# Generator Coordinate Method with proton-neutron pairing amplitudes

## <u>Nobuo Hinohara</u>

Center for Computational Sciences, Univ. of Tsukuba, Japan National Superconducting Cyclotron Laboratory, Michigan State Univ., USA





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





Jun. 26, 2015

The Future of multi-reference density functional theory

# Outline

#### GCM with pn-pairing coordinates

NH and Engel, Phys. Rev. C90, 031301 (2014)

- Introduction, double-beta decay, QRPA, generator coordinate method, proton-neutron correlations
- □ application to SO(8) model, <sup>76</sup>Ge double-beta decay
- □ future plans
- □ summary

□ Finite-amplitude method for Nambu-Goldstone modes

- NH, in preparation
- □ Introduction
- □ formulation
- center of mass modes
- D pairing rotation
- □ summary

#### Double-beta decay



Review: Avignone, et al., Rev. Mod. Phys. 80, 481 (2008)

#### Nuclear Matrix Element

0v half life

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

$$M_{0\nu} \approx M_{0\nu}^{\rm GT} - \frac{g_V^2}{g_A^2} M_{0\nu}^F$$

Closure approximation

$$M_{0\nu}^{F} = \langle f | \sum_{a,b} H(r_{ab}, \bar{E}) \tau_{a}^{+} \tau_{b}^{+} | i \rangle$$
$$M_{0\nu}^{GT} = \langle f | \sum_{a,b} H(r_{ab}, \bar{E}) \vec{\sigma}_{a} \cdot \vec{\sigma}_{b} \tau_{a}^{+} \tau_{b}^{+} | i \rangle$$

H: neutrino potential ~ 1/r

Neutron-proton QRPA



-M<sup>(0)</sup>

QRPA is valid when the mean field approximation is good for ground states and system is not too close to the phase transition

# Going beyond small-amplitude approximation

#### **Generator Coordinate Method**

superposition of the projected mean fields along generator coordinates q

 $|\Psi(N,Z,I=0,M=0)\rangle = \sum_{\substack{q \ \text{weight function}}} f_k(q) \phi_{I=0,M=0}^{N,Z}(q)\rangle$ 

□ correlations along important coordinates (q: collective property: deformation, pairing...)

□ weight function is determined from variational equation (Hill-Wheeler equation)

mean field breaks symmetries and correlations are included:
 symmetry restoration: particle number and angular momentum projection

"shell model" using a small set of collective non-orthogonal basis only

Large model space based on mean field approximation

#### Phase transition / fluctuation

including order parameters in the generator coordinates

# Generator coordinate method (Gogny D1S)



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

generator coordinate: axial quadrupole deformation  $\beta$ 



Yao et al. Phys. Rev. C **91**, 024316 (2015) Song et al., Phys. Rev. C **90**,054309 (2014)

#### Neutron-proton correlation



#### GCM for nuclear matrix element

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

Generalized Hartree-Bogoliubov (spherical 3D HO basis)  $\hat{a}_{k}^{\dagger} = \sum_{l} \left( U_{lk}^{(n)} \hat{c}_{l}^{(n)\dagger} + V_{lk}^{(n)} \hat{c}_{k}^{(n)} + U_{lk}^{(p)} \hat{c}_{l}^{(p)\dagger} + V_{lk}^{(p)} \hat{c}_{k}^{(p)} \right)$   $a_{k} |\phi(q)\rangle = 0$ 

GCM with deformation and isovector np pairing



GCM with deformation and isoscalar np pairing

reliable framework for the nuclear matrix elements with neutron-proton correlation

#### Comparison with SO(8) model

SO(8) Hamiltonian: isovector, isoscalar pairing, spin-isospin ph int.  $\Omega$ =12, A=24 2nu GT matrix element of T=4 $\rightarrow$ T=2



□ Generator coordinate: isoscalar pairing  $P_0$  (S<sub>z</sub>=0, 1-dimensinoal GCM) □ Exact solution: isospin symmetric: GCM basis breaks isospin symmetry

## <sup>76</sup>Ge $\rightarrow$ <sup>76</sup>Se 0 $\nu$ matrix element (1D GCM)

NH and J. Engel, Phys.Rev.C90, 031301(R) (2014) Hamiltonian: sp energy + SO(8) + QQ force (three indep isovector pairing strengths) parameters: fitted to Skyrme SkO'/SkM\* deformation, gap g<sub>ph</sub>: GT- resonance peak of <sup>76</sup>Ge,(Skyrme HFB) g<sub>pp</sub>: exp B(GT+) of <sup>76</sup>Se pf + sdg two major shells



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

Skyrme	no gph/ g <sup>T=0</sup>	no g <sup>T=0</sup>	1D full	QRPA
SkO'	14.0	9.5	5.4	5.6
SkM*	11.8	9.4	4.1	3.5

# <sup>76</sup>Ge $\rightarrow$ <sup>76</sup>Se 0 $\nu$ matrix element (1D GCM)





matrix element is large at the same deformation

off-diagonal part of the matrix element important negative region at large isoscalar paring of final state isoscalar pairing shifts the wave function to isoscalar region

# Inclusion of quadrupole deformation (2D GCM)



#### Future plans for systematic calculation

things to be improved: effective interaction

# Alternative approach to shell model for heavier system Extension to Skyrme-DFT



#### Comparison with shell model in pf-shell nuclei

J. Menendez, NH, J. Engel, in preparation

Shell model: KB3G interaction (black)

PT1+PT0+QQ P+Q derived from Dufour and Zuker prescription (green)

Shell model without isoscalar pairing (blue)

GCM: generator coordinate: isoscalar pairing and axial deformation (red)

Dufour and Zuker, Phys. Rev. C54, 1641 (1996)



"collective" degrees of freedom (isoscalar pairing) play major role even in light systems.

alternative solution of a shell model Hamiltonian diagonalization for heavier system

# Extension to Skyrme DFT

neutron-proton DFT for generating GCM basis

isospin-invariant DFT: Perlinska et al., Phys. Rev. C 69, 014316 (2004)

current status:

neutron-proton mixing in particle-holes (HFODD/HFBTHO)

K. Sato, et al. Phys. Rev. C88, 061301 (2013) J. Sheikh, NH, et al. Phys. Rev. C89, 054317 (2014)

pairing part in progress

projection problem: regularization schemes Lacroix, Duguet, Bender Phys. Rev. C**79** (2009) Satula and Dobaczewski Phys. Rev. C**90**, 054303 (2014) ...

T=11 isobaric analogue states



## Summary

- Double-beta decay nuclear matrix elements are calculated using generator coordinate method including both axial quadrupole deformation and isoscalar/isovector protonneutron pairing degrees of freedom.
- □ Future plans
- alternative approach to shell model for heavier system
   Extension to Skyrme-DFT

Finite amplitude method for Nambu-Goldstone modes

NH, in preparation

#### Spontaneous symmetry breaking

Nambu-Goldstone (NG) mode appears as a solution of self-consistent QRPA when mean field (DFT) breaks continuous symmetries which the original EDF has

broken symmetry	mean field	NG mode in the QRPA	Kπ
translational (Galilean invariance)	center of mass fixed to the origin	center of mass motion	0-, 1-
rotational	deformation (axial or triaxial)	rotation	1+, (2+)
particle number (gauge symmetry)	pairing condensation (BCS)	pairing rotation	0+
neutron-proton (isospin symmetry)	neutron-proton mixing	isospin rotation	0+

NG mode restores the broken symmetry in the QRPA level

$$[\hat{H}_{QRPA}, \hat{\mathcal{P}}_{NG}] = i\Omega_{NG}^2 M_{TV} \hat{\mathcal{Q}}_{NG} = 0$$
  
 $[\hat{H}_{QRPA}, \hat{\mathcal{Q}}_{NG}] = -\frac{i}{M_{TV}} \hat{\mathcal{P}}_{NG}$   
 $M_{NG}$ : broken symmetry (momentum operator)

**Thouless-Valatin inertia from QRPA** 

$$[\hat{H}_{\text{QRPA}}, \hat{\mathcal{Q}}_{\text{NG}}] = -\frac{\imath}{M_{\text{TV}}} \hat{\mathcal{P}}_{\text{NG}}$$

 $M_{TV}$ : Thouless-Valatin inertia

Q<sub>NG</sub>: canonical conjugate coordinate op.

Thouless-Valatin inertia from QRPA

$$M_{\rm TV} = 2P_{\rm NG}(A+B)^{-1}P_{\rm NG}$$

Conjugate coordinate operator (not known except for center of mass motion)

$$Q_{\rm NG} = i M_{\rm NG}^{-1} (A+B)^{-1} P_{\rm NG} \ ({\rm Im} \ P_{\rm NG} = 0),$$

$$Q_{\rm NG} = -iM_{\rm NG}^{-1}(A-B)^{-1}P_{\rm NG} \ ({\rm Re} P_{\rm NG} = 0).$$

Required for spurious mode removal (FAM/iterative Arnoldi)

$$\delta\rho_{\rm cal}(\omega) = \delta\rho_{\rm phy}(\omega) + \lambda_P \delta\rho_P + \lambda_R \delta\rho_R$$
$$\delta\rho_R \equiv i[R, \rho_0] = \sum_i (|\bar{R}_i\rangle\langle\phi_i| + |\phi_i\rangle\langle\bar{R}_i|),$$



Nakatsukasa et al PRC76,024318(2007)

# **Thouless-Valatin inertia from FAM**

Strength function in PQ representation

$$S(\hat{F},\omega) = \sum_{i} \frac{1}{\omega^2 - \Omega_i^2} \left\{ \frac{1}{M_i} |\langle P_i | \hat{F} | 0 \rangle|^2 + M_i \Omega_i^2 |\langle Q_i | \hat{F} | 0 \rangle|^2 + \omega [QP]_i(\hat{F}) \right\}$$

$$[QP]_{i}(\hat{F}) \equiv i\left(\langle Q_{i}|\hat{F}|0\rangle^{*}\langle P_{i}|\hat{F}|0\rangle - \langle P_{i}|\hat{F}|0\rangle^{*}\langle Q_{i}|\hat{F}|0\rangle\right)$$

#### FAM for NG modes: (Blaizot and Ripka)

$$S(\hat{F},\omega)_{\rm NG} = \sum_{i,\Omega_i=0} \frac{1}{\omega^2} \left\{ \frac{1}{M_i} |\langle P_i | \hat{F} | 0 \rangle|^2 + \omega [QP]_i(\hat{F}) \right\}$$

external field  $F = Q_{NG}$ 

Thouless-Valatin inertia from the energy-weighted sum rule of the conjugate coordinate operator

$$M_{\rm TV}^{-1} = 2m_1(\hat{\mathcal{Q}}_{\rm NG}) = \frac{2}{2\pi i} \int_D \omega S(\hat{\mathcal{Q}}_{\rm NG}, \omega) d\omega$$

external field  $F = P_{NG}$ 

Thouless-Valatin inertia from a linear response calculation at zero energy, using a broken-symmetry operator (related to inverse energy-weighted sum rule)

$$S(\hat{\mathcal{P}}_{\mathrm{NG}},\omega) = \begin{cases} 0 & (\omega \neq \pm \Omega_i) \\ -M_{\mathrm{NG}} & (\omega = 0) \end{cases}$$

Coordinate operator is computed from the amplitudes

$$Q_{\rm NG} = iM_{\rm NG}^{-1}(A+B)^{-1}P_{\rm NG} = i\frac{X(0)+Y(0)}{2S(\hat{\mathcal{P}}_{\rm NG},0)} \quad ({\rm Im} \, P_{\rm NG}=0),$$
$$Q_{\rm NG} = -iM_{\rm NG}^{-1}(A-B)^{-1}P_{\rm NG} = i\frac{X(0)-Y(0)}{2S(\hat{\mathcal{P}}_{\rm NG},0)} \quad ({\rm Re} \, P_{\rm NG}=0).$$

Center of mass mode

trivial case 
$$\hat{\boldsymbol{Q}}_{\text{CM}} = \frac{1}{A} \sum_{i=1}^{A} \hat{\boldsymbol{r}}_{i}, \quad \hat{\boldsymbol{P}}_{\text{CM}} = -i \sum_{i=1}^{A} \hat{\boldsymbol{\nabla}}_{i} \quad M_{\text{CM}} = mA$$

finite HO basis:

translational mode is not at zero energy

$$S(\hat{\mathcal{P}}_{\rm NG}, \omega) \sim \frac{M_{\rm NG}\Omega_{\rm NG}^2}{\omega^2 - \Omega_{\rm NG}^2}$$
$$\Omega_{\rm NC}^2 = \frac{1}{1 + 1}$$

$$P_{\mathrm{NG}}^{z} = \frac{1}{S(\hat{\mathcal{P}}_{\mathrm{NG}}, 0)S(\hat{\mathcal{Q}}_{\mathrm{NG}}, 0)}$$

Response to momentum operator



HFBTHO, SLy4+volume pairing, 26Mg (oblate)

$N_{ m sh}$	$1/2m$ from $(\hat{\boldsymbol{Q}}_{\mathrm{CM}})_z$	$1/2m$ from $(\hat{P}_{\rm CM})_z$	Inglis-Belyaev	$\Omega_{\rm CM}~{\rm MeV}$	$\langle [(\hat{oldsymbol{Q}}_{ ext{CM}})_z, (\hat{oldsymbol{P}}_{ ext{CM}})_z]  angle / i$
5	20.69748	20.74676	26.04977	1.346	0.998836
10	20.78073	20.82140	25.87571	0.889	0.999310
15	20.73573	20.73232	25.73650	0.151	1.000026
20	20.73946	20.73666	25.74138	0.146	1.000041
exact	20.73553	20.73553	-	0	1

$$1/2m = A/2M_{CM}$$

Inglis-Belyaev cranking inertia does not reproduce the mass

## Pairing rotational mode

SLy4+volume pairing, 26Mg (oblate, proton number broken) Nsh=5



### Pairing rotations : realistic cases



ground states form "pairing rotational bands" proton pairing: effect of residual Coulomb significant Mixing of neutron and proton pairing rotations

when neutron and proton are in a superconducting phase

broken symmetries: neutron number and proton number NG modes (QRPA eigenmodes): two, but mixing of two TV inertias from two NG modes → three moments of inertia QRPA eigenmodes

$$\hat{N}_1 = \hat{N}_n \cos \theta + \alpha \hat{N}_p \sin \theta,$$
$$\hat{N}_2 = -\hat{N}_n \sin \theta + \alpha \hat{N}_p \cos \theta,$$

$$\hat{\Theta}_1 = \hat{\Theta}_n \cos \theta + \frac{1}{\alpha} \hat{\Theta}_p \sin \theta$$
$$\hat{\Theta}_2 = -\hat{\Theta}_n \sin \theta + \frac{1}{\alpha} \hat{\Theta}_p \cos \theta$$

Thouless-Valatin mass of eigenmodes

$$M_{1} = -S(\hat{N}_{n}, \hat{N}_{n}) \cos^{2} \theta - \alpha^{2} S(\hat{N}_{p}, \hat{N}_{p}) \sin^{2} \theta$$
$$-2\alpha S(\hat{N}_{n}, \hat{N}_{p}) \sin \theta \cos \theta,$$
$$M_{2} = -S(\hat{N}_{n}, \hat{N}_{n}) \sin^{2} \theta - \alpha^{2} S(\hat{N}_{p}, \hat{N}_{p}) \cos^{2} \theta$$
$$+2\alpha S(\hat{N}_{n}, \hat{N}_{p}) \sin \theta \cos \theta,$$

constraint from orthogonality of two modes:

$$S(\hat{N}_n, \hat{N}_n) = -2N_n(A+B)^{-1}N_n$$
  

$$S(\hat{N}_n, \hat{N}_p) = -2N_n(A+B)^{-1}N_p$$
  

$$S(\hat{N}_p, \hat{N}_p) = -2N_p(A+B)^{-1}N_p$$

 $\tan 2\theta = \frac{2\alpha S(\hat{N}_n, \hat{N}_p)}{S(\hat{N}_n, \hat{N}_n) - \alpha^2 S(\hat{N}_p, \hat{N}_p)}$ 

## Mixing of neutron and proton pairing rotations

TV inertias from two NG modes  $\rightarrow$  three moments of inertia



Recent development of finite-amplitude method for NG modes

□ Thouless-Valatin inertia

 $\square$  Coordinate operator  $\rightarrow$  useful for decoupling the spurious modes

Outlook

- paring collective Hamiltonian
- □ rotational moment of inertia, E(2+) systematics
- □ isorotation

# Collaborators

- Double-beta decay
  - □ Jon Engel (UNC-Chapel Hill, USA)
  - Javier Menendez (Tokyo, Japan)

DFT

- Javid Sheikh (Kashmir, India)
- Koichi Sato (RIKEN, Japan)
- Takashi Nakatsukasa (Tsukuba/RIKEN, Japan)
- Jacek Dobaczewski (York/Warsaw/Jyvaskyla)
- Witold Nazarewicz (NSCL/FRIB, MSU, USA)

#### □ FAM

- Markus Kortelainen (Jyvaskyla, Finland)
- Erik Olsen (MSU, USA)
- U Witold Nazarewicz

#### Calculation

Killdevil, UNC-Chapel Hill





KRAKEN XT5 (NICS,UT)



