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

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Outline

- Introduction
- Generator coordinate method
- Application to SO(8) model, $^{76}$Ge double-beta decay
- Future plans
- Summary
Status of nuclear matrix element calculations


\[
\frac{1}{T_{1/2}^{0\nu}} = G_{0\nu}(Q_{\beta\beta}, Z) |M_{0\nu}|^2 \left< m_{\beta\beta} \right>^2
\]
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 $q$

$$
|\Psi(N, Z, I = 0, M = 0)\rangle = \sum f_k(q)|\phi_{I=0, M=0}^{N, Z}(q)\rangle
$$

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

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

Norm kernel

$$\mathcal{I}(q, q') = \langle \phi_{I=0, M=0}^{N, Z}(q)|\phi_{I=0, M=0}^{N, Z}(q')\rangle$$
Three steps for GCM calculations

Generator Coordinate Method

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

\[
|\Psi(N, Z, I = 0, M = 0)\rangle = \sum_{q} f_k(q) |\phi_{I=0, M=0}^{N, Z}(q)\rangle
\]

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) \( \rightarrow \) projections

step 2: projected two-body matrix elements

\[
\mathcal{H}(q, q') = \langle \phi_{I=0, M=0}^{N, Z}(q) | \hat{H} | \phi_{I=0, M=0}^{N, Z}(q') \rangle
\]

\[
\mathcal{I}(q, q') = \langle \phi_{I=0, M=0}^{N, Z}(q) | \phi_{I=0, M=0}^{N, Z}(q') \rangle
\]

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

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

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

$$f = \mathcal{I}^{-1/2} g$$

no physical meaning 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


covariant density functional theory
GCM collective wave functions (2-dim)

GC: axial quadrupole deformation and isovector like-particle pairing

Normalized nuclear matrix elements

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

\[ = \sum_{qq'} \frac{f_F^*(q)T(q, q')f_I(q')}{\sqrt{\mathcal{I}_F(q, q)\mathcal{I}_I(q', q')}} \]

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

- Quadrupole deformation
  - Gogny D1S

- Isovector pairing
  - Gogny D1S

- Octupole deformation
  - Covariant DFT

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**

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

\( \lambda_n \) and \( \lambda_p \) are determined simultaneously to satisfy the particle number expectation values.
Projections

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

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

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

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 \(\rightarrow\) 1-dim if axial symmetric Gauss-Legendre integration

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

\[ |\phi_{I = 0, M = 0}^N Z(q)\rangle = \hat{P}^N \hat{P}^Z \hat{P}^I_{M = 0 K = 0} |\phi(q)\rangle \]

- The most computationally demanding part
- performed in the two-body matrix elements calculations
**Test calculation using SO(8) solvable model**

**SO(8) Hamiltonian**

\[
\hat{H}_{SO(8)} = -g \frac{1 + x}{2} \sum_{\nu} \hat{S}^\dagger_{\nu} \hat{S}_{\nu} - g \frac{1 - x}{2} \sum_{\mu} \hat{P}^\dagger_{\mu} \hat{P}_{\mu} + g_{ph} \sum_{\mu \nu} \hat{F}^\dagger_{\mu} \hat{F}_{\nu}
\]

- Isovector pairing
- Isoscalar pairing
- Sigma-tau force

Interaction parameter: \( x(g_{pp}), g_{ph} \)

\[
x = 1 \quad \text{or} \quad g_{pp} = 0 \quad : \quad \text{Isovector phase}
\]

\[
x = 0 \quad \text{or} \quad g_{pp} = g_{\text{pair}} \quad : \quad \text{SU(4) spin-isospin symmetric}
\]

\[
x = -1 \quad \text{or} \quad g_{pp} = \infty \quad : \quad \text{Isoscalar phase}
\]

\[
g_{pp} / g_{\text{pair}} = (1-x) / (1+x)
\]

Ground state energy \((g_{ph}=0)\)

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

**initial state** : \(T=4(N=16,Z=8)\)

**final state** : \(T=2(N=14,Z=10)\)

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.
$2\nu$ closure GT matrix element ($g_{ph}=1.5g_{pair}$)

$\Omega=12, A=24$ $2\nu$ closure GT matrix element of $T=4\rightarrow T=2$

The graph shows the $M_{GT}^{2\nu}$ as a function of $g_{pp}/g_{pair} = (1-x)/(1+x)$ for different models:
- exact
- GCM
- PNP GCM
- AMP GCM
- PNP+AMP GCM
- QRPA

GCM with neutron-proton pairing generator coordinate works well.
$0\nu\beta\beta$ nuclear matrix element calculation

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

generator coordinates to be considered (important correlations)

- quadrupole deformation (axial deformation $\beta$, triaxial deformation $\gamma$)
- isovector pairing amplitudes (like-particle, $nn$ and $pp$)
- isovector pairing amplitude ($np$)
- isoscalar pairing amplitudes ($np$, three spin components)
- Gamow-Teller correlation (particle-hole $\sigma\tau$, 9 components)

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

Fermi matrix element: $\beta$ and isovector np amplitude
Gamow-Teller matrix element: $\beta$ and isoscalar np amplitude ($S_z=0$)
### Hamiltonian

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

### Parameters:

- **Sp energy**
- **Isovector pairing**
- **Quadrupole (QQ) interaction**
- **Isoscalar pairing**
- **Gamow-Teller interaction**

### Single-particle model space:

- HO $N_{sh}=3, 4$ (pf + sdg) shells, $\Omega=50$

### 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 $2\nu$ closure Fermi matrix element
  - From SU(4) symmetry
- Gamow-Teller interaction $g_{ph}$: GT- resonance peak energy of $^{76}\text{Ge}$ (Skyrme QRPA)
- $T=0$ pn pairing: from total $\beta^+$ strength of $^{76}\text{Se}$
$^{76}$Ge$\rightarrow^{76}$Se 0ν matrix element (1D GCM)


generator coordinate: isoscalar pairing only, without QQ force

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

\[ g_{pp} = 1.47 (\text{SkO}') , 1.56 (\text{SkM}^*) \]

QRPA: collapse near the phase transition \( g_{pp} = g^{T=0}/g^{T=1} \sim 1.6 \)

GCM: smooth dependence on isoscalar pairing

<table>
<thead>
<tr>
<th>Skyrme</th>
<th>no gph/$g^{T=0}$</th>
<th>no $g^{T=0}$</th>
<th>1D full</th>
<th>QRPA</th>
</tr>
</thead>
<tbody>
<tr>
<td>SkO'</td>
<td>14.0</td>
<td>9.5</td>
<td>5.4</td>
<td>5.6</td>
</tr>
<tr>
<td>SkM*</td>
<td>11.8</td>
<td>9.4</td>
<td>4.1</td>
<td>3.5</td>
</tr>
</tbody>
</table>

+ στ correlation     + isoscalar pairing correlation
$\textbf{76Ge} \rightarrow \textbf{76Se} \text{ 0v matrix element (1D GCM)}$

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

matrix element and collective wave function squared

```
g^T=0 \neq 0\quad g^T=0 = 0
```

generator coordinate: $\phi = \langle P_0 + P_0^T \rangle$

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

similar plot for $\beta$
(Rodriguez et al. PPNP66 2011)
Inclusion of quadrupole deformation (2D GCM)

collective wave function squared

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

Rodríguez and Martinez-Pinedo

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)

<table>
<thead>
<tr>
<th>Skyrme</th>
<th>1D full</th>
<th>2D full</th>
<th>spherical QRPA</th>
</tr>
</thead>
<tbody>
<tr>
<td>SkO'</td>
<td>5.4</td>
<td>4.7</td>
<td>5.6</td>
</tr>
<tr>
<td>SkM*</td>
<td>4.1</td>
<td>4.7</td>
<td>3.5</td>
</tr>
</tbody>
</table>
Future plans

things to be improved: **effective interaction**

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

Extension to Skyrme DFT

neutron-proton Skyrme DFT for GCM

  - pairing part: in progress.. (HFBTHO)

- determination of relevant coupling constants
  - optimization

- projection problem
  - when density-dependent term is present

- Regularization schemes

T=11 isobaric analogue states

\[ \langle \hat{T}_z \rangle \]
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)


- collective degrees of freedom (isoscalar pairing) play major role even in light systems
- suppression of the nuclear matrix element due to the isoscalar pairing
Can we use GCM as an alternative to shell model for heavier system?

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

- GCM with isoscalar pairing: good approximation to shell model
  - heavier system such as $^{136}\text{Xe}$, $^{150}\text{Nd}$
- 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