Recent progress in the nuclear matrix element calculation using the finite-amplitude method for QRPA

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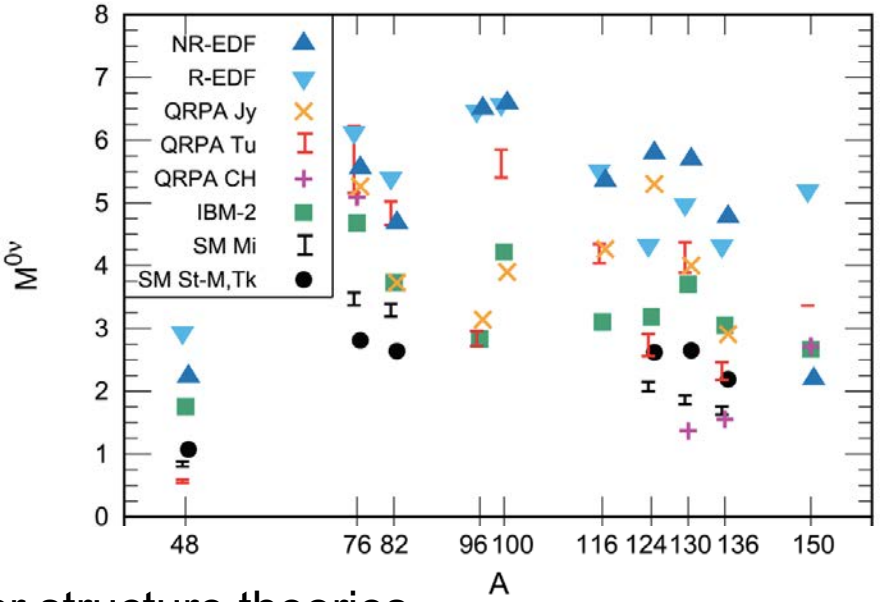
Nuclear matrix element and QRPA

$$(T_{1/2}^{0\nu})^{-1} = G_{0\nu}(Q_{\beta\beta}, Z)|M_{0\nu}|^2\langle m_{\beta\beta}\rangle^2$$

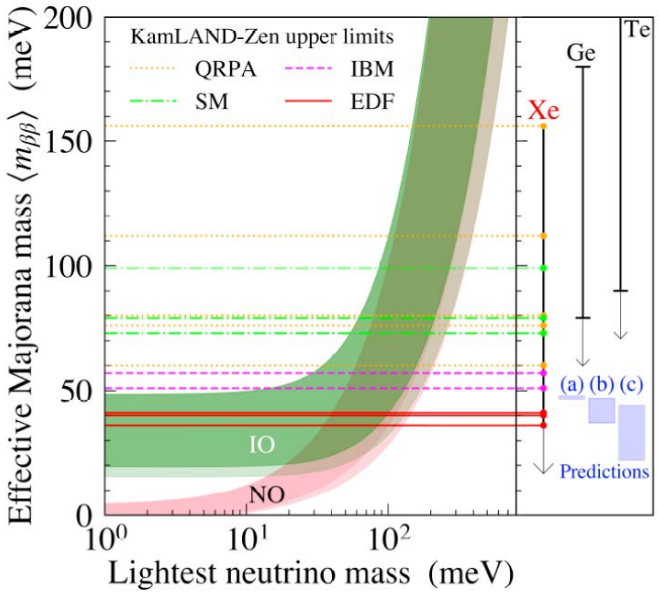


nuclear structure theories

NR/R EDF: generator coordinate method
QRPA:quasiparticle random-phase approx.
IBM2:interacting boson model
SM: shell model

Engel and Menéndez, Rep. Prog. Phys. **80**, 046301 (2017)

KamLAND-Zen(^{136}Xe)
$T_{1/2}^{0\nu} > 2.3 \times 10^{26}$ y



Abe et al., Phys. Rev. Lett. **130**. 051801 (2023)

a factor of 2-3 deviation

Quasiparticle random-phase approximation (QRPA)

QRPA: Microscopic theory for excited states of nuclei based on the nuclear DFT

QRPA equation (non-Hermitian eigenvalue problem)

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^i \\ Y^i \end{pmatrix} = \Omega_i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^i \\ Y^i \end{pmatrix}$$

A: Hermitian matrix
B: symmetric matrix
Ω: excitation energy
(X,Y): wave functions

dimension: 10^5-10^6 full diagonalization is computationally demanding

Physics applications: giant resonances – nuclear matter properties
low-energy vibrational collective excitation
beta decay (eigenvalues below Q value)
double-beta decay (contribution with a ~1/|Ω| factor)
fission inertia (inertia for collective motion)
moment of inertia/ pairing rotational inertia

Solutions of QRPA:

basis reduction: truncation in the two-quasiparticle space (standard)
Lanczos method (Johnson, et al. Comp. Phys. Commun. **120**, 155 (1999)
iterative Arnoldi method (Toivanen et al. Phys. Rev. C **81**, 034312 (2010))

iteration: **finite-amplitude method** (Nakatsukasa et al., Phys. Rev. C **76**, 024318 (2007))

2vββ NME within pnQRPA

$$[T^{2\nu}_{1/2}]^{-1} = G_{2\nu}(Q_{\beta\beta}, Z)\,|M^{2\nu}|^2$$

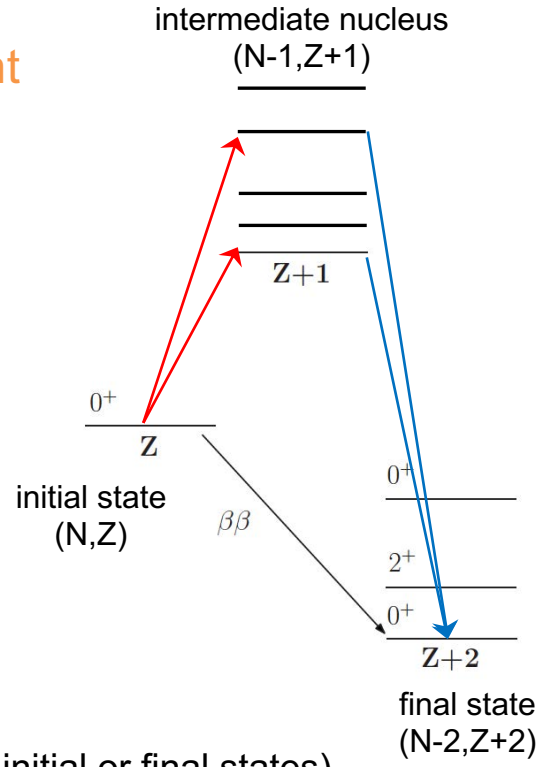
phase space factor

nuclear matrix element

$$M^{2\nu} = M^{2\nu}_{\mathrm{GT}} - \frac{g_V^2}{g_A^2} M^{2\nu}_{\mathrm{F}} \approx M^{2\nu}_{\mathrm{GT}}$$

$$M^{2\nu}_{\mathrm{GT}} = \sum_n \frac{\langle 0^+_f | \sum_a \boldsymbol{\sigma}_a \tau^-_a | n\rangle \cdot \langle n | \sum_b \boldsymbol{\sigma}_b \tau^-_b | 0^+_i\rangle}{E_n - \frac{M_i + M_f}{2}}$$

$$M^{2\nu}_{\mathrm{GT}} = \sum_{n_i n_f} \frac{\langle 0^+_f | \sum_a \boldsymbol{\sigma}_a \tau^-_a | n_f\rangle \langle n_f | n_i\rangle \langle n_i | \sum_b \boldsymbol{\sigma}_b \tau^-_b | 0^+_i\rangle}{E_n - \frac{M_i + M_f}{2}}$$



All $J^\pi=1^+$ states in the intermediate states are required

($J^\pi=1^+$ (or $K^\pi=0,1^+$ when deformed) excited states from the initial or final states)

single Gamow-Teller matrix element <n|σT|0> have strong correlation with:

spin-isospin interaction (g_{ph}) and isoscalar spin-triplet pairing interaction (g_{pp})

g_{pp} is often fitted to 2vββ half-life: Impossible to predict 2vββ/ECEC half-life

Globally fitted g_{ph} and g_{pp}

g_{ph} and g_{pp} in nuclear EDF

Mustonen and Engel, Phys. Rev. C **93**, 014304 (2016)

g_{ph} : isovector time-odd EDF

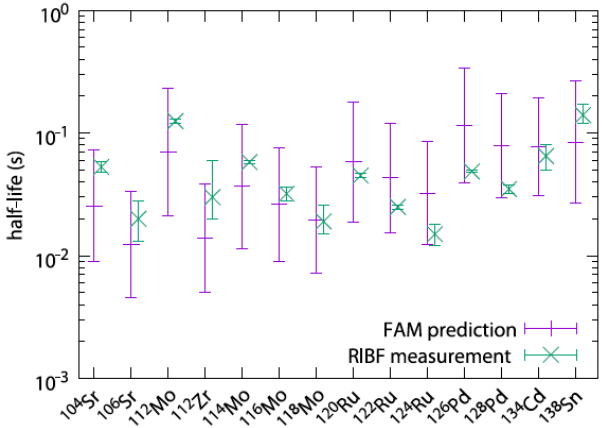
$$\chi_1^{\mathrm{odd}}(\boldsymbol{r}) = C_1^s[\rho_0]\boldsymbol{s}_1^2 + C_1^{\Delta s}\boldsymbol{s}_1 \cdot \Delta\boldsymbol{s}_1 + C_1^j\boldsymbol{j}_1^2 + C_1^T\boldsymbol{s}_1 \cdot \boldsymbol{T}_1 + C_1^{\nabla j}\boldsymbol{s}_1 \cdot \boldsymbol{\nabla} \times \boldsymbol{j}_1 + C_1^F\boldsymbol{s}_1 \cdot \boldsymbol{F}_1 + C_1^{\nabla s}(\boldsymbol{\nabla} \cdot \boldsymbol{s}_1)^2,$$

g_{pp}: mixed-type isoscalar pairing

$$V_{\mathrm{pp}} = (V_0\hat{\Pi}_{T=0} + V_1\hat{\Pi}_{T=1})\left[1 - \alpha\frac{\rho_{00}(\mathbf{r})}{\rho_c}\right]\delta(\mathbf{r})$$

Experimental data used for fitting

Set	GT resonances	SD resonances	β-decay half-lives
A	^{208}Pb, ^{112}Sn, ^{76}Ge, ^{130}Te, ^{90}Zr, ^{48}Ca	None	^{48}Ar, ^{60}Cr, ^{72}Ni, ^{82}Zn, ^{92}Kr, ^{102}Sr, ^{114}Ru, ^{126}Cd, ^{134}Sn, ^{148}Ba
B	Same as A	None	^{52}Ti, ^{74}Zn, ^{92}Sr, ^{114}Pd, ^{134}Te, ^{156}Sm, ^{180}Yb, ^{200}Pt, ^{226}Rn, ^{242}U
C	Same as A	None	^{52}Ti, ^{72}Ni, ^{92}Sr, ^{114}Ru, ^{134}Te, ^{156}Nd, ^{180}Yb, ^{204}Pt, ^{226}Rn, ^{242}U
D	Those of A and ^{150}Nd	None	^{58}Ti, ^{78}Zn, ^{98}Kr, ^{126}Cd, ^{152}Ce, ^{166}Gd, ^{204}Pt
E	Same as D	^{90}Zr, ^{208}Pb	^{58}Ti, ^{78}Zn, ^{98}Kr, ^{126}Cd, ^{152}Ce, ^{166}Gd, ^{226}Rn



10 parameters in proton-neutron channel (ph and pp)
based on Skyrme SkO' and SV-min
fitted to β decay half-life, Gamow-Teller and spin-dipole resonance energies
→ prediction of 2νββ NME is possible

Globally fitted g_{ph} and g_{pp}

g_{ph} and g_{pp} in nuclear EDF

$$\chi_1^{\text{odd}}(\boldsymbol{r}) = C_1^s[\rho_0]\boldsymbol{s}_1^2 + C_1^{\Delta s}\boldsymbol{s}_1 \cdot \Delta\boldsymbol{s}_1 + C_1^j \boldsymbol{j}_1^2 + C_1^T \boldsymbol{s}_1 \cdot \boldsymbol{T}_1 + C_1^{\nabla j}\boldsymbol{s}_1 \cdot \boldsymbol{\nabla} \times \boldsymbol{j}_1 + C_1^F \boldsymbol{s}_1 \cdot \boldsymbol{F}_1 + C_1^{\nabla s}(\boldsymbol{\nabla} \cdot \boldsymbol{s}_1)^2,$$

Mustonen and Engel, Phys. Rev. C **93**, 014304 (2016)

$$V_{\text{pp}} = (V_0 \hat{\Pi}_{T=0} + V_1 \hat{\Pi}_{T=1})\left[1 - \alpha \frac{\rho_{00}(\mathbf{r})}{\rho_c}\right]\delta(\mathbf{r})$$

TABLE III. The Jacobian matrix, evaluated at the result of the two-parameter fit 1E. All parameters except for the strength of isoscalar pairing are expressed in natural units. The strength of isoscalar pairing has been scaled by the strength of isovector pairing. The derivatives of the $\log_{10} t$ values are hence dimensionless and those of the resonance energies are in the units of MeV.

$\mathcal{O}$	$d\mathcal{O}/dC_1^s$	$d\mathcal{O}/dV_0$	$d\mathcal{O}/dC_1^F$	$d\mathcal{O}/dC_1^T$	$d\mathcal{O}/dC_1^{\nabla s}$	$d\mathcal{O}/dC_1^{\Delta s}$	$d\mathcal{O}/dC_1^j$	$d\mathcal{O}/dC_1^{\nabla j}$
^{208}Pb E_{GTR}	57.261	−0.000	2.434	5.869	0.429	−1.002	0.000	0.143
^{112}Sn E_{GTR}	29.498	−1.032	1.432	2.863	0.286	−0.573	0.000	0.000
^{76}Ge E_{GTR}	45.115	−7.225	2.004	4.295	0.429	−1.145	0.000	0.000
^{130}Te E_{GTR}	53.790	−3.096	2.434	5.297	0.429	−1.002	0.143	0.000
^{90}Zr E_{GTR}	29.498	−1.032	1.288	2.720	0.429	−1.002	−0.143	0.143
^{48}Ca E_{GTR}	32.968	−0.000	1.432	3.149	0.573	−1.288	0.000	0.000
^{208}Pb E_{SDR}	52.055	−0.000	2.291	4.008	0.286	−1.575	−0.143	−0.143
^{90}Zr E_{SDR}	29.498	−0.000	1.575	2.004	0.286	−1.432	−0.286	−0.143
^{58}Ti $\log_{10} t$	4.749	−4.318	0.203	0.445	0.045	−0.109	−0.011	−0.002
^{78}Zn $\log_{10} t$	6.889	−2.922	0.256	0.589	0.164	−0.382	0.253	−0.025
^{98}Kr $\log_{10} t$	5.410	−3.252	0.265	0.559	0.050	−0.116	−0.012	−0.003
^{126}Cd $\log_{10} t$	5.583	−4.641	0.252	0.496	0.017	−0.050	0.001	0.007
^{152}Ce $\log_{10} t$	5.409	−2.474	0.293	0.540	0.051	−0.120	0.003	−0.009
^{166}Gd $\log_{10} t$	5.081	−2.924	0.250	0.497	0.035	−0.132	−0.007	−0.010
^{204}Pt $\log_{10} t$	3.755	−3.340	−0.015	0.160	−0.018	−0.316	−0.076	0.026

isoscalar pairing strength (g_{pp}~V_0) is well constrained by the data set

Finite amplitude method (FAM)

original QRPA eigenvalue problem

Nakatsukasa et al., Phys. Rev. C **76**, 024318 (2007)
Avogadro and Nakatsukasa, Phys. Rev. C **84**, 014314 (2011)

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^i \\ Y^i \end{pmatrix} = \Omega_i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^i \\ Y^i \end{pmatrix}$$

large-dimensional eigenvalue problem: model space truncation necessary

finite-amplitude method (iterative solution)

Linear response theory: QRPA under an external field F with a complex energy ω

$$\left[\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] \begin{pmatrix} X(\omega) \\ Y(\omega) \end{pmatrix} = - \begin{pmatrix} F^{20} \\ F^{02} \end{pmatrix}$$

external field

X(ω, F) and Y(ω, F) can be computed efficiently without truncation
FAM solves the linear equation of X and Y by iteration
FAM computes AX+BY and B*X+A*Y without computing A and B explicitly
it avoids explicit calculation of A and B matrices

Relation between the FAM XY and QRPA XY (eigenvectors)

$$X_{\mu\nu}(\omega, \hat{F}) = -\sum_i \left\{ \frac{X^i_{\mu\nu} \langle i|\hat{F}|0\rangle}{\Omega_i - \omega} + \frac{Y^{i*}_{\mu\nu} \langle 0|\hat{F}|i\rangle}{\Omega_i + \omega} \right\}$$

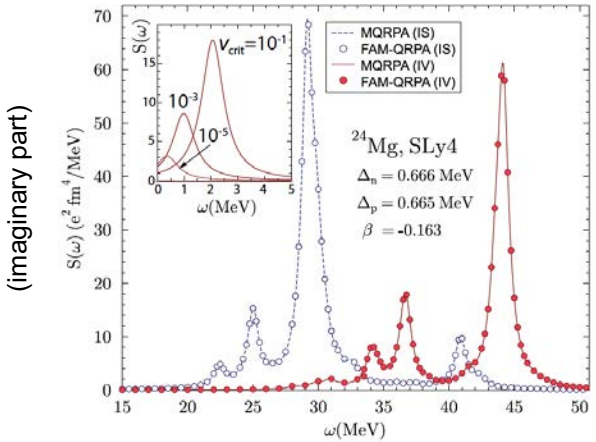
$$Y_{\mu\nu}(\omega, \hat{F}) = -\sum_i \left\{ \frac{Y^i_{\mu\nu} \langle i|\hat{F}|0\rangle}{\Omega_i - \omega} + \frac{X^{i*}_{\mu\nu} \langle 0|\hat{F}|i\rangle}{\Omega_i + \omega} \right\}$$

Finite amplitude method (FAM)

Strength function

$$S(\hat{F},\omega) = \sum_{\mu<\nu} F^{20}_{\mu\nu} X_{\mu\nu}(\omega) + F^{02}_{\mu\nu} Y_{\mu\nu}(\omega)$$

$$-\frac{1}{\pi}\mathrm{Im}\, S(\hat{F},\omega+i\gamma) = \frac{\gamma}{\pi}\sum_i \left[\frac{|\langle i|\hat{F}|0\rangle|^2}{(\omega-\Omega_i)^2+\gamma^2} - \frac{|\langle i|\hat{F}^\dagger|0\rangle|^2}{(\omega+\Omega_i)^2+\gamma^2}\right]$$

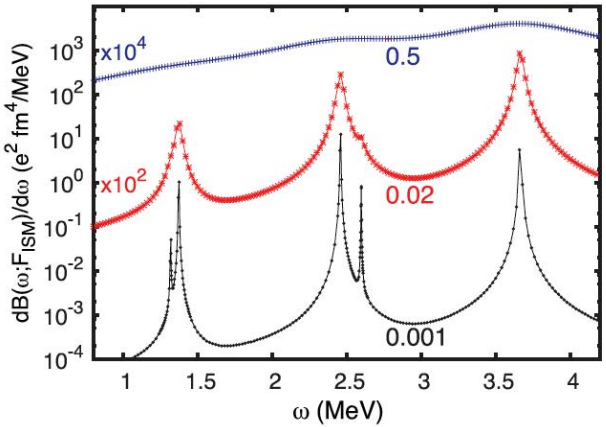


Stoitsov et al., Phys. Rev. C **84**, 04135(R) (2011)

Eigenvalues/Eigenvectors

FAM amplitudes has a first-order pole at QRPA energies(Ω_i)

$$\frac{1}{2\pi i}\oint_{C_i} X_{\mu\nu}(\omega)d\omega = e^{i\theta}|\langle i|\hat{F}|0\rangle|X^i_{\mu\nu}$$



NH, Kortelainen, Nazarewicz, Phys. Rev. C **87**, 064309 (2013)

FAM for 2νββ NME

NH and Engel, Phys. Rev. C **105**, 044314 (2022)

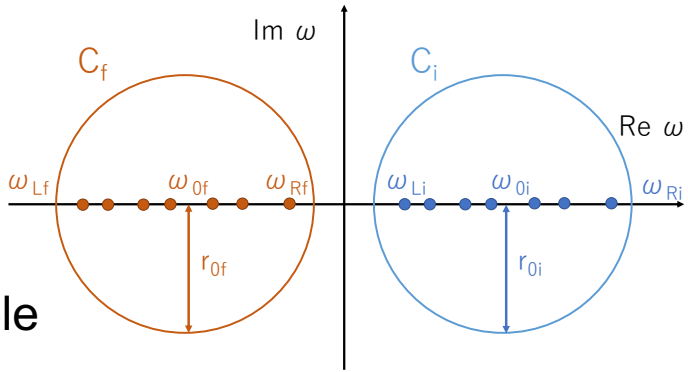
$$X_{\mu\nu}(\omega,\hat{F}) = -\sum_i \left\{ \frac{X^i_{\mu\nu}\langle i|\hat{F}|0\rangle}{\Omega_i-\omega} + \frac{Y^{i*}_{\mu\nu}\langle 0|\hat{F}|i\rangle}{\Omega_i+\omega} \right\} \qquad Y_{\mu\nu}(\omega,\hat{F}) = -\sum_i \left\{ \frac{Y^i_{\mu\nu}\langle i|\hat{F}|0\rangle}{\Omega_i-\omega} + \frac{X^{i*}_{\mu\nu}\langle 0|\hat{F}|i\rangle}{\Omega_i+\omega} \right\}$$

$$\mathcal{T}(\omega_i,\omega_f) = \sum_K (-1)^K \sum_{pn} \left[\bar{Y}^{(f)}_{pn}(\omega_f,\hat{F}^{\mathrm{GT}-}_{-K}) \bar{X}^{(i)}_{pn}(\omega_i,\hat{F}^{\mathrm{GT}-}_{K}) - \alpha \bar{X}^{(f)}_{pn}(\omega_f,\hat{F}^{\mathrm{GT}-}_{-K}) \bar{Y}^{(i)}_{pn}(\omega_i,\hat{F}^{\mathrm{GT}-}_{K}) \right]$$

FAM from final state FAM from initial state

(Ybar, Xbar includes part of overlap matrix between initial and final HFB states)

$$M^{2\nu}_{\mathrm{GT}} = \left(\frac{1}{2\pi i}\right)^2 \oint_{C_i} d\omega_i \oint_{C_f} d\omega_f \frac{2\mathcal{T}(\omega_i,\omega_f)}{\omega_i-\omega_f}$$



double contour integration
initial state: στ- external field
final state: στ- external field (take the backward part)
FAM calculation with different ω and F are parallelizable
α controls the overlap (α=0 QTDA, α=1 QRPA)

Fermi and Gamow-Teller sum rule

NH and Engel, Phys. Rev. C **105**, 044314 (2022)

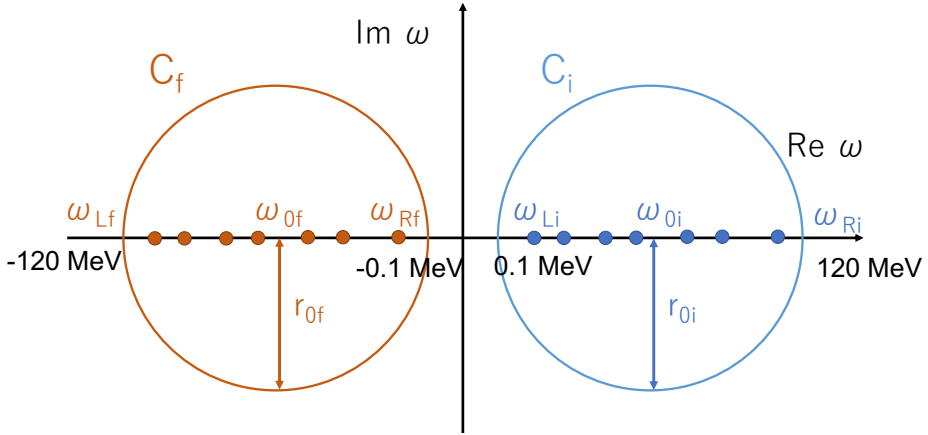
- initial=final and setting the final state FAM external field to (σ)τ+, without denominator provides sum rule
- pnFAM(HFBTHO) Mustonen et al., Phys. Rev. C **90**, 024308 (2014)
- SkM*+Volume pairing, Nsh=20, integration up to 120 MeV

$$|\langle n_i|\sum_a \sigma_a^K \tau_a^-|0^+_{\rm gs}\rangle|^2 = \langle 0^+_{\rm gs}|\sum_b \sigma_b^{-K}\tau_b^+|n_i\rangle\langle n_i|\sum_a \sigma_a^K\tau_a^-|0^+_{\rm gs}\rangle$$

	$\frac{m(\mathrm{F}-)-m(\mathrm{F}+)}{N-Z}$	$\frac{m(\mathrm{GT}-)-m(\mathrm{GT}+)}{3(N-Z)}$
^{76}Ge	0.9995	0.9992
^{76}Se	0.9994	0.9992
^{130}Te	0.9996	0.9993
^{130}Xe	0.9996	0.9993
^{136}Xe	0.9998	0.9997
^{136}Ba	0.9996	0.9994
^{150}Nd	0.9996	0.9994
^{150}Sm	0.9996	0.9995

Discretization of the contour integration

double integration along the contours C_i and C_f

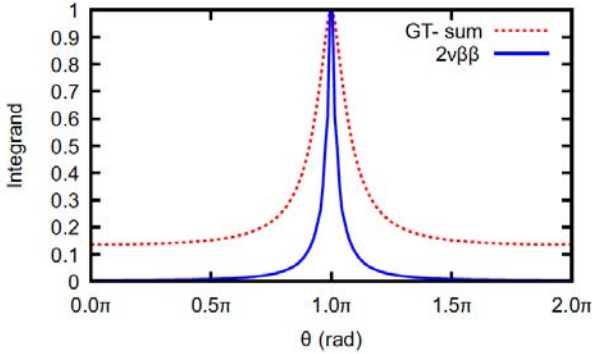


main contribution is from around ω_{Li}

$$\theta_k = \left(m + x_k^{\gamma}\right)\pi,$$

$$x_k = -1 + 2\frac{k-1}{n_r - 1} \quad (k = 1, 2, \ldots, n_r),$$

NH and Engel, Phys. Rev. C **105**, 044314 (2022)



angle along Ci

γ	1	3	5	7
$m(\mathrm{F}-)$	12.0213	12.0209	12.0201	12.0189
$m(\mathrm{F}+)$	0.0252	0.0255	0.0260	0.0269
$m(\mathrm{F}-) - m(\mathrm{F}+)$	11.9961	11.9954	11.9940	11.9920
$m(\mathrm{GT}-)$	37.5860	37.5837	37.5811	37.5774
$m(\mathrm{GT}+)$	1.6065	1.6070	1.6085	1.6109
$m(\mathrm{GT}-) - m(\mathrm{GT}+)$	35.9795	35.9767	35.9726	35.9664
$M^{2\nu} m_e c^2$	0.1802	0.1574	0.1574	0.1575

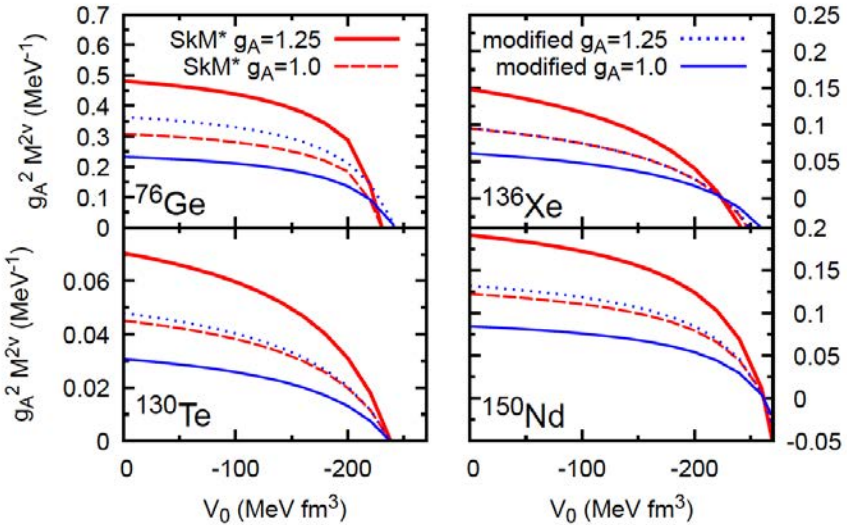
$n_r = 202$, $\gamma = 5$ is used

Benchmark calculation with matrix diagonalization

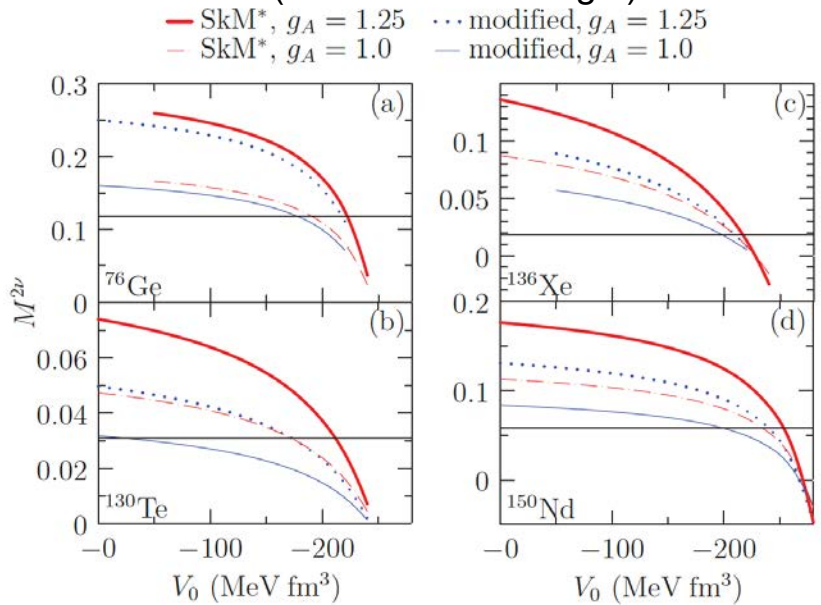
SkM*+Volume pairing

NH and Engel, Phys. Rev. C **105**, 044314 (2022)

FAM



Matrix diagonalization
(Mustonen and Engel)



Mustonen and Engel Phys. Rev. C **87**, 064302 (2013)

- A factor about two difference in ^{76}Ge, other three almost agree
- QTDA overlap for intermediate states
- Mustonen and Engel: 2D coordinate-basis HFB
- FAM: HFBTHO(2D HO basis)
- pairing strength fitted to OES

Dimension and Computational Time

QRPA(matrix diagonalization)

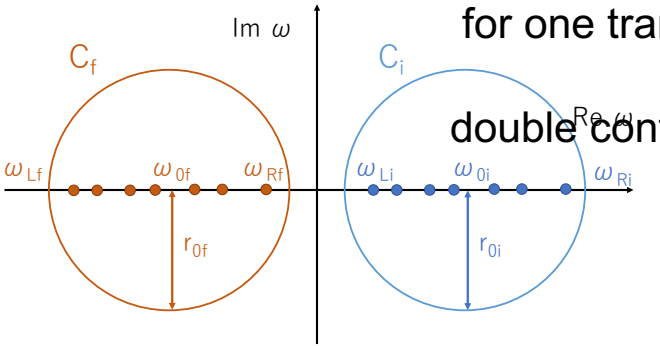
Mustonen and Engel (2013)
2qp space of 500,000 dim → truncated to 15,000 dim

FAM(iteration)

HFBTHO(20 HO major shell model space, axial symmetry)
1qp dimension～1,771 (with time-reversal symmetry)
pnFAM 2qp dimension：257,686 ($K^{\pi}=0^{+}$)、256,025 ($K^{\pi}=\pm1^{+}$)

Computational time

Oakforest-PACS: 25 processes in 1 node (MPI)
contour discretized with 200 points ~ 2-3 hrs (1FAM calc 15min)
size of FAM amplitude (X,Y)：4.8GB
(including 200 pts on the contour, GT K=0,±1, initial and final
for one transition for a give EDF, 1200 FAM calculations)

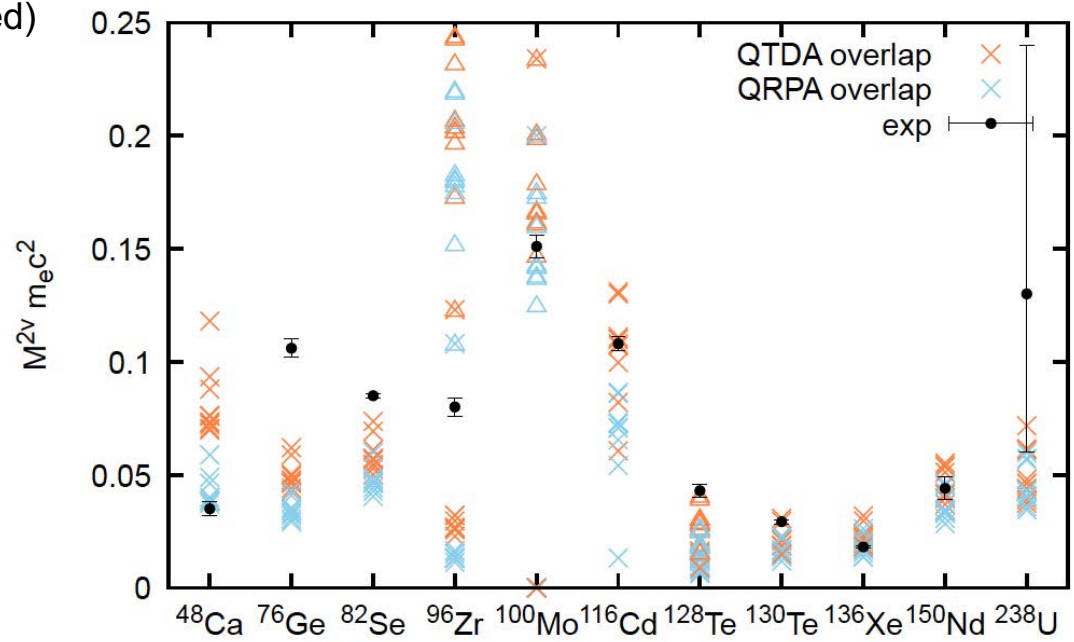


double contour integration (w/o parallelization)：15 min for 200 pts

2vNME from Globally fitted EDF (pnQRPA)

NH and Engel, Phys. Rev. C **105**, 044314 (2022)

10 parameter sets (1A,1B,1C,1D,1E,2,3A,3B,4,5) based on SkO' and SV-min
two overlap integral (QTDA and QRPA)
g_A=1.0 (quenched)

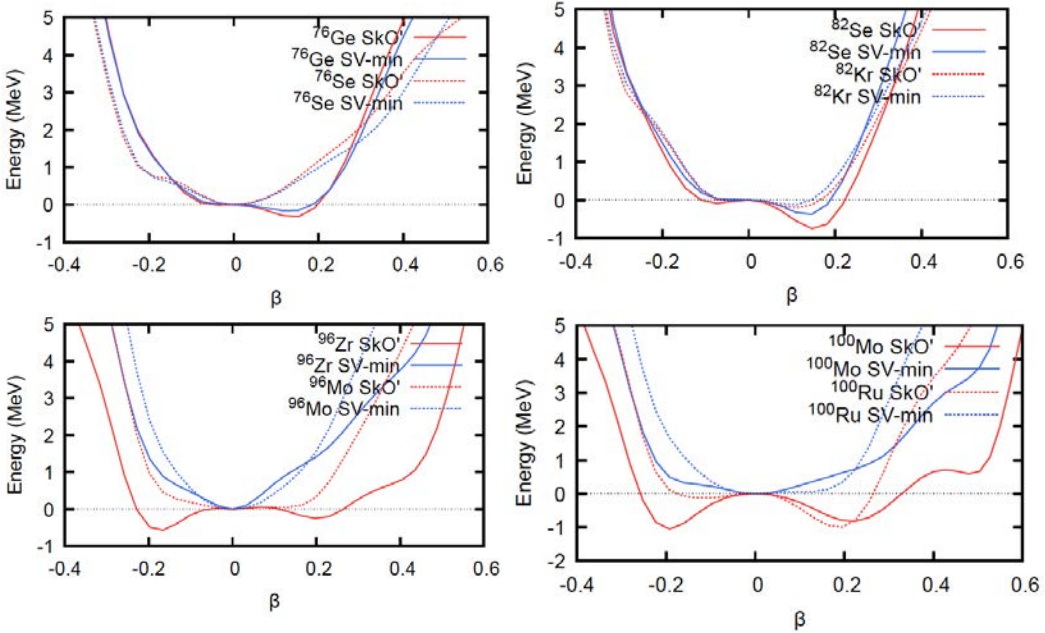


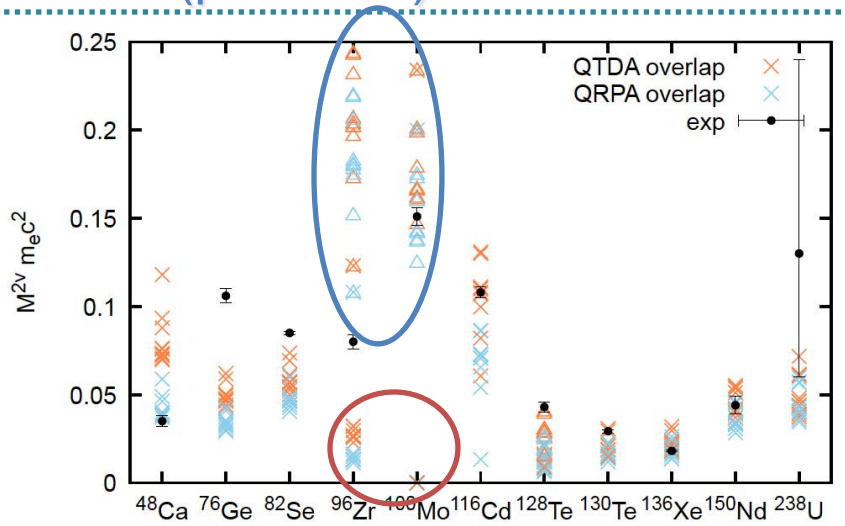
better agreement with experimental data in heavier nuclei (A≧128)
parameter dependence and deviation from data is large in lighter nuclei

2νNME from Globally fitted EDF (pnQRPA)

^{48}Ca, ^{116}Cd: NME depends on EDF parameters
→ fitting including them may improve EDF

Shape dependence





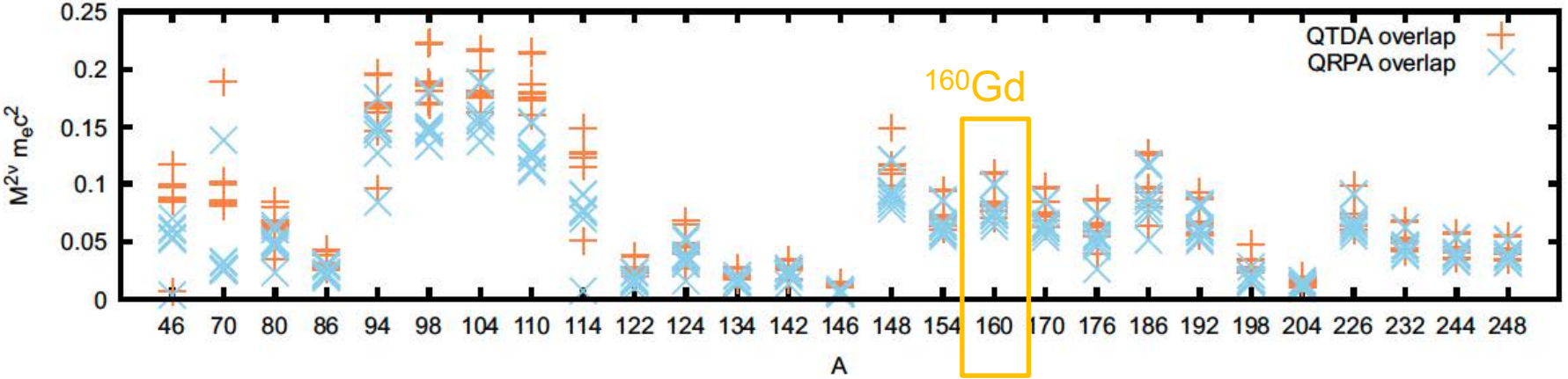
^{76}Ge, ^{82}Se, ^{96}Zr, ^{100}Mo:
^{96}Zr, ^{100}Mo (SkO'):shape coexistence
X: oblate initial state (^{96}Zr, ^{100}Mo)
△ : spherical(^{96}Mo) prolate(^{100}Mo) initial state

Correlation beyond pnQRPA become important
if initial and final states have different deformation

Predictions for possible 2νββ decay nuclei

NH and Engel, Phys. Rev. C **105**, 044314 (2022)

Globally fitted EDF (including g_{pp}) enables us prediction of 2νββ NME



(^{46}Ca,^{70}Zn,^{80}Se,^{86}Kr,^{94}Zr,^{98}Mo,^{104}Ru,^{110}Pd,^{114}Cd,^{122}Sn,^{124}Sn,
^{134}Xe,^{142}Ce,^{146}Nd,^{148}Nd,^{154}Sm,^{160}Gd,^{170}Er,^{176}Yb,^{186}W,^{192}Os,
^{198}Pt,^{204}Hg,^{226}Ra,^{232}Th,^{244}Pu,^{248}Cm)

Takashi Iida et al. (Tsukuba)

Toward 0νββ NME

In the FAM we need to decompose the operator into two one-body ops.

2νββ/DGT : $\sum_a \boldsymbol{\sigma}_a \tau_a^- \cdot \sum_b \boldsymbol{\sigma}_b \tau_b^-$ three terms (K=0, ±1)

0νββ :

$$M^{0\nu} = M^{0\nu}_{\rm GT} - \frac{g_V^2}{g_A^2} M^{0\nu}_{\rm F} + M^{0\nu}_{\rm T},$$

$$M^{0\nu}_{\rm F} = \frac{2R}{\pi g_A^2} \int_0^\infty q dq \frac{h_{\rm F}(q)}{q + \bar{E} - (E_i + E_f)/2} \langle f | \sum_{ab} j_0(q r_{ab}) \tau_a^- \tau_b^- | i \rangle$$

$$M^{0\nu}_{\rm GT} = \frac{2R}{\pi g_A^2} \int_0^\infty q dq \frac{h_{\rm GT}(q)}{q + \bar{E} - (E_i + E_f)/2} \langle f | \sum_{ab} j_0(q r_{ab}) \boldsymbol{\sigma}_a \cdot \boldsymbol{\sigma}_b \tau_a^- \tau_b^- | i \rangle \qquad \boldsymbol{r}_{ab} = \boldsymbol{r}_a - \boldsymbol{r}_b$$

$$M^{0\nu}_{\rm T} = \frac{2R}{\pi g_A^2} \int_0^\infty q dq \frac{h_{\rm T}(q)}{q + \bar{E} - (E_i + E_f)/2} \langle f | \sum_{ab} j_2(q r_{ab}) [3(\boldsymbol{\sigma}_j \cdot \hat{\boldsymbol{r}}_{ab})(\boldsymbol{\sigma}_k \cdot \hat{\boldsymbol{r}}_{ab}) - \boldsymbol{\sigma}_a \cdot \boldsymbol{\sigma}_b] \tau_a^- \tau_b^- | i \rangle,$$

$$j_0(q r_{ab}) = 4\pi \sum_{l=0}^{\infty} j_l(q r_a) j_l(q r_b) \sum_{m=-l}^{l} Y^*_{lm}(\hat{\boldsymbol{r}}_a) Y_{lm}(\hat{\boldsymbol{r}}_b)$$

summations over: momentum q, l,m, and spins

numbers of FAM double integrations necessary

Reduced basis method for the FAM

NH, Zhang, Engel, in preparation

We regard complex energy ω as a parameter

$$\begin{pmatrix} X_{\mu\nu}(\omega) \\ Y_{\mu\nu}(\omega) \end{pmatrix} = \sum_{k=1}^{n} a_k(\omega) \begin{pmatrix} X_{\mu\nu}(\omega_k) \\ Y_{\mu\nu}(\omega_k) \end{pmatrix} + b_k(\omega) \begin{pmatrix} Y^*_{\mu\nu}(\omega_k) \\ X^*_{\mu\nu}(\omega_k) \end{pmatrix}$$

$X(\omega_k)$, $Y(\omega_k)$: FAM solutions at the training energies (ω_k, k=1,..., n)

emulated FAM amplitudes satisfy the FAM equation

$$\left[\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] \begin{pmatrix} X(\omega) \\ Y(\omega) \end{pmatrix} = - \begin{pmatrix} F^{20} \\ F^{02} \end{pmatrix}$$

weights are given by Rayleigh-Ritz variational method

$$\sum_k (\mathcal{H}_{jk} - \omega \mathcal{N}_{jk}) \begin{pmatrix} a_k(\omega) \\ b_k(\omega) \end{pmatrix} = - \begin{pmatrix} S^*_j \\ S'_j \end{pmatrix} = -\boldsymbol{S}^*$$

$$S_j = S(\hat{F}, \omega_j)$$
$$S'_j = S(\hat{F}^\dagger, \omega_j)$$

strengths at training energies

N: norm kernel (overlap)
H: Hamiltonian kernel

same as the Hill-Wheeler equation (Schrödinger equation for non-orthogonal basis) in the generator coordinate method (GCM)

differences with GCM: Norm kernel is not positive definite
collective Hamiltonian is non-Hermitian

Reduced basis method for nuclear DFT response

Emulator for X and Y at an arbitrary value of ω

NH, Zhang, Engel, in preparation

$$X_{\mu\nu}(\omega) = \sum_{k=1}^{n} a_k(\omega) X_{\mu\nu}(\omega_k) + b_k(\omega) Y^*_{\mu\nu}(\omega_k) + c_k(\omega) X^*_{\mu\nu}(\omega_k) + d_k(\omega) Y_{\mu\nu}(\omega_k)$$

$$Y_{\mu\nu}(\omega) = \sum_{k=1}^{n} a_k(\omega) Y_{\mu\nu}(\omega_k) + b_k(\omega) X^*_{\mu\nu}(\omega_k) + c_k(\omega) Y^*_{\mu\nu}(\omega_k) + d_k(\omega) X_{\mu\nu}(\omega_k)$$

ω_k: energies at training points

Test calculation: ^{24}Mg (oblate) isoscalar monopole mode (like-particle QRPA)

training: 11 FAM amplitudes (ω_k=0~10+ i MeV)

energy(MeV)		strength(e^2 fm^4)	
QRPA	RBM	QRPA	RBM
1.318	1.318	5.771E-04	4.612E-04
1.373	1.373	1.510E-02	1.515E-02
2.458	2.458	1.781E-01	1.781E-01
2.598	2.598	3.061E-03	3.044E-03
3.667	3.667	5.782E-01	5.782E-01
5.119	5.119	3.740E-04	3.736E-04
7.411	7.411	4.879E-01	4.879E-01
7.890	7.890	8.755E-03	8.823E-02
7.960	7.961	3.295E-02	3.291E-02
8.929	8.929	8.598E-02	8.597E-02
9.128	9.128	2.342E-03	2.346E-03
10.24	10.25	2.246E-04	2.160E-04

Reduced basis method

Frame et al., Phys. Rev. Lett. **121**, 032501 (2018)
Bonilla et al., Phys. Rev. C **106**, 054322 (2022)
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Talk by Xilin Zhang at TRIUMF workshop (2023)

Summary and outlook

Summary

- Systematic calculation of 2vββ (QRPA) NME using globally-fitted EDF
- All two-quasiparticle excitations within the model space (~250,000) are included
- Different parameter set give similar NME in heavy nuclei
- pnQRPA is not good when initial and final deformation are different (and shape coexistence)

Outlook

- Reduced basis method for 0vββ NME