\lambda}_{pqrs} \frac{[[a^{\dagger}_{p}a^{\dagger}_{q}]^{J_1}[\tilde{a}_{s}\tilde{a}_{r}]^{J_2}]^{\lambda}_{\mu}}{\sqrt{2\lambda+1}}$$

The operator can be transformed consistently with the Hamiltonian by using the same VS-IMSRG transformation:

$$\hat{O}_{eff} = e^{\Omega}\hat{\mathcal{O}}^{\lambda}e^{-\Omega}$$

In the transformation of NMEs, we using the Omega derived from the VS-IMSRG transformation for either the parent nuclei or the daughter nuclei.

Projected generator coordinate method (PGCM)

We assume that the many-body wave function can be expressed as a superposition of the angular-momentum and particle-number projected reference states constrained to various amounts of expectation values for collective operators, such as axial deformation, triaxial deformation, and isoscalar pairing.

$$|\Psi^J_{NZ\sigma}\rangle = \sum_{K,q} f^{JK}_{q,\sigma} |JMK; NZ; q\rangle$$

where $|JMK; NZ; q\rangle \equiv \hat{P}^J_{MK} \hat{P}^N \hat{P}^Z |\varphi(q)\rangle$,and q is short for the set of all expectation values.The $\hat{P}$'s are angular-momentum and particle-number projection operators:

$$\begin{aligned} \hat{P}^J_{MK} &= \frac{2J+1}{8\pi^2} \int D^{J*}_{MK}(\Omega) R(\Omega) d\Omega \\ \hat{P}^{A_0} &= \frac{1}{\pi} \int_0^\pi d\varphi e^{i\varphi(\hat{A}-A_0)} \end{aligned}$$

Projected generator coordinate method (PGCM)

Starting from the variational principle of Ritz, we derive the Hill–Wheeler equation, whose solution allows us to evaluate the fluctuations of collectivity:

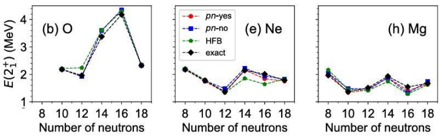
$$\sum_{K',q'} [\mathcal{H}^J_{KK'}(q,q') - E^J_\sigma \mathcal{N}^J_{KK'}(q,q')] f^{JK'}_{q',\sigma} = 0$$

where

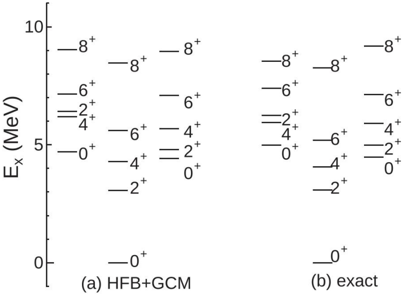
$$\begin{aligned}
\mathcal{H}^J_{KK'}(q,q') &= \langle \varphi(q) | H_{eff} \hat{P}^J_{KK'} \hat{P}^N \hat{P}^Z | \varphi(q') \rangle \\
\mathcal{N}^J_{KK'}(q;q') &= \langle \varphi(q) | \hat{P}^J_{KK'} \hat{P}^N \hat{P}^Z | \varphi(q') \rangle
\end{aligned}$$

After solving the Hill–Wheeler equation, we can obtain the expectation of any operators.

PGCM compared to shell model



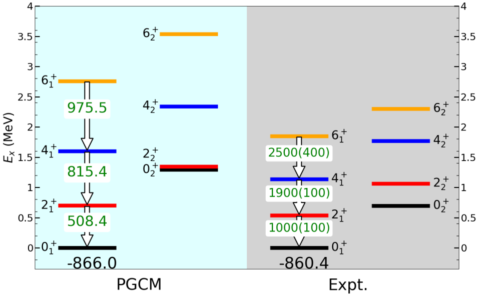
Phys. Rev. C 104,054306 (2021)



Phys. Rev. C 103, 064302 (2021)

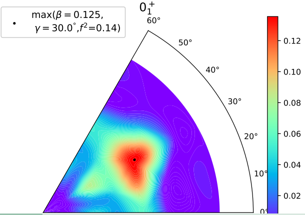
PGCM provides a good approximation to the shell model.

VS-IM-GCM results using EM(1.8/2.0) interaction

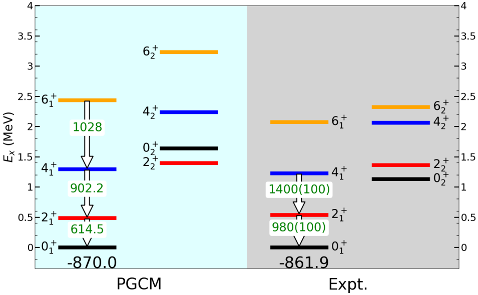


Experimental and calculated spectra of ^{100}Mo

Our calculated spectra are in good agreement with experimental data. The collective wavefuntion of ground state and 2_1^+ state are both triaxially deformed.

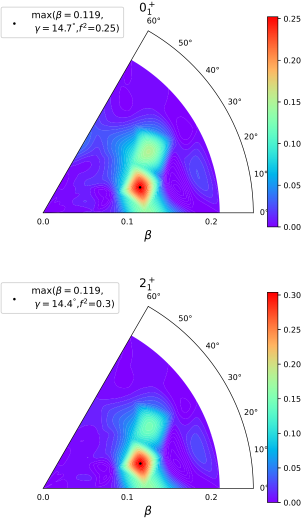


VS-IM-GCM results using EM(1.8/2.0) interaction



Experimental and calculated spectra of ^{100}Ru

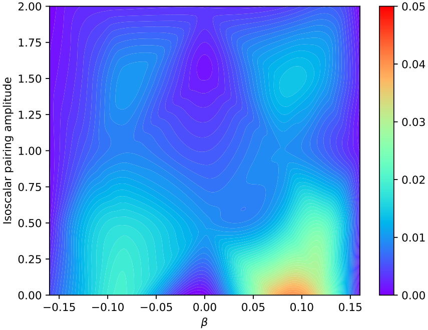
Our calculated energy levels are in good agreement with experimental data. The collective wavefuntion indicates ground state exists shape mixing.



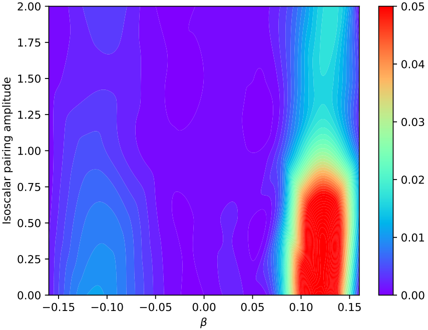
VS-IM-GCM results using EM(1.8/2.0) interaction

While calculating NME, the influence of the isoscalar pairing (ISP) can't be ignored. Here are the collective wave function as function of deformation β and ISP amplitude.

^{100}Mo



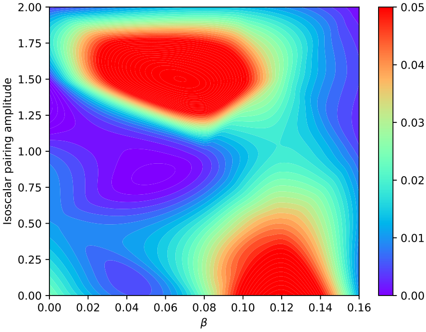
^{100}Ru



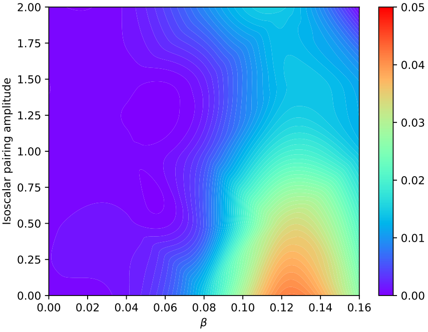
VS-IM-GCM results using EM(1.8/2.0) interaction

Since these two nuclei are both triaxial deformed, here are the collective wave function as function of deformation β in $\gamma = 30^\circ$ and ISP amplitude.

^{100}Mo



^{100}Ru



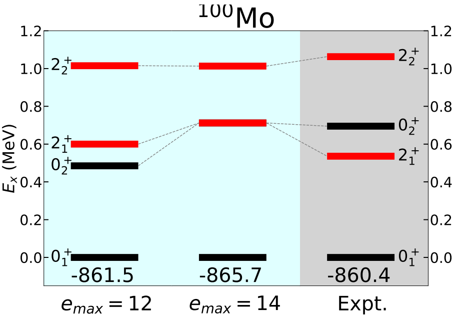
VS-IM-GCM results using EM(1.8/2.0) interaction

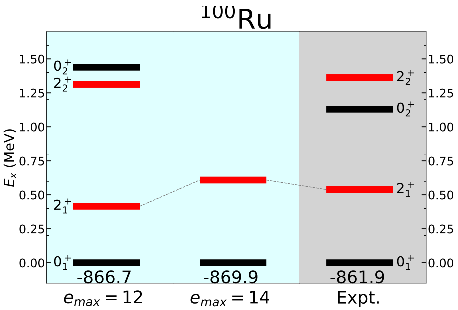
Calculated values of $M^{0\nu}$ for the decay of the ^{100}Mo ground state to ^{100}Ru ground state compared with other calculations.

	$M^{0\nu}_{GT}$	$M^{0\nu}_{F}$	$M^{0\nu}_{T}$	$M^{0\nu}_{CT}$	$M^{0\nu}$
triaxial w/o ISP	1.254(30)	-1.246(4)	-0.291(8)	1.004(17)	2.735(20)
axial w/o ISP	1.492(9)	-1.59(1)	-0.341(11)	1.117(20)	3.25(2)
triaxial w/ ISP	0.86(3)	$-1.31(1)$	$-0.31(1)$	1.03(5)	2.38(1)
SM (bare)	3.418	-0.878	0.002		3.962
SM (effective)	1.634	-0.970	0.007		2.240
IBM-2	3.73	-0.48	0.19		4.22
EDF	5.361	-1.986			6.588
BMF-CDFT					5.08
pnQRPA	4.950	-2.367	-0.571		5.850
pnQRPA	3.13	-1.03	-0.26		3.90

VS-IM-GCM results using $\triangle$N2LO$_{GO}$ (394) interaction

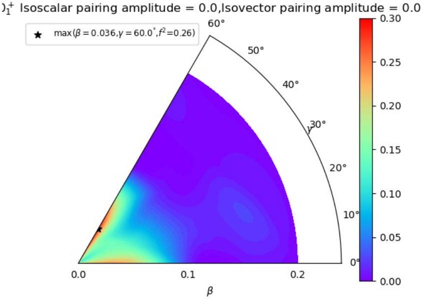
The results here don't include isoscalar pairing yet.



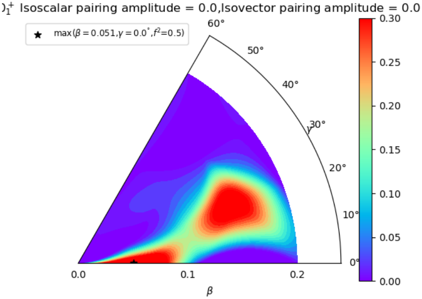


	$M_{GT}^{0\nu}$	$M_F^{0\nu}$	$M_T^{0\nu}$	$M_{CT}^{0\nu}$	$M^{0\nu}$
$e_{max} = 12$	0.353(30)	-0.537(9)	-0.379(5)	0.506(6)	0.817(36)
$e_{max} = 14$	0.335(9)	-0.099(3)	-0.096(2)	0.353(4)	0.653(12)

The collective wavefunction of ground state of ^{100}Mo and ^{100}Ru of $e_{max} = 14$.



^{100}Mo



^{100}Ru

The parent nucleus is close to a spherical shape, while the daughter nucleus exhibits shape mixing between triaxial and prolate deformations.

Summary

- ⋆ For the first time, we perform the *ab initio* calculations for the NME of ^{100}Mo $\rightarrow^{100}$ Ru $0\nu\beta\beta$ decay.
- ⋆ Both ^{100}Mo and ^{100}Ru are triaxially deformed nuclei, and the triaxial deformation effect impacts the NME by about 15%.
- ⋆ Isoscalar pairing significantly affects the Gamow–Teller term, but has little impact on other components.

Thank you for your attention!