

Angular-momentum-projection
 method to approach nuclear
 many-body result

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### Nuclear structure models

- Shell-model diagonalization method
  - Based on quantum mechanical principles
  - Growing computer power helps extending applications
  - A single configuration contains no physics
  - Huge basis dimension required, severe limit in applications
- Mean-field approximations
  - Applicable to any size of systems
  - Fruitful physics around minima of energy surfaces
  - No configuration mixing, results depend on quality of mean-field
  - States with broken symmetry, cannot study transitions
- Algebraic models
  - Based on symmetries, simple and elegant
  - Serve as important guidance for complicated calculations

### How to treat deformed nuclei

- Most nuclei in the nuclear chart are deformed. To describe a deformed nucleus, a spherical shell model loses advantages.
- One can start from a deformed basis by breaking the rotational symmetry spontaneously.
- Then apply angular-momentum-projection technique to recover the symmetry.
  - important correlations prepared through a better mean-field
  - intrinsic states classified with well-defined physical meanings
  - these states transformed to the laboratory frame
  - diagonalization performed in the (angular-momentum) projected basis
  - results may be interpreted by algebraic models

#### Deformed basis vs spherical basis

#### Rotational spectrum in <sup>48</sup>Cr

- Exp. data:
  - Brandolini et al, NPA 642 (1998) 387
- PSM:
  - Hara, Sun and Mizusaki, *PRL* 83 (1999) 1922
  - Deformed basis with a.-m. projection;
     Basis states ~ 50
- pf-SM:
  - Caurier et al., PRL 75 (1995) 2466
  - Conventional M-scheme spherical shell model; Basis states ~ 2 million



#### A method related to mean-field and shell models

- Angular-momentum projection method based on deformed mean-field solutions
  - Start from intrinsic bases (e.g. solutions of deformed meanfield) and select most relevant configurations
  - Use angular momentum projection technique to transform them to laboratory basis (many-body technique)
  - Diagonalize Hamiltonian in the projected basis (configuration mixing, a shell-model concept)
- It is an efficient way, and probably the only way to treat heavy, deformed nuclei microscopically in a shell model concept
- Example: Projected Shell Model
  - K. Hara, Y. Sun, Int. J. Mod. Phys. E 4 (1995) 637

## Projected Shell Model (PSM)

- Take a set of deformed (quasi)particle states (e.g. solutions of HF, HFB or Nilsson + BCS)
- Select configurations (qp vacuum + multi-qp states near the Fermi level)
- Project them onto good angular momentum (if necessary, also parity, particle number) to form a basis in lab frame
- If necessary, superimpose configurations belonging to different qp representations (the GCM-concept)
- Diagonalize a two-body Hamiltonian in projected basis

## Comparison with other models

- Comparison with spherical shell model
  - No problem with basis size
  - PSM basis constructed by physical guidance
- Comparison with mean-field models
  - Violated symmetries restored
  - Configuration mixing implemented
- Comparison with algebraic models
  - Do not require a symmetry to start with
  - Yet the PSM results can be discussed with symmetry ideas
- Comparison with the Tuebingen, Tokyo approaches
  - Different in preparation of basis and in effective interactions

#### Emergence of SU(3) symmetry

- Nearly perfect SU(3) symmetry emerges from a.-m.-projection
  - Project on separate BCS vacuum of  $|\phi_{V}\rangle$  and  $|\phi_{\pi}\rangle$ , then couple the projected states  $|I_{\sigma}\rangle = N^{I}\hat{P}^{I}|\phi_{\sigma}\rangle$ to form the basis  $|(I_{V} \otimes I_{\pi})I\rangle$
  - Diagonalize the Hamiltonian in the coupled basis
  - Multi-phonon scissors mode is predicted
  - Sun, Wu, Guidry *et al.*, *PRL* 80 (1998) 672; *NPA* 703 (2002) 130



#### • • • $\gamma$ -vibrational states

- γ-vibration states cannot be obtained when axial symmetry in the basis states is assumed
- Need 3-dimensional angular-momentum projection performed on a triaxially deformed basis



Y. Sun et al. Phys. Rev. C 61 (2000) 064323

#### γ-deformed multi-qp excitations

- 0-phonon (K=0), 1-phonon (K=2), 2-phonon (K=4) γ-vibrational bands
  - Y. Sun et al, Phys. Rev. C61 (2000) 064323
- Each phonon γ-vibrational mode can couple with qp states – generalization of the usual concept of γvibration
  - Sheikh *et al.*, Phys. Rev. C77 (2008) 034313; Nucl. Phys. A824 (2009) 58



## Basic structure

• Ansatz of wavefunction:  $\Psi_{M}^{I} = \sum_{\kappa} f_{\kappa} \hat{P}_{MK_{\kappa}}^{I} |\phi_{\kappa}\rangle$ 

with the projector: 
$$\hat{P}_{MK}^{I} = \frac{2I+1}{8\pi^{2}} \int d\Omega D_{MK}^{I}(\Omega) \hat{D}(\Omega)$$

• The eigenvalue equation:  $\sum_{\kappa} \left( H_{\kappa\kappa'}^{I} - E N_{\kappa\kappa'}^{I} \right) f_{\kappa'} = 0$ 

with matrix elements:  $H_{\kappa\kappa'}^{I} = \langle \phi_{\kappa} | \hat{H} \hat{P}_{\kappa\kappa'}^{I} | \phi_{\kappa'} \rangle \qquad N_{\kappa\kappa'}^{I} = \langle \phi_{\kappa} | \hat{P}_{\kappa\kappa'}^{I} | \phi_{\kappa'} \rangle$ 

• The Hamiltonian is diagonalized in the projected basis  $\left\{ \hat{P}_{\scriptscriptstyle MK}^{\scriptscriptstyle I} \big| \phi_{\scriptscriptstyle \kappa} \right\}$ 

#### a.-m.-projected multi-quasi-particle states based on a fixed deformation

• Even-even nuclei:

 $\left\{ \hat{P}_{MK}^{I} | 0 \rangle, \hat{P}_{MK}^{I} \alpha_{\nu}^{+} \alpha_{\nu}^{+} | 0 \rangle, \hat{P}_{MK}^{I} \alpha_{\pi}^{+} \alpha_{\pi}^{+} | 0 \rangle, \hat{P}_{MK}^{I} \alpha_{\nu}^{+} \alpha_{\nu}^{+} \alpha_{\pi}^{+} \alpha_{\pi}^{+} | 0 \rangle, \ldots \right\}$ 

• Odd-odd nuclei:

 $\left\{\hat{P}_{MK}^{I}\alpha_{v}^{+}\alpha_{\pi}^{+}\big|0\right\rangle, \hat{P}_{MK}^{I}\alpha_{v}^{+}\alpha_{v}^{+}\alpha_{v}^{+}\alpha_{\pi}^{+}\big|0\right\rangle, \hat{P}_{MK}^{I}\alpha_{v}^{+}\alpha_{\pi}^{+}\alpha_{\pi}^{+}\big|0\right\rangle, \hat{P}_{MK}^{I}\alpha_{v}^{+}\alpha_{v}^{+}\alpha_{v}^{+}\alpha_{v}^{+}\alpha_{\pi}^{+}\alpha_{\pi}^{+}\big|0\right\rangle, \ldots\right\}$ 

- Odd-neutron nuclei:  $\left\{ \hat{P}_{MK}^{I} \alpha_{\nu}^{+} |0\rangle, \hat{P}_{MK}^{I} \alpha_{\nu}^{+} \alpha_{\pi}^{+} \alpha_{\pi}^{+} |0\rangle, \hat{P}_{MK}^{I} \alpha_{\nu}^{+} \alpha_{\nu}^{+} \alpha_{\nu}^{+} \alpha_{\pi}^{+} \alpha_{\pi}^{+} |0\rangle, \ldots \right\}$
- Odd-proton nuclei:  $\left\{ \hat{P}_{MK}^{I} \alpha_{\pi}^{+} | 0 \rangle, \hat{P}_{MK}^{I} \alpha_{\nu}^{+} \alpha_{\nu}^{+} \alpha_{\pi}^{+} | 0 \rangle, \hat{P}_{MK}^{I} \alpha_{\nu}^{+} \alpha_{\nu}^{+} \alpha_{\pi}^{+} \alpha_{\pi}^{+} \alpha_{\pi}^{+} | 0 \rangle, \ldots \right\}$

# Hamiltonian and single particle space

- Hamiltonian  $H = H_0 \sum_{\lambda} \frac{\chi_{\lambda}}{2} \sum_{\mu} Q_{\lambda\mu}^+ Q_{\lambda\mu} G_M P^+ P G_Q \sum_{\mu} P_{\mu}^+ P_{\mu}$  Interaction strengths  $\chi$  is related to deformation  $\varepsilon$  by  $\chi_{\tau\tau'} = \frac{2/3 \varepsilon \hbar \omega_{\tau} \hbar \omega_{\tau'}}{\hbar \omega_n \langle Q_0 \rangle_n + \hbar \omega_p \langle Q_0 \rangle_p}$ 
  - $G_{\rm M}$  is determined by observed even-odd mass difference
  - $G_{\rm O}$  is assumed to be proportional to  $G_{\rm M}$  with a ratio ~ 0.20
- Single particle space
  - Three major shells for neutrons or protons (normally deformed) four major shells for neutrons or protons (super-deformed)
  - For example, for rare-earth nuclei, N = 4, 5, 6 for neutrons N = 3, 4, 5 for protons

#### Example of a deformed rotor

- Angular-momentum-projected energy calculation shows a deep prolate minimum for a superheavy nucleus
  - A very good rotor with axially-symmetric deformed shape
  - Quasi-particle excitations based on the same deformed potential



#### Multi-quasiparticle excitations

- 0-, 2-, 4-qp states of <sup>178</sup>Hf
- Data:
  - S.M. Mullins *et al*, *Phys. Lett.* B 393 (1997) 279
- Theory:
  - Y. Sun *et al*, *Phys. Lett.* B 589 (2004) 83



#### Calculation of matrix elements for multi-quasiparticle states

• If a multi-quasiparticle state is written as  $|\Phi_{\kappa}\rangle$ , then the central task is to calculate  $\mathcal{H}_{\kappa\kappa'} = \langle \Phi_{\kappa} | \hat{H}[\Omega] | \Phi_{\kappa'} \rangle$ ,

with 
$$[\Omega] = \frac{\hat{R}(\Omega)}{\langle \Phi | \hat{R}(\Omega) | \Phi \rangle}$$

• For example, a norm matrix element

$$\mathcal{N}_{\kappa\kappa'} = \langle \Phi | a_1 \cdots a_n [\Omega] a_{1'}^{\dagger} \cdots a_{n'}^{\dagger} | \Phi \rangle$$

can be written as combinations of

$$A_{\nu\nu'}(\Omega) \equiv \langle \Phi | [\Omega] a_{\nu}^{\dagger} a_{\nu'}^{\dagger} | \Phi \rangle = (V^*(\Omega) U^{-1}(\Omega))_{\nu\nu'},$$
  

$$B_{\nu\nu'}(\Omega) \equiv \langle \Phi | a_{\nu} a_{\nu'}[\Omega] | \Phi \rangle = (U^{-1}(\Omega) V(\Omega))_{\nu\nu'},$$
  

$$C_{\nu\nu'}(\Omega) \equiv \langle \Phi | a_{\nu}[\Omega] a_{\nu'}^{\dagger} | \Phi \rangle = (U^{-1}(\Omega))_{\nu\nu'},$$

#### Multi-quasiparticle computation using the Pfaffian algorithm

- Calculation of projected matrix elements usually uses the generalized Wick theorem
- A matrix element having n (n') qp creation or annihilation operators respectively on the left- (right-) sides of the rotation operator contains (n + n - 1)!! terms in the expression – a problem of combinatorial complexity
- Use of the Pfaffian algorithm:
  - L.M. Robledo, Phys. Rev. C 79 (2009) 021302(R).
  - L.M. Robledo, Phys. Rev. C 84 (2011) 014307.
  - T. Mizusaki, M. Oi, Phys. Lett. B 715 (2012) 219.
  - M. Oi, T. Mizusaki, Phys. Lett. B 707 (2012) 305.
  - T. Mizusaki, M. Oi, F.-Q. Chen, Y. Sun, Phys. Lett. B 725 (2013) 175



L.-J. Wang et al. *Phys. Rev.* C90 (2014) 011303(R)

#### Example for very high-spin states



# Example of softness – no definite shapes



Mean-field calculation shows a spherical shape.

Projected calculation shows shallow minima separated by a low energy barrier.

Shapes may be developed with rotation.





Angular-momentum-projected energy surfaces as functions of  $\epsilon$  and  $\gamma$ 

#### Description of a system with soft potential surfaces

- A spherical nucleus described by spherical shell model.
- A deformed nucleus described by deformed shell model.
- Transitional ones are *difficult*. A better wavefunction is a superposition of many states of deformation parameter β.

$$\begin{split} \left| \Psi^{I} \right\rangle &= \int f^{I}(\beta) \left| \Phi^{I}(\beta) \right\rangle d\beta \\ \left| \Phi^{I}(\beta) \right\rangle &= \hat{P}^{I} \left| \phi(\beta) \right\rangle \end{split}$$



Schematic energy potential for spherical (red), transitional (dashed), and deformed (blue) nuclei.

$$\{\boldsymbol{\beta}\} = \{\boldsymbol{\beta}_1, \boldsymbol{\beta}_2, \boldsymbol{\beta}_3, \dots\}$$

# Generate Coordinate Method (GCM)

• GCM starts with a general ansatz for a trail wave function

$$\left|\Psi\right\rangle = \int da f(a) \left|\Phi(a)\right\rangle$$

with  $\{a\} = a_1, a_2, \dots, a_i$  being generate coordinates

• f(a) is a weight function, determined by solving the Hill-Wheeler Equation

$$\mathcal{H}f = E\mathcal{N}f$$

with the overlap functions

$$\mathcal{H}(a,a') = \left\langle \Phi(a) | \hat{H} | \Phi(a') \right\rangle, \mathcal{N}(a,a') = \left\langle \Phi(a) | \Phi(a') \right\rangle$$

#### Projected Generate Coordinate Method (PGCM)

• Choosing generate coordinate as  $\mathcal{E}_2$ , an improved wave function

$$\left|\Psi^{I,N}\right\rangle = \int d\varepsilon_2 f^{I,N}(\varepsilon_2) \left|\Phi^{I,N}(\varepsilon_2)\right\rangle$$
$$\left|\Phi^{I,N}(\varepsilon_2)\right\rangle = \hat{P}^I \hat{P}^N \left|\Phi_0(\varepsilon_2).\right\rangle$$

• Hamiltonian

$$\hat{H} = \hat{H}_0 - \frac{\chi}{2} \sum_{\mu} \hat{Q}^+_{\mu} \hat{Q}_{\mu} - G_M \hat{P}^+ \hat{P} - G_Q \sum_{\mu} \hat{P}^+_{\mu} \hat{P}_{\mu}$$

with a fixed set of parameters (fixed  $\chi$ ,  $G_M$ , and  $G_Q$ ) is diagonalized for a chain of isotopes.

F.-Q. Chen, Y. Sun, P. Ring, Phys. Rev. C88 (2013) 014315

#### Energy levels

- Comparison of energy levels of 2<sub>1</sub><sup>+</sup>, 4<sub>1</sub><sup>+</sup>, and 6<sub>1</sub><sup>+</sup> of ground band and excited 0<sub>2</sub><sup>+</sup> state
  - Exp data (filled squares)
  - Calculations (open circles)

for isotopes from N=90 (transitional) to N=98 (well-deformed) nuclei



## Spherical-deformed shape phase transition

- Drastic changes in electric quadrupole transition B(E2, 2<sup>+</sup> → 0<sup>+</sup>) from vibrator <sup>152</sup>Gd (N=88), to critical point <sup>154</sup>Gd (N=90), to rotor <sup>156-160</sup>Gd (N>90).
- Black squares show if use only one fixed deformation  $\varepsilon_2$  in the calculation, transitional feature cannot be reproduced.



# Distribution function

- The Hill-Wheeller Equation diagonalizes the Hamiltonian in a non-orthogonal basis, and therefore,  $f(\varepsilon_2)$  is not a proper quantity to analyze the GSM wave function.
- Transformation of  $f(\varepsilon_2)$  to an orthogonal basis gives

$$g(\boldsymbol{\varepsilon}_2) = \int \mathscr{N}^{1/2}(\boldsymbol{\varepsilon}_2, \boldsymbol{\varepsilon}_2') f(\boldsymbol{\varepsilon}_2') d\boldsymbol{\varepsilon}_2'$$

which can be used to present the distribution of the GCM wave functions.

•  $g^2(\varepsilon_2)$  represent the probability function.

#### Distribution function of deformation



Calculated distribution function of deformation for the first three 0<sup>+</sup> states in <sup>154</sup>Gd and <sup>160</sup>Gd

#### Probability function of deformation



Calculated probability function of deformation for ground state  $0_1^+$  and excited  $0_2^+$  state in <sup>154</sup>Gd and <sup>160</sup>Gd.

## Probability function of deformation

- Peak of the Gaussian defines deformation
  - <sup>160</sup>Gd being more deformed than <sup>154</sup>Gd
- The distribution is wider for <sup>154</sup>Gd
  - reflecting the softness of this nucleus
- The distribution for  $0_2^+$  is much more fragmented
  - reflecting a vibrational nature of these states
- For 0<sub>1</sub><sup>+</sup>, system stays mainly at system's deformation with the largest probability
- For 0<sub>2</sub><sup>+</sup>, system shows two peaks having different heights lying separately at both sides of the equilibrium
  - indicating an anharmonic oscillation
  - prefering to have a larger probability in the site of larger deformation

## β-decay & electron-capture in stars (with temperature)

- Stellar weak-interaction rates are important for resolving astrophysical problems
  - for nucleosynthesis calculations
  - for core collapse supernova modeling
- Calculation of transition matrix element
  - essentially a nuclear structure problem
  - necessary to connect thermally excited parent states with many daughter states
  - for both allowed and forbidden GT transitions



#### Stellar enhancement of decay rate

• A stellar enhancement can result from the thermal population of excited states

$$\lambda_{\beta} = \sum_{i} \left( p_{i} \times \sum_{j} \lambda_{\beta i j} \right)$$
$$p_{i} = \frac{\left(2I_{i} + 1\right) \times \exp\left(-E_{i} / kT\right)}{\sum_{m} \left(2I_{m} + 1\right) \times \exp\left(-E_{m} / kT\right)}$$

• Examples in the s-process

F. Kaeppeler, Prog. Part. Nucl. Phys. 43 (1999) 419



# Transition matrix elements in the projected basis

• Gamow-Teller rate 
$$B(GT) = \frac{2I_f + 1}{2I_i + 1} \left\langle \psi_{I_f} \middle| \hat{\beta}^{\pm} \middle| \psi_{I_i} \right\rangle^2$$

• Wavefunction  $\Psi_{M}^{I} = \sum_{\kappa} f_{\kappa} \hat{P}_{MK_{\kappa}}^{I} |\phi_{\kappa}\rangle$ 

• e-e system 
$$|\phi_e(\varepsilon_e)\rangle = \{ |\varepsilon_e\rangle, b_v^+ b_v^+|\varepsilon_e\rangle, b_\pi^+ b_\pi^+|\varepsilon_e\rangle, b_v^+ b_v^+ b_\pi^+|\varepsilon_e\rangle, \cdots \}$$

• o-o system 
$$|\phi_o(\varepsilon_o)\rangle = \{ a_v^+ a_\pi^+ | \varepsilon_o\rangle, a_v^+ a_v^+ a_\nu^+ a_\pi^+ | \varepsilon_o\rangle, a_v^+ a_\pi^+ a_\pi^+ a_\pi^+ | \varepsilon_o\rangle, \cdots \}$$

• Overlapping matrix element (K. Tanabe *et al.*, *PRC* 59 (1999) 2494).  $\langle \phi_o(\varepsilon_o) | \hat{O} \hat{P}^I_{K_o K_e} | \phi_e(\varepsilon_e) \rangle \sim \int d\Omega D^I_{K_o K_e}(\Omega) \langle \phi_o(\varepsilon_o) | \hat{O} \hat{R}(\Omega) | \phi_e(\varepsilon_e) \rangle$ 

# The interactions

• Total Hamiltonian  $\hat{H} = \hat{H}_0 + \hat{H}_{QP} + \hat{H}_{GT}$ 

Quadrupole + monopole-pairing + quadrupole-pairing

$$\hat{H}_{QP} = -\frac{1}{2}\chi_{QQ}\sum_{\mu}\hat{Q}_{2\mu}^{\dagger}\hat{Q}_{2\mu} - G_M\hat{P}^{\dagger}\hat{P} - G_Q\sum_{\mu}\hat{P}_{2\mu}^{\dagger}\hat{P}_{2\mu}$$

• Charge-exchange (Gamow-Teller)

$$\hat{H}_{GT} = + 2\chi_{GT} \sum_{\mu} \hat{\beta}_{1\mu}^{-} (-1)^{\mu} \hat{\beta}_{1-\mu}^{+} - 2\kappa_{GT} \sum_{\mu} \hat{\Gamma}_{1\mu}^{-} (-1)^{\mu} \hat{\Gamma}_{1-\mu}^{+}$$
$$\hat{\beta}_{1\mu}^{-} = \sum_{\pi,\nu} \langle \pi | \sigma_{\mu} \tau_{-} | \nu \rangle c_{\pi}^{\dagger} c_{\nu}, \quad \hat{\beta}_{1\mu}^{+} = (-)^{\mu} (\beta_{1-\mu}^{-})^{\dagger}$$
$$\hat{\Gamma}_{1\mu}^{-} = \sum_{\pi,\nu} \langle \pi | \sigma_{\mu} \tau_{-} | \nu \rangle c_{\pi}^{\dagger} c_{\bar{\nu}}^{\dagger}, \quad \hat{\Gamma}_{1\mu}^{+} = (-)^{\mu} (\Gamma_{1-\mu}^{-})^{\dagger}$$

• Kuz'min & Soloviev, Nucl. Phys. A 486 (1988) 118

#### Distribution of B(GT)

- Initial state: ground state in even-even nucleus
- Final states: all 1<sup>+</sup> states in odd-odd nucleus
- Ikeda sum-rule fulfilled

$$S(\mathrm{GT}^{-}) - S(\mathrm{GT}^{+})$$

$$= \sum_{f} B(GT^{-}, i \to f) - \sum_{f} B(GT^{+}, i \to f)$$

$$= \sum_{f,\mu} |\langle \Psi_{f} | \hat{\beta}_{1\mu}^{-} | \Psi_{i} \rangle|^{2} - \sum_{f,\mu} |\langle \Psi_{f} | \hat{\beta}_{1\mu}^{+} | \Psi_{i} \rangle|^{2}$$

$$= 3(N - Z).$$



#### • • • | B(GT) and log *ft* in <sup>164</sup>Ho $\rightarrow$ <sup>164</sup>Dy



Z.-C. Gao, Y. Sun, Y.-S. Chen, PRC 74 (2006) 054303



### • • • Summary

- Angular momentum projection is an efficient way to approach the nuclear many-body problem with the shell model concept.
- Projected Shell Model is a practical example.
  - Start from Nilsson + BCS quasiparticle states
  - Perform angular-momentum-projection on (multi-quasiparticle) states
  - Improve the PSM wave function by superimposing projected states with different deformation
  - Diagonalize the Hamiltonian in the projected basis
- Phaffian algorithm can help to simplify numerical calculations
  - Computer code can be developed when large number of quasiparticle excitations are included.

## Collaboration

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