Recent development of projected shell model based on many-body techniques

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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 depending 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

### Deformed basis vs spherical basis

- Most nuclei are deformed. To describe a deformed nucleus, a spherical shell model needs a huge configuration space, thus has no obvious advantage.
- J.P. Elliott was the first to take the advantage of a deformed many-body basis and developed the SU(3) shell model.
- For heavy nuclei, the original Elliott SU(3) scheme is no longer valid;
  - one may use generalized SU(3) schemes if symmetries exist.
  - or more generally, one can start from a deformed basis and apply angular-momentum-projection technique.

# • • • A method related to mean-field, shell model, algebraic models

- Angular-momentum projection method based on 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)
  - Numerical results can be discussed using algebraic models

The Projected Shell Model:

• K. Hara, Y. Sun, Int. J. Mod. Phys. E 4 (1995) 637

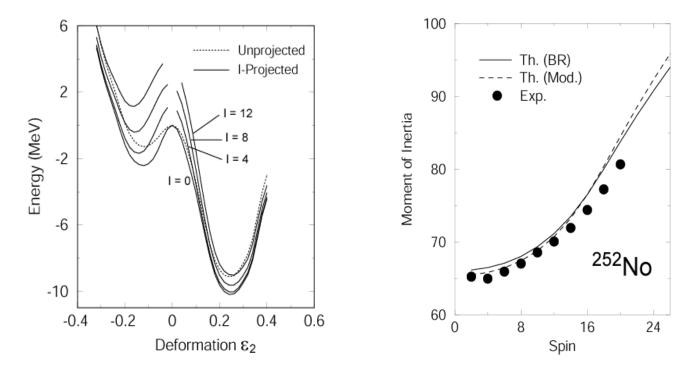
## • • The procedure

- Take a set of quasiparticle states at a fixed deformation (e.g. solutions of HF, HFB or HF + 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 laboratory frame
- Diagonalize a two-body Hamiltonian in the projected basis
- This model has worked well for spectrum description for nuclei with stable deformation (and super-deformation or superheavy nuclei)

K. Hara, Y. Sun, Int. J. Mod. Phys. E 4 (1995) 637

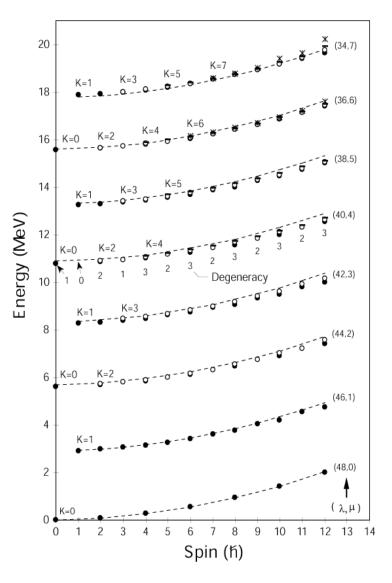
# Example of a good axially-deformed rotor

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



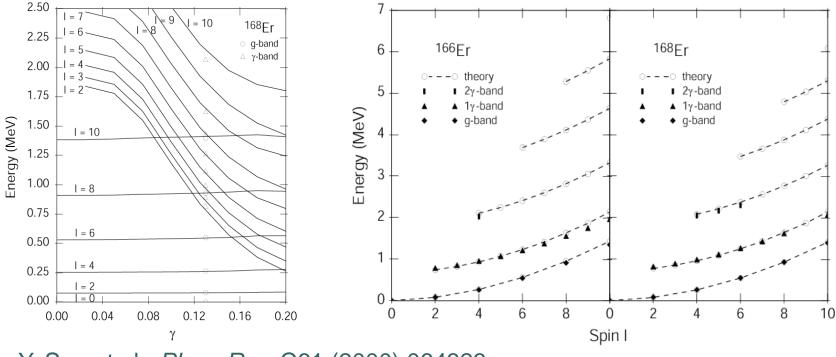
#### Emergence of SU(3) symmetry

- Nearly perfect SU(3) symmetry emerges from a.-m.-projection
  - Project on separate BCS vacuum of  $|\phi_{\nu}\rangle$  and  $|\phi_{\pi}\rangle$ , then couple the projected states  $|I_{\sigma}\rangle = N^{I}\hat{P}^{I}|\phi_{\sigma}\rangle$ to form the basis  $|(I_{\nu} \otimes I_{\pi})I\rangle$
  - Diagonalize the Hamiltonian in the coupled basis
  - Multi-phonon scissors mode is predicted
  - Y. Sun *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. C61 (2000) 064323

## γ-vibrations

#### Calculated transition rates confirm the multi-phonon structure

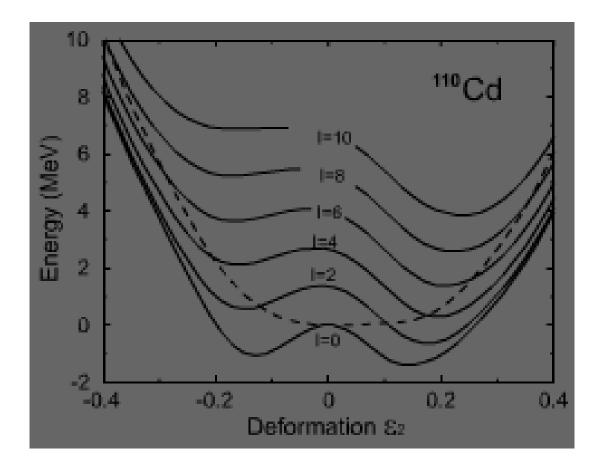
**Table 1.** Comparison of all known experimental in-band and inter-band B(E2) values (associated errors in parenthesis) and calculated ones in W.u. for <sup>168</sup>Er.  $K = 4^+$  lifetimes from ref. [2],  $K = 0^+$ , and  $K = 2^+$  lifetimes and B(E2) values from ref. [8] and all the references therein.

$(I,K)_{\rm i} \to (I,K)_{\rm f}$	$B(E2)_{\rm exp}$ (W.u.)	$B(E2)_{\text{TPSM}}$ (W.u.)
$(2,0)_i \to (0,0)_f$	207~(6)	228.6
$(4,0)_i \rightarrow (2,0)_f$	318(12)	326.9
$(6,0)_i \rightarrow (4,0)_f$	$440^{(a)}$ (30)	361.2
$(8,0)_i \rightarrow (6,0)_f$	350(20)	380.0
$(10,0)_{i} \to (8,0)_{f}$	302(21)	393.0

P. Boutachkov et al. *Eur. Phys. J.* A15 (2002) 455

$(2,2)_i \rightarrow (0,0)_f$	4.80(17)	2.7
$(2,2)_i \rightarrow (2,0)_f$	8.5(4)	4.5
$(2,2)_i \rightarrow (4,0)_f$	0.62(4)	0.3
$(3,2)_i \rightarrow (2,0)_f$	> 0.19	4.9
$(3,2)_i \rightarrow (4,0)_f$	> 0.13	2.7
$(4,2)_{i} \to (2,0)_{f}$	1.7(4)	1.3
$(4,2)_i \rightarrow (4,0)_f$	8.7 (18)	5.5
$(4,2)_{i} \to (6,0)_{f}$	1.13(25)	0.7
$(5,2)_{i} \rightarrow (4,0)_{f}$		3.9
$(5,2)_{i} \to (6,0)_{f}$		3.7
$(6,2)_{i} \to (4,0)_{f}$	0.78(19)	0.8
$(6,2)_{i} \to (6,0)_{f}$	6.4(16)	5.7
$(6,2)_{i} \to (8,0)_{f}$	2.4(7)	1.1
$(7,2)_{i} \to (6,0)_{f}$		3.3
$(7,2)_{i} \to (8,0)_{f}$		4.4
$(8,2)_{i} \to (6,0)_{f}$	1.3(6)	0.5
$(8,2)_{i} \to (8,0)_{f}$	1.8 (8)	5.7
$(8,2)_{i} \to (10,0)_{f}$	120(50)	1.4
$(4,4)_{i} \rightarrow (2,2)_{f}$	3.4(19)	11.9
$(4,4)_{i} \to (3,2)_{f}$	2.2(13)	7.1
$(4,4)_{i} \to (4,2)_{f}$	$1.7^{(b)}$ (9)	2.7
$(4,4)_{i} \to (5,2)_{f}$	$0.7^{(b)}$ (3)	0.6
$(4,4)_i \rightarrow (6,2)_f$	2.0(13)	0.1
$(5,4)_{i} \rightarrow (3,2)_{f}$	5(5)	7.7
$(5,4)_{i} \to (4,2)_{f}$	4(3)	8.6
$(5,4)_{i} \to (5,2)_{f}$	1.8(15)	4.6
$(5,4)_{i} \rightarrow (6,2)_{f}$	0.8(7)	1.3
$(5,4)_{i} \to (7,2)_{f}$	7 (6)	0.2

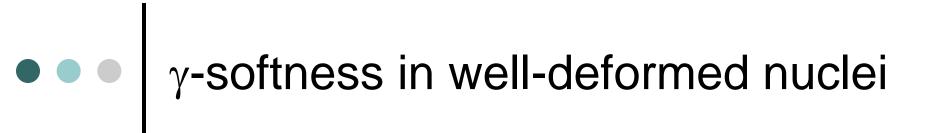
# Example of softness – no definite shapes

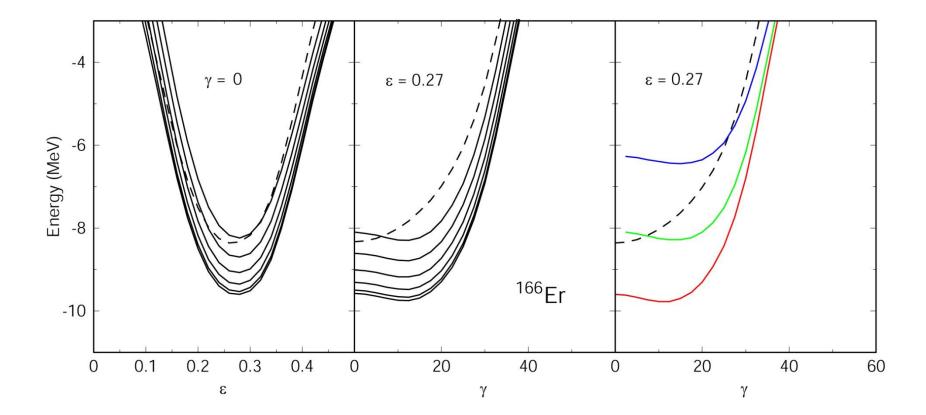


Mean-field calculation shows a spherical shape.

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

Shapes may be developed with rotation.



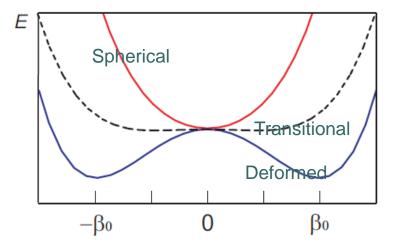


Angular-momentum-projected energy surfaces as functions of  $\epsilon$  and  $\gamma$ 

### 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)

o 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

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

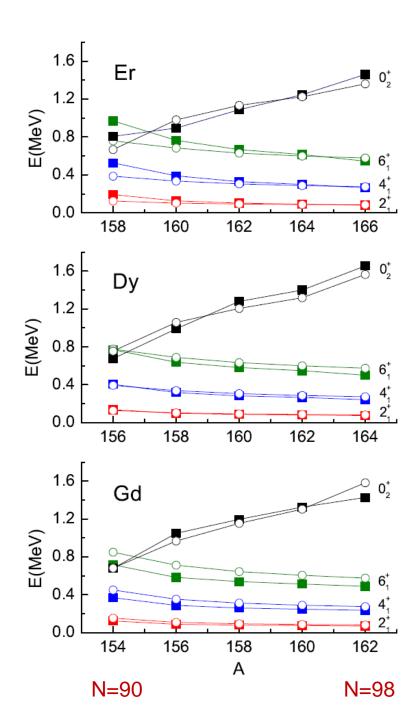
with a fixed set of parameters (fixed  $\chi$ ,  $G_M$ , and  $G_Q$ ) is diagonalized for a chain of isotopes.

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

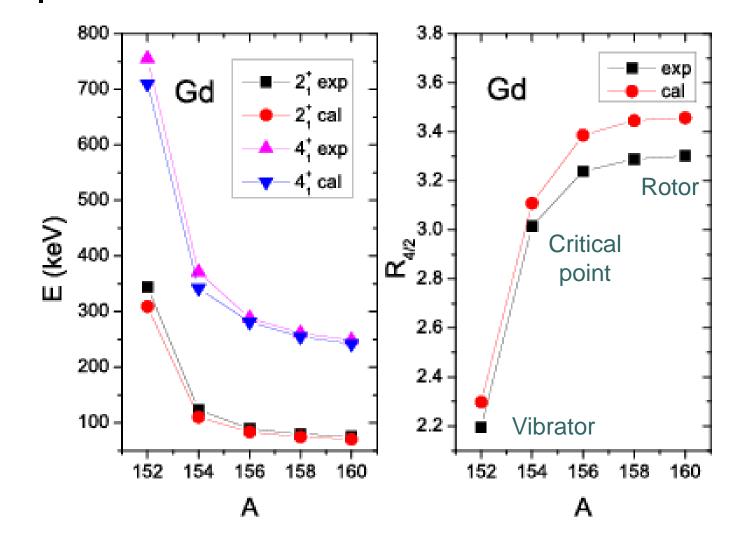
#### Energy levels

- 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

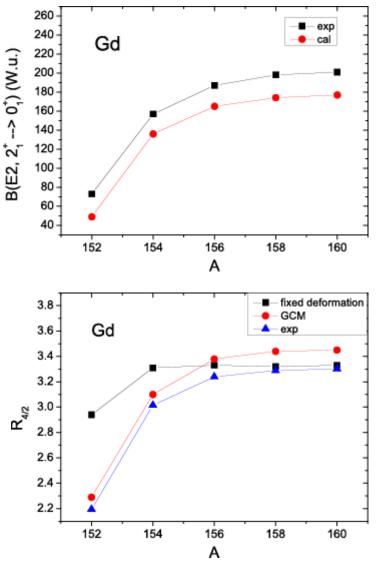


## Spherical-deformed shape phase transition



# 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

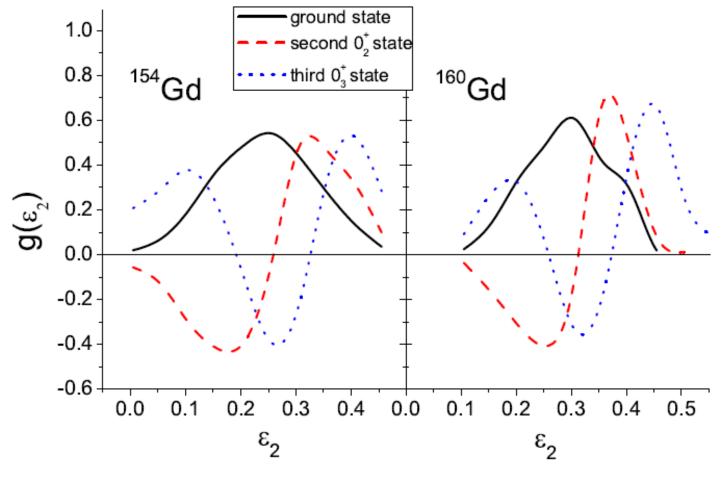
- The Hill-Wheeller Equation diagonalizes the Hamiltonian in a non-orthogonal basis, and therefore,  $f(\varepsilon_2)$  is not a proper quantity to analyze the GSM wave function.
- Transformation of  $f(\varepsilon_2)$  to an orthogonal basis gives

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

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

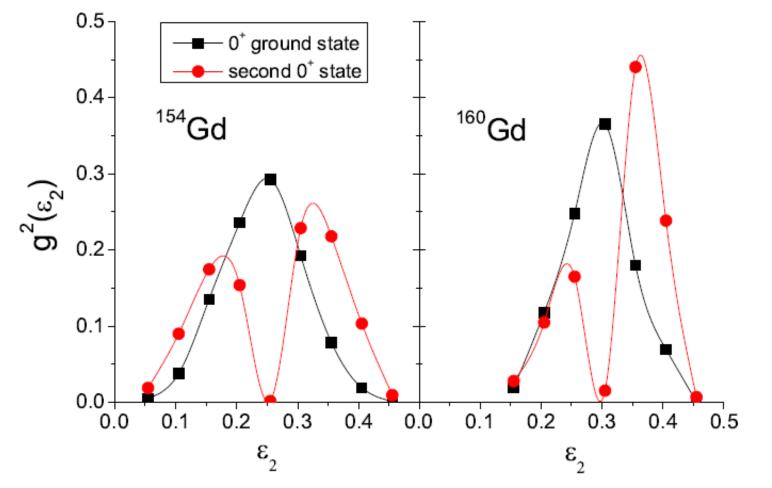
•  $g^2(\varepsilon_2)$  represent the probability function.

### 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



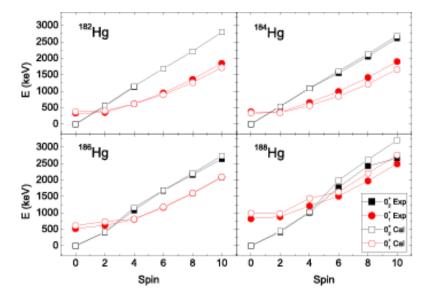
Calculated probability function of deformation for ground state  $0_1^+$  and excited  $0_2^+$  state in <sup>154</sup>Gd and <sup>160</sup>Gd.

## 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

### Hg isotopes

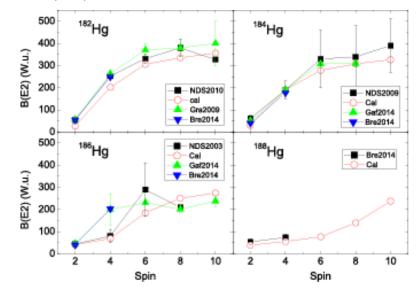
#### Energy levels for two 0<sup>+</sup> bands



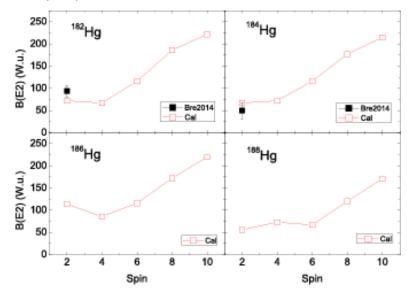
Main features can not be described when superposition is taken only for prolate deformation.

Need superposition for both prolate and oblate deformations.

#### B(E2) for first 0<sup>+</sup> band



B(E2) for second 0<sup>+</sup> band



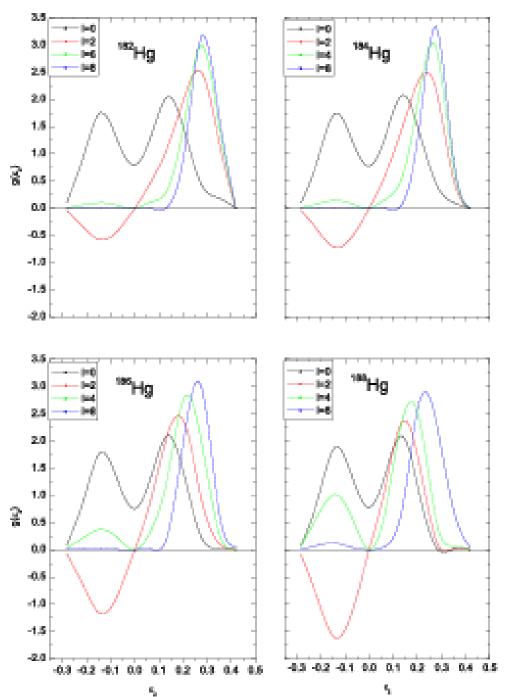
### Hg isotopes

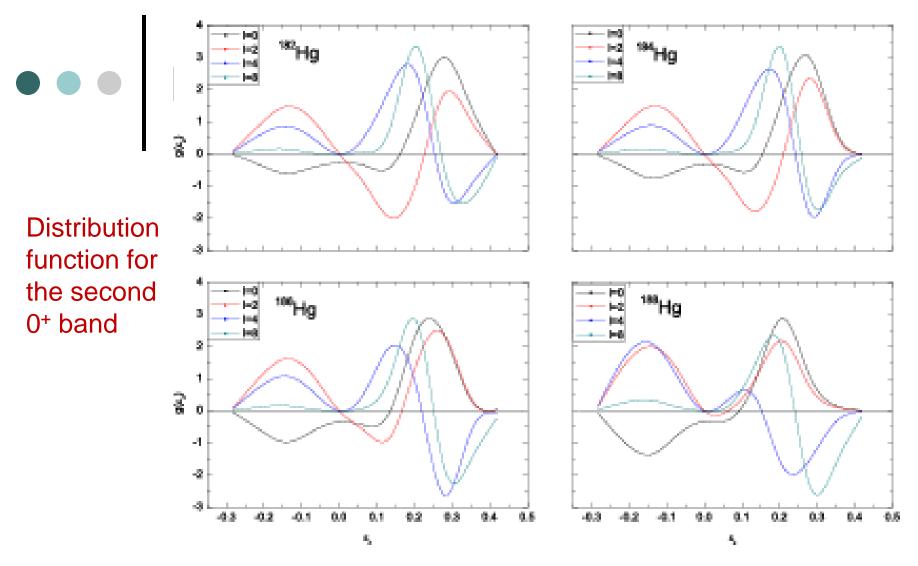
Distribution function for the first 0<sup>+</sup> band

I=0: nearly spherical, two peaks distributed around zero deformation

I=2: has one node, but distributed more on prolate side

I=4 or higher: mainly peaked on the prolate side





I=0: nearly prolately deformed

I=2: has two nodes, but developed to co-existing shapes at <sup>188</sup>Hg
 I=4 or higher: shape developed rapidly. Finally mainly peaked on the prolate side with one node

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

• Even-even nuclei:

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

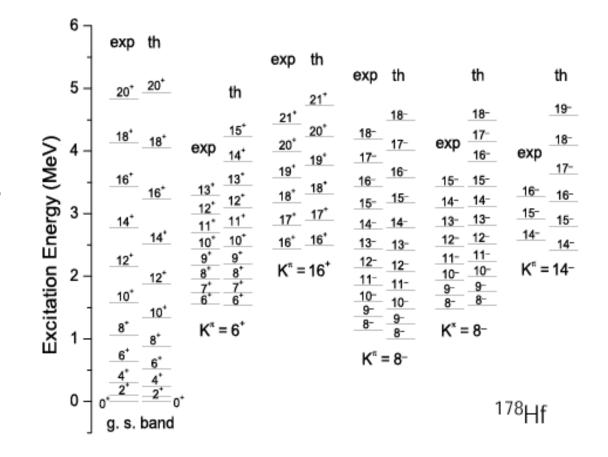
• Odd-odd nuclei:

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

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

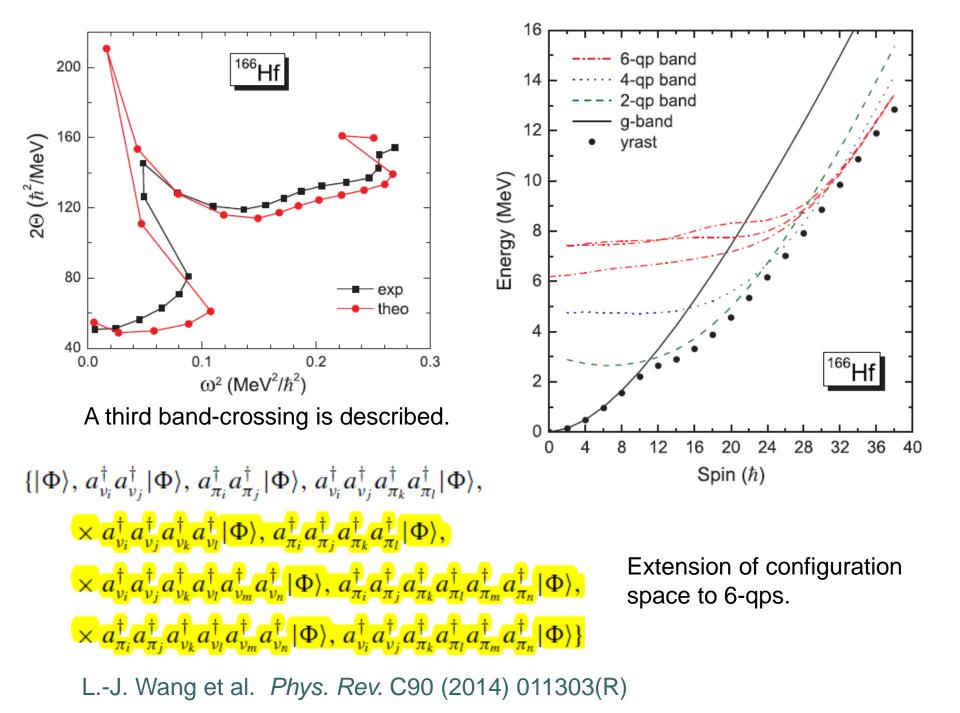
### Multi-quasiparticle excitations

- 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

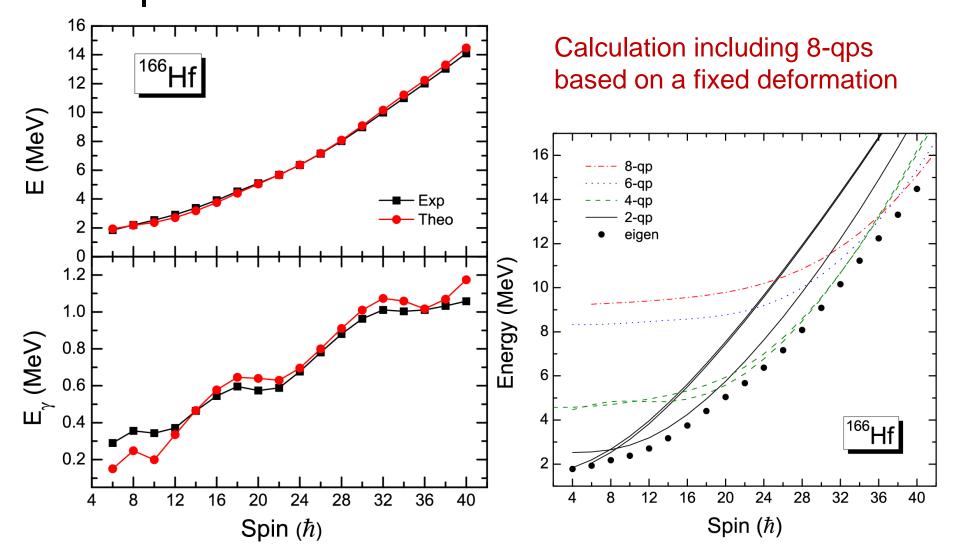


### Multi-quasiparticle computation using the Pfaffian algorithm

- 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



#### Example for very high-spin states



### • • • Summary

• New development in the Projected Shell Model:

- We improved the PSM wave function by superimposing (angular-momentum and particle-number) projected states with different deformation ε<sub>2</sub>
- The method can be applied to problems of soft nuclei, shape co-existence, phase transition, etc.
- excited 0<sup>+</sup> states can be described together with the ground state in an equal footing
- High order multi-quasiparticle states using the Phaffian algorithm
  - To overcome the problem in the classical Wick's theorem for matrix-element calculation
  - Computer code can be developed when large number of quasiparticle excitations are included.



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