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

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 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 $^{48}\text{Cr}$
  - Exp. data:
  - PSM:
    - Deformed basis with a.-m. projection; Basis states $\sim$ 50
  - pf-SM:
    - Caurier *et al.*, *PRL* 75 (1995) 2466
    - Conventional M-scheme spherical shell model; Basis states $\sim$ 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 mean-field) 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
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 $|\phi_r\rangle$ and $|\phi_\pi\rangle$, then couple the projected states $|I_\sigma\rangle = N^I \hat{P}^I |\phi_\sigma\rangle$ to form the basis $|(I_r \otimes I_\pi)I\rangle$
  - Diagonalize the Hamiltonian in the coupled basis
  - Multi-phonon scissors mode is predicted
γ-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

\( \gamma \)-deformed multi-qp excitations

- 0-phonon \((K=0)\), 1-phonon \((K=2)\), 2-phonon \((K=4)\) \(\gamma\)-vibrational bands
- Each phonon \(\gamma\)-vibrational mode can couple with qp states – generalization of the usual concept of \(\gamma\)-vibration
Basic structure

- Ansatz of wavefunction: \( \psi^I_M = \sum_\kappa f_\kappa \hat{P}^I_{MK \kappa} | \phi_\kappa \rangle \)

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

- The eigenvalue equation: \( \sum_\kappa \left( H^I_{\kappa \kappa'} - E N^I_{\kappa \kappa'} \right) f_{\kappa'} = 0 \)

  with matrix elements: \( H^I_{\kappa \kappa'} = \langle \phi_\kappa | \hat{H} \hat{P}^I_{KK} | \phi_{\kappa'} \rangle \) \( N^I_{\kappa \kappa'} = \langle \phi_\kappa | \hat{P}^I_{KK} | \phi_{\kappa'} \rangle \)

- The Hamiltonian is diagonalized in the projected basis \( \{ \hat{P}^I_{MK} | \phi_\kappa \rangle \} \)
a.-m.-projected multi-quasi-particle states based on a fixed deformation

- Even-even nuclei:
  \[ \{ \hat{P}_{MK}^I \alpha_v^+ \alpha_v^+ | 0 \}, \hat{P}_{MK}^I \alpha_v^+ \alpha_v^+ \alpha_v^+ | 0 \}, \hat{P}_{MK}^I \alpha_v^+ \alpha_v^+ \alpha_v^+ \alpha_v^+ | 0 \}, \ldots \} \]

- Odd-odd nuclei:
  \[ \{ \hat{P}_{MK}^I \alpha_v^+ \alpha_v^+ | 0 \}, \hat{P}_{MK}^I \alpha_v^+ \alpha_v^+ \alpha_v^+ \alpha_v^+ \alpha_v^+ | 0 \}, \hat{P}_{MK}^I \alpha_v^+ \alpha_v^+ \alpha_v^+ \alpha_v^+ \alpha_v^+ \alpha_v^+ | 0 \}, \ldots \} \]

- Odd-neutron nuclei:
  \[ \{ \hat{P}_{MK}^I \alpha_v^+ | 0 \}, \hat{P}_{MK}^I \alpha_v^+ \alpha_v^+ \alpha_v^+ | 0 \}, \hat{P}_{MK}^I \alpha_v^+ \alpha_v^+ \alpha_v^+ \alpha_v^+ | 0 \}, \ldots \} \]

- Odd-proton nuclei:
  \[ \{ \hat{P}_{MK}^I \alpha_v^+ | 0 \}, \hat{P}_{MK}^I \alpha_v^+ \alpha_v^+ \alpha_v^+ | 0 \}, \hat{P}_{MK}^I \alpha_v^+ \alpha_v^+ \alpha_v^+ \alpha_v^+ | 0 \}, \ldots \} \]
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
    \[ \chi_{\tau\tau'} = \frac{2/3 \varepsilon \hbar \omega_{\tau} \hbar \omega_{\tau'}}{\hbar \omega_n \langle Q_0 \rangle_n + \hbar \omega_p \langle Q_0 \rangle_p} \]
  - \( G_M \) is determined by observed even-odd mass difference
  - \( G_Q \) is assumed to be proportional to \( G_M \) with a ratio \( \sim 0.20 \)

- 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

Herzberg et al., Nature 442 (2006) 896
Multi-quasiparticle excitations

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

Data:

Theory:
Calculation of matrix elements for multi-quasiparticle states

- If a multi-quasiparticle state is written as $|\Phi_k\rangle$, then the central task is to calculate

$$\mathcal{H}_{kk'} = \langle \Phi_k | \hat{H}[\Omega] | \Phi_{k'} \rangle,$$

$$\mathcal{N}_{kk'} = \langle \Phi_k | [\Omega] | \Phi_{k'} \rangle,$$

with

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

- For example, a norm matrix element

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

can be written as combinations of

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

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

$$C_{vv'}(\Omega) \equiv \langle \Phi | a_v [\Omega] a_{v'}^{\dagger} | \Phi \rangle = (U^{-1}(\Omega))_{vv'}$$
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:
A third band-crossing is described.

\[
\{ |\Phi\rangle, a^\dagger_{v_i} a^\dagger_{v_j} |\Phi\rangle, a^\dagger_{\pi_i} a^\dagger_{\pi_j} |\Phi\rangle, a^\dagger_{v_i} a^\dagger_{v_j} a^\dagger_{\pi_k} a^\dagger_{\pi_l} |\Phi\rangle, \\
\times a^\dagger_{v_i} a^\dagger_{v_j} a^\dagger_{v_k} a^\dagger_{v_l} |\Phi\rangle, a^\dagger_{\pi_i} a^\dagger_{\pi_j} a^\dagger_{\pi_k} a^\dagger_{\pi_l} |\Phi\rangle, \\
\times a^\dagger_{v_i} a^\dagger_{v_j} a^\dagger_{v_k} a^\dagger_{v_l} a^\dagger_{v_m} a^\dagger_{v_n} |\Phi\rangle, a^\dagger_{\pi_i} a^\dagger_{\pi_j} a^\dagger_{\pi_k} a^\dagger_{\pi_l} a^\dagger_{\pi_m} a^\dagger_{\pi_n} |\Phi\rangle, \\
\times a^\dagger_{\pi_i} a^\dagger_{\pi_j} a^\dagger_{\pi_k} a^\dagger_{\pi_l} a^\dagger_{\pi_m} a^\dagger_{\pi_n} |\Phi\rangle \}
\]

Extension of configuration space to 6-qps.
Example for very high-spin states

Calculation including 8-qps based on a fixed deformation
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 $\varepsilon$ 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 $\beta$.

$$|\Psi^I\rangle = \int f^I(\beta) |\Phi^I(\beta)\rangle d\beta$$

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

$\{\beta\} = \{\beta_1, \beta_2, \beta_3, \ldots \}$
Generate Coordinate Method (GCM)

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

\[ |\Psi\rangle = \int da f(a) |\Phi(a)\rangle \]

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

\[ \mathcal{H} f = EN f \]

with the overlap functions

\[ \mathcal{H}(a, a') = \langle \Phi(a) | \hat{H} | \Phi(a') \rangle, \]
\[ N(a, a') = \langle \Phi(a) | \Phi(a') \rangle \]
Choosing generate coordinate as $\varepsilon_2$, an improved wave function

$$|\Psi^{I,N}\rangle = \int d\varepsilon_2 f^{I,N}(\varepsilon_2) |\Phi^{I,N}(\varepsilon_2)\rangle$$

$$|\Phi^{I,N}(\varepsilon_2)\rangle = \hat{P}^I \hat{P}^N |\Phi_0(\varepsilon_2)\rangle.$$

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.

Energy levels

- Comparison of energy levels of $2_1^+$, $4_1^+$, and $6_1^+$ of ground band and excited $0_{2^+}$ state
  - Exp data (filled squares)
  - Calculations (open circles)

for isotopes from N=90 (transitional) to N=98 (well-deformed) nuclei
Drastic changes in electric quadrupole transition $B(E2, 2^+ \rightarrow 0^+)$ from vibrator $^{152}$Gd (N=88), to critical point $^{154}$Gd (N=90), to rotor $^{156-160}$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-Wheeler 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

$$g(\varepsilon_2) = \int \mathcal{N}^{1/2}(\varepsilon_2, \varepsilon'_2) f(\varepsilon'_2) d\varepsilon'_2$$

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 $0^+$ states in $^{154}\text{Gd}$ and $^{160}\text{Gd}$
Calculated probability function of deformation for ground state $0_1^+$ and excited $0_2^+$ state in $^{154}$Gd and $^{160}$Gd.
Probability function of deformation

- Peak of the Gaussian defines deformation
  - $^{160}\text{Gd}$ being more deformed than $^{154}\text{Gd}$
- The distribution is wider for $^{154}\text{Gd}$
  - reflecting the softness of this nucleus
- The distribution for $0_{2^+}$ is much more fragmented
  - reflecting a vibrational nature of these states
- For $0_{1^+}$, system stays mainly at system’s deformation with the largest probability
- For $0_{2^+}$, system shows two peaks having different heights lying separately at both sides of the equilibrium
  - indicating an anharmonic oscillation
  - preferring to have a larger probability in the site of larger deformation
\( \beta \)-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

$$\lambda_\beta = \sum_i \left( p_i \times \sum_{ij} \lambda_{bij} \right)$$

$$p_i = \frac{(2I_i + 1) \times \exp(-E_i / kT)}{\sum_m (2I_m + 1) \times \exp(-E_m / kT)}$$

- Examples in the s-process

Transition matrix elements in the projected basis

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

- Wavefunction
  \[ \psi^I_M = \sum_k f^I_K P^I_{MKK} | \phi_k \rangle \]

- e-e system
  \[ | \phi_e (\varepsilon_e) \rangle = \{ | \varepsilon_e \rangle, b_v^+ b_v^+ | \varepsilon_e \rangle, b_{\pi}^+ b_{\pi}^+ | \varepsilon_e \rangle, b_v^+ b_v^+ b_{\pi}^+ b_{\pi}^+ | \varepsilon_e \rangle, \ldots \} \]

- o-o system
  \[ | \phi_o (\varepsilon_o) \rangle = \{ | a_v^+ a_{\pi}^+ | \varepsilon_o \rangle, a_v^+ a_v^+ a_{\pi}^+ a_{\pi}^+ | \varepsilon_o \rangle, a_v^+ a_{\pi}^+ a_{\pi}^+ a_{\pi}^+ | \varepsilon_o \rangle, \ldots \} \]

  \[ \left\langle \phi_o (\varepsilon_o) | \hat{O}^I P^I_{K_0K_e} | \phi_e (\varepsilon_e) \right\rangle \sim \int d\Omega D^I_{K_0K_e} (\Omega) \left\langle \phi_o (\varepsilon_o) | \hat{O} \hat{R} (\Omega) | \phi_e (\varepsilon_e) \right\rangle \]
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)
  \[ \hat{H}_{GT} = + 2 \chi_{GT} \sum_{\mu} \beta_{1\mu} (-1)^\mu \beta_{1-\mu}^+ - 2 \kappa_{GT} \sum_{\mu} \Gamma_{1\mu}^- (-1)^\mu \Gamma_{1-\mu}^+ \]
  \[ \beta_{1\mu}^- = \sum_{\pi,\nu} \langle \pi | \sigma_{\mu} \tau_- | \nu \rangle c_{\pi}^\dagger c_\nu, \quad \beta_{1\mu}^+ = (-)^\mu (\beta_{1-\mu}^-)^\dagger \]
  \[ \Gamma_{1\mu}^- = \sum_{\pi,\nu} \langle \pi | \sigma_{\mu} \tau_- | \nu \rangle c_{\pi}^\dagger c_{\nu}^\dagger, \quad \Gamma_{1\mu}^+ = (-)^\mu (\Gamma_{1-\mu}^-)^\dagger \]

Distribution of $B(GT)$

- Initial state: ground state in even-even nucleus
- Final states: all $1^+$ states in odd-odd nucleus
- Ikeda sum-rule fulfilled

$$S(GT^-) - S(GT^+) = \sum_f B(GT^-, i \rightarrow f) - \sum_f B(GT^+, i \rightarrow f)$$

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

$$= 3(N - Z).$$
B(GT) and log ft in $^{164}$Ho $\rightarrow$ $^{164}$Dy

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

Summary
Collaboration

- (Students) Y.-C. Yang (杨迎春), Y.-X. Liu (刘艳鑫)
  H. Jin (金华), F.-Q. Chen (陈芳祁)
  L.-J. Wang (王龙军), Q.-L. Hu (胡庆丽)
- (China) Z.-C. Gao (高早春)
- (Japan) T. Mizusaki (水崎高浩)
  M. Oi
- (USA) M. Guidry
- (Germany) P. Ring