Beyond Mean-Field Boson-Fermion Model for Odd Nuclei

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Calculation of odd nuclei — Motivation

- Variety of mean-field approaches based on energy density functional

- Quantitative study of spectroscopy necessitates inclusion of beyond-mean-field effects, — e.g., by GCM

- Extension to odd systems — i.e., time-reversal symmetry, blocking at each deformation

Q. Develop a model that allows a systematic and computationally feasible description of odd nuclei?
The method

Self-consistent mean-field (SCMF) within nuclear DFT

Construct Particle-Core coupling Hamiltonian

- Even-even core nucleus → bosonic degrees of freedom (interacting boson model IBM)
- Particle-core coupling → interacting boson-fermion model (IBFM)
This talk

... mainly discusses the methodology

Three parts:

(i) Even-even

(ii) Odd-A

(iii) Odd-A with octupole
Even-even nuclei
Synopsis of IBM

✓ simple phenomenological description of heavy nuclei by the drastic reduction of Hilbert space: boson ≈ valence nucleon pairs

✓ use of group theory — i.e., U(5)-vibrator, SU(3)-rotor, SO(6)-γ -soft rotor

- Shell model: \( \sim O(10^{14}) \) 2+ states
- IBM: 26 2+ states

Dimension:

- e.g., \(^{154}\text{Sm} \): 22 valence nucleons (12 protons + 10 neutrons)
More microscopic consideration

Otsuka, Arima, Iachello (1978)

(1) Truncation to smaller (S, D pair) subspace

(2) Mapping of Hamiltonian matrix

(3) Eigenvalue problem in (s, d) boson space

... this prescription was limited to spherical shapes

→ Why not construct the IBM Hamiltonian based on DFT?
Step 1/2. Self-consistent mean-field

Energy surface: semi-classical description of shapes (not observables)

excitation spectra and transition rates $\rightarrow$ IBM Hamiltonian
Mapping SCMF surface onto expectation value of the IBM Hamiltonian in the boson condensate completely determines strength parameters of the Hamiltonian.

- essential boson Hamiltonian

\[ \hat{H} = \epsilon \hat{n}_d + \kappa \hat{Q} \cdot \hat{\bar{Q}} \]

- Spherical driving
- Deformation driving

\[ \hat{n}_d = d^\dagger \cdot \bar{d}, \quad \hat{Q} = s^\dagger \bar{d} + d^\dagger s + \chi [d^\dagger \times d]^{(2)} \]

- energy surface

\[ E_{IBM}(\beta, \gamma) = \langle \phi_B(\beta\gamma) | \hat{H} | \phi_B(\beta, \gamma) \rangle \]

- boson condensate

\[ |\phi_B(\beta, \gamma)\rangle \approx \left(s^\dagger + \beta \cos \gamma d_0^\dagger + \frac{1}{\sqrt{2}} \beta \sin \gamma (d_2^\dagger + d_{-2}^\dagger)\right)^N |0\rangle \]

- relation to collective model

\[ \beta_{IBM} = c\beta \quad (C > 1) \quad \gamma_{IBM} = \gamma \]

Parameters (\( \epsilon, \kappa, \chi \)) are determined to reproduce the topology of the SCMF surface around the mean-field minimum. \( E_{SCMF}(\beta, \gamma) \approx E_{IBM}(\beta, \gamma) \)

Boson Hamiltonian is derived only from nucleonic d.o.f.
✓ ... IBM calculation with strength parameters determined by the mapping: no need for phenomenological fit
✓ ... systematic and economic description of excitation spectra
$\gamma$ -soft nucleus

Quadrupole-octupole shape transitions in Th isotopes


spectroscopic properties → quadrupole-octupole IBM Hamiltonian with octupole $f_3$ boson ($J=3^-$)
\[ \hat{H}_B = \hat{H}_{sd} + \hat{H}_f + \hat{H}_{sdf} \]

- sdf-bocon Hamiltonian:

\[ \hat{H}_B = \epsilon_d \hat{n}_d + \epsilon_f \hat{n}_f + \kappa_2 \hat{Q} \cdot \hat{Q} + \kappa'_2 \hat{L} \cdot \hat{L} + \kappa_3 : \hat{V}_3^\dagger \cdot \hat{V}_3 : \]

\[ \hat{Q} = s^\dagger \tilde{d} + d^\dagger \tilde{s} + \chi_{dd}[d^\dagger \times \tilde{d}]^{(2)} + \chi_{ff}[f^\dagger \times \tilde{f}]^{(2)}. \]

\[ \hat{L} = \sqrt{10}[d^\dagger \times \tilde{d}]^{(1)} \]

\[ \hat{V}_3^\dagger = s^\dagger \tilde{f} + \chi_{df}[d^\dagger \times \tilde{f}]^{(3)} \]

- Parameters: \( \epsilon_d, \epsilon_f, \kappa_2, \chi_{dd}, \chi_{ff}, \kappa'_2, \kappa_3, \chi_{df} \)

- Operators:

\[ \hat{T}^{(E2)} = e_B^{(2)} \hat{Q} \]

\[ \hat{T}^{(E3)} = e_B^{(3)} (\hat{V}_3^\dagger + \hat{V}_3) \]

\[ \hat{T}^{(E1)} = e_B^{(1)} [d^\dagger \times \tilde{f} + f^\dagger \times \tilde{d}]^{(1)} \]
Spectroscopic properties

(a) Positive parity
- $2^+$
- $4^+$
- $6^+$
- $8^+$
- $10^+$

(b) Negative parity
- $1^-$
- $3^-$
- $5^-$
- $7^-$
- $9^-$

Soft octupole shape
Rigid octupole shape

(a) E3
- $B(E3; 3^- \rightarrow 0^+)$ (W.u.)

(b) E1
- $B(E1; 1^- \rightarrow 0^+)$ (W.u.)
$^{226}$Th: rigid octupole deformation

![Diagram showing the excitation energy (MeV) for $^{226}$Th with experimental and theoretical states labeled.](image)

- Experimental states:
  - $12^+$
  - $11^-$
  - $10^+$
  - $9^-$
  - $8^+$
  - $7^-$
  - $6^+$
  - $5^-$
  - $4^+$
  - $3^-$
  - $2^+$
  - $1^-$
  - $0^+$

- Theoretical states:
  - $12^+$
  - $11^-$
  - $10^+$
  - $9^-$
  - $8^+$
  - $7^-$
  - $6^+$
  - $5^-$
  - $4^+$
  - $3^-$
  - $2^+$
  - $1^-$
  - $0^+$

The diagram includes a contour plot labeled $^{226}$Th and DD-PC1, with axes $\beta_2$ and $\beta_3$. The plot is color-coded with varying intensities indicating different energy levels.
Octupoles in rare-earth region


✓ compare the Gogny-D1M GCM results, to a similar degree of accuracy
Odd-A nuclei
$^{151-155}$Eu isotopes: particle + axially-deformed core

Even-even boson core

$^{146-154}$Sm (7–11 bosons outside of $^{132}$Sn doubly magic nucleus)

Odd proton orbitals

full $Z=50$–82 proton major shell:

- $1g_{7/2}$, $2d_{5/2}$, $2d_{3/2}$, $3s_{1/2}$ for positive parity
- $1h_{11/2}$ for negative parity
IBFM Hamiltonian:

\[ \hat{H} = \hat{H}_B + \hat{H}_F + \hat{H}_{BF} \]

\[ \hat{H}_B = \epsilon_d \hat{n}_d + \kappa \hat{Q}_B \cdot \hat{Q}_B + \kappa' \hat{L}_B \cdot \hat{L}_B \]

\[ \hat{Q}_B = s^\dagger \hat{d} + d^\dagger s + \chi (d^\dagger \times \hat{d})^{(2)} \]

\[ \hat{H}_F = \sum_j \epsilon_j [a_j^\dagger \times \tilde{a}_j]^{(0)} \]

\[ \hat{H}_{BF} = \sum_{jj'} \Gamma_{jj'} \hat{Q}_B \cdot [a_{j'}^\dagger \times \tilde{a}_{j'}]^{(2)} + \sum_{jj'j''} \Lambda_{jj''}^{jj'} : [d^\dagger \times \tilde{a}_j]^{(j''')} \times [a_j^\dagger \times \tilde{d}]^{(j''')} : + \sum_j A_j [a^\dagger \times \tilde{a}_j]^{(0)} \hat{n}_d, \]

\begin{align*}
\text{dynamical term} & \text{ exchange term} & \text{monopole term} \\
\end{align*}

\[ \Gamma_{jj'} = \Gamma_0 (u_j u_{j'} - v_j v_{j'}) Q_{jj'} \]

\[ \Lambda_{jj''}^{jj'} = -2 \Lambda_0 \sqrt{\frac{5}{2j''} + 1} (u_j v_{j'} + v_j u_{j'}) (u_{j'} v_{j'''} + v_{j'} u_{j'''}) Q_{jj'} Q_{j'j''} \]

\[ A_j = -\sqrt{2j + 1} A_0 \]

Parameters: \( \epsilon_d, \kappa, \chi, \kappa', \epsilon_j, v_j^2, \Gamma_0, \Lambda_0, A_0 \)
Constructing boson-fermion interaction

\[ H = H_B + H_F + H_{BF} \]

- **Even-even boson (IBM) core**, determined by the mapping from SCMF energy surface
- **Odd (unpaired) fermion**: \( \varepsilon_j \)
- **Boson-fermion coupling**: \( v_j^2, \Gamma_0, \Lambda_0, A_0 \)

- Single-particle energies \( \varepsilon_j \) and occupation probabilities \( v_j^2 \) are calculated by the SCMF constrained at zero deformation.

- Three strength parameters for \( H_{BF} \) \( (\Gamma_0, \Lambda_0, A_0) \) are fitted to data...
Collective wave functions for the lowest $\pi=+1$ and $\pi=-1$ states

As a result of including $H_{BF}$, one obtains solutions peaked around the minimum ($\beta = \beta_{\text{min}} \neq 0$) of the energy surface of boson core.

Input: S.P.E. & $v_j^2$ at zero deformation ($\beta = 0$)
Comparison with “phenomenological” parameters for Eu

Considerable differences in magnitude and trend (esp. in $\Lambda_0^+$)

cf. Phenomenological parameters taken from O. Scholten, in “Interacting Bose-Fermi Systems in Nuclei” (F. Iachello ed.)
The deviation comes mainly from different single-particle energies and occupations — e.g.,

\[ \varepsilon(d_{5/2}) - \varepsilon(g_{7/2}) \approx 3 \text{ MeV (ours)} \]

\[ < 0.5 \text{ MeV (Scholten)} \]

\[ v^2(g_{7/2}) \approx 0.96 \text{ (ours)} \]

\[ \approx 0.6 \text{ (Scholten)} \]

\[ v^2(h_{11/2}) \approx 0.13 \text{ (ours)} \]

\[ \approx 0.35 \text{ (Scholten)} \]
Energy spectra in odd-A Eu
Strong prolate deformed core

K=5/2^± and 3/2^± rotational bands following the J(J+1) rule, with the ΔJ=1 systematics in the strong-coupling limit
Core is soft (transitional)
Positive-parity bands showing the $\Delta J=1$ systematics in the strong-coupling limit
Negative-parity bands with the $\Delta J=2$ systematics, decoupled from the core
γ -soft cases

✓ γ -soft Ba core + odd neutron in full sdg shell
✓ 134,135 Ba: in proximity to the E(5) critical-point symmetry of U(5)-O(6) phase transition

Odd nuclei with octupole
Octupole-octupole degrees of freedom in \( ^{142,144,146}\text{Ba} \) mapped onto quadrupole-octupole IBM Hamiltonian.
low-energy positive and negative-parity (one f-boson) band connected by the large E3 decay from 3− to 0+ states

Boson-fermion Hamiltonian with octupole

\[ \hat{H}_{BF} = \hat{H}_{BF}^{sd} + \hat{H}_{BF}^{f} + \hat{H}_{BF}^{sdf}. \]

\( \hat{H}_{BF}^{sd} = \sum_{j_a,j_b} \gamma_{j_a,j_b}^{sd} \hat{Q}_{sd}^{(2)} \cdot [\hat{a}_{j_a}^\dagger \times \hat{\bar{a}}_{j_b}]^{(2)} + \sum_{j_a,j_b,j_c} \Lambda_{j_a,j_b,j_c}^{dd} :[[\hat{a}_{j_a}^\dagger \times \hat{d}]^{(j_c)} \times [\hat{d}^\dagger \times \hat{\bar{a}}_{j_b}]^{(j_c)}]^{(0)} : + \sum_{j_a} A_{j_a}^{d} [\hat{a}_{j_a}^\dagger \times \hat{\bar{a}}_{j_a}]^{(0)} \hat{n}_d, \)

\( \hat{H}_{BF}^{f} = \sum_{j_a,j_b} \gamma_{j_a,j_b}^{ff} \hat{Q}_{ff}^{(2)} \cdot [\hat{a}_{j_a}^\dagger \times \hat{\bar{a}}_{j_b}]^{(2)} + \sum_{j_a,j_b,j_c} \Lambda_{j_a,j_b,j_c}^{ff} :[[\hat{a}_{j_a}^\dagger \times \hat{f}]^{(j_c')} \times [\hat{f}^\dagger \times \hat{\bar{a}}_{j_b}]^{(j_c')} ]^{(0)} : + \sum_{j_a} A_{j_a}^{f} [\hat{a}_{j_a}^\dagger \times \hat{\bar{a}}_{j_a}]^{(0)} \hat{n}_f, \)

\( \hat{H}_{BF}^{sdf} = \sum_{j_a,j_b,j'_b} \gamma_{j_a,j_b}^{sdf} \hat{V}_3 \cdot [\hat{a}_{j_a}^\dagger \times \hat{\bar{a}}_{j'_b}]^{(3)} + \sum_{j_a,j_b,j_c} \Lambda_{j_a,j_b,j_c}^{df} :[[\hat{a}_{j_a}^\dagger \times \hat{d}]^{(j_c)} \times [\hat{f}^\dagger \times \hat{\bar{a}}_{j'_b}]^{(j_c)} ]^{(0)} :+(H.C.). \)

✓ similar \( v_j \) dependence of the coefficients
✓ 3p_{1/2,3/2} 2f_{5/2,7/2} 1h_{9/2} 21i_{13/2} major shell, boson-fermion parameters determined separately for normal- and unique-parity configs.
✓ No octupole deformation in ground state for both parity
✓ Octupole bands built on $15/2^-$ and $7/2^+$ states are predicted

... supporting experimental situation [PRC86, 044324 (2012)]
... algebraic (IBM/IBFM) Hamiltonian for nuclear spectroscopy is determined by mapping from SCMF calculation within DFT;

... allows an accurate and computationally feasible description of shapes and excitations;

... opens up possibilities of investigating a large number of heavy, odd nuclei in a systematic way.

... can boson-fermion coupling constants be determined only from SCMF?
✓ simple description of heavy nuclei by the drastic reduction of Hilbert space: boson $\approx$ valence nucleon pairs

✓ Connection to collective model — i.e., U(5)-vibrator, SU(3)-deformed rotor, SO(6)-$\gamma$-soft rotor

✓ Hamiltonian is diagonalized in lab frame, thus providing observables

✓ in itself phenomenological, so it needs a microscopic input

→ Why not construct the IBM Hamiltonian based on DFT?
Coupling constants in terms of $v^2$

- **$sd$-boson part:**

$$A^d_j = -A_0^d \sqrt{2j + 1}$$

$$\Gamma^{sd}_{ja, jb} = \Gamma_0^{sd}(u_{ja} u_{jb} - v_{ja} v_{jb})Q_{ja, jb}^{(2)}$$

$$\Lambda^{dd}_{ja, jb, j_c} = -2\Lambda_0^{dd} \sqrt{\frac{5}{2j_c + 1}}(u_{ja} v_{jc} + v_{ja} u_{jc})Q_{ja, j_c}^{(2)}(u_{jb} v_{jc} + v_{jb} u_{jc})Q_{jb, j_c}^{(2)}$$

- **$f$-boson part:**

$$A^f_j = -A_0^f \sqrt{2j + 1}$$

$$\Gamma^{ff}_{ja, jb} = \Gamma_0^{ff}(u_{ja} u_{jb} - v_{ja} v_{jb})Q_{ja, jb}^{(2)}$$

$$\Lambda^{ff}_{ja, jb, j'_c} = -2\Lambda_0^{ff} \sqrt{\frac{7}{2j'_c + 1}}(u_{ja} v_{jc} + v_{ja} u_{jc})Q_{ja, j'_c}^{(2)}(u_{jb} v_{jc} + v_{jb} u_{jc})Q_{jb, j'_c}^{(2)}$$

- **$sdf$-boson part:**

$$\Gamma^{sf}_{ja, j'_b} = \Gamma_0^{sf}(u_{ja} u_{j'_b} - v_{ja} v_{j'_b})Q_{ja, j'_b}^{(3)}$$

$$\Lambda^{df}_{ja, j'_b, j_c} = -2\Lambda_0^{df} \sqrt{\frac{7}{2j_c + 1}}(u_{ja} v_{jc} + v_{ja} u_{jc})Q_{ja, j'_b}^{(2)}(u_{j'_b} v_{jc} + v_{j'_b} u_{jc})Q_{jb, j'_c}^{(3)}$$

**Parameters:**

- $\Gamma_0^{sd}, \Gamma_0^{ff}, \Lambda_0^{dd}, \Lambda_0^{ff}, A_0^d, A_0^f$

- $\Gamma_0^{sf}, \Lambda_0^{df}$

for each of unique-parity ($i_{13/2}$) and normal-parity ($p_{1/2, 3/2} f_{5/2, 7/2} h_{9/2}$) configs.