Application of generator coordinate method with neutron-proton pairing amplitudes to nuclear matrix elements

Nobuo Hinohara

Center for Computational Sciences,
University of Tsukuba, Japan

筑波大学
University of Tsukuba

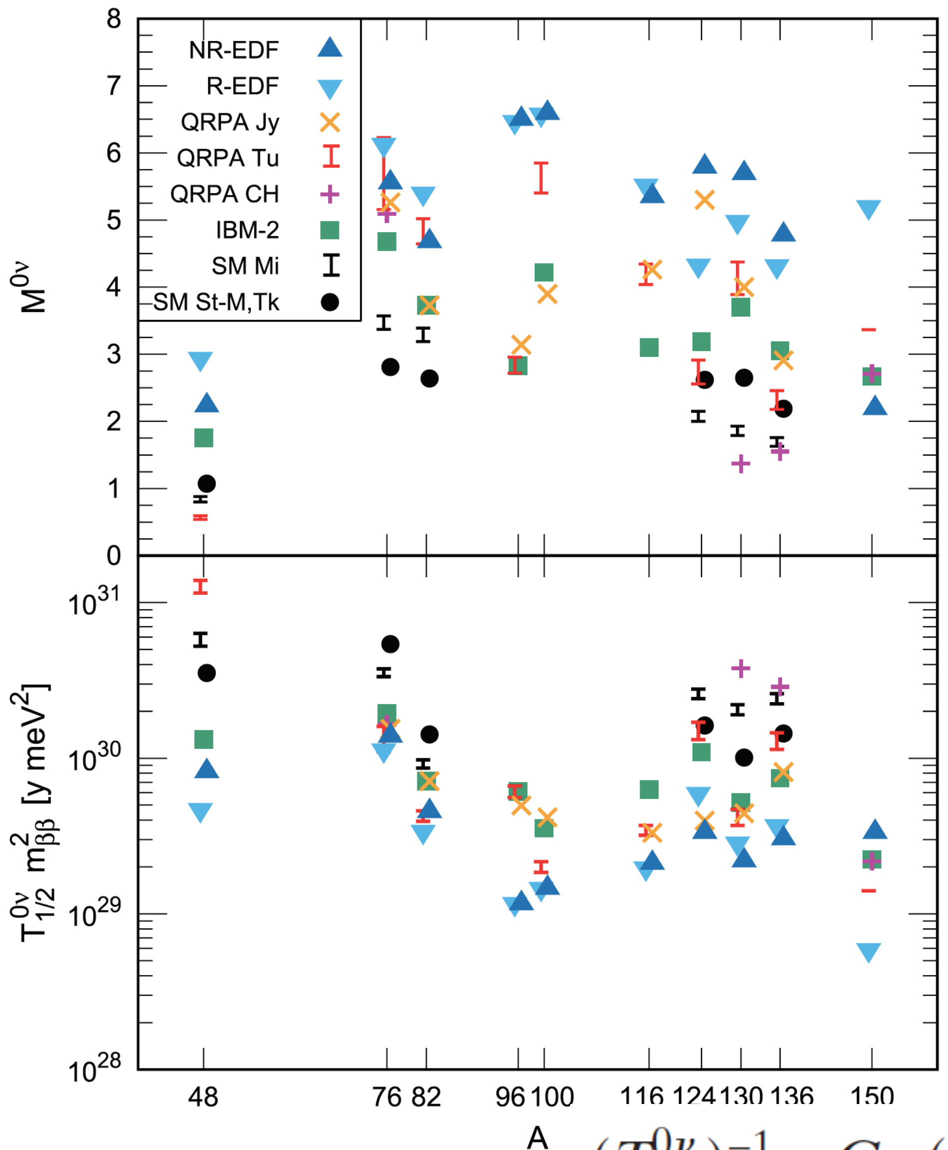
筑波大学
計算科学研究センター
Center for Computational Sciences

Outline

- Introduction
- Generator coordinate method
- Application to SO(8) model, ^{76}Ge double-beta decay
- Future plans
- Summary

Status of nuclear matrix element calculations

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



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

Origin of differences

- decay operator
- many-body theory (correlations)
- single-particle model space
- effective interaction

Origin of differences

- Shell model
  - full many-body correlations
  - relatively small single-particle model space
  - effective interaction
- Quasiparticle random-phase approximation (QRPA)
  - two-quasiparticle correlations
    - breaks down at the phase transition
  - large single-particle model space
  - effective interaction/EDF
  - neutron-proton pairing
- Generator coordinate method (GCM)
  - selected collective correlations (basically quadrupole)
  - large single-particle model space
  - closure approximation necessary
  - effective interaction/EDF

Generator coordinate method

Generator Coordinate Method

superposition of the projected mean fields (GCM basis) along generator coordinates q

$$|\Psi(N,Z,I=0,M=0)\rangle = \sum_q f_k(q)|\phi^{N,Z}_{I=0,M=0}(q)\rangle$$

initial/final ground state — weight function

Hill-Wheeler equation: Schrödinger eq. for many-body states

$$\hat{H}|\Psi_k\rangle = E_k|\Psi_k\rangle$$

⇩

$$\sum_{q'}\{\mathcal{H}(q,q') - E_k\mathcal{I}(q,q')\}f_k(q') = 0$$

Hamiltonian kernel $\quad \mathcal{H}(q,q') = \langle\phi^{N,Z}_{I=0,M=0}(q)|\hat{H}|\phi^{N,Z}_{I=0,M=0}(q')\rangle$

Norm kernel $\quad \mathcal{I}(q,q') = \langle\phi^{N,Z}_{I=0,M=0}(q)|\phi^{N,Z}_{I=0,M=0}(q')\rangle$

Three steps for GCM calculations

Generator Coordinate Method

superposition of the projected mean fields (GCM basis) along generator coordinates q

$$|\Psi(N,Z,I=0,M=0)\rangle = \sum_q f_k(q)|\phi^{N,Z}_{I=0,M=0}(q)\rangle$$

initial/final ground state — weight function

step 1: constrained HFB calculation to generate GCM basis

correlations along important coordinates
(q: collective properties, deformation, pairing, ...)
mean field breaks symmetries (rotational, particle-number)→ projections

step 2: projected two-body matrix elements

$$\mathcal{H}(q,q') = \langle\phi^{N,Z}_{I=0,M=0}(q)|\hat{H}|\phi^{N,Z}_{I=0,M=0}(q')\rangle \qquad \mathcal{I}(q,q') = \langle\phi^{N,Z}_{I=0,M=0}(q)|\phi^{N,Z}_{I=0,M=0}(q')\rangle$$

$$\mathcal{T}(q,q') = \langle\phi^{N-2,Z+2}_{I=0,M=0}(q)|\hat{M}_{0\nu}|\phi^{N,Z}_{I=0,M=0}(q')\rangle$$

step 3: Hill-Wheeler eq. to determine f(q) for the ground states

$$\sum_{q'}\left\{\mathcal{H}(q,q')f_k(q') - E_k\mathcal{I}(q,q')\right\}f_k(q') = 0$$

Remarks

Generator Coordinate Method

superposition of the projected mean fields (GCM basis) along generator coordinates q

$$|\Psi(N,Z,I=0,M=0)\rangle = \sum_q f_k(q)|\phi^{N,Z}_{I=0,M=0}(q)\rangle$$

initial/final ground state — weight function

GCM basis is not orthogonal

Hill-Wheeler equation $\mathcal{H}f_k = E_k \mathcal{I} f_k$

weight function
no physical meaning → $f = \mathcal{I}^{-1/2} g$ ← collective wave function

Hill-Wheeler equation
for collective wave function $(\mathcal{I}^{-1/2}\mathcal{H}\mathcal{I}^{-1/2})g_k = E_k g_k$

small norm problem

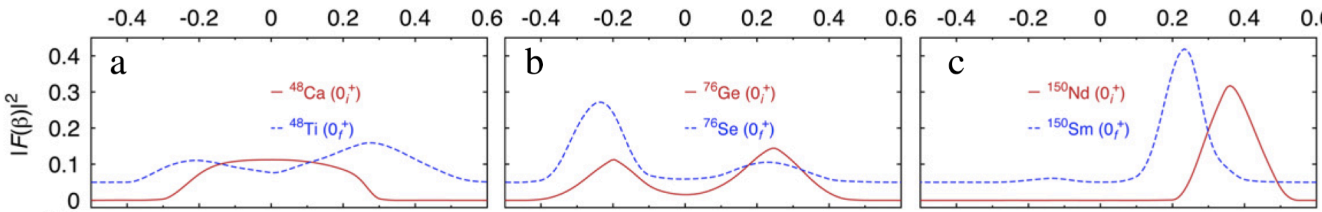
small (zero) eigenvalues in norm kernel cause numerical instability
cutoff is introduced in norm eigenvalues to avoid the problem

GCM collective wave functions (1-dim)

Generator coordinate: axial quadrupole deformation

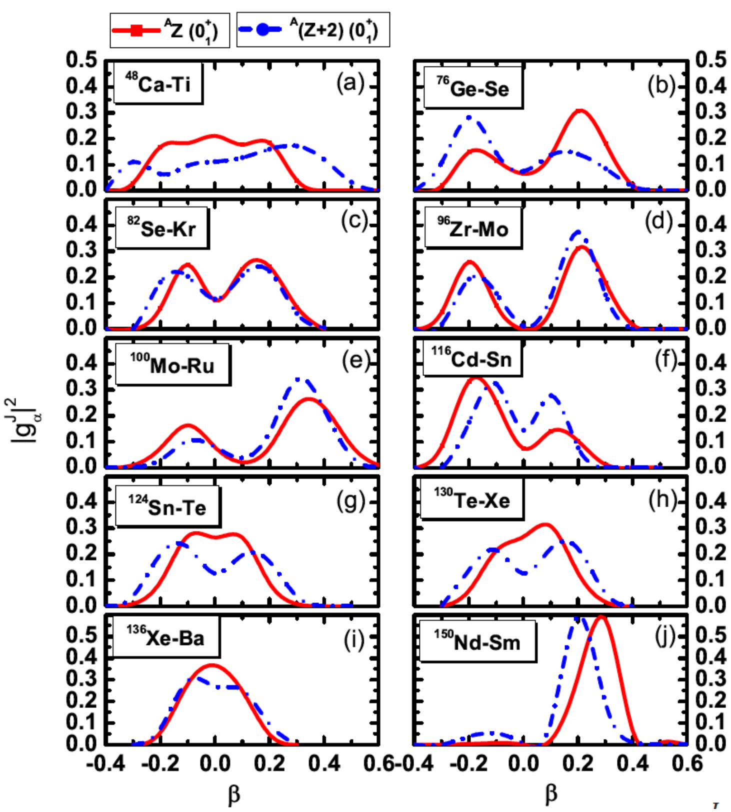
Gogny D1S

T. Rodriguez and G. Martinez-Pinedo, Prog. Part. Nucl. Phys. **66**, 436 (2011)



covariant density functional theory

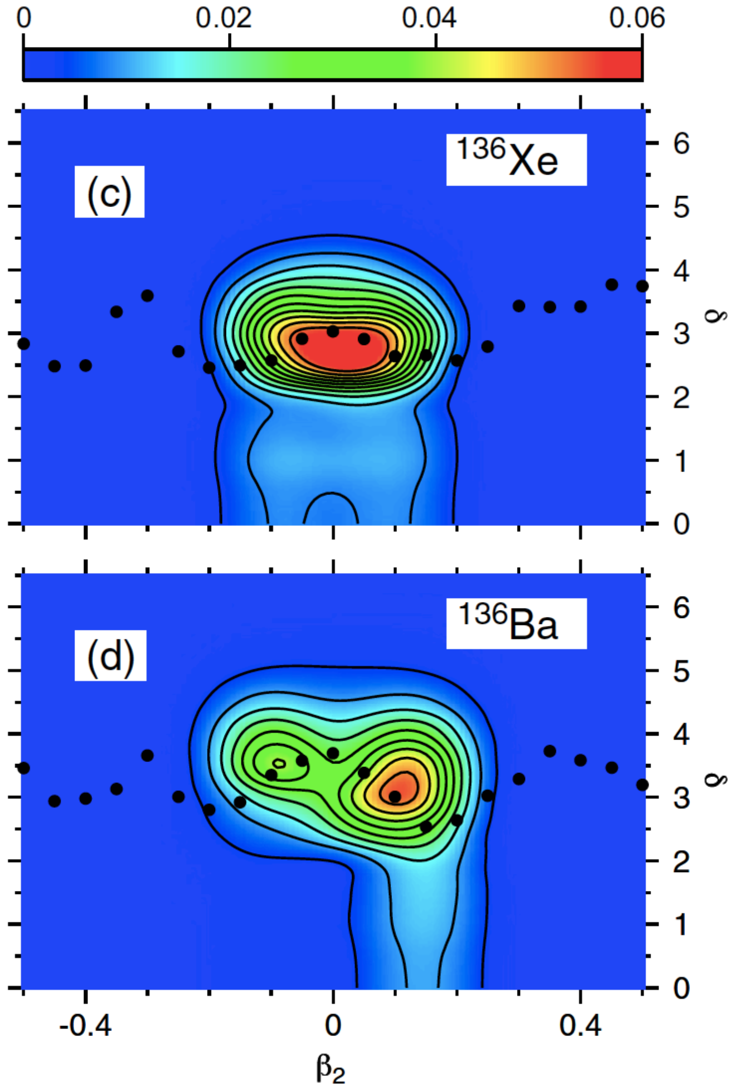
Yao et al. Phys. Rev. C **91**, 024316 (2015)



GCM collective wave functions (2-dim)

GC: axial quadrupole deformation and isovector like-particle pairing

Vaquero, Rodriguez, Egido, Phys. Rev. Lett. **111**,142501 (2013)



Normalized nuclear matrix elements

$$M^{0\nu} = \langle N-2, Z+2, I=0 | \hat{M}^{0\nu} | N, Z, I=0 \rangle$$

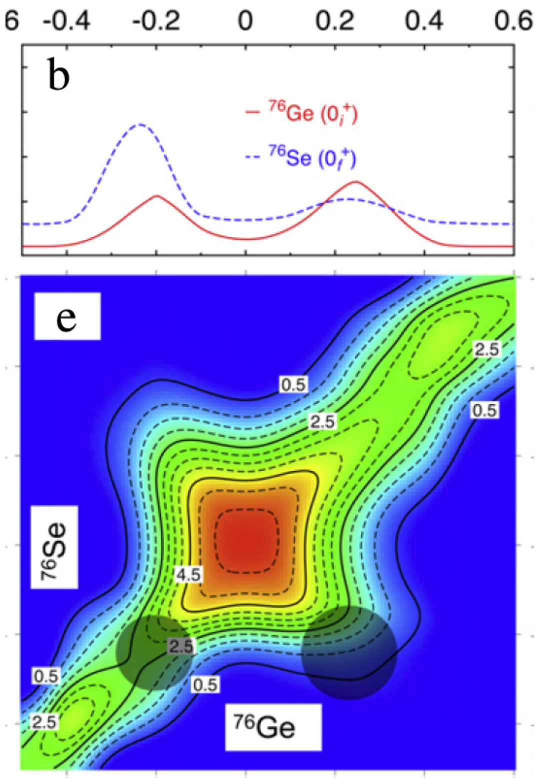
$$\mathcal{T}(q,q') = \langle \phi^{N-2,Z+2}_{I=0,M=0}(q) | \hat{M}_{0\nu} | \phi^{N,Z}_{I=0,M=0}(q') \rangle$$

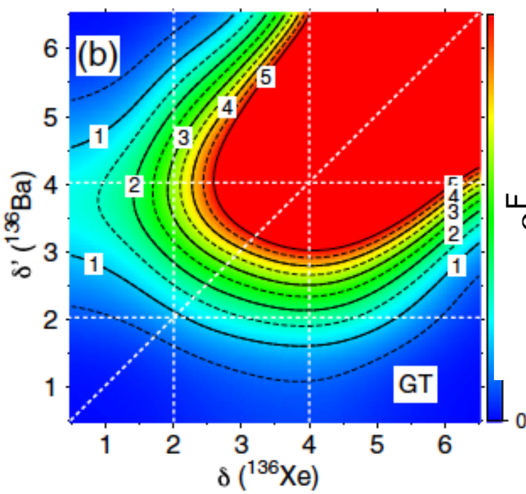
$$= \sum_{qq'} \frac{f^*_F(q)\mathcal{T}(q,q')f_I(q')}{\sqrt{\mathcal{I}_F(q,q)\mathcal{I}_I(q',q')}} = \sum_{qq'} f^*_F(q)\tilde{\mathcal{T}}(q,q')f_I(q')$$

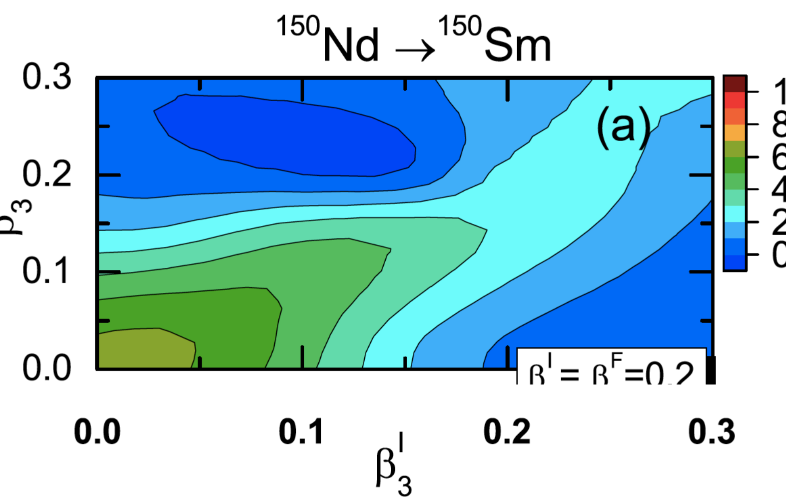
quadrupole deformation
Gogny D1S

isovector pairing
Gogny D1S

octupole deformation
covariant DFT





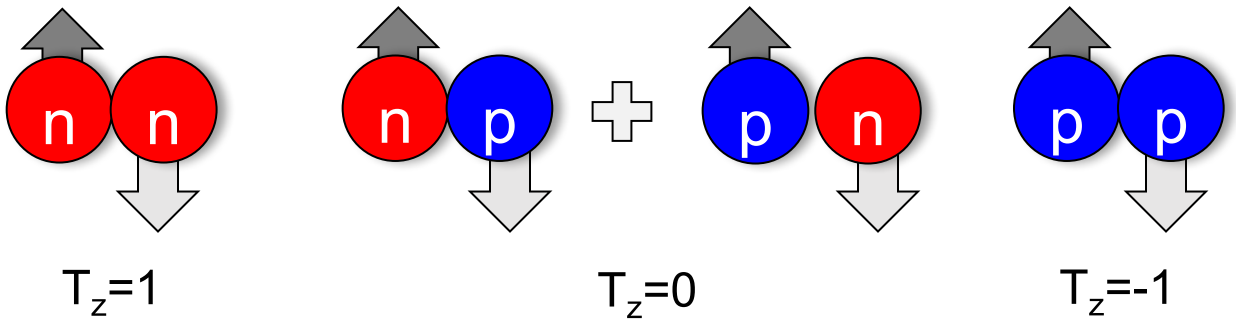


T. Rodriguez and G. Martinez-Pinedo, Prog. Part. Nucl. Phys. **66**, 436 (2011)
Vaquero, Rodriguez, Egido, Phys. Rev. Lett. **111**,142501 (2013)
Yao and Engel, Phys. Rev. C **94**, 014306 (2016)

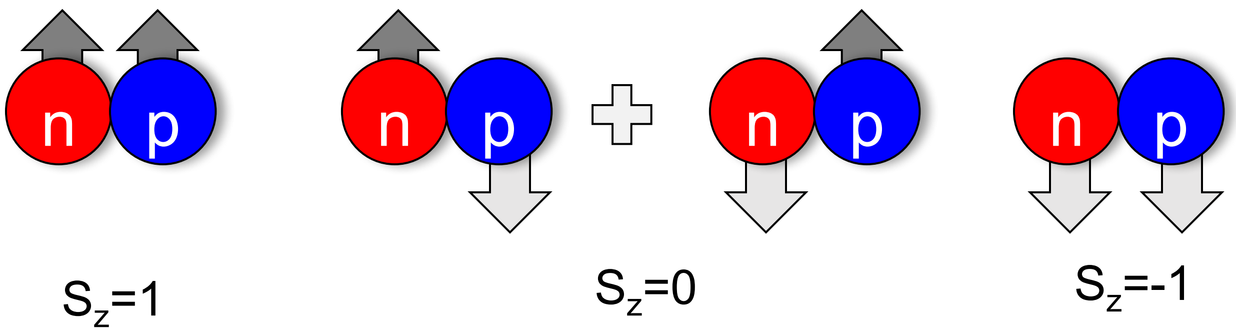
Neutron-proton correlation

neutron-proton pairing

Isovector (T=1, S=0) pairings → Fermi matrix element



Isoscalar (T=0, S=1) pairings → Gamow-Teller matrix element



στ (Gamow-Teller type) particle-hole (T=1, S=1)
→ Gamow-Teller matrix element

neutron-proton pairing suppresses the nuclear matrix elements (QRPA)
neutron-proton pairing and στ correlations are not included in GCM (REDF/NREDF)

GCM for nuclear matrix element

GCM with quadrupole deformation and
np pairing degrees of freedom
with a simple shell model interaction (P+Q model)

GCM basis with neutron-proton pairing generator coordinate

Generalized Hartree-(Fock)-Bogoliubov (spherical 3D HO basis)

$$\hat{a}_k^\dagger = \sum_l \left(U_{lk}^{(n)} \hat{c}_l^{(n)\dagger} + V_{lk}^{(n)} \hat{c}_k^{(n)} + U_{lk}^{(p)} \hat{c}_l^{(p)\dagger} + V_{lk}^{(p)} \hat{c}_k^{(p)} \right)$$

$$a_k |\phi(q)\rangle = 0$$

Hartree-(Fock)-Bogoliubov equation

$$\begin{pmatrix} h_{nn} - \lambda_n & \Delta_{nn} & h_{np} & \Delta_{np} \\ -\Delta_{nn}^* & -h_{nn} + \lambda_n & -\Delta_{np}^* & -h_{np}^* \\ h_{pn} & \Delta_{pn} & h_{pp} - \lambda_p & \Delta_{pp} \\ -\Delta_{pn}^* & -h_{pn}^* & -\Delta_{pp}^* & -h_{pp}^* + \lambda_p \end{pmatrix} \begin{pmatrix} U_k^{(n)} \\ V_k^{(n)} \\ U_k^{(p)} \\ V_k^{(p)} \end{pmatrix} = E_k \begin{pmatrix} U_k^{(n)} \\ V_k^{(n)} \\ U_k^{(p)} \\ V_k^{(p)} \end{pmatrix}$$

λ_n and λ_p are determined simultaneously to satisfy the particle number expectation values

Projections

pairing condensation and deformation break particle number (gauge) symmetry and rotational symmetry

$$|\phi(q)\rangle = \cdots + |N-2\rangle + |N-1\rangle + |N\rangle + |N+1\rangle + |N+2\rangle + \cdots$$

$$|\phi(q)\rangle = |I=0\rangle + |I=1\rangle + |I=2\rangle + \cdots$$

eigenstates of number/angular momentum

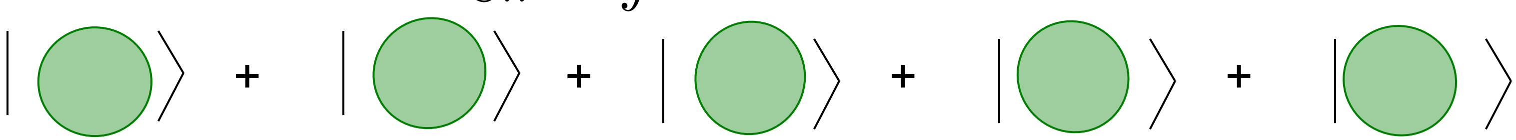
Particle number projection (PNP): method of residue (Fomenko method)

$$\hat{P}^N|\phi(q)\rangle = \frac{1}{2\pi}\int_0^{2\pi} d\phi e^{i\phi(\hat{N}-N)}|\phi(q)\rangle = |N\rangle$$

Angular momentum projection (AMP): 3-dim integration→1-dim if axial symmetric

Gauss-Legendre integration

$$\hat{P}^J_{MK}|\phi(q)\rangle = \frac{2J+1}{8\pi^2}\int d\Omega \mathcal{D}^J_{MK}\hat{R}(\Omega)|\phi(q)\rangle$$



$$|\phi^{N,Z}_{I=0,M=0}(q)\rangle = \hat{P}^N\hat{P}^Z\hat{P}^{I=0}_{M=0K=0}|\phi(q)\rangle$$

- ☐ The most computationally demanding part
- ☐ performed in the two-body matrix elements calculations

Test calculation using SO(8) solvable model

SO(8) Hamiltonian

Model: Evans et al., Nucl. Phys. A **367** (1981) 77.

$$\hat{H}_{\mathrm{SO}(8)} = -g\frac{1+x}{2}\sum_{\nu}\hat{S}^{\dagger}_{\nu}\hat{S}_{\nu} - g\frac{1-x}{2}\sum_{\mu}\hat{P}^{\dagger}_{\mu}\hat{P}_{\mu} + g_{\mathrm{ph}}\sum_{\mu\nu}\hat{\mathcal{F}}^{\mu\dagger}_{\nu}\hat{\mathcal{F}}^{\mu}_{\nu}$$

isovector pairing　　isoscalar pairing　　sigma-tau force

$$\hat{S}^{\dagger}_{\mu} = \frac{1}{\sqrt{2}}\sum_{l}\sqrt{2l+1}[c^{\dagger}_{l}c^{\dagger}_{l}]^{L=0}_{S=0,(T,T_z)=(1,\mu)}$$

$$\hat{P}^{\dagger}_{\mu} = \frac{1}{\sqrt{2}}\sum_{l}\sqrt{2l+1}[c^{\dagger}_{l}c^{\dagger}_{l}]^{L=0}_{(S,S_z)=(1,\mu),T=0}$$

$$\hat{\mathcal{F}}^{\mu}_{\nu} = \frac{1}{\sqrt{2}}\sum_{l}\sqrt{2l+1}[c^{\dagger}_{l}\bar{c}_{l}]^{L=0}_{(S,S_z)=(1,\mu),T=(1,\nu)}$$

$$\bar{c}_{l,m_l,m_s,m_\tau} = (-1)^{l+1+m_l+m_s+m_\tau}c_{l,-m_l,-m_s,-m_\tau}$$

interaction parameter : $x(g_{pp})$, g_{ph}

$x=1$ or $g_{pp}=0$: isovector phase

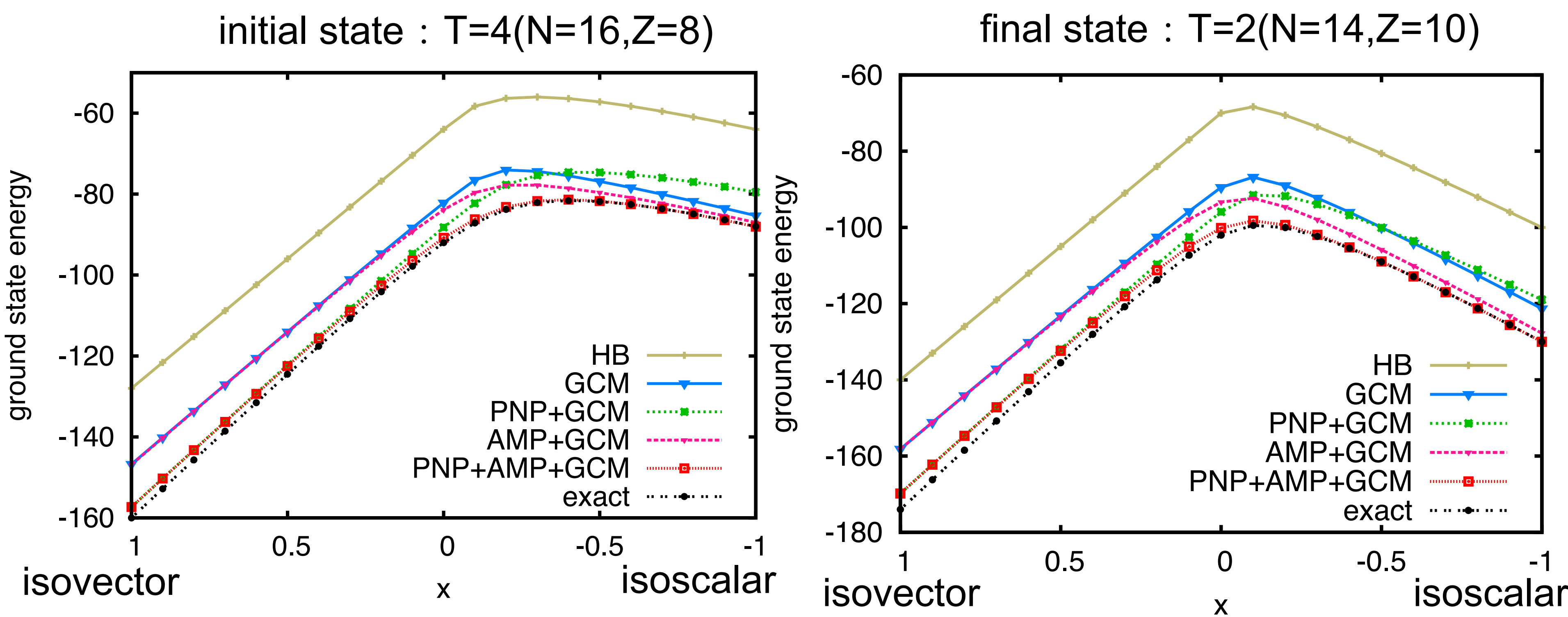
$x=0$ or $g_{pp}=g_{pair}$: SU(4) spin-isospin symmetric

$x=-1$ or $g_{pp}=\infty$: isoscalar phase

$g_{pp}/g_{pair} = (1-x) / (1+x)$

Ground state energy (g_{ph}=0)

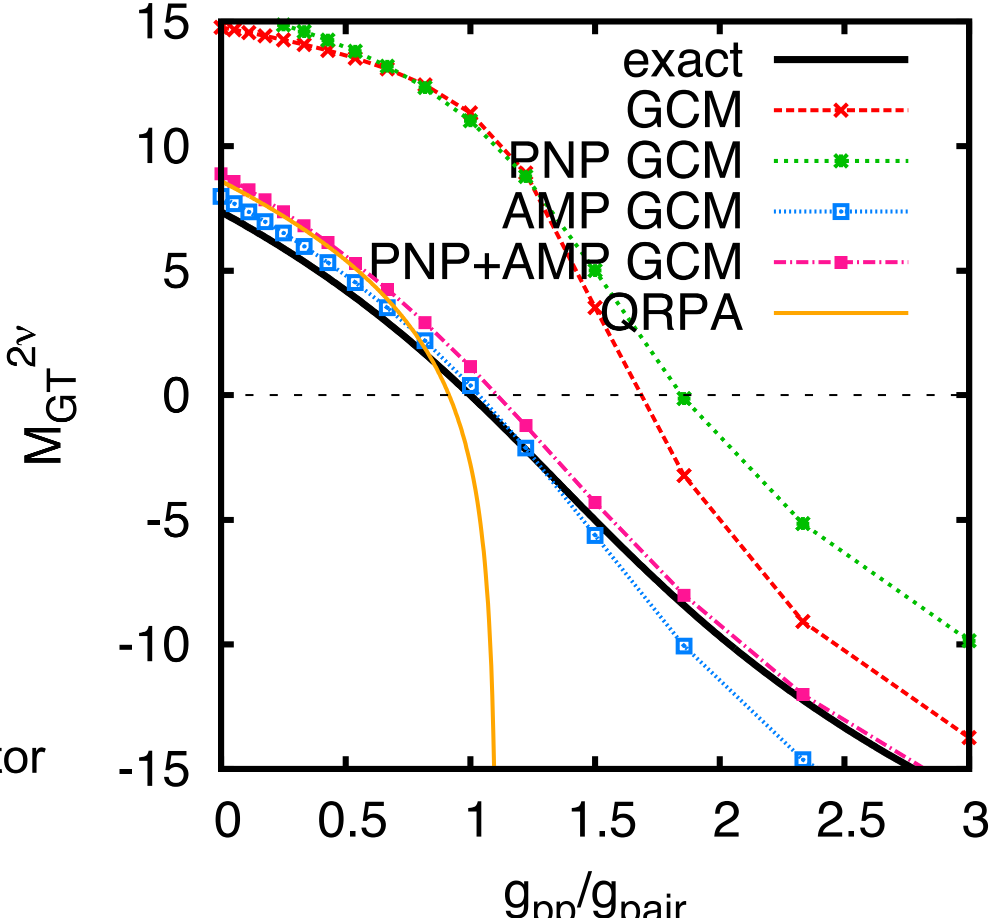
generator coordinate: isoscalar pairing P_0 (1-dim GCM)



GCM works even after the isovector-isoscalar phase transition (g.s. energy/NME)
isospin projection would be necessary to reproduce the isovector phase in this model

2ν closure GT matrix element ($g_{ph}=1.5g_{pair}$)

Ω=12、A=24 2ν closure GT matrix element of T=4→T=2



isovector isoscalar

$g_{pp}/g_{pair}=(1-x)/(1+x)$

GCM with neutron-proton pairing generator coordinate works well

0νββ nuclear matrix element calculation

$$\langle f | M_{0\nu} | i \rangle \approx \langle f | M_{0\nu}^{\mathrm{GT}} | i \rangle - \frac{g_V^2}{g_A^2} \langle f | M_{0\nu}^{\mathrm{F}} | i \rangle$$

generator coordinates to be considered (important correlations)

- ☐ quadrupole deformation (axial deformation β, triaxial deformation γ)
- ☐ isovector pairing amplitudes (like-particle, nn and pp)
- ☐ isovector pairing amplitude (np)
- ☐ isoscalar pairing amplitudes (np, three spin components)
- ☐ Gamow-Teller correlation (particle-hole στ, 9 components)

We assume axial symmetry of the system and
evaluate the Fermi and GT matrix elements separately

Fermi matrix element : β and isovector np amplitude
Gamow-Teller matrix element : β and isoscalar np amplitude (S_z=0)

$^{76}Ge \rightarrow {}^{76}Se$ ββ decay

NH and J. Engel, Phys. Rev. C **90**, 031301(R) (2014)

Hamiltonian

$$H = h_0 - \sum_{\mu=-1}^{1} g_\mu^{T=1} S_\mu^\dagger S_\mu - \frac{\chi}{2}\sum_{K=-2}^{2} Q_{2K}^\dagger Q_{2K} - g^{T=0}\sum_{\nu=-1}^{1} P_\nu^\dagger P_\nu + g_{ph}\sum_{\mu,\nu=-1}^{1} F_\nu^{\mu\dagger} F_\nu^\mu$$

sp energy | isovector pairing | quadrupole (QQ) interaction | isoscalar pairing | Gamow-Teller interaction

single-particle model space: HO N_{sh}=3, 4 (pf + sdg) shells, Ω=50

parameters：

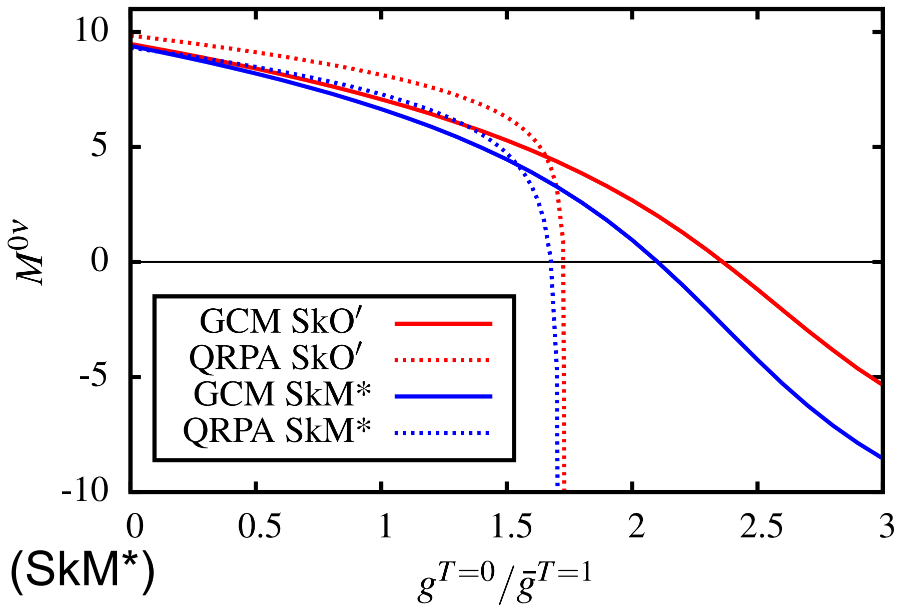
- sp energies、T=1 pp,nn pairing strength (indep.)、QQ force strength：
    - fitted to reproduce the Skyrme-HFB gaps and deformation (SkO' and SkM*)
- T=1 pn pairing strength: value that vanishes 2v closure Fermi matrix element
    - from SU(4) symmetry
- Gamow-Teller interaction g_{ph}：GT- resonance peak energy of ^{76}Ge (Skyrme QRPA)
- T=0 pn pairing: from total β+ strength of ^{76}Se

$^{76}Ge \rightarrow ^{76}Se$ 0v matrix element (1D GCM)

NH and J. Engel, Phys. Rev. C **90**, 031301(R) (2014)

generator coordinate: isoscalar pairing only, without QQ force

$$\phi = \frac{\langle P_0 + P_0^\dagger \rangle}{2}$$



g_{pp} = 1.47(SkO'), 1.56 (SkM*)

QRPA: collapse near the phase transition $g_{pp}=g^{T=0}/g^{T=1}$ ~ 1.6
GCM: smooth dependence on isoscalar pairing

Skyrme	no gph/$g^{T=0}$	no $g^{T=0}$	1D full	QRPA
SkO'	14.0	9.5	5.4	5.6
SkM*	11.8	9.4	4.1	3.5

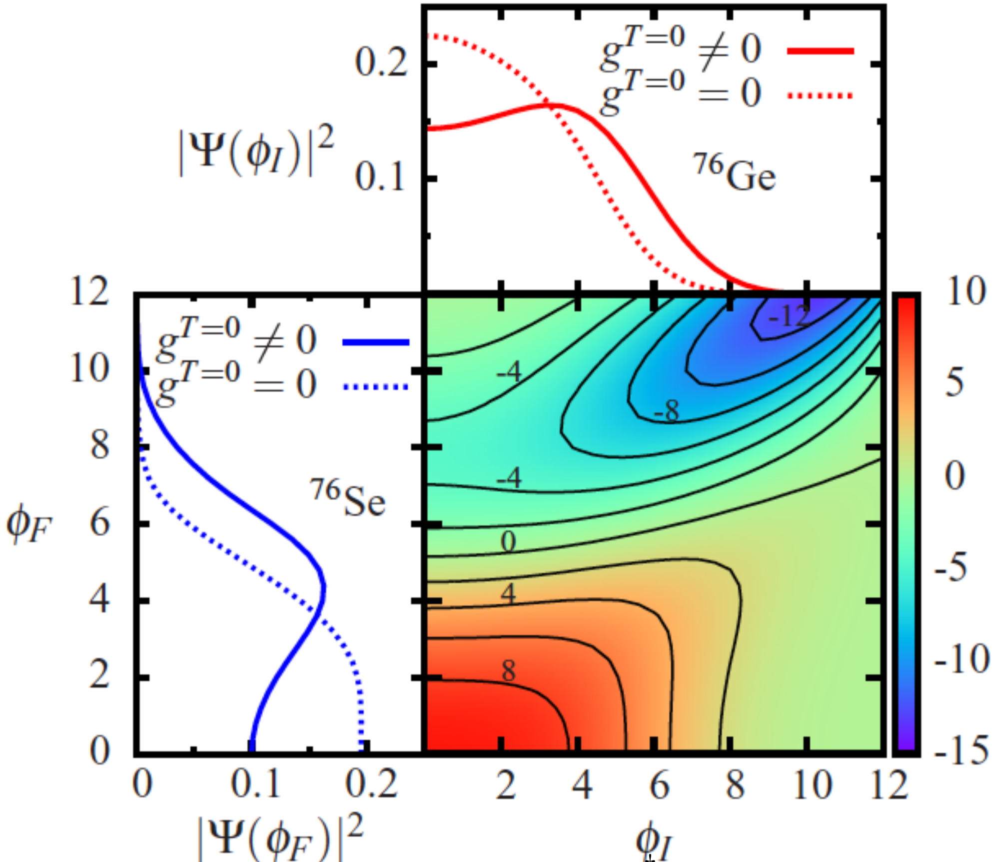
+ στ correlation

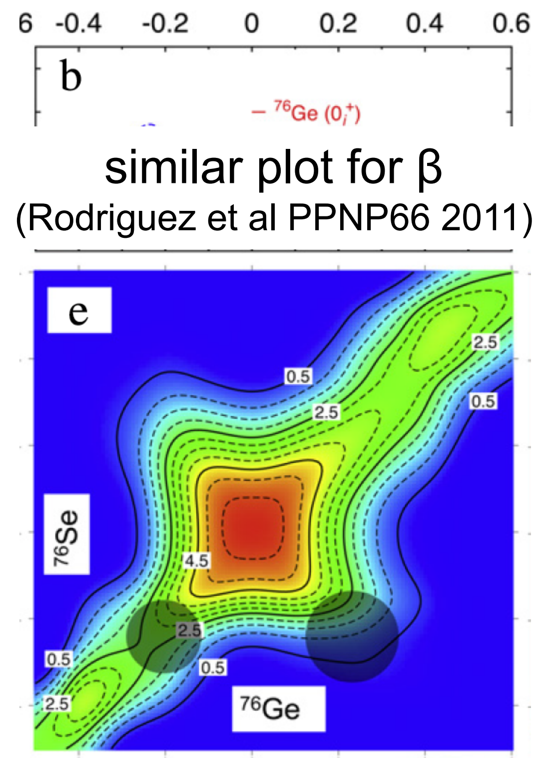
+ isoscalar pairing correlation

^{76}Ge→^{76}Se 0ν matrix element (1D GCM)

$$M^{0\nu} = \langle N-2, Z+2, I=0|\hat{M}^{0\nu}|N, Z, I=0\rangle = \sum_{qq'} \frac{f_F^*(q)\mathcal{T}(q,q')f_I(q')}{\sqrt{\mathcal{I}_F(q,q)\mathcal{I}_I(q',q')}} = \sum_{qq'} f_F^*(q)\tilde{\mathcal{T}}(q,q')f_I(q')$$

matrix element and collective wave function squared





similar plot for β
(Rodriguez et al PPNP66 2011)

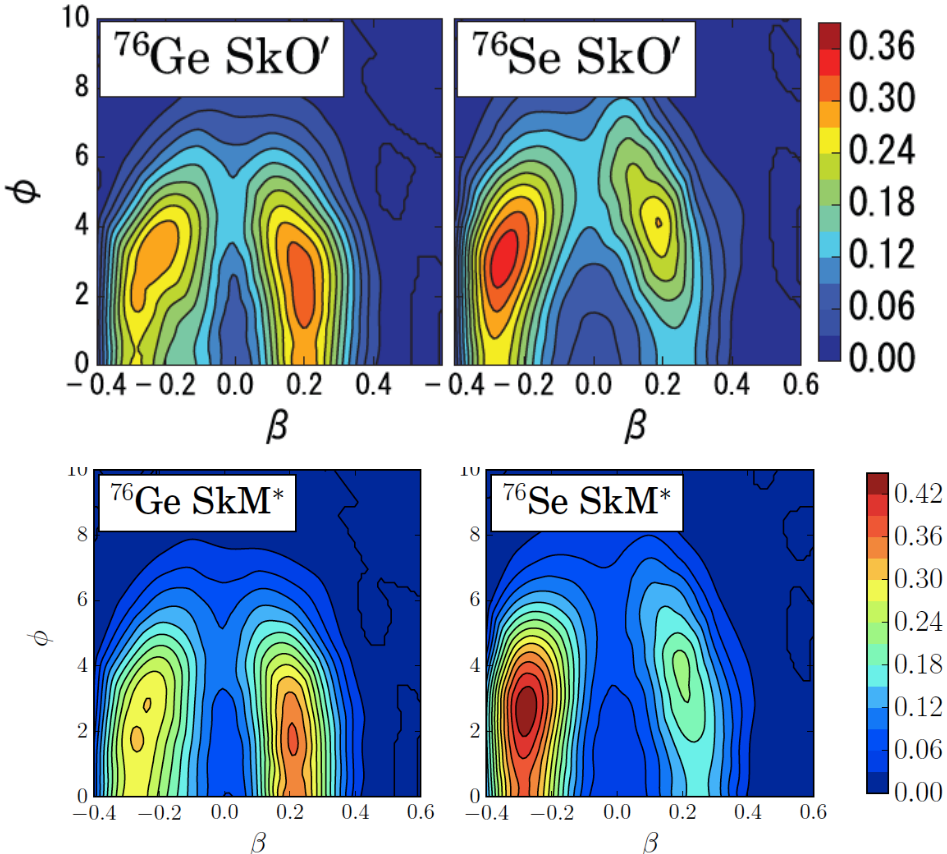
matrix element is large at the same deformation

generator coordinate: $\phi = \frac{\langle P_0 + P_0^\dagger \rangle}{2}$

- deformation: reduces the matrix element due to small initial/final state overlap
- isoscalar pairing: reduces the matrix element due to negative contribution

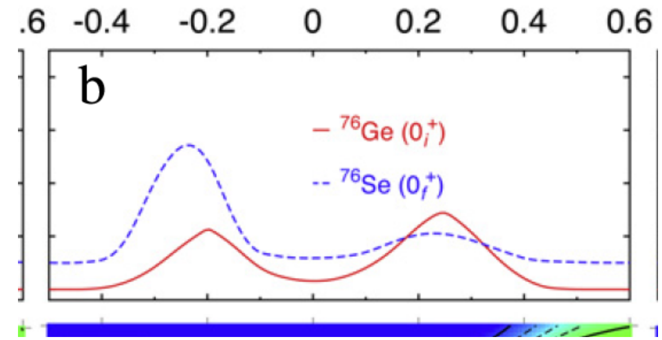
Inclusion of quadrupole deformation (2D GCM)

collective wave function squared



g_{pp} = 1.75(SkO'), 1.51 (SkM*)

Rodríguez and Martinez-Pinedo
Prog. Part. Nucl. Phys. 66 (2011) 436.



matrix element

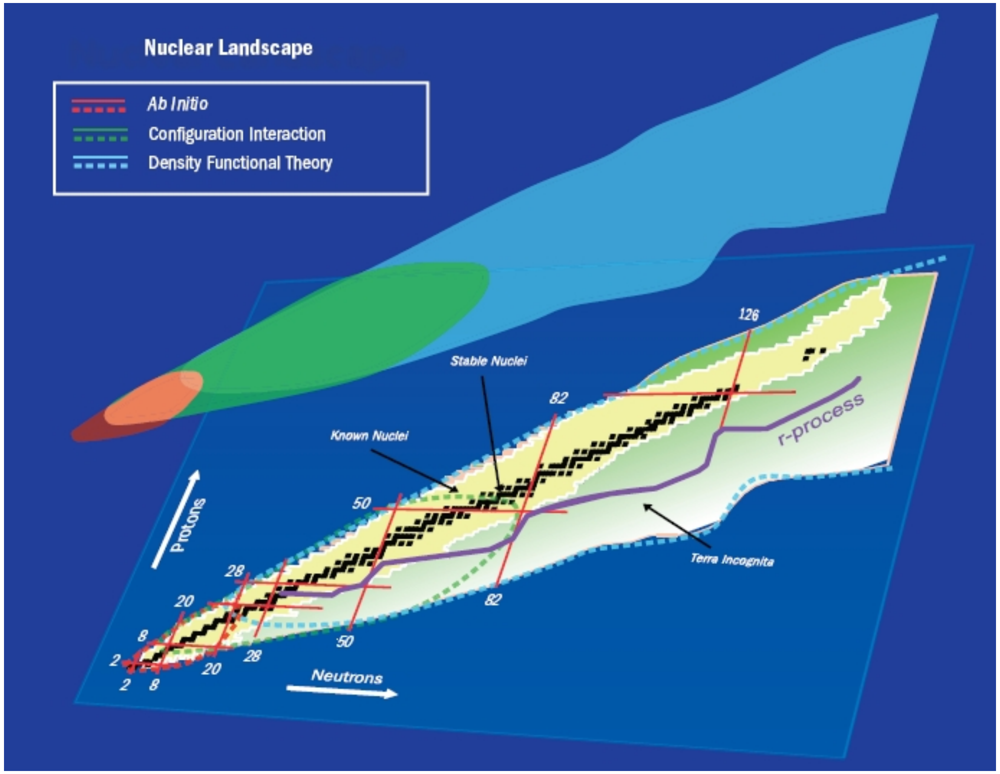
Skyrme	1D full	2D full	spherical QRPA
SkO'	5.4	4.7	5.6
SkM*	4.1	4.7	3.5

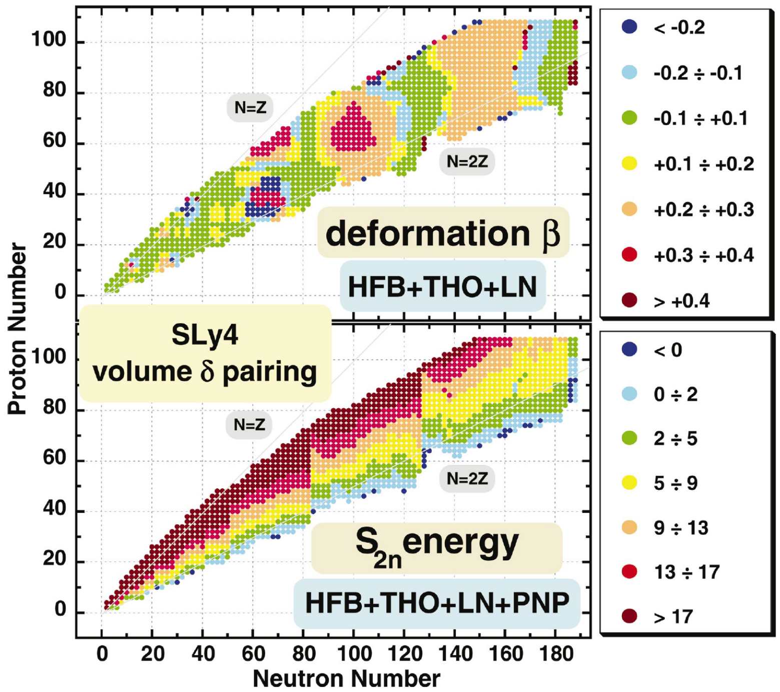
Gogny beta-GCM: 4.60
PRL **105**, 252503(2010)
Gogny beta+delta GCM: 5.55
PRL **111**, 142501(2013)
Skyrme pnQRPA SkM*: 5.1
PRC **87**, 064302(2013)
Covariant DFT beta-GCM: 6.13
PRC **91**, 024316(2015)

Future plans

things to be improved: effective interaction

1) Extension to Skyrme-DFT
2) Alternative approach to shell model for heavier system





Stoitsov et al., Phys. Rev. C **68**,054312 (2003)

Extension to Skyrme DFT

neutron-proton Skyrme DFT for GCM

- isospin-invariant DFT (formulation : Perlińska et al., Phys. Rev. C **69**, 014316 (2004))
  - ph part: HFODD Sato, et al. Phys. Rev. C **88**, 061301 (2013)
  - HFBTHO Sheikh, NH et al., Phys. Rev. C **89**, 054317 (2014)
  - pairing part: in progress.. (HFBTHO)

- determination of relevant coupling constants
  - optimization

    Mustonen and Engel, Phys. Rev. C **93**,104304 (2016)

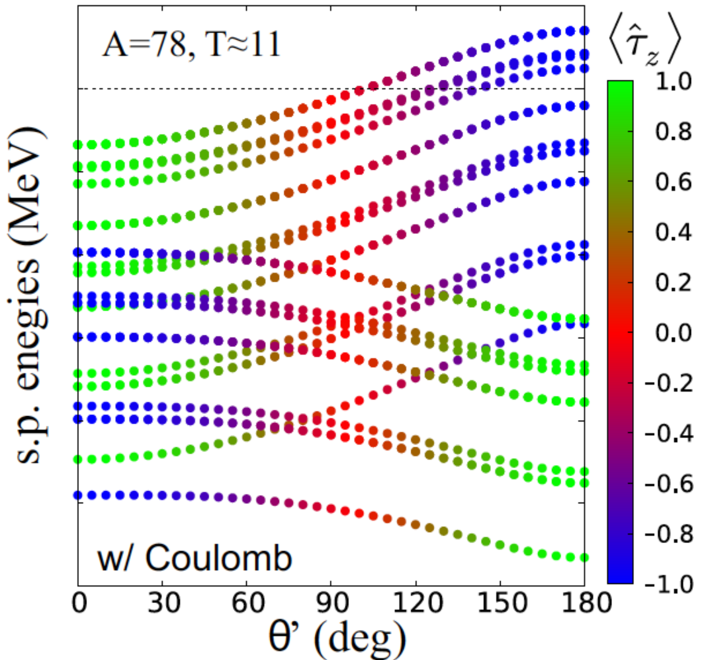
- projection problem
  - when density-dependent term is present

    Dobaczewski et al., Phys. Rev. C **76**, 054315 (2007)

  - Regularization schemes

    Lacroix, Duguet, Bender Phys. Rev. C **79** (2009)
    Satula and Dobaczewski Phys. Rev. C **90**, 054303 (2014)

T=11 isobaric analogue states



^{78}Ni ^{78}Sn

Isoscalar pairing in shell model

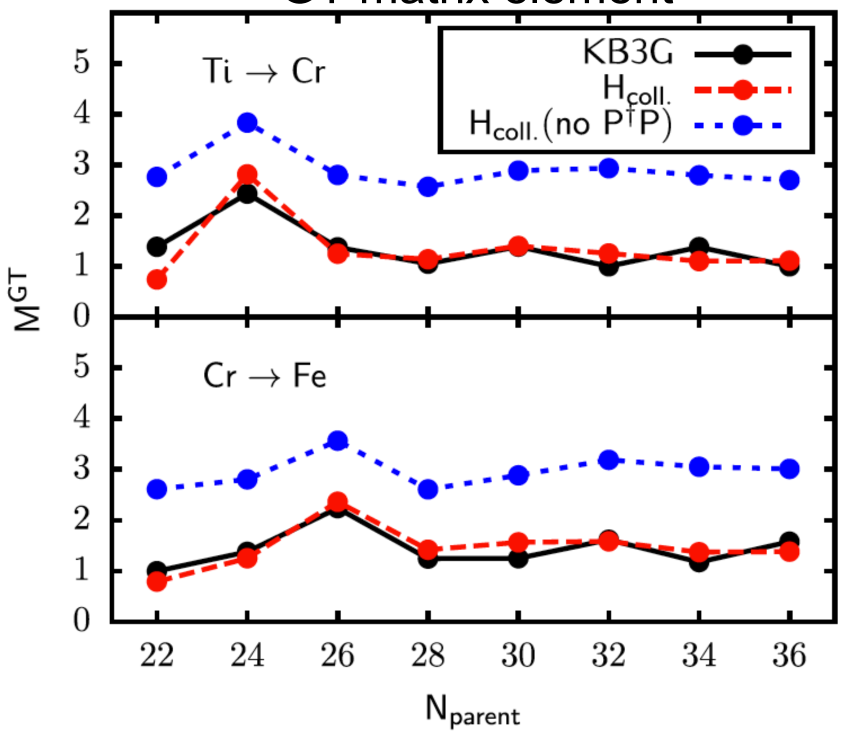
Menéndez, NH et al., Phys. Rev. C **93**, 014305 (2016)

What is the contribution of the isoscalar pairing in the shell model calculation?

Shell model: KB3G interaction (black)
separable interaction derived from KB3G using Dufour and Zuker prescription (red)
Shell model without isoscalar pairing (blue)

Dufour and Zuker, Phys. Rev. C **54**, 1641 (1996)

GT matrix element



- ☐ collective degrees of freedom (isoscalar pairing) play major role even in light systems
- ☐ suppression of the nuclear matrix element due to the isoscalar pairing

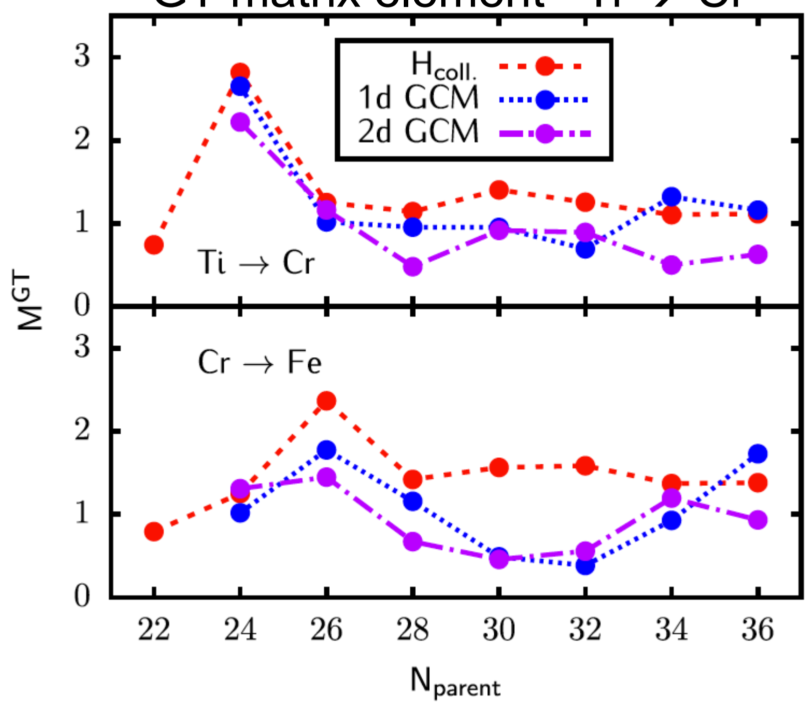
Comparison with shell model and GCM

Menéndez, NH et al., Phys. Rev. C **93**, 014305 (2016)

Can we use GCM as an alternative to shell model for heavier system?

H_{coll}: shell model(separable interaction by Dufour and Zuker) (red)
1d GCM: isoscalar pairing (blue)
2d GCM: isoscalar pairing and quadrupole deformation (purple)

GT matrix element Ti → Cr



- GCM with isoscalar pairing: good approximation to shell model
  - heavier system such as ^{136}Xe, ^{150}Nd
- deviation around magic number: improvement necessary for the no-pairing gap states

Summary

- Generator coordinate method with neutron-proton pairing
  - large-amplitude approach for NME
  - large single-particle model space
  - suppression with neutron-proton pairing

- Extension to Skyrme-DFT GCM

- Comparison with shell model approach

Collaborators

- double-beta decay
  - Jonathan Engel (UNC-CH, USA)
  - Javier Menéndez (U. Tokyo, Japan)
  - Gabriel Martínez-Pinedo (GSI, Germany)
  - Tomás Rodríguez (Madrid, Spain)
- pnDFT
  - Javid Sheikh (Kashmir Univ, India)
  - Koichi Sato (Osaka City Univ. Japan)
  - Takashi Nakatsukasa (Univ. Tsukuba, Japan)
  - Jacek Dobaczewski (York, GB/Warsaw, Poland/Jyvaskyla, Finland)
  - Witek Nazarewicz (NSCL/FRIB, MSU, USA)

Computational Resources

COMA(PACS-IX)
Center for Computational Sciences, Univ. Tsukuba