Nuclear matrix element for double-beta decay within density functional theory

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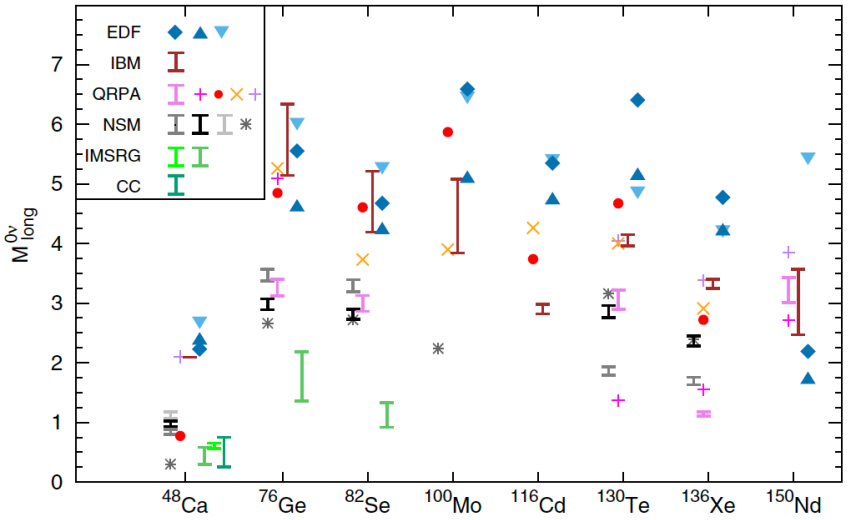
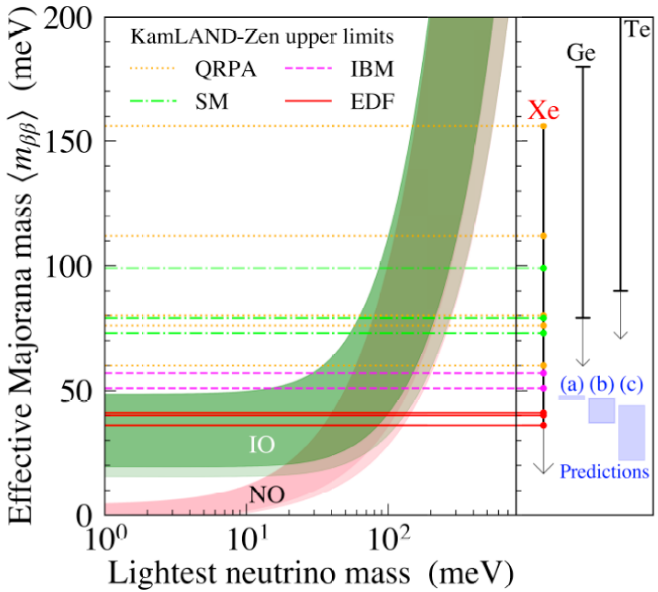
Nuclear matrix element

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

Phase space factor　　NME



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



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

nuclear structure theories

Agostini et al. Rev. Mod. Phys. **95**, 025002 (2023)

EDF: generator coordinate method based on energy density functional
IBM: interacting boson model
QRPA: quasiparticle random-phase approximation
NSM: shell model
IMSRG: In-mediums similarity renormalization group
CC: coupled-cluster theory

a factor of 2-3 deviation

Phase space factor: see poster P28(Kanai)

Nuclear density functional theory

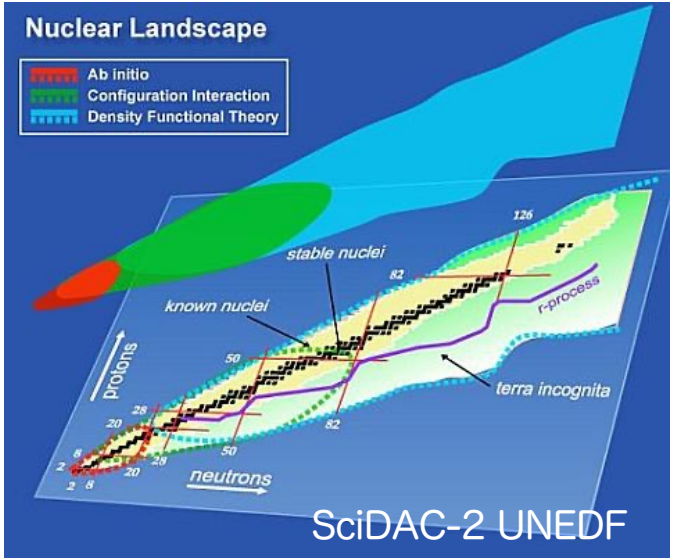
Density functional theory (DFT)

- idea developed in electron systems: There exists an energy density functional (E[ρ]) that gives exact density of the ground state and the energy (Hohenberg and Kohn)
- extension of this idea to nuclear ground state (and excited states)
- applicable to all mass region (even neutron matter in neutron star)
- EDF is determined phenomenologically by using experimental data (mass, radius, etc)

NME within DFT

correlations beyond DFT(mean field) are important:
treated in a perturbative (QRPA) or non-perturbative (GCM) way

- neutron-proton pairing (included in QRPA)
- shape coexistence/fluctuation (included in GCM)
- no DFT calculation including both



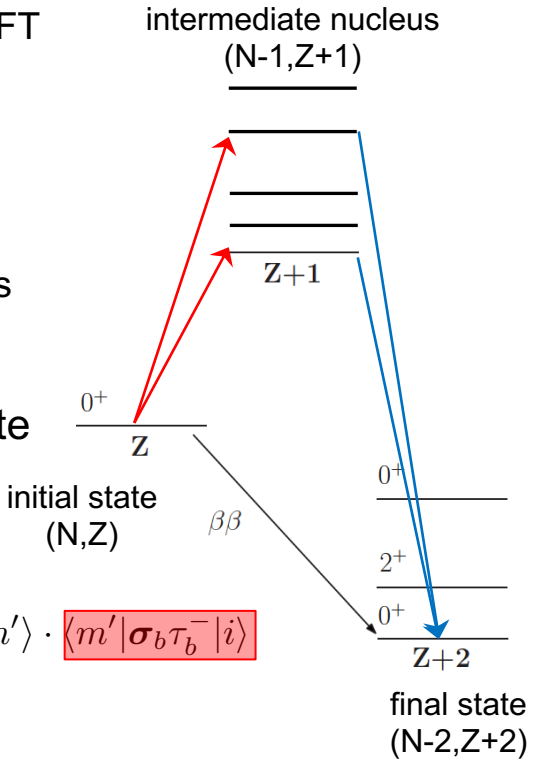
Quasiparticle random-phase approximation (QRPA)

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



- proton-neutron excitation:
  regard intermediate nucleus as an excited state of initial/final state

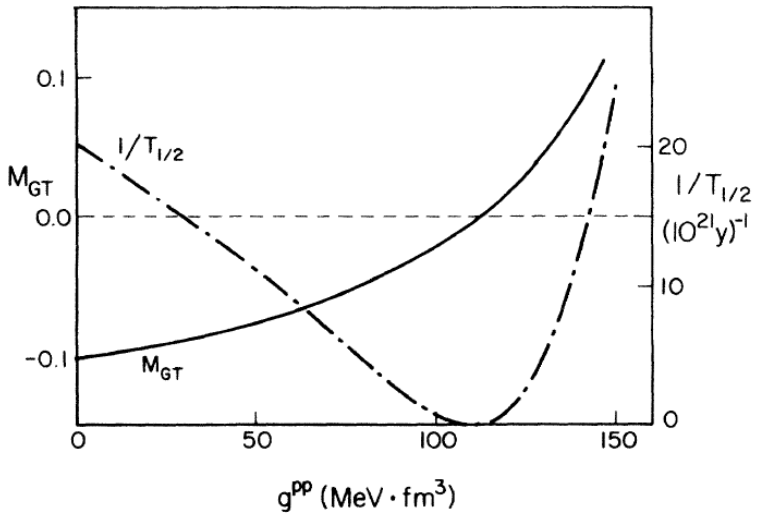
- NME

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

transition to the intermediate state is calculated with QRPA correlation
correlations are included both in initial/final state and intermediate states

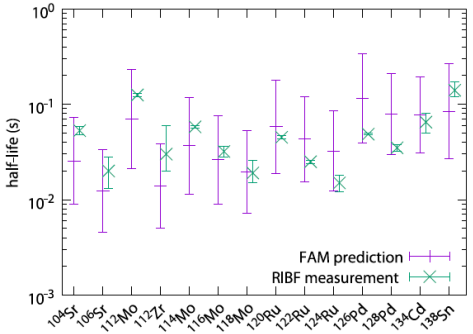
g_{pp} and g_{ph}

- NME is sensitive to g_{pp} (isoscalar neutron-proton pairing strength) and g_{ph} (neutron-proton Gamow-Teller (GT) interaction strength)
- Both cannot be determined from ground-state information
- Conventionally g_{pp} is fitted to 2νββ half-life for each isotope before computing 0νββ NME → impossible to predict 2νββ half-life
- Globally fitted EDF with g_{pp} and g_{ph}: fitted to β decay half-life and GT resonance energy



Vogel and Zirnbauer Phys. Rev. Lett. **57**, 3148 (1986)

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



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

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)

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

dimension: 10^5-10^6 (with axial deformation)
full diagonalization is computationally demanding. model space truncation necessary

finite-amplitude method (iterative solution)

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

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

⟸ 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)

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

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

FAM for 2νββ NME

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

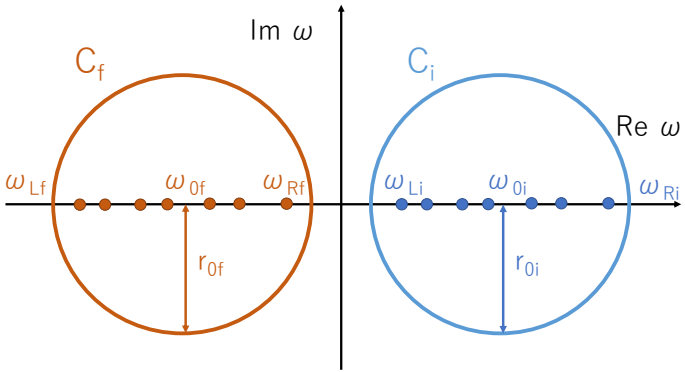
$$X_{\mu\nu}(\omega,\hat{F}) = -\sum_i \left\{ \frac{X^i_{\mu\nu}\langle i|\hat{F}|0\rangle}{\Omega_i-\omega} + \frac{Y^{i*}_{\mu\nu}\langle 0|\hat{F}|i\rangle}{\Omega_i+\omega} \right\} \qquad Y_{\mu\nu}(\omega,\hat{F}) = -\sum_i \left\{ \frac{Y^i_{\mu\nu}\langle i|\hat{F}|0\rangle}{\Omega_i-\omega}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

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

FAM from final state FAM from initial state

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

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



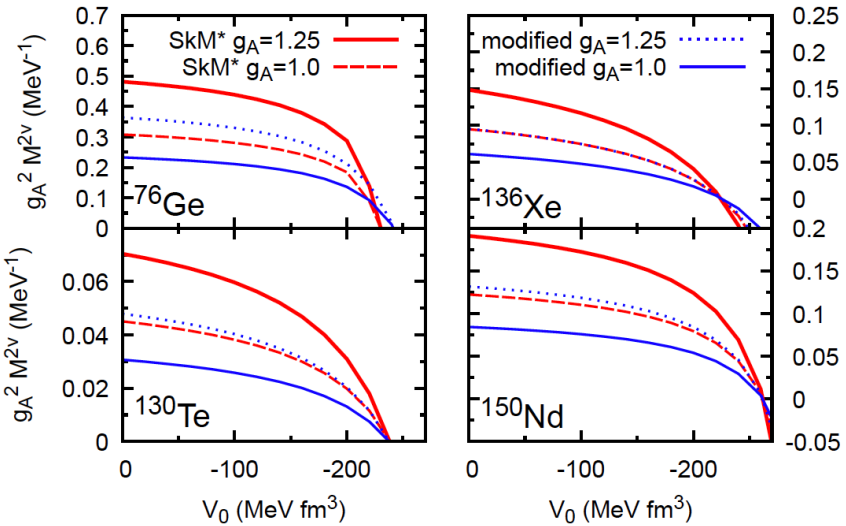
double contour integration
initial state: σ⊤- external field
final state: σ⊤- external field (take the backward part)
FAM calculation with different ω and F are parallelizable
α controls the overlap (α=0 QTDA, α=1 QRPA)

Benchmark calculation with matrix diagonalization

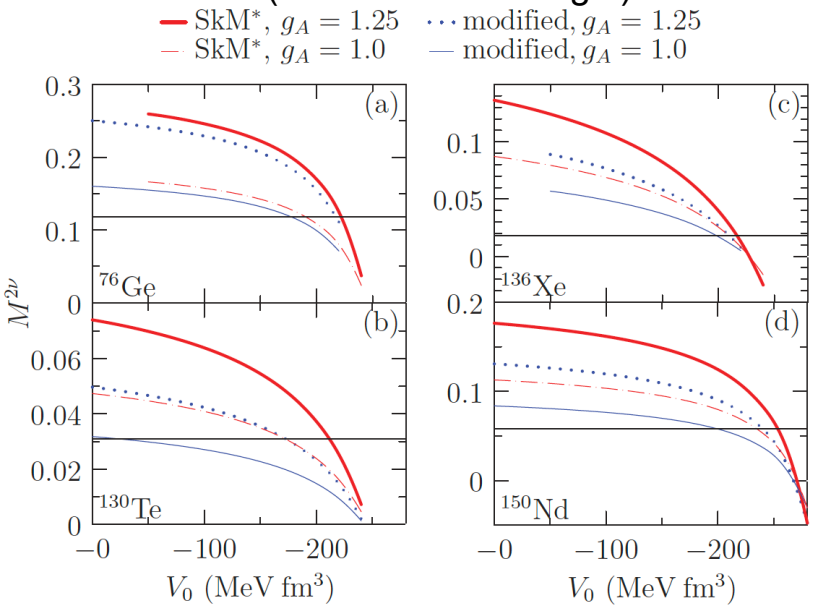
SkM*+Volume pairing

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)

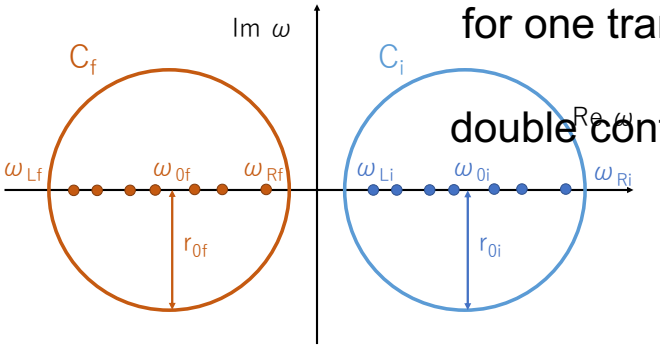
Mustonen and Engel (2013)
2qp space of 500,000 dim → truncated to 15,000 dim

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)

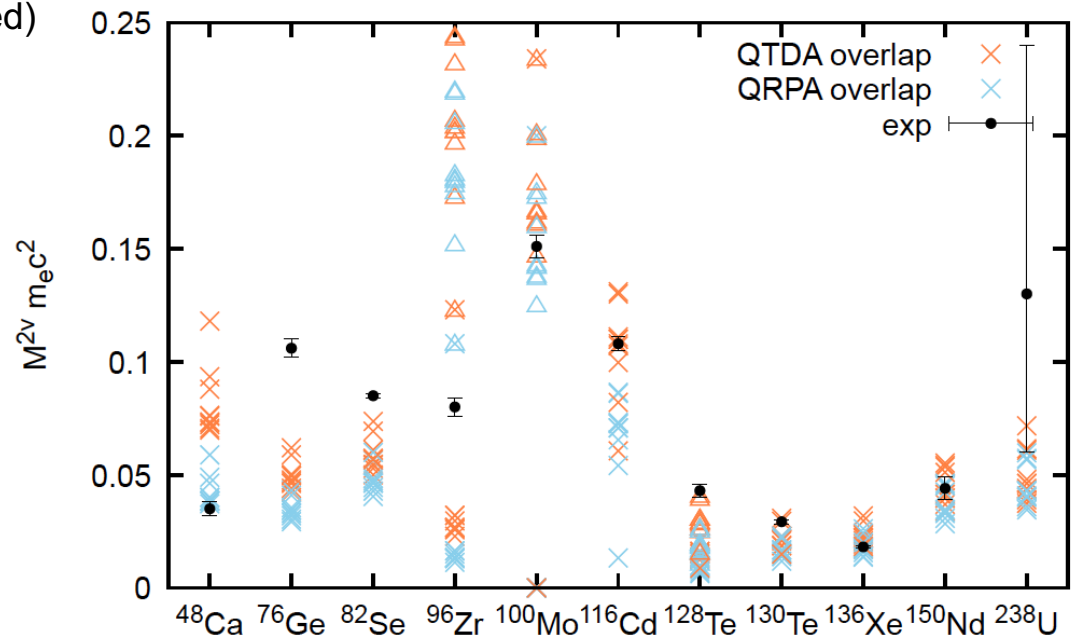


double contour integration (w/o parallelization)：15 min for 200 pts

2νββ NME 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)

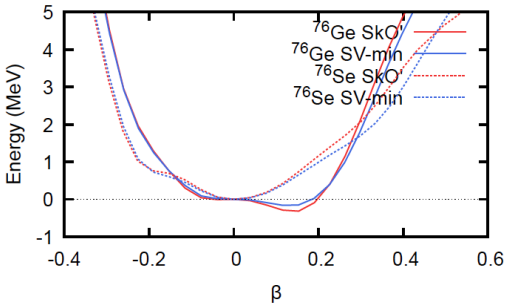


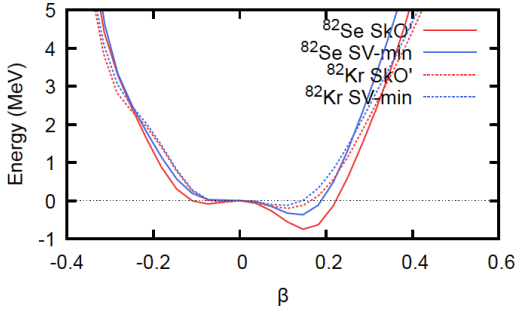
better agreement with experimental data in heavier nuclei (A≧128)
parameter dependence and deviation from data is large in lighter nuclei

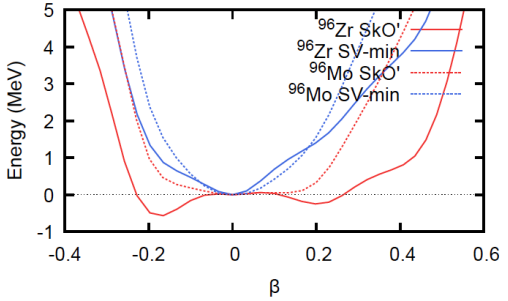
2vNME from Globally fitted EDF (pnQRPA)

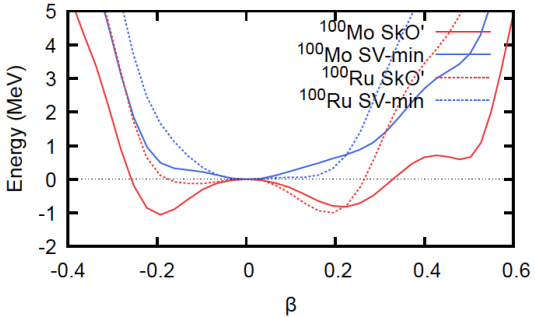
^{48}Ca, ^{116}Cd: NME depends on EDF parameters
→ fitting including them may improve EDF

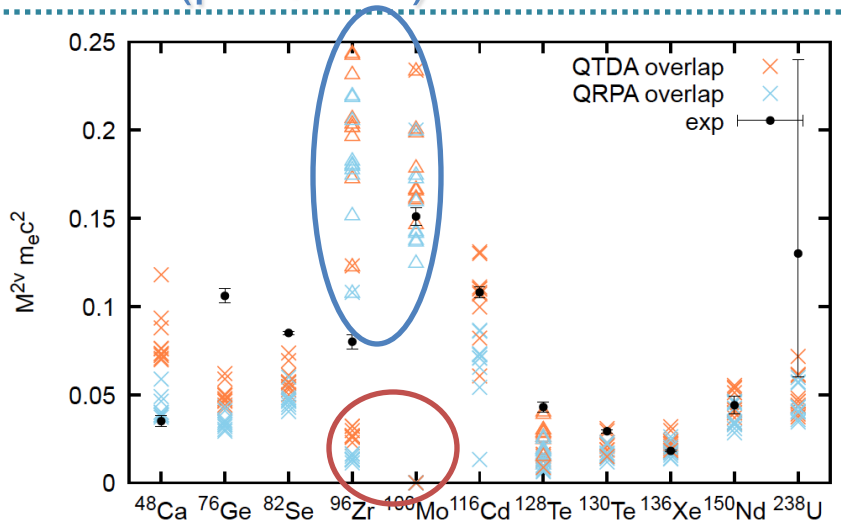
Shape dependence











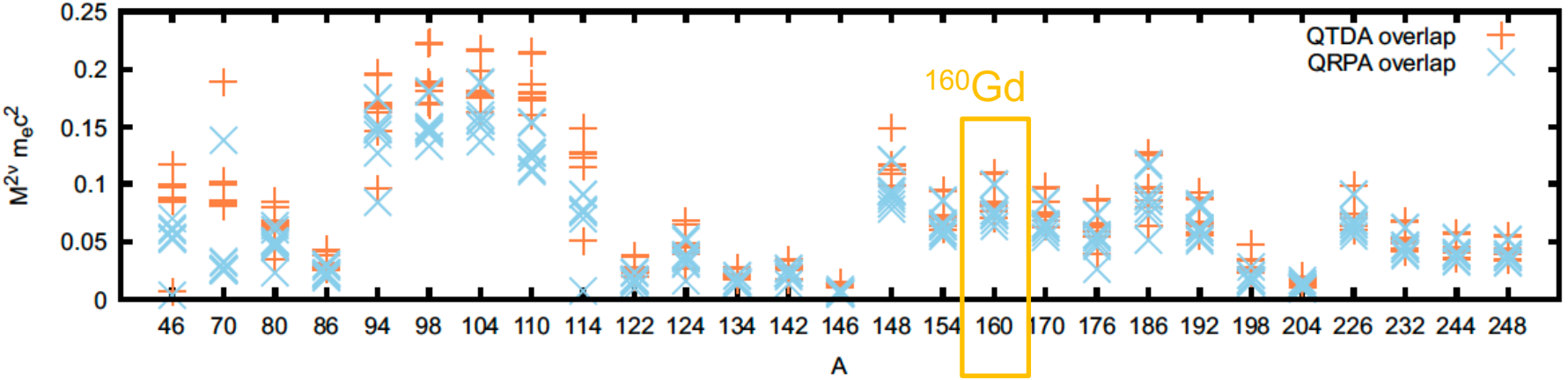
^{76}Ge, ^{82}Se, ^{96}Zr, ^{100}Mo:
^{96}Zr, ^{100}Mo (SkO'):shape coexistence
X: oblate initial state (^{96}Zr, ^{100}Mo)
△ : spherical(^{96}Mo) prolate(^{100}Mo) initial state

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)

Next talk by Takashi Iida (Tsukuba)

Toward 0νββ NME

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

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

0νββ(GT): $\int dq f(q) \sum_{ab} j_0(qr_{ab}) \boldsymbol{\sigma}_a \tau_a^- \cdot \boldsymbol{\sigma}_b \tau_b^-$

$$= 4\pi \int dq f(q) \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left[\sum_a j_l(qr_a) Y_{lm}^*(\hat{\boldsymbol{r}}_a) \boldsymbol{\sigma}_a \tau_a^- \right] \cdot \left[\sum_a j_l(qr_b) Y_{lm}(\hat{\boldsymbol{r}}_b) \boldsymbol{\sigma}_b \tau_b^- \right]$$

$$j_0(qr_{ab}) = 4\pi \sum_{l=0}^{\infty} j_l(qr_a) j_l(qr_b) \sum_{m=-l}^{l} Y_{lm}^*(\hat{\boldsymbol{r}}_a) Y_{lm}(\hat{\boldsymbol{r}}_b) \qquad r_{ab} = |\boldsymbol{r}_a - \boldsymbol{r}_b|$$

summations over: momentum q, l,m, and spins
large numbers of FAM double integrations necessary

Reduced basis method for nuclear DFT response

We regard complex energy ω as a parameter.
Emulator for X and Y at an arbitrary value of ω is

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)
Drischler et al., Front. Phys. **10**, 1092931 (2023)
Talk by Xilin Zhang at TRIUMF workshop (2023)

0v Fermi transition (Very preliminary)

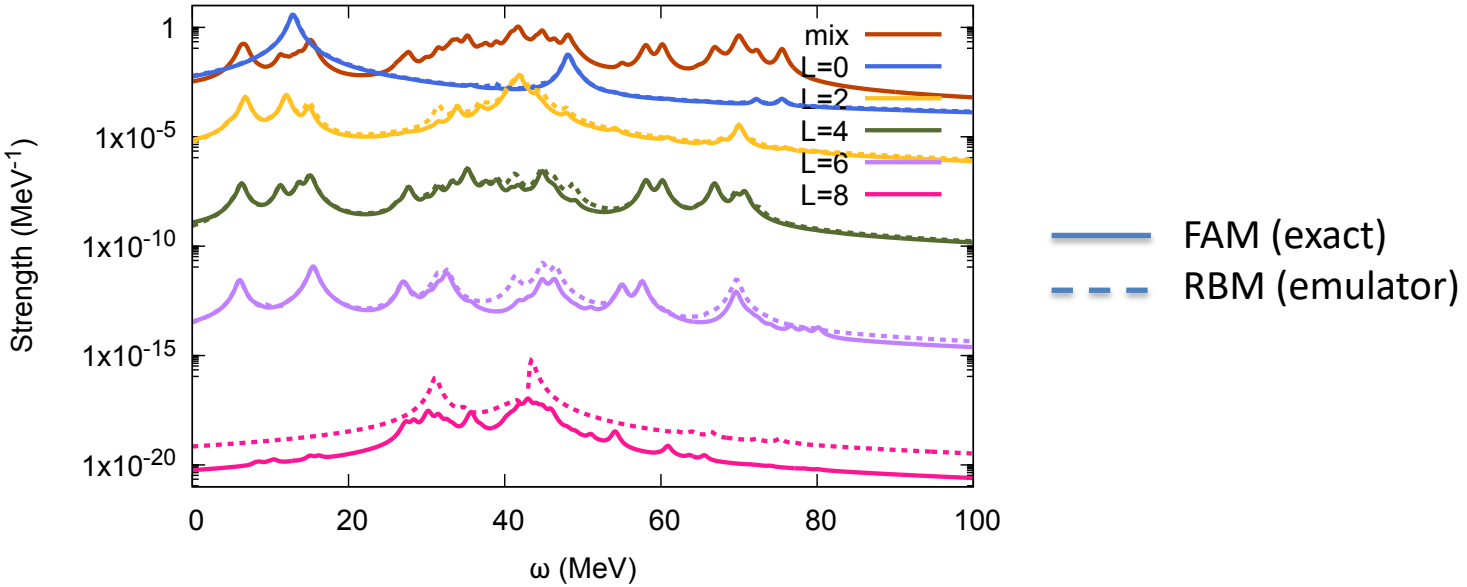
$^{48}Ca \rightarrow {}^{48}Sc$ by one-body part of the 0v Fermi mode, in a small model space (N_{sh}=5)

training: neutrino momentum q = 1.0 fm^{-1}, m = 0

one mixed operator (L=0) + (L=2)*1.5^2 + (L=4)*1.5^4 + …

50 energy points (0 - 98+0.5i MeV, 2 MeV interval) → energies are the parameters

evaluation at q = 0.2 fm^{-1}, m=0 for each L-operator in 0v Fermi transition



50-100 FAM training calculations may produce the emulator valid for a wide range of L and q

Summary and outlook

Summary

- Systematic calculation of 2νββ (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

- Emulator using reduced basis method for 0νββ NME