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

## Yang Sun

Shanghai Jiao Tong University, China

## 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- For heavy nuclei, the original Elliott $\operatorname{SU}(3)$ scheme is no longer valid;
- one may use generalized $\mathrm{SU}(3)$ 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 $\mathrm{SU}(3)$ symmetry

- Nearly perfect SU(3) symmetry emerges from a.-m.-projection
- Project on separate BCS vacuum of $\left|\phi_{\nu}\right\rangle$ and $\left|\phi_{\pi}\right\rangle$, then couple the projected states $\left|I_{\sigma}\right\rangle=N^{I} \hat{P}^{\prime}\left|\phi_{\sigma}\right\rangle$ to form the basis $\left|\left(I_{\nu} \otimes I_{\pi}\right) I\right\rangle$
- 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

- $\gamma$-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


## $\gamma$-vibrations

- Calculated transition rates confirm the multi-phonon structure

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

| $(I, K)_{\mathrm{i}} \rightarrow(I, K)_{\mathrm{f}}$ | $B(E 2)_{\exp }$ (W.u.) | $B(E 2)_{\text {TPSM }}$ (W.u.) |
| :---: | :---: | :---: |
| $(2,0)_{\mathrm{i}} \rightarrow(0,0)_{\mathrm{f}}$ | $207(6)$ | 228.6 |
| $(4,0)_{\mathrm{i}} \rightarrow(2,0)_{\mathrm{f}}$ | $318(12)$ | 326.9 |
| $(6,0)_{\mathrm{i}} \rightarrow(4,0)_{\mathrm{f}}$ | $440^{\text {(a) }}(30)$ | 361.2 |
| $(8,0)_{\mathrm{i}} \rightarrow(6,0)_{\mathrm{f}}$ | $350(20)$ | 380.0 |
| $(10,0)_{\mathrm{i}} \rightarrow(8,0)_{\mathrm{f}}$ | $302(21)$ | 393.0 |

P. Boutachkov et al.

Eur. Phys. J. A15 (2002) 455

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

## $\gamma$-softness in well-deformed nuclei



Angular-momentum-projected energy surfaces as functions of $\varepsilon$ 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 $\beta$.


Schematic energy potential for
$\left|\Psi^{I}\right\rangle=\int f^{I}(\beta)\left|\Phi^{I}(\beta)\right\rangle d \beta$ spherical (red), transitional (dashed), and deformed (blue) nuclei.

$$
\left|\Phi^{I}(\beta)\right\rangle=\hat{P}^{I}|\phi(\beta)\rangle
$$

$$
\{\beta\}=\left\{\beta_{1}, \beta_{2}, \beta_{3}, \ldots\right\}
$$

## Generate Coordinate Method (GCM)

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

$$
|\Psi\rangle=\int \operatorname{daf}(a)|\Phi(a)\rangle
$$

with $\{a\}=a_{1}, a_{2}, \ldots, a_{i}$ being generate coordinates

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

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

with the overlap functions

$$
\begin{aligned}
\mathscr{H}\left(a, a^{\prime}\right) & =\langle\Phi(a)| \hat{H}\left|\Phi\left(a^{\prime}\right)\right\rangle \\
\mathscr{N}\left(a, a^{\prime}\right) & =\left\langle\Phi(a) \mid \Phi\left(a^{\prime}\right)\right\rangle
\end{aligned}
$$

## Projected Generate Coordinate Method (PGCM)

- Choosing generate coordinate as $\varepsilon_{2}$, an improved wave function

$$
\begin{gathered}
\left|\Psi^{I, N}\right\rangle=\int d \varepsilon_{2} f^{I, N}\left(\varepsilon_{2}\right)\left|\Phi^{I, N}\left(\varepsilon_{2}\right)\right\rangle \\
\left|\Phi^{I, N}\left(\varepsilon_{2}\right)\right\rangle=\hat{P}^{l} \hat{P}^{N}\left|\Phi_{0}\left(\varepsilon_{2}\right) \cdot\right\rangle
\end{gathered}
$$

- 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 $2_{1}{ }^{+}, 4_{1}{ }^{+}$, and $6_{1}{ }^{+}$ of ground band and excited $\mathrm{O}_{2}{ }^{+}$state
- Exp data (filled squares)
- Calculations (open circles)
for isotopes from $\mathrm{N}=90$ (transitional) to $\mathrm{N}=98$ (well-deformed) nuclei





## Spherical-deformed shape phase transition



## Spherical-deformed shape phase transition

- Drastic changes in electric quadrupole transition $\mathrm{B}\left(\mathrm{E} 2,2^{+}\right.$ $\rightarrow 0^{+}$) from vibrator ${ }^{152} \mathrm{Gd}$ ( $\mathrm{N}=88$ ), to critical point ${ }^{154} \mathrm{Gd}$ ( $\mathrm{N}=90$ ), to rotor ${ }^{156-160} \mathrm{Gd}(\mathrm{N}>90)$.

- 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, $f\left(\varepsilon_{2}\right)$ is not a proper quantity to analyze the GSM wave function.
- Transformation of $f\left(\varepsilon_{2}\right)$ to an orthogonal basis gives

$$
g\left(\varepsilon_{2}\right)=\int \mathscr{N}^{1 / 2}\left(\varepsilon_{2}, \varepsilon_{2}^{\prime}\right) f\left(\varepsilon_{2}^{\prime}\right) d \varepsilon_{2}^{\prime}
$$

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

- $g^{2}\left(\varepsilon_{2}\right)$ represent the probability function.


## Distribution function of deformation



Calculated distribution function of deformation for the first three $0^{+}$states in ${ }^{154} \mathrm{Gd}$ and ${ }^{160} \mathrm{Gd}$

## Probability function of deformation



Calculated probability function of deformation for ground state $\mathrm{O}_{1}{ }^{+}$and excited $\mathrm{O}_{2}{ }^{+}$state in ${ }^{154} \mathrm{Gd}$ and ${ }^{160} \mathrm{Gd}$.

## Probability function of deformation

- Peak of the Gaussian defines deformation
- ${ }^{160} \mathrm{Gd}$ being more deformed than ${ }^{154} \mathrm{Gd}$
- The distribution is wider for ${ }^{154} \mathrm{Gd}$
- reflecting the softness of this nucleus
- The distribution for $\mathrm{O}_{2}{ }^{+}$is much more fragmented
- reflecting a vibrational nature of these states
- For $\mathrm{O}_{1}{ }^{+}$, system stays mainly at system's deformation with the largest probability
- For $\mathrm{O}_{2}{ }^{+}$, 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


## $-\quad \mathrm{Hg}$ isotopes

Energy levels for two $0^{+}$bands


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

Need superposition for both prolate and oblate deformations.
$B(E 2)$ for first $0^{+}$band

$B(E 2)$ for second $0^{+}$band


## Hg isotopes

Distribution function for the first $0^{+}$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


Distribution function for the second $0^{+}$band


I=0: nearly prolately deformed
$\mathrm{I}=2$ : has two nodes, but developed to co-existing shapes at ${ }^{188 \mathrm{Hg}}$
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

o Even-even nuclei:

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

- Odd-odd nuclei:

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

- Odd-neutron nuclei:

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

- Odd-proton nuclei:

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

## Multi-quasiparticle excitations

- 0-, 2-, 4-qp states of ${ }^{178} \mathrm{Hf}$
- 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


A third band-crossing is described.

$\left\{|\Phi\rangle, a_{v_{i}}^{\dagger} a_{v_{j}}^{\dagger}|\Phi\rangle, a_{\pi_{i}}^{\dagger} a_{\pi_{j}}^{\dagger}|\Phi\rangle, a_{v_{i}}^{\dagger} a_{v_{j}}^{\dagger} a_{\pi_{k}}^{\dagger} a_{\pi_{l}}^{\dagger}|\Phi\rangle\right.$,

Extension of configuration space to 6-qps.
$\times a_{v_{i}}^{\dagger} a_{v_{j}}^{\dagger} a_{v_{k}}^{\dagger} a_{v_{l}}^{\dagger}|\Phi\rangle, a_{\pi_{i}}^{\dagger} a_{\pi_{j}}^{\dagger} a_{\pi_{k}}^{\dagger} a_{\pi_{l}}^{\dagger}|\Phi\rangle$,
$\times a_{v_{i}}^{\dagger} a_{v_{j}}^{\dagger} a_{v_{k}}^{\dagger} a_{v_{l}}^{\dagger} a_{v_{m}}^{\dagger} a_{v_{n}}^{\dagger}|\Phi\rangle, a_{\pi_{i}}^{\dagger} a_{\pi_{j}}^{\dagger} a_{\pi_{k}}^{\dagger} a_{\pi_{l}}^{\dagger} a_{\pi_{m}}^{\dagger} a_{\pi_{n}}^{\dagger}|\Phi\rangle$,
$\left.\times a_{\pi_{i}}^{\dagger} a_{\pi_{j}}^{\dagger} a_{v_{k}}^{\dagger} a_{v_{l}}^{\dagger} a_{v_{m}}^{\dagger} a_{v_{n}}^{\dagger}|\Phi\rangle, a_{v_{i}}^{\dagger} a_{v_{j}}^{\dagger} a_{\pi_{k}}^{\dagger} a_{\pi_{l}}^{\dagger} a_{\pi_{m}}^{\dagger} a_{\pi_{n}}^{\dagger}|\Phi\rangle\right\}$
L.-J. Wang et al. Phys. Rev. C90 (2014) 011303(R)

## Example for very high-spin states



Calculation including 8-qps based on a fixed deformation


## 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 $\varepsilon_{2}$
- The method can be applied to problems of soft nuclei, shape co-existence, phase transition, etc.
- excited $0^{+}$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.


## Collaborators

Fang-Qi Chen
Long-Jun Wang
(Shanghai Jiao Tong University, China)
T. Mizusaki (Senshu University, Japan)
M. Oi (Senshu University, Japan)
P. Ring (TU Munich, Germany)

