Application of quantum number projection method to tetrahedral shape and high-spin states in nuclei

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Contents

- Efficient method of projection calculation
- Application to tetrahedral shape
  what kind of rotational spectra?
- Application to high-spin states
  cranking versus J-projection?
  wobbling and chiral rotational band

Efficient method of projection calculation

S.Tagami and Y.R.Shimizu,
Prog.Theor.Phys.127 (2012),79.

General quantum number projection and configuration mixing (GCM)

Final wave function

number parity

$$|\Psi^{INZ(\pm)}_{M;\alpha}\rangle = \sum_{K,n} \underbrace{g^{INZ(\pm)}_{Kn,\alpha}}_{\text{amplitude}} \hat{P}^I_{MK}\hat{P}^N\hat{P}^Z\hat{P}_\pm \underline{|\Phi_n\rangle}$$

several symmetry broken HFB-type states

projectors:

$$\hat{P}^I_{MK} = \frac{2I+1}{8\pi^2}\int d^3\omega D^{I\,*}_{MK}(\omega)\underline{\hat{R}(\omega)}, \quad \hat{P}^N = \frac{1}{2\pi}\int d\varphi\, \underline{e^{i\varphi(\hat{N}-N)}}$$

ω =Euler angle (α , β , γ)

Hill-Wheeler equation (generalized eigenvalue problem)

$$\sum_{K',n'} \mathcal{H}^{INZ(\pm)}_{Kn;K'n'}\, \underline{g^{INZ(\pm)}_{K'n',\alpha}} = E^{INZ(\pm)}_{\alpha} \sum_{K',n'} \mathcal{N}^{INZ(\pm)}_{Kn;K'n'}\, \underline{g^{INZ(\pm)}_{K'n',\alpha}}$$

energy eigenvalue

kernels:

$$\begin{pmatrix} \mathcal{H}^{INZ(\pm)}_{Kn;K'n'} \\ \mathcal{N}^{INZ(\pm)}_{Kn;K'n'} \end{pmatrix} = \langle\Phi_n| \begin{pmatrix} \hat{H} \\ 1 \end{pmatrix} \hat{P}^I_{KK'}\hat{P}^N\hat{P}^Z\hat{P}_\pm|\Phi_{n'}\rangle$$

Projection calculation

kernels: $\begin{pmatrix} \mathcal{H}^{INZ(\pm)}_{Kn;K'n'} \\ \mathcal{N}^{INZ(\pm)}_{Kn;K'n'} \end{pmatrix} = \langle \Phi_n | \begin{pmatrix} \hat{H} \\ 1 \end{pmatrix} \hat{P}^I_{KK'} \hat{P}^N \hat{P}^Z \hat{P}_\pm | \Phi_{n'} \rangle$

$$\hat{P}^I_{MK} = \frac{2I+1}{8\pi^2} \int d^3\omega D^{I\,*}_{MK}(\omega) \underline{\hat{R}(\omega)}, \quad \hat{P}^N = \frac{1}{2\pi} \int d\varphi \, \underline{e^{i\varphi(\hat{N}-N)}}$$

$$\hat{R}(\alpha,\beta,\gamma) \equiv e^{i\gamma \hat{J}_z} e^{i\beta \hat{J}_y} e^{i\alpha \hat{J}_z}$$

General projection

$$|\alpha\rangle = \hat{P}_\alpha |\Phi\rangle, \qquad \hat{P}_\alpha = \int g_\alpha(\boldsymbol{x}) \underline{\hat{D}(\boldsymbol{x})} d\boldsymbol{x}.$$

multi-dim. numerical integration

unitary transformation

need to calculate:

$\langle \Phi | \hat{P}_\alpha \underline{\hat{O}} \hat{P}_{\alpha'} | \Phi' \rangle$ or $\langle \Phi | \hat{D}(\boldsymbol{x}) \hat{O} \hat{D}(\boldsymbol{x}') | \Phi' \rangle$

arbitrary observable

or $\boxed{\langle \Phi | \hat{O} \hat{D}(\boldsymbol{x}) | \Phi' \rangle}$ between HFB-type states

Efficient method of projection and GCM

Calculation of $\boxed{\langle\Phi|\hat{O}\hat{D}(\boldsymbol{x})|\Phi'\rangle}$ HFB-type states with large basis size

- Truncation in terms of canonical basis

c.f. P.Bonche et al., NPA510(1990),466. Appendix.

$|\Phi\rangle \leftrightarrow (U,V)$

quasiparticle $\beta_k|\Phi\rangle = 0 \ (k=1,2,...,M)$

original basis (spherical HO) $c_l|0\rangle = 0 \ (l=1,2,...,M)$ $\quad \beta_k^\dagger = \sum_l (U_{lk}c_l^\dagger + V_{lk}c_l)$

canonical basis → diagonalize $\rho_{l'l} = \langle\Phi|c_l^\dagger c_{l'}|\Phi\rangle$ density matrix

$$b_k^\dagger = \sum_l W_{lk}c_l^\dagger, \qquad \langle\Phi|b_k^\dagger b_{k'}|\Phi\rangle = \delta_{kk'}\underline{v_k^2}$$

occupation probabilities

Q=1-P $\quad$ P-space: $k=1,2,...,L_p(\epsilon);\ v_k^2 > \epsilon$

by the way, in the canonical basis,
a HFB-type state can be written:

$$|\Phi\rangle = \prod_{i>0,\neq B} (u_i + v_i b_i^\dagger b_{\tilde{i}}^\dagger) \prod_{i_B} b_{i_B}^\dagger |0\rangle$$ canonical form

(Bloch-Messiah Theorem)

pair of orbits with small v_i does not
contribute to HFB-type mean-field!

Efficient method of projection and GCM

Calculation of $\boxed{\underline{\langle\Phi|}\hat{O}\hat{D}(\boldsymbol{x})\underline{|\Phi'\rangle}}$ HFB-type states with large basis size

Truncation in terms of canonical basis

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occupation probabilities

Q=1-P $\quad$ P-space: $k=1,2,...,L_p(\epsilon);\ v_k^2 > \epsilon$

Utilize Thouless amplitude with respect to a Slater-determinantal state

$$|\phi_0\rangle = \prod_{k=1}^{N} b_k^\dagger|0\rangle$$

N :particle number

$$|\Phi\rangle = \exp\left(\sum_{ll'}\underline{Z_{ll'}}a_l^\dagger a_{l'}^\dagger\right)|\phi_0\rangle \qquad a_k^\dagger = \begin{cases} b_k & (1\le k\le N) \\ b_k^\dagger & (N+1\le k\le M)\end{cases}$$

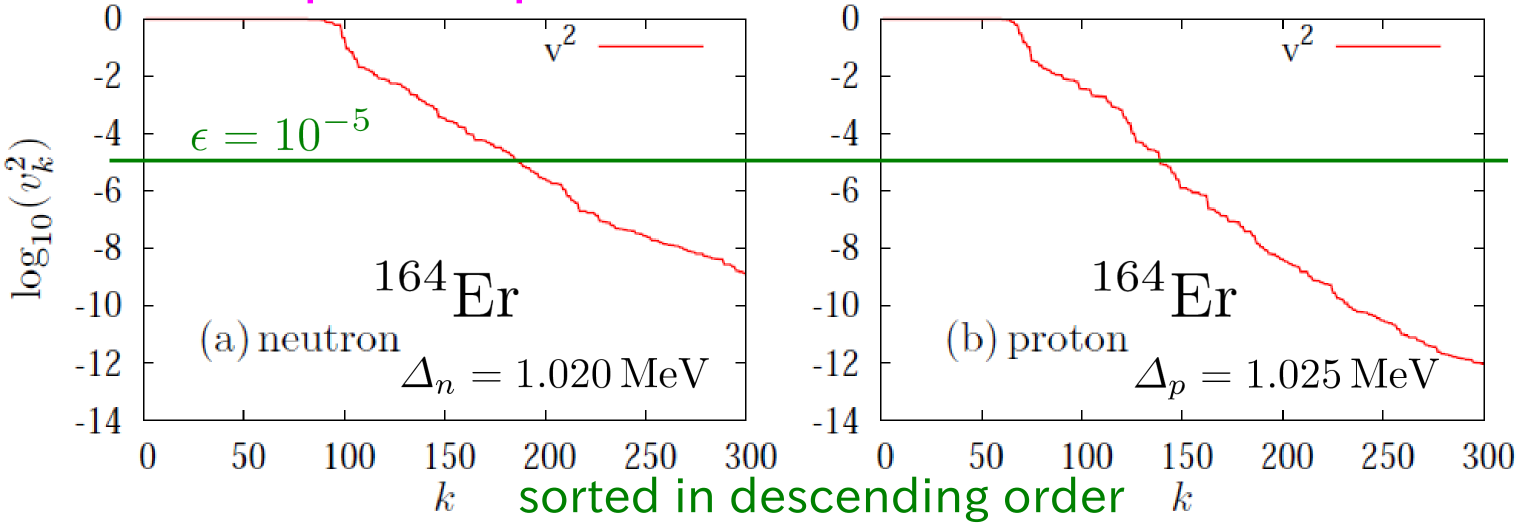
Truncation in canonical basis (1)

$$b_k^\dagger = \sum_l W_{lk} \underline{c_l^\dagger}, \qquad \langle \Phi | b_k^\dagger b_{k'} | \Phi \rangle = \delta_{kk'} \underline{v_k^2}$$

spherical HO

original-basis
=spherical-HO

occupation probabilities of canonical basis



$\beta_k |\Phi\rangle = 0$
$(k = 1, 2, \ldots, M)$

total num.
M =3,542 !!
for $N_{\mathrm{osc}}^{\max} = 20$

P-space: $k = 1, 2, \ldots, \underline{L_p}(\epsilon); \; v_k^2 > \epsilon$ ➡ L_p is much smaller !!

$$\beta_k^\dagger = \sum_l (U_{lk} c_l^\dagger + V_{lk} c_l)$$

$$U = W\bar{U}C, \quad V = W^* \bar{V} C$$

(Bloch-Messiah Theorem)

$$\bar{U} = \underbrace{\begin{pmatrix} \overbrace{\bar{U}_{pp}}^{L_p} & 0 \\ 0 & 1 \end{pmatrix}}_{M}, \quad \bar{V} = \begin{pmatrix} \bar{V}_{pp} & 0 \\ 0 & 0 \end{pmatrix}$$

Thouless form

$$|\Phi\rangle = \exp\left(\sum_{ll'} Z_{ll'} b_l^\dagger b_{l'}^\dagger \right) |0\rangle$$

canonical basis

$$Z \equiv (\bar{V}\bar{U}^{-1})^* = \begin{pmatrix} Z_{pp} & 0 \\ 0 & 0 \end{pmatrix}$$

Truncation in canonical basis (2)

D:transformation matrix
in original HO basis

Calculation of norm overlap

$$\tilde{D} \equiv W^\dagger \underline{D} W' = \begin{pmatrix} \tilde{D}_{pp} & \tilde{D}_{pq} \\ \tilde{D}_{qp} & \tilde{D}_{qq} \end{pmatrix}$$

$$\langle \Phi | \hat{D} | \Phi' \rangle = \langle 0 | \hat{D} | 0 \rangle \left(\det \tilde{D} \underline{\det \bar{\mathcal{U}}_D^*} \right)^{1/2}$$

$$\bar{\mathcal{U}}_D = \bar{U}^\dagger \tilde{D} \bar{U}' + \bar{V}^\dagger \tilde{D}^* \bar{V}'$$

$$\bar{U} = \begin{pmatrix} \bar{U}_{pp} & 0 \\ 0 & 1 \end{pmatrix}$$

$$\bar{V} = \begin{pmatrix} \bar{V}_{pp} & 0 \\ 0 & 0 \end{pmatrix}$$

$$\bar{\mathcal{U}}_D = \begin{pmatrix} \bar{U}_{pp}^\dagger \tilde{D}_{pp} \bar{U}_{pp} + \bar{V}_{pp}^\dagger \tilde{D}_{pp}^* \bar{V}_{pp} & \bar{U}_{pp}^\dagger \tilde{D}_{pq} \\ \tilde{D}_{qp} \bar{U}_{pp} & \tilde{D}_{qq} \end{pmatrix} \equiv \begin{pmatrix} \bar{\mathcal{U}}_{pp} & \bar{\mathcal{U}}_{pq} \\ \bar{\mathcal{U}}_{qp} & \bar{\mathcal{U}}_{qq} \end{pmatrix}$$

D mixes P- and Q-spaces!

MxM determinant!
(*2Mx2M* pfaffian)

But, using Thouless amplitude

$$\langle \Phi | \hat{D} | \Phi' \rangle = \langle 0 | \hat{D} | 0 \rangle |\det \bar{U} \det \bar{U}'|^{1/2} \left(\underline{\det \left[1 + Z^\dagger Z'_D \right]} \right)^{1/2}$$

$$Z = \begin{pmatrix} Z_{pp} & 0 \\ 0 & 0 \end{pmatrix} \qquad Z'_D = \tilde{D} Z' \tilde{D}^T = \begin{pmatrix} Z'_{Dpp} & Z'_{Dpq} \\ Z'_{Dqp} & Z'_{Dqq} \end{pmatrix}, \quad 1 + Z^\dagger Z_D = \begin{pmatrix} 1 + Z_{pp}^\dagger Z_{Dpp} & Z_{pp}^\dagger Z_{Dpq} \\ 0 & 1 \end{pmatrix}$$

$$\langle \Phi | \hat{D} | \Phi' \rangle = \langle 0 | \hat{D} | 0 \rangle |\det \bar{U}_{pp} \det \bar{U}'_{pp}|^{1/2} \left(\det \left[1 + Z_{pp}^\dagger Z'_{Dpp} \right] \right)^{1/2}$$

LpxLp determinant!

The matrix dimension reduced from *MxM* to *LpxLp*
Here $M \approx O(1,000)$ $L_p \approx O(100)$!!

Including one-body operator, $\langle \Phi | \hat{O} \hat{D}(\boldsymbol{x}) | \Phi' \rangle$, it can be shown that the calculational effort: $O(M^3) \rightarrow O(M L_p^2)$

LARGE REDUCTION OF CALCULATION $\sim$ 100times by the way, the actual calculation is performed with using the pfaffian rather than determinant,

$$\hat{D}|\Phi\rangle \to |\Phi_D\rangle$$ another HFB-type state

generally for overlap of two HFB-type states

$$\langle\Phi|\Phi'\rangle = |\det \bar{U} \det \bar{U}'|^{1/2} \underline{\left(\det\left[1+Z^\dagger Z'\right]\right)^{1/2}}$$

square-root of complex number!
→ "sign-problem"

$$\left(\det\left[1+Z^\dagger Z'\right]\right)^{1/2} = \left[\det\begin{pmatrix} Z' & -1 \\ 1 & Z^\dagger \end{pmatrix}\right]^{1/2}$$

$$\Rightarrow (-)^{M(M+1)/2}\, \underbrace{\mathrm{pf}\begin{pmatrix} Z' & -1 \\ 1 & Z^\dagger \end{pmatrix}}_{\text{pfaffian}}$$

For 2Nx2N anti-symmetric matrix R,

$$\mathrm{pf}(R) \equiv \frac{1}{2^n n!} \sum_{\sigma\in S_{2N}} \mathrm{sgn}(\sigma) \prod_{i=1}^{N} R_{\sigma(2i-1)\sigma(2i)}$$

L.M.Robledo, PRC79(2009),021302(R).

In order to calculate pfaffian, Thouless form is necessary!

Utilize Thouless form with Slater-det.(1)

Slater-determinant in canonical basis: $|\phi_0\rangle = \prod_{k=1}^{N} b_k^\dagger |0\rangle$

$$|\Phi\rangle = \exp\left(\sum_{ll'} (Z_a)_{ll'} a_l^\dagger a_{l'}^\dagger\right)|\phi_0\rangle$$

$$|\Phi\rangle = \exp\left(\sum_{ll'} (Z_b)_{ll'} b_l^\dagger b_{l'}^\dagger\right)|0\rangle$$

N :neutron/proton number

$$a_k^\dagger = \begin{cases} b_k & (1 \le k \le N) \\ b_k^\dagger & (N+1 \le k \le M) \end{cases}$$

$Z_a = (V_a U_a^{-1})^* \longleftrightarrow$ pairing correlations

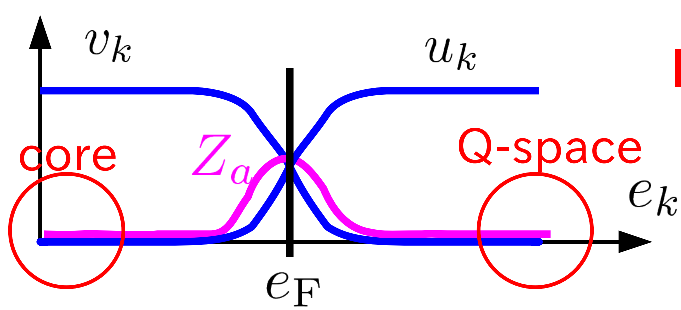
$u_k \leftrightarrow v_k$ for hole states $(k = 1, 2, ..., N)$

$Z_a \to 0$ as $\Delta \to 0$ while $Z_b \to \infty$ as $\Delta \to 0$

$u_k^2 = 1 - v_k^2$

One can take the no-pairing limit !!

Furthermore,



→ additional truncation: core (deep hole) contributions

core-space: $k = 1, 2, ..., L_o(\epsilon);\ u_k^2 < \epsilon$

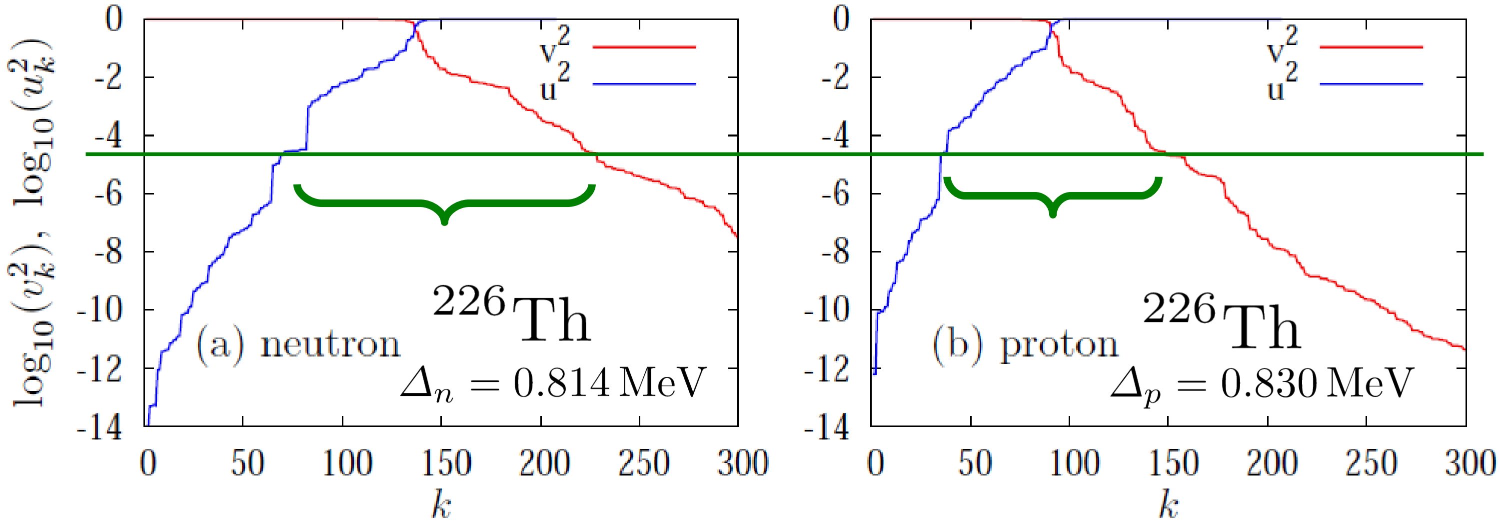
$$Z_a = \begin{array}{c} \overbrace{}^{L_o} \qquad\qquad L_p - L_o \\ \underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 0 & Z_{\bar{p}\bar{p}} & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{L_p} \end{array} \Big\} M$$

Reduction by core truncation is restricted (need to calculate $\langle\phi_0|\hat{O}\hat{D}(\boldsymbol{x})|\phi_0'\rangle$), but effective for heavy nuclei !!

projection from HF states

Utilize Thouless form with Slater-det.(2)

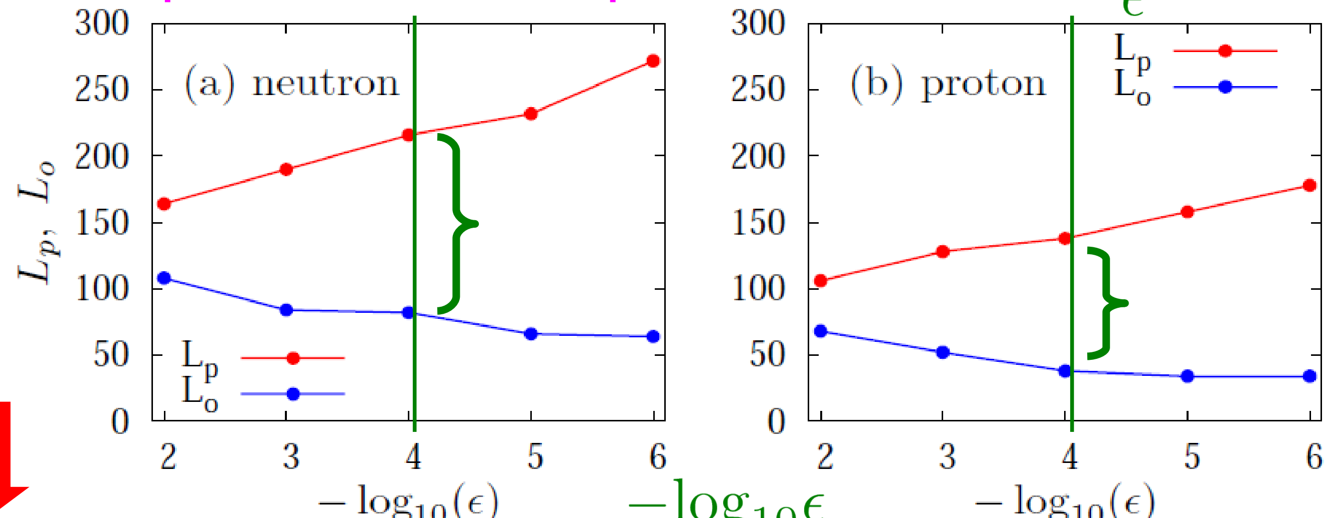
occupation and emplty probabilities of canonical basis



$\epsilon \approx 10^{-4}$

P-spce and core-space dimentions

ϵ



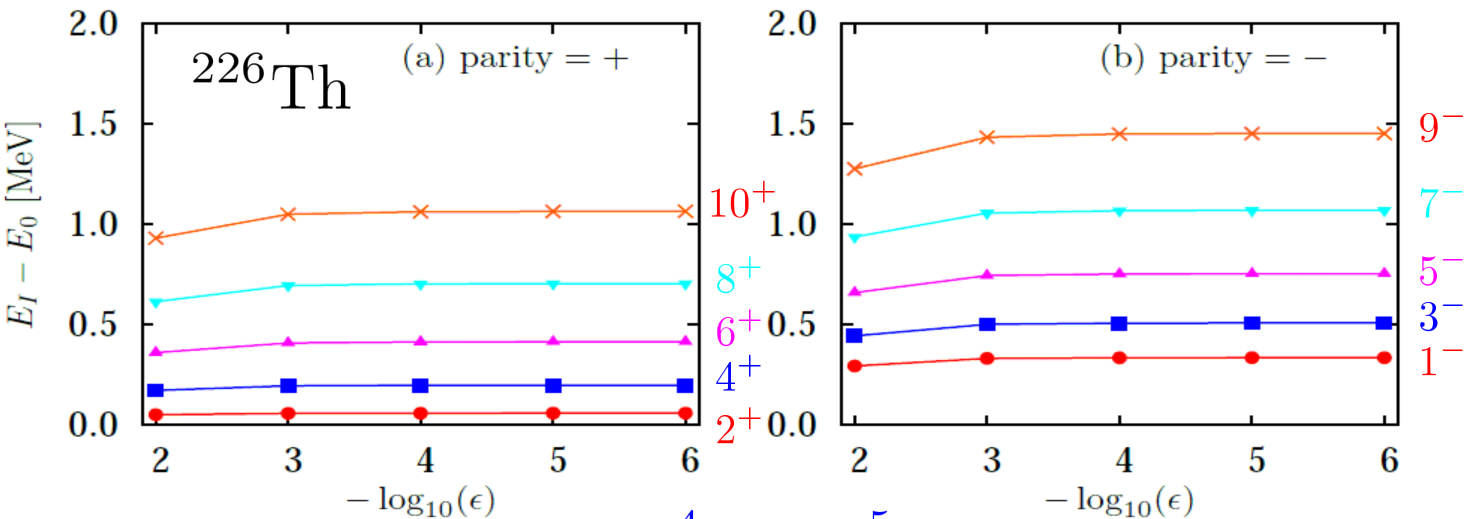
$-\log_{10}\epsilon$

Reduction of effective number of space:

$M \approx 3,000 \Rightarrow L_p - L_o \approx 100$ about 2-3 orders of magnitude!

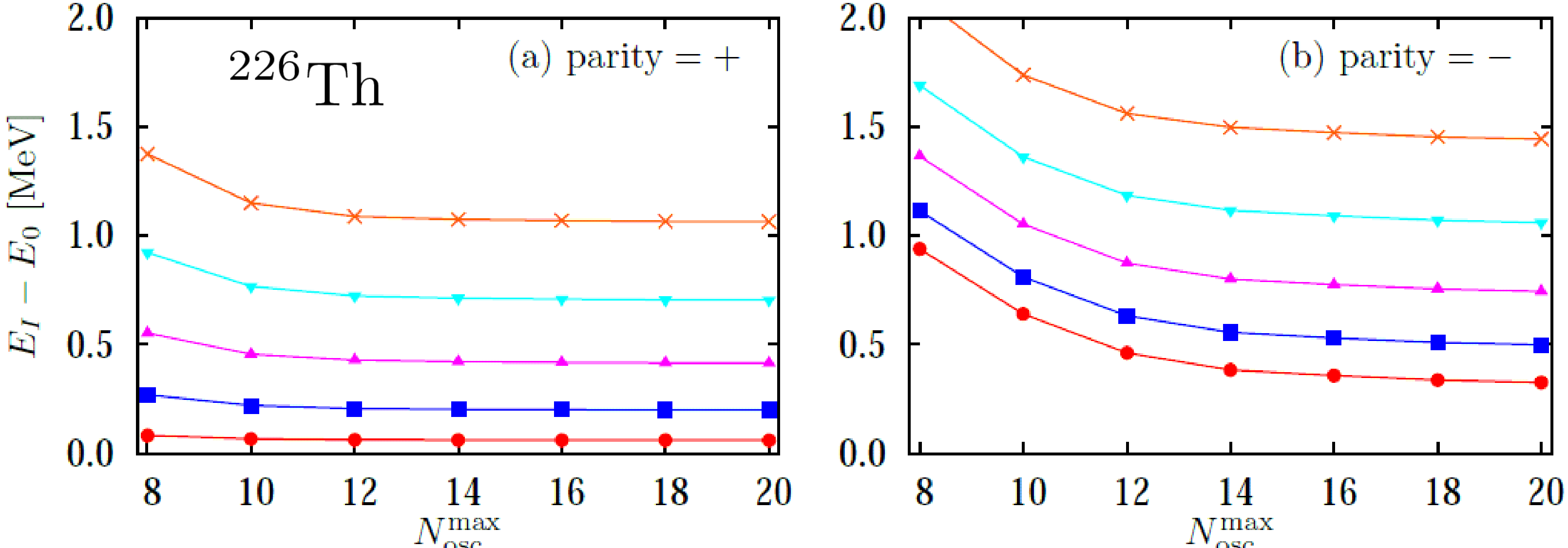
Test of convergence

Rotational excitation spectra: $^{226}\mathrm{Th}$ octupole deformed



ang.mom.,
number,
parity,
-projections

$\epsilon \approx 10^{-4} - 10^{-5}$ is enough



$N_{\mathrm{osc}}^{\mathrm{max}} \approx 16 - 18$ is enough

Choice of hamiltonian

Skyrme,Gogny : density-dep.
$\rightarrow$ some problems

Schematic multi-separable type,
consistent with Woods-Saxon mean-field

$$\hat{H} = \hat{h} + \hat{H}_F + \hat{H}_G, \qquad \hat{h} = \sum_{\tau=\mathrm{n,p}} \left(\hat{t}_\tau + \underline{\hat{V}^\tau_{\mathrm{WS}}} \right),$$

particle-hole channel
$\lambda = 2, 3, 4$

$$\hat{H}_F = -\frac{1}{2}\chi \sum_{\lambda \geq 2} : \hat{F}_\lambda \cdot \hat{F}_\lambda :, \qquad \hat{F}_{\lambda\mu} = \sum_{\tau=\mathrm{n,p}} \sum_{ij} \langle i|\hat{F}^\tau_{\lambda\mu}|j\rangle \hat{c}^\dagger_i \hat{c}_j$$

isoscalar

$$F^\tau_{\lambda\mu}(\boldsymbol{r}) \equiv R^\tau_0 \underline{\frac{dV^\tau_c}{dr}} Y_{\lambda\mu}(\theta,\phi), \quad V^\tau_c, R^\tau_0 \text{ :WS cental pot., radius}$$

Bohr-Mottelson textbook Vol.II

$$\chi = \chi_{\mathrm{self}} = (\kappa_n + \kappa_p)^{-1}, \quad \kappa_\tau \equiv (R^\tau_0)^2 \int \rho^\tau_0(r) \frac{d}{dr}\left(r^2 \frac{dV^\tau_c(r)}{dr} \right) dr$$

pairing channel
$\lambda = 0, 2$

$$\hat{H}_G = -\sum_{\tau,\lambda \geq 0} g^\tau_\lambda \hat{G}^{\tau\dagger}_\lambda \cdot \hat{G}^\tau_\lambda, \qquad \hat{G}^{\tau\dagger}_{\lambda\mu} \equiv \frac{1}{2} \sum_{ij} \langle i|\tilde{G}^\tau_{\lambda\mu}|j\rangle \hat{c}^\dagger_i \hat{c}^\dagger_{\tilde{j}},$$

$$\tilde{G}_{\lambda\mu}(\boldsymbol{r}) \equiv \left(\frac{r}{\bar{R}_0} \right)^\lambda \sqrt{\frac{4\pi}{2\lambda+1}} Y_{\lambda\mu}(\theta,\phi), \quad \bar{R}_0 = 1.2A^{1/3}\ \mathrm{fm}$$

g^τ_0 :even-odd mass diff. $\quad g^\tau_2/g^\tau_0 = 13.6$:moment of inertia

Mean-field state $|\Phi\rangle$ is generated with cranking

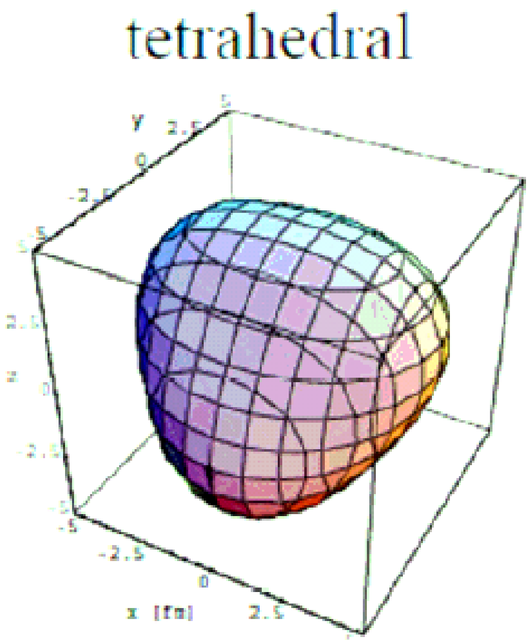
deformation by Woods-Saxon -Strutinsky cal.

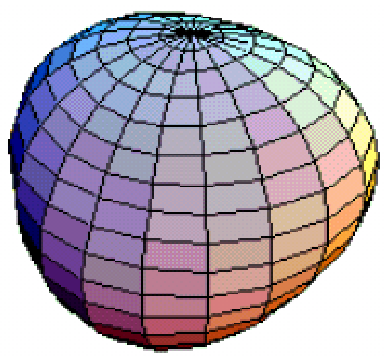
$$\hat{h}' = \underline{\hat{h}_{\mathrm{def}}} - \sum_{\tau=\mathrm{n,p}} \Delta_\tau \left(\hat{P}^\dagger_\tau + \hat{P}_\tau \right) - \sum_{\tau=\mathrm{n,p}} \lambda_\tau \hat{N}_\tau - \underline{\omega_{\mathrm{rot}} \hat{J}_x},$$

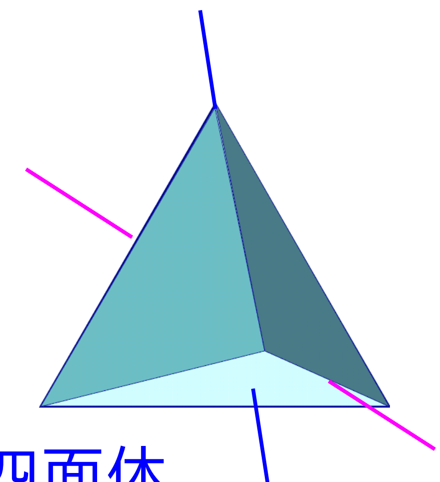
Monopole pair field

Application to tetrahedral shape

S.Tagami, Y.R.Shimizu, and J.Dudek,
arXiv: 1301.3278, 1301.3279.







正四面体

one of regular polyhedron

Tetrahedral nuclear states

Usual quadrupole def. ⟷ D_{2h}-symmetry

Higher point-group symmetry in nuclei ?

symmetry ⟷ degeneracies of single-particle orbits ⟷ stability (shell-effect)

nuclear shape : $R(\theta,\varphi) = R_0 c_v(\{\alpha\})\Big(1 + \sum_{\lambda,\mu} \underline{\alpha^*_{\lambda\mu}} Y_{\lambda\mu}(\theta,\varphi)\Big)$

Tetrahedral T_d : only $\alpha_{32} \equiv t_3$ (no $\alpha_{2\mu}, \alpha_{4\mu}, \alpha_{5\mu}, \alpha_{6\mu}$)

➡ 4-fold degenerate orbits appears (usually 2-fold !)

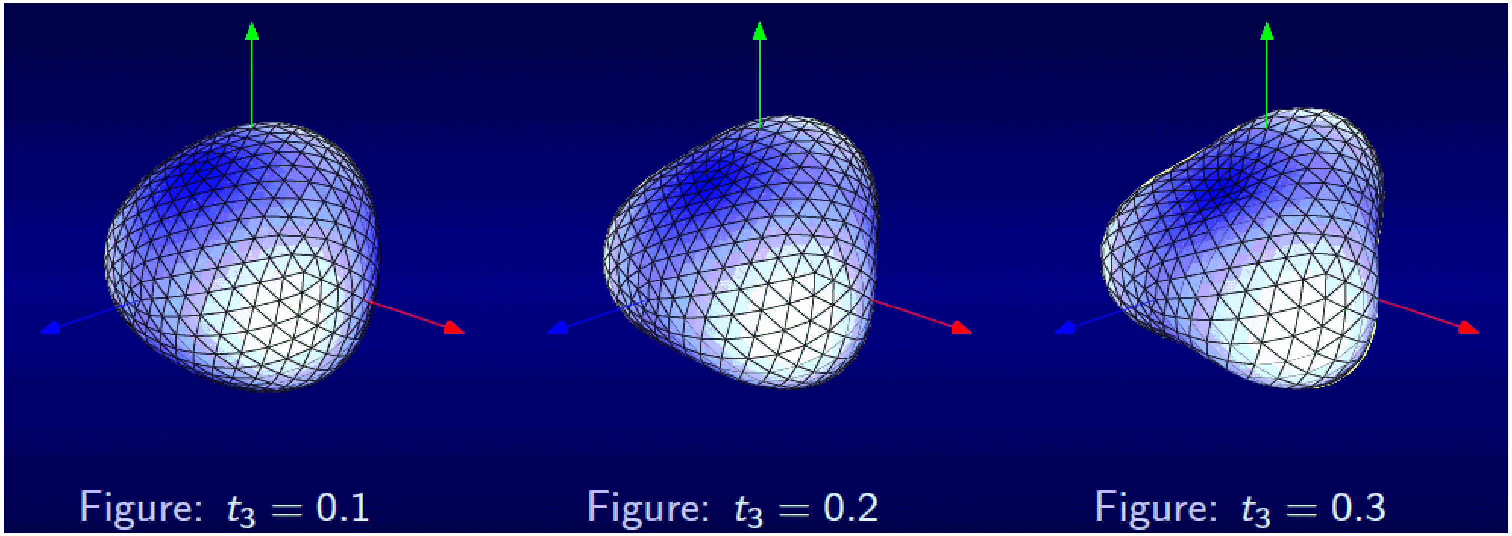
X.Li and J.Dudek, PRC49(1994),R1250.

Various predictions so far:

- Onishi-Shline, NPA165(1971),180. $^{16}\mathrm{O}$ 4-α states
- Takami-Yabana-Matsuo, PLB431(1998),242. Skyrme HF/HFB
- Yamagami-Matsuyanagi-Matsuo, NPA693(2001),579. $^{80}\mathrm{Zr}$
- J.Dudek et al., PRL88(2002),252502; PRL97(2006),072501.

  systematic calculations with
  Woods-Saxon Strutinsky and Skyrme HF/HFB approaches

Tetrahedral shape and magic numbers

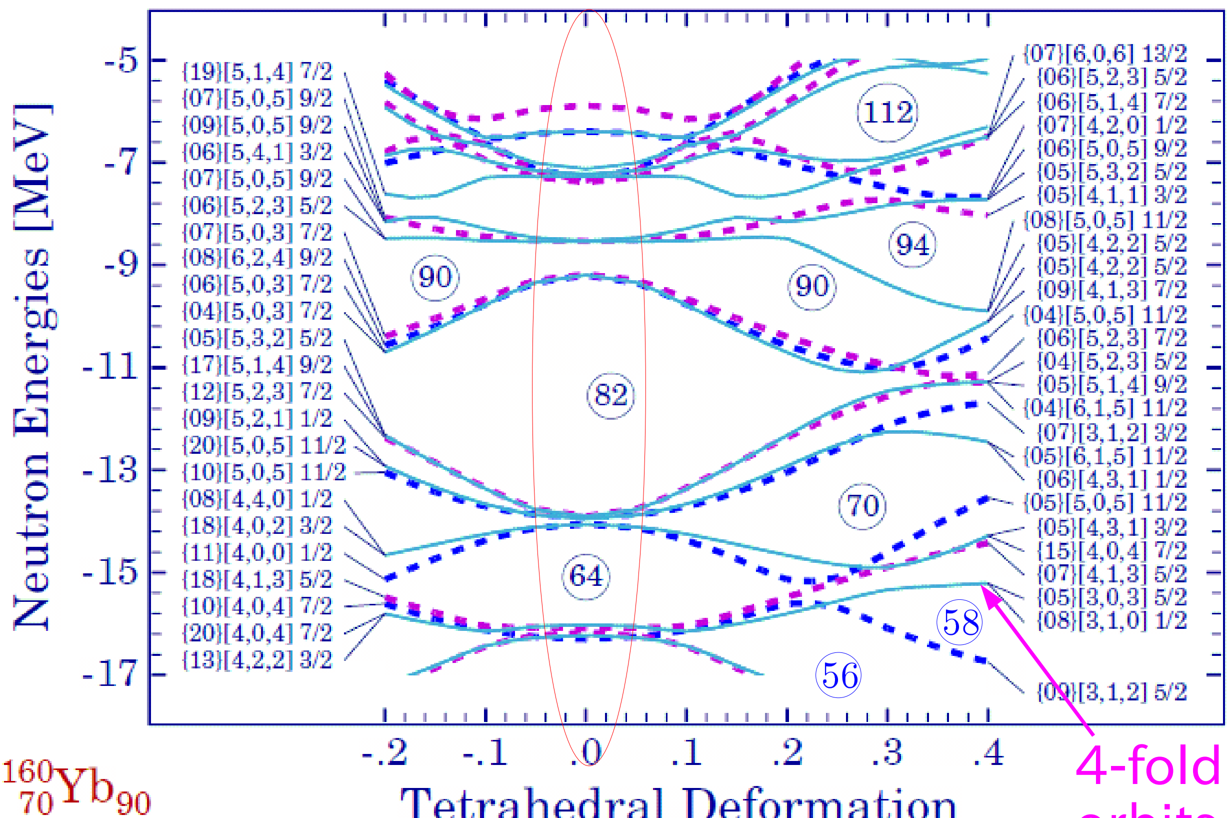


$t_3 = \alpha_{32}$

$\alpha_{\lambda\mu}$

λ:odd, $\mu \neq 0$

parity broken and non-axial deformation



$^{160}_{70}\mathrm{Yb}_{90}$

4-fold orbits

Tetrahedral Magic numbers:

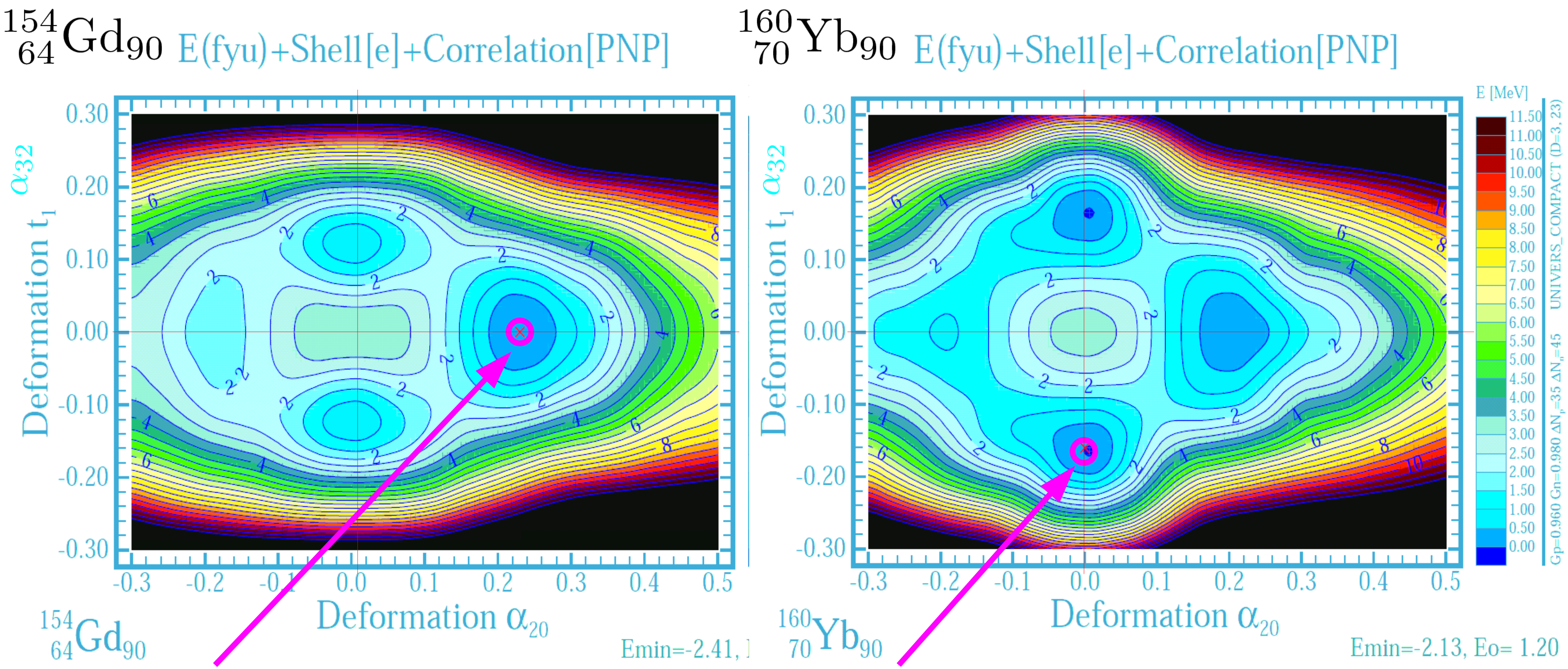
16,20,32,40, 56(58),64,70, 90,112,136

$^{64}_{32}\mathrm{Ge}_{32}$, $^{72}_{32}\mathrm{Ge}_{40}$, $^{88}_{32}\mathrm{Ge}_{56}$, $^{80}_{40}\mathrm{Zr}_{40}$, $^{110}_{40}\mathrm{Zr}_{70}$, $^{112}_{56}\mathrm{Ba}_{56}$, $^{126}_{56}\mathrm{Ba}_{70}$, $^{146}_{56}\mathrm{Ba}_{90}$, $^{134}_{64}\mathrm{Gd}_{70}$, $^{154}_{64}\mathrm{Gd}_{90}$, $^{160}_{70}\mathrm{Yb}_{90}$, $^{222}_{90}\mathrm{Th}_{136}$

Example of potential surface calculations

Woods-Saxon universal-compact potential,
Strutinsky cal. with finite-range droplet model

Projection of Multi-dimensional (λ <9) surface to $(\alpha_{32}, \alpha_{20})$
(Strasbourg-Lublin-Krakow collaboration)

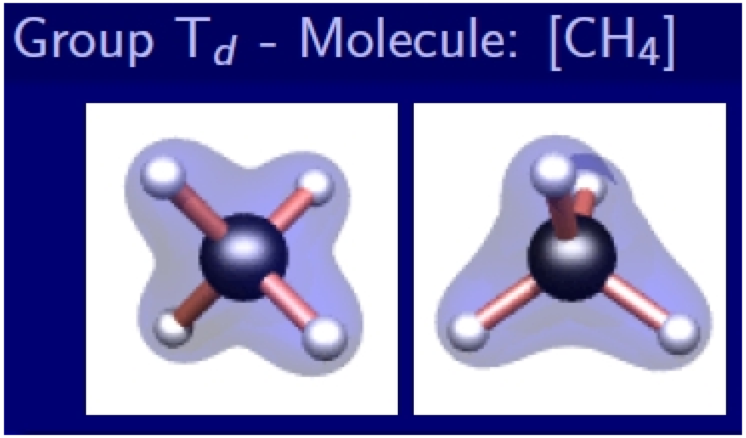


Quadrupole ground state!

Tetrahedral ground state!
(Z=70,N=90)

What kind of spectra is expected for tetrahedral rotor?

methane



Known in molecules

deformation → quantum rotor,
but "spherical rotor" in a sense,

$$\mathcal{J}_1 = \mathcal{J}_2 = \mathcal{J}_3 = \mathcal{J}, \qquad E(I) = \frac{I(I+1)}{2\mathcal{J}}$$

But, no quadrupole moment Q_2, no E2 transitions at all !

Group theory consideration

(irreducible representations of point-group T_d)

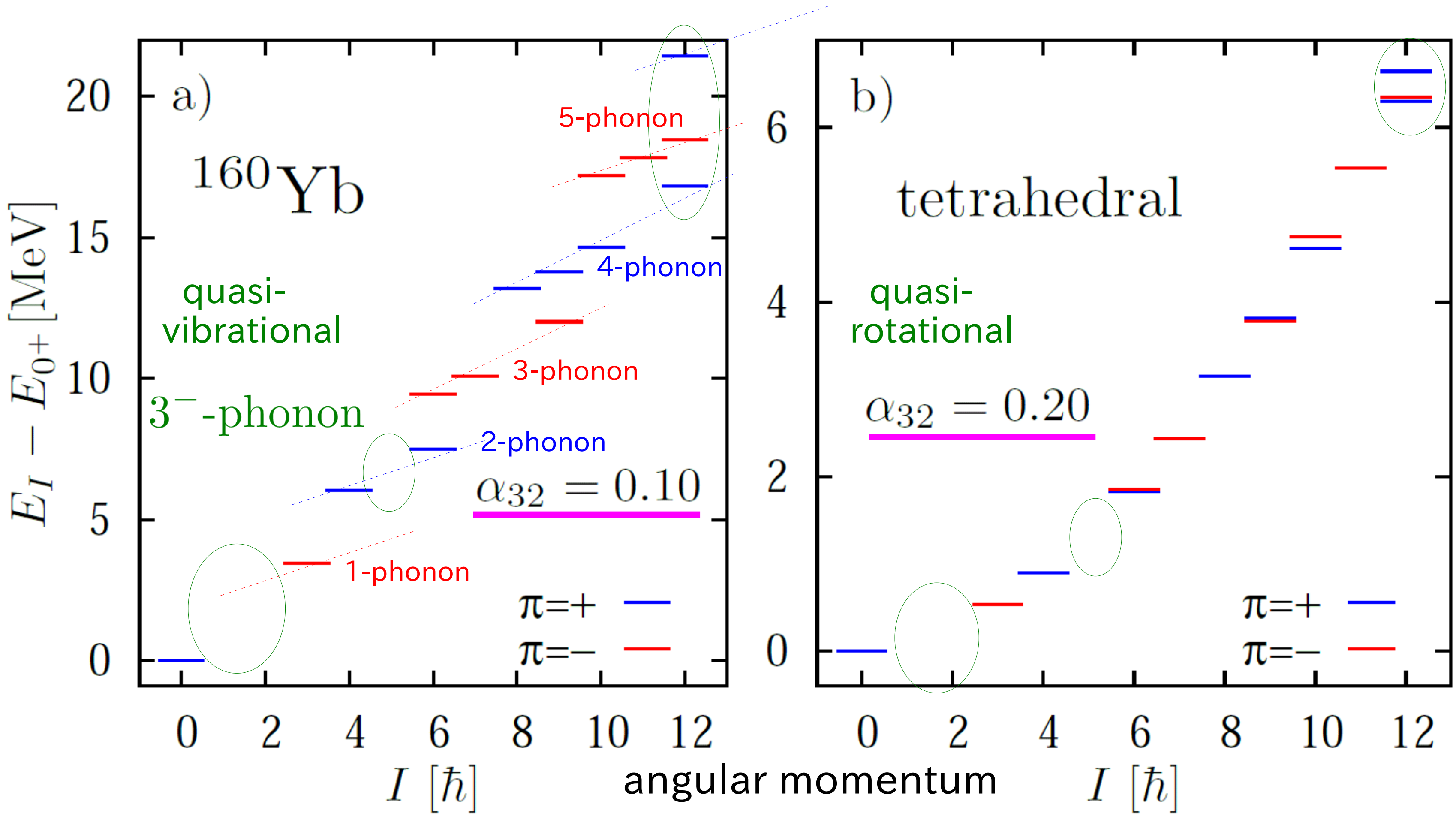
five irrep.'s
A_1,A_2,
E,
F_1,F_2

even-even nucleus with pairing

$$\boxed{A_1 : \quad \begin{array}{l} 0^+,\, 3^-,\, 4^+,\, 6^+,\, 6^-,\, 7^-,\, 8^+,\, 9^+,\, 9^-, \\ 10^+,\, 10^-,\, 11^-,\, 2\times 12^+,\, 12^-,\, \cdots . \end{array}}$$

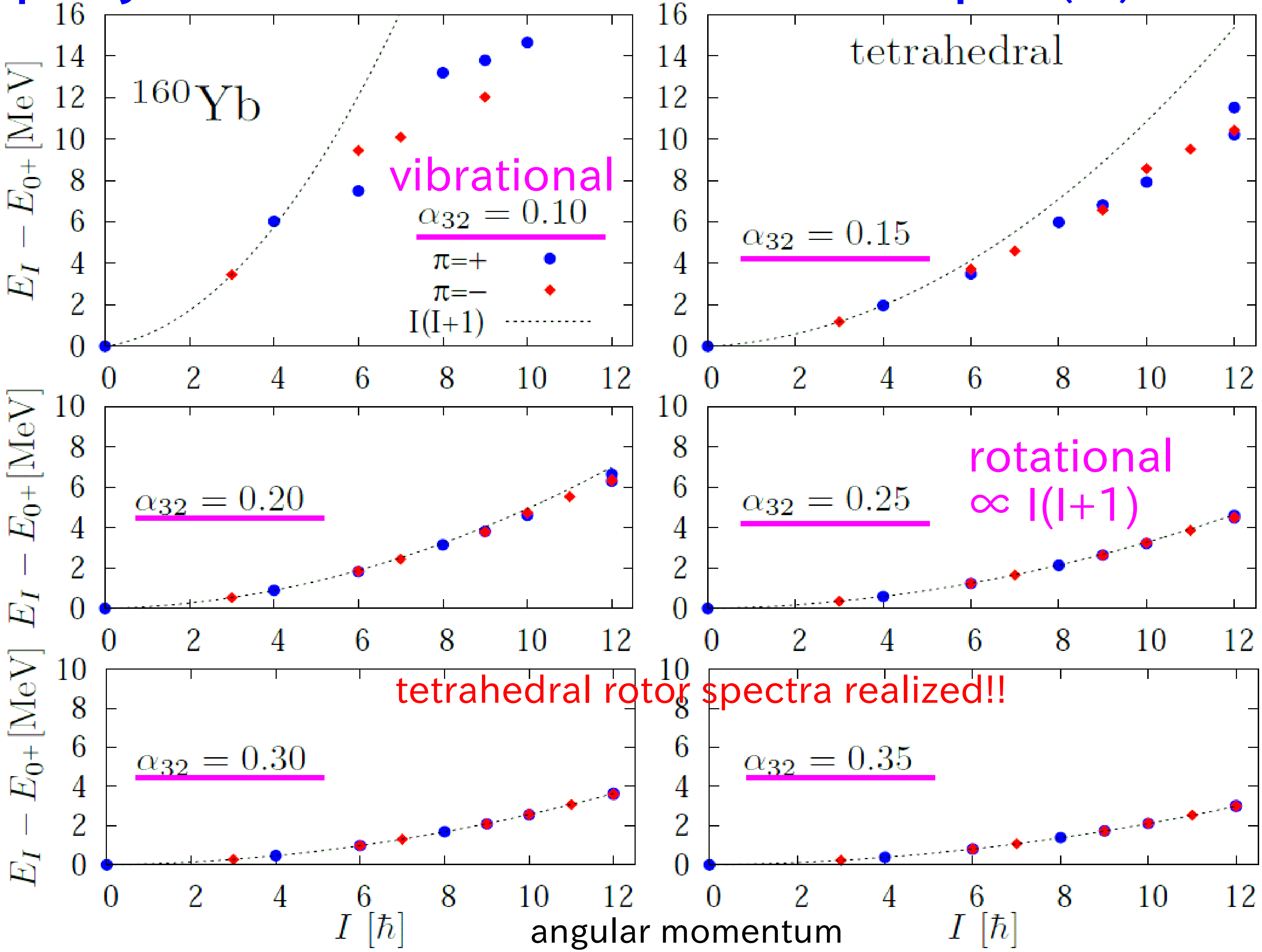
as the lowest band

Result of angular momentum and parity projection for tetrahedral shape (1)



$$A_1 : \quad 0^+, 3^-, 4^+, 6^+, 6^-, 7^-, 8^+, 9^+, 9^-, \\ 10^+, 10^-, 11^-, 2 \times 12^+, 12^-, \cdots .$$

Result of angular momentum and parity projection for tetrahedral shape (2)



What kind of spectra is expected for tetrahedral rotor? (2)

Group theory consideration

odd nuclei (half-integer spins)

completely different from quadrupole rotor!

three irrep.'s

$$E_{1/2}: \quad \frac{1}{2}^+, \frac{5}{2}^-, \frac{7}{2}^+, \frac{7}{2}^-, \frac{9}{2}^+, \frac{11}{2}^+, \frac{11}{2}^-, \frac{13}{2}^+, 2\times\frac{13}{2}^-, \frac{15}{2}^+, \frac{15}{2}^-, \cdots.$$

parity conjugate

two-fold states

$$E_{5/2}: \quad \frac{1}{2}^-, \frac{5}{2}^+, \frac{7}{2}^-, \frac{7}{2}^+, \frac{9}{2}^-, \frac{11}{2}^-, \frac{11}{2}^+, \frac{13}{2}^-, 2\times\frac{13}{2}^+, \frac{15}{2}^-, \frac{15}{2}^+, \cdots.$$

$$G_{3/2}: \quad \frac{3}{2}^+, \frac{3}{2}^-, \frac{5}{2}^+, \frac{5}{2}^-, \frac{7}{2}^+, \frac{7}{2}^-, 2\times\frac{9}{2}^+, 2\times\frac{9}{2}^-, 2\times\frac{11}{2}^+, 2\times\frac{11}{2}^-, 2\times\frac{13}{2}^+, 2\times\frac{13}{2}^-, \cdots.$$

parity doublets

four-fold states

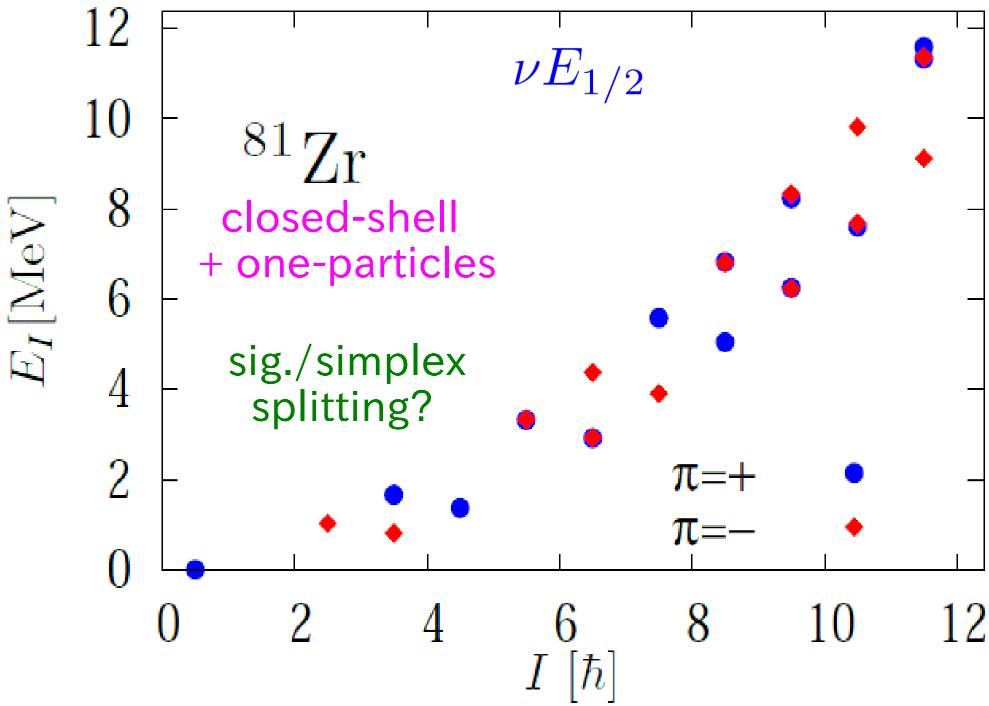
which becomes lowest depends on the last odd-nucleon orbit!

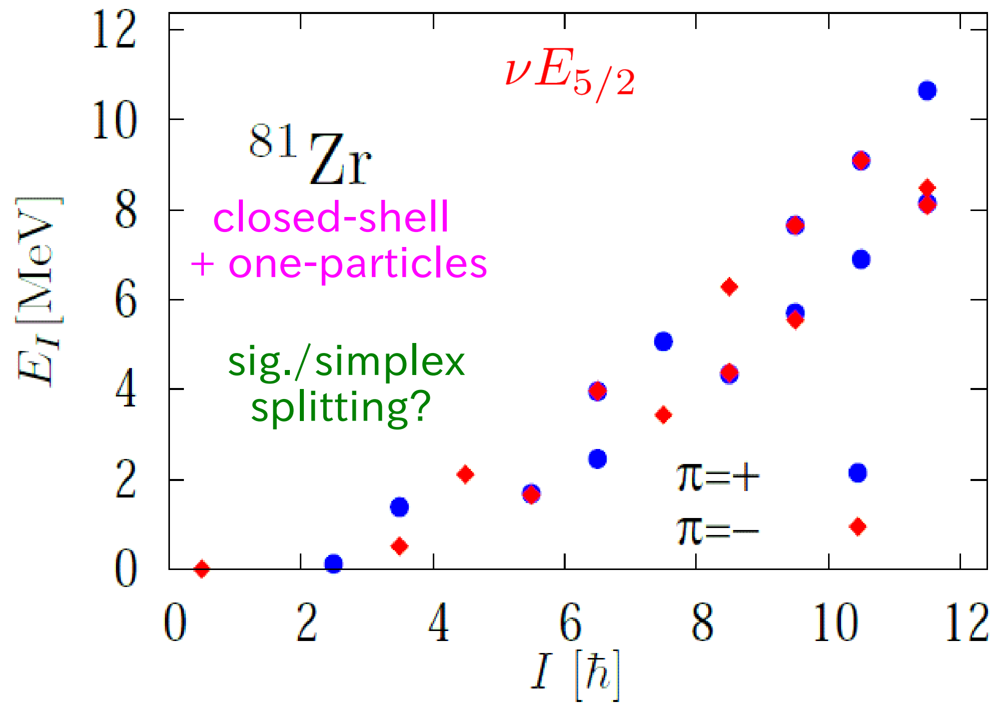
Example of calculations (1)

Very new!

odd nuclear states around ^{80}Zr (N=Z=40)

α_{32}=0.4 and without pairing (Δ=0)





$$E_{1/2}: \quad \frac{1}{2}^+, \frac{5}{2}^-, \frac{7}{2}^+, \frac{7}{2}^-, \frac{9}{2}^+, \frac{11}{2}^+, \frac{11}{2}^-, \frac{13}{2}^+, 2\times\frac{13}{2}^-, \frac{15}{2}^+, \frac{15}{2}^-, \cdots.$$

$$E_{5/2}: \quad \frac{1}{2}^-, \frac{5}{2}^+, \frac{7}{2}^-, \frac{7}{2}^+, \frac{9}{2}^-, \frac{11}{2}^-, \frac{11}{2}^+, \frac{13}{2}^-, 2\times\frac{13}{2}^+, \frac{15}{2}^-, \frac{15}{2}^+, \cdots.$$

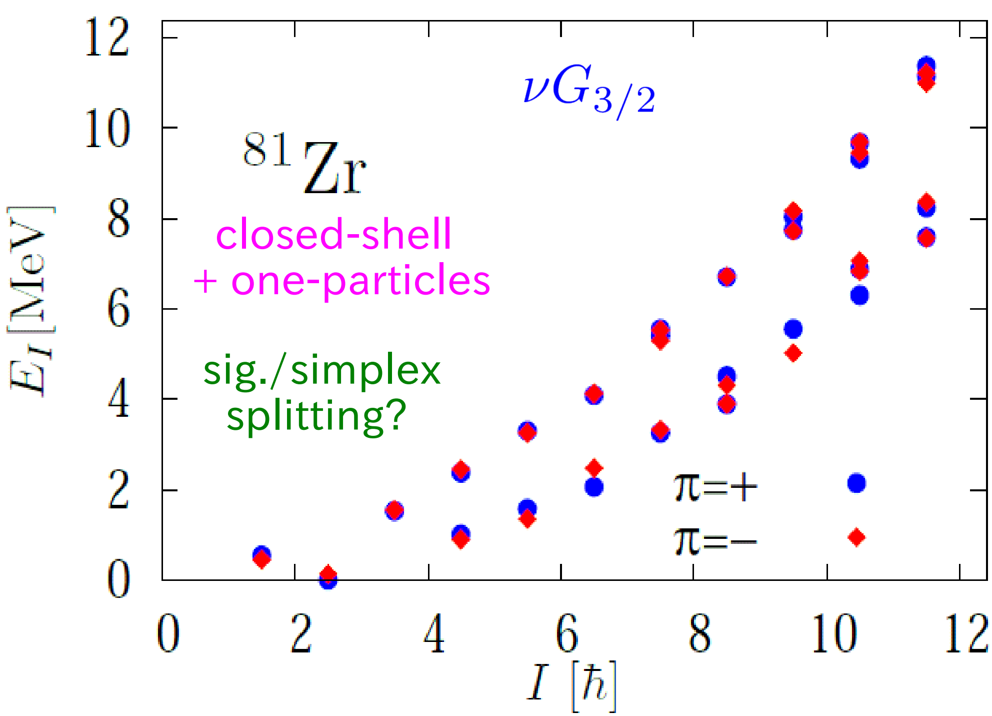
Group theory consideration OK,
but projection necessary for precise spectra !!

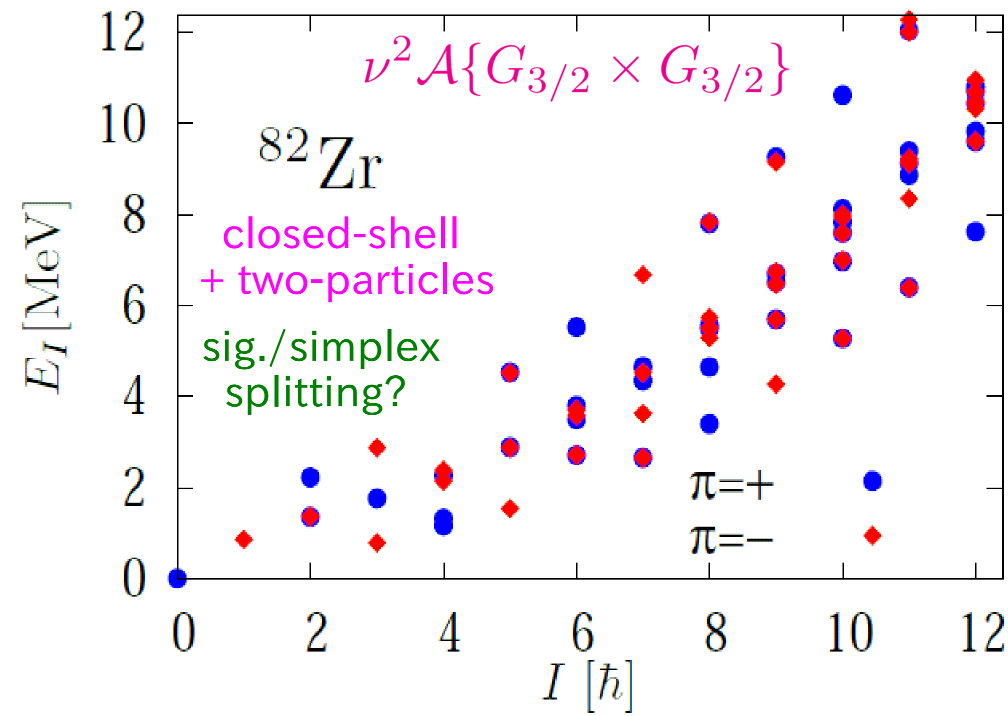
Example of calculations (2)

Very new!

odd and two-particle states around ^{80}Zr (N=Z=40)

α_{32}=0.4 and without pairing (Δ=0)





$$G_{3/2}: \quad \frac{3}{2}^+, \frac{3}{2}^-, \frac{5}{2}^+, \frac{5}{2}^-, \frac{7}{2}^+, \frac{7}{2}^-, 2\times\frac{9}{2}^+, 2\times\frac{9}{2}^-, 2\times\frac{11}{2}^+, 2\times\frac{11}{2}^-, 2\times\frac{13}{2}^+, 2\times\frac{13}{2}^-, \cdots.$$

$$\mathcal{A}\{G_{3/2} \times G_{3/2}\} = A_1 + E + F_2$$

F_2 seems split into three bands

Group theory consideration OK,
but projection necessary for precise spectra !!

Irreducible representations of T_d-rotor for even-even nuclei (integer spins)

$$A_1 : \begin{array}{l} 0^+, 3^-, 4^+, 6^+, 6^-, 7^-, 8^+, 9^+, 9^-, \\ 10^+, 10^-, 11^-, 2\times 12^+, 12^-, \cdots . \end{array}$$

parity conjugate

$$A_2 : \begin{array}{l} 0^-, 3^+, 4^-, 6^-, 6^+, 7^+, 8^-, 9^-, 9^+, \\ 10^-, 10^+, 11^-, 2\times 12^-, 12^+, \cdots . \end{array}$$

$$E : \begin{array}{l} 2^+, 2^-, 4^+, 4^-, 5^+, 5^-, 6^+, 6^-, 7^+, 7^-, \\ 2\times 8^+, 2\times 8^-, 9^+, 9^-, 2\times 10^-, 2\times 10^+, \cdots . \end{array}$$

$$F_1 : \begin{array}{l} 1^+, 2^-, 3^+, 3^-, 4^+, 4^-, 2\times 5^+, 5^-, 6^+, 2\times 6^-, \\ 2\times 7^+, 2\times 7^-, 2\times 8^+, 2\times 8^-, 3\times 9^+, 2\times 9^-, \cdots . \end{array}$$

parity conjugate

$$F_2 : \begin{array}{l} 1^-, 2^+, 3^-, 3^+, 4^-, 4^+, 2\times 5^-, 5^+, 6^-, 2\times 6^+, \\ 2\times 7^-, 2\times 7^+, 2\times 8^-, 2\times 8^+, 3\times 9^-, 2\times 9^+, \cdots . \end{array}$$

How demanding for computer

Full angular momentum projection is demanding!
because of three dimensional integrals

Typical tetrahedral calculation with cranking:
all the symmetries broken

Medium heavy nuclei with mesh of Euler angles,

$$N_\alpha = N_\beta = N_\gamma \approx 100$$

(for sizable tetrahedral deformation)

Two to three days: 50 — 70 hours by a machine
with Xeon E5645(6cores)x2=12 CPU cores

c.f. If the system is nearly axially symmetric,
then the calculation is much faster!

Application to high-spin states

Y.Fujioka master thesis, Mar. 2012

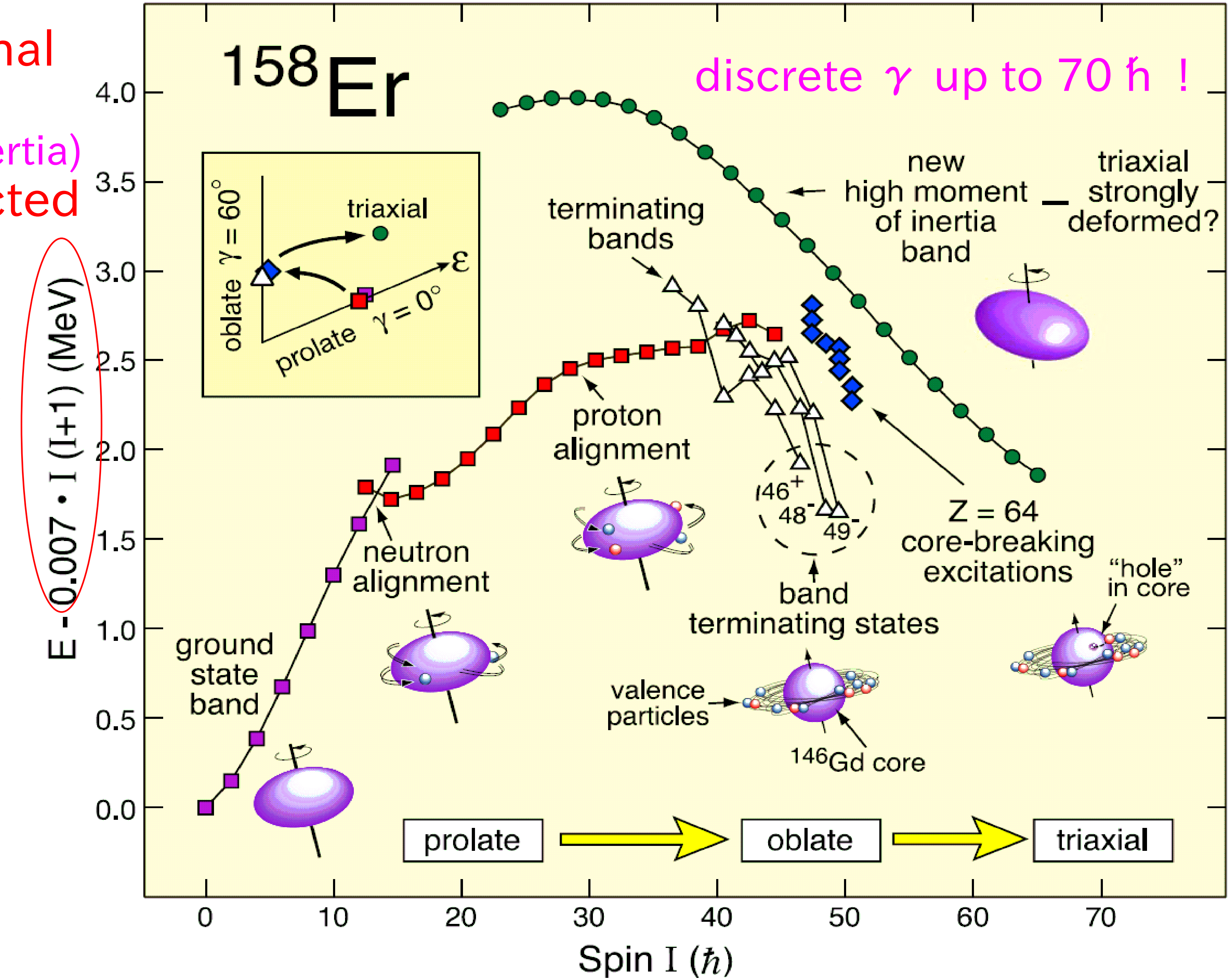
・" Problem" of projection from cranked mean-field

・Wobbling rotational band
・Chiral doublet band

State-of-the-art high-spin yrast spectra

E.S.Paul et al., PRL 98,012501(2007)

bulk rotational energy (rigid inertia) subtracted



Application to high-spin states

Mean-field approximation
⟷ Cranking method

Mean-field state $|\Phi\rangle$ is generated with cranking

$$\hat{h}' = \hat{h}_{\rm def} - \sum_{\tau={\rm n,p}} \Delta_\tau \left(\hat{P}_\tau^\dagger + \hat{P}_\tau\right) - \sum_{\tau={\rm n,p}} \lambda_\tau \hat{N}_\tau - \underline{\omega_{\rm rot}\hat{J}_x},$$

rotational frequency

$\omega_{\rm rot} \to {\rm large} \quad \Leftrightarrow \quad \langle \hat{J}_x \rangle = I(\omega_{\rm rot}) \to {\rm large}$ high-spin states

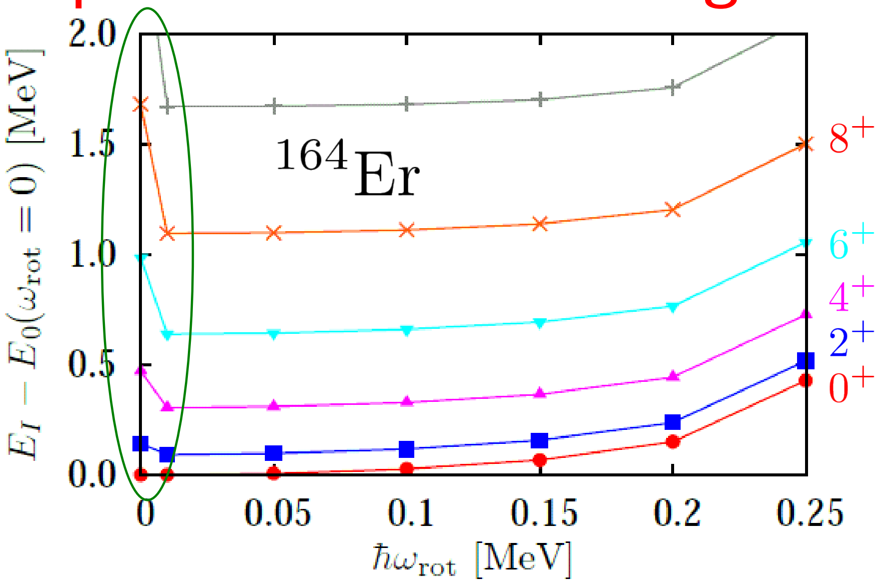
$|\Psi_{IM=I}\rangle \approx |\Phi(\omega_{\rm rot})\rangle$ semiclassical quantization

Angular momentum projection
→ rotational band:
how about high-spin states?

Some results of projection calculation

(no configuration-mixing!)

Importance of cranking for moment of inertia



difference between $\omega_{\rm rot}=0$ and $\omega_{\rm rot}\neq 0$

$\omega_{\rm rot}=0 \rightarrow E_I = \mathcal{H}^I_{00}/\mathcal{N}^I_{00}$

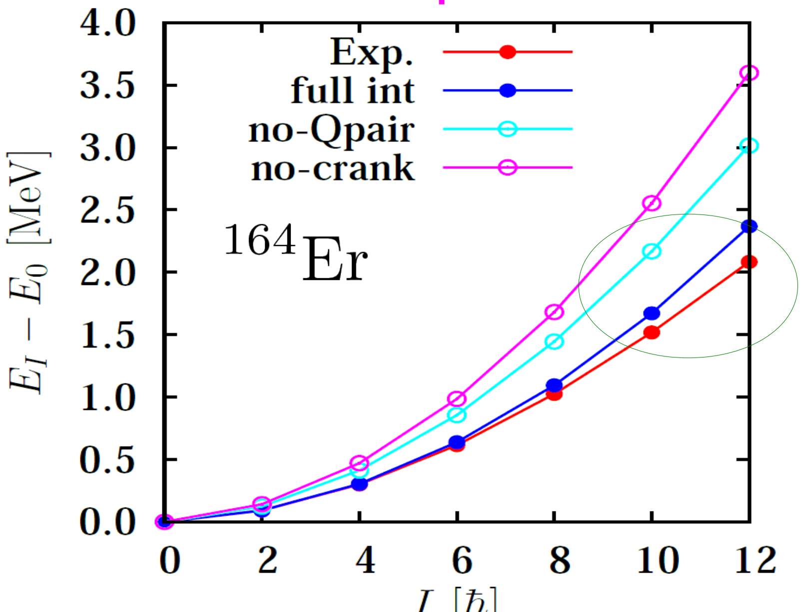
only K=0 contributes (axially symm.), but

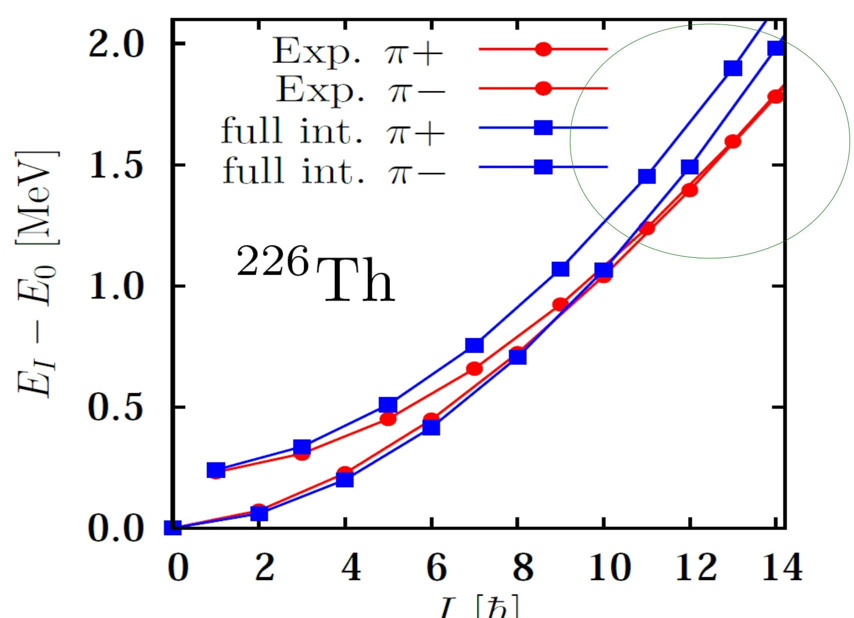
$\omega_{\rm rot}\neq 0 \rightarrow \det\left(\mathcal{H}^I_{KK'} - E_I\mathcal{N}^I_{KK'}\right)=0$

K-mixing contributes, even if $\omega_{\rm rot}\rightarrow 0$ → larger mom. of inertia

small $\omega_{\rm rot}$ is enough

Rotational spectra



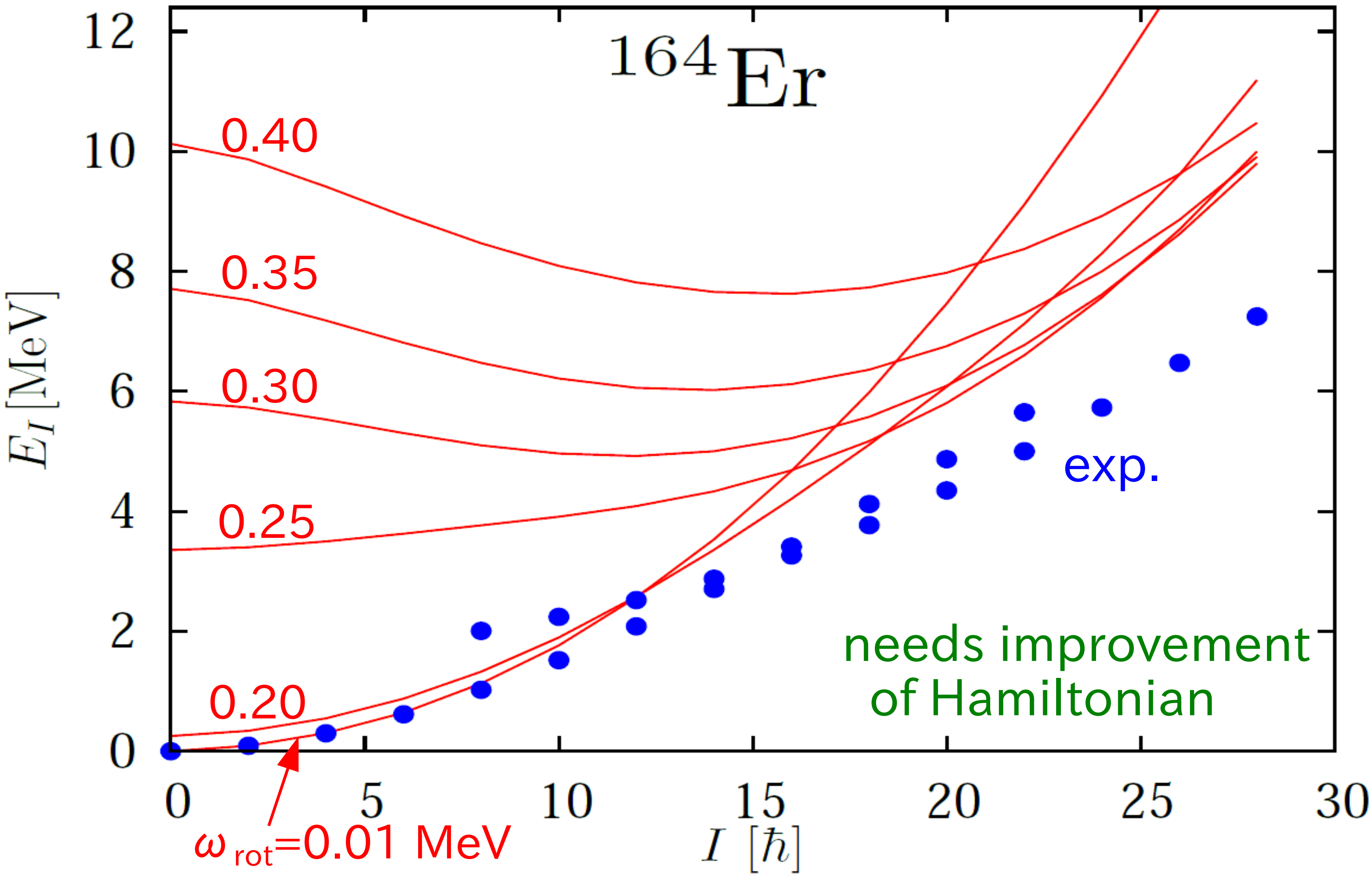


"Problem" of projection from cranked mean-field

Which frequency $\omega_{\rm rot}$ should be used?

$$|\Psi_{IM}(\omega_{\rm rot})\rangle = \sum_K g_K^I \; \hat{P}_{MK}^I \, |\Phi(\omega_{\rm rot})\rangle$$

extra-ambiguity!



Possible solutions

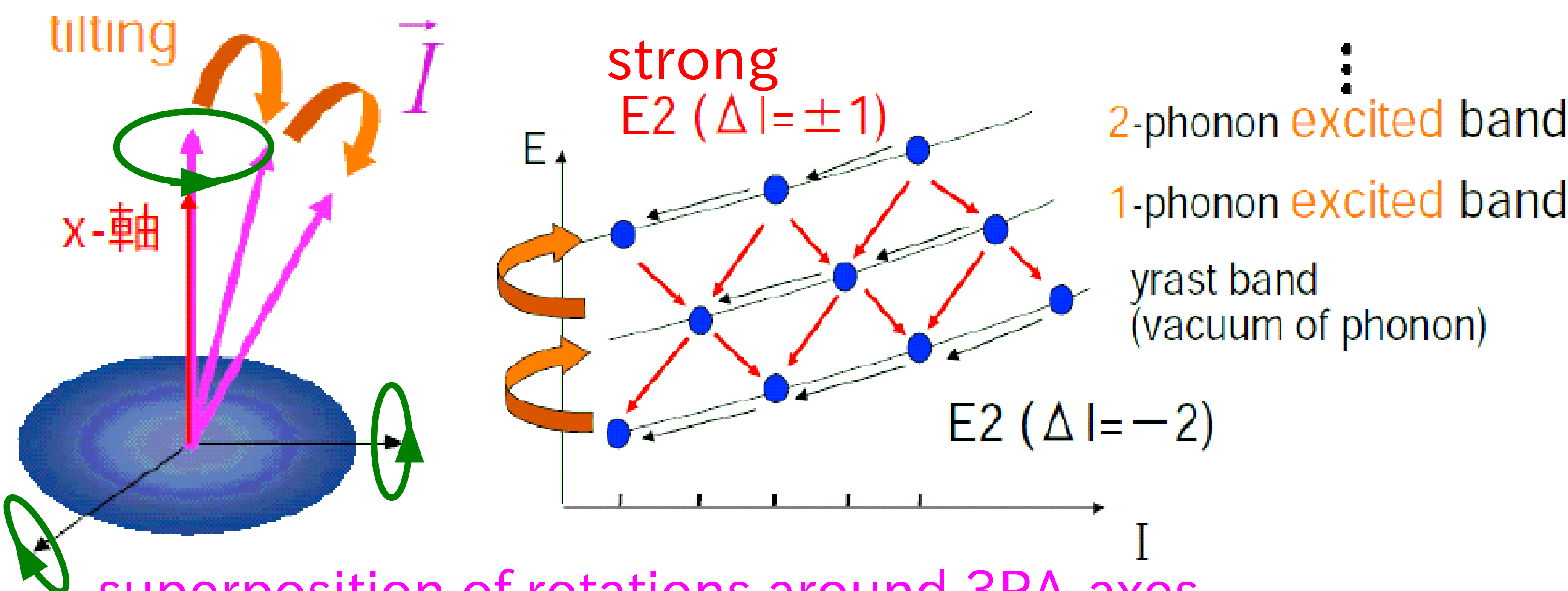
- Variation after projection:
  search best ω_{rot} for each spin-values
  → different projection calculation for each spin
  (very inefficient!)
- Do not use cranking!
  use projection to generate basis for shell model
  (not only 0-q.p. but 2,4,...-q.p. states coupled)
  → Projected Shell Model (PSM)
  by K.Hara and Y.Sun and collaborators

  Most successfull application of projection
- No other possibility?
  e.g., use two mean-field states for g- and s-bands

Wobbling rotational bands

Quantum mechanical motions of asymmetric-top
→ How triaxial nucleus rotates collectively?

strong triaxial def. → coll.rot. around three PA-axes
→ phonon-like multiple bands
from one intrinsic configuration

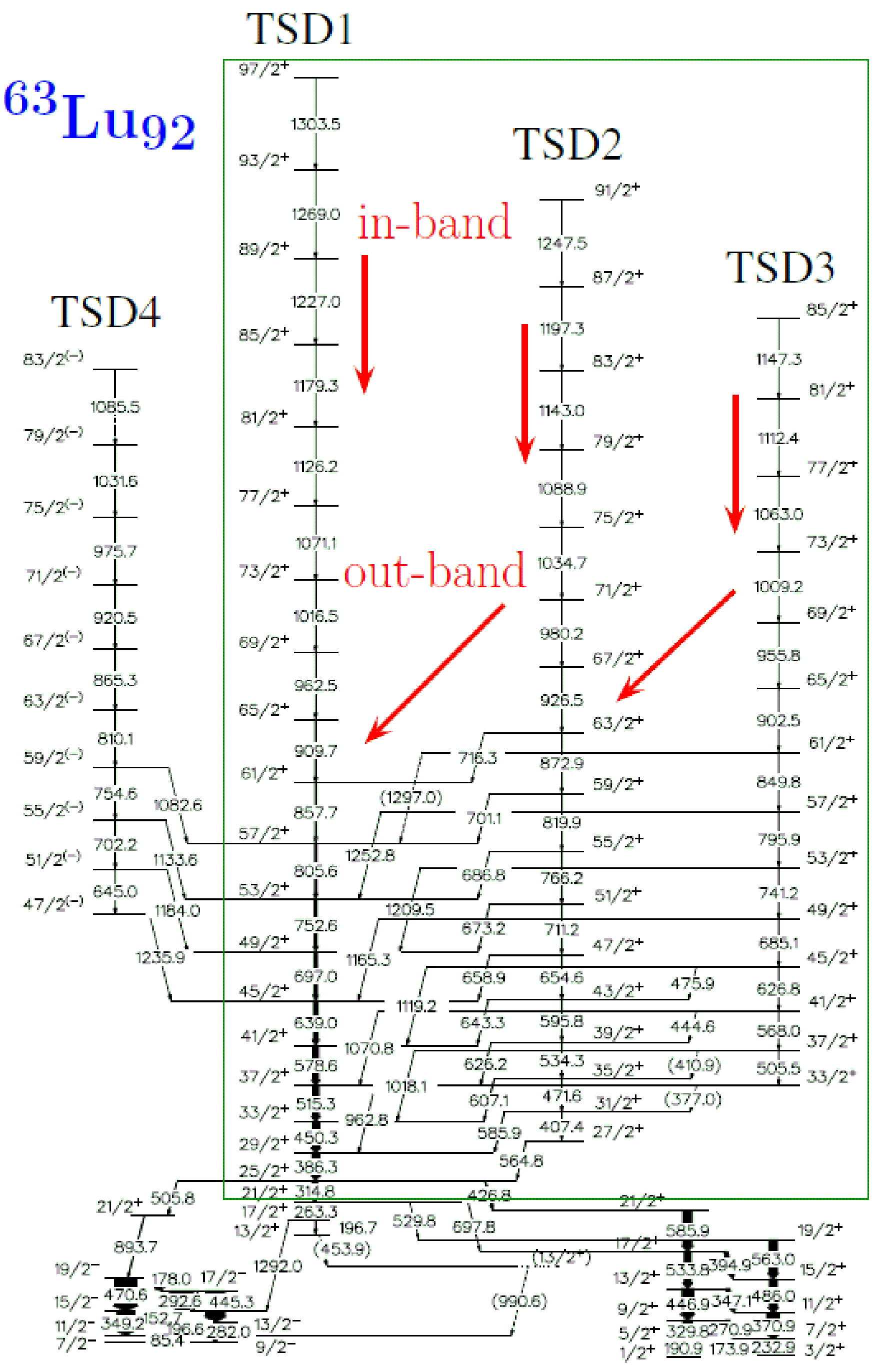


superposition of rotations around 3PA-axes
→ rotation-axis tilts and precesses

No-breaking of chiral symm.

TSD: triaxial superdeformed

$^{163}\mathrm{Lu}_{92}$



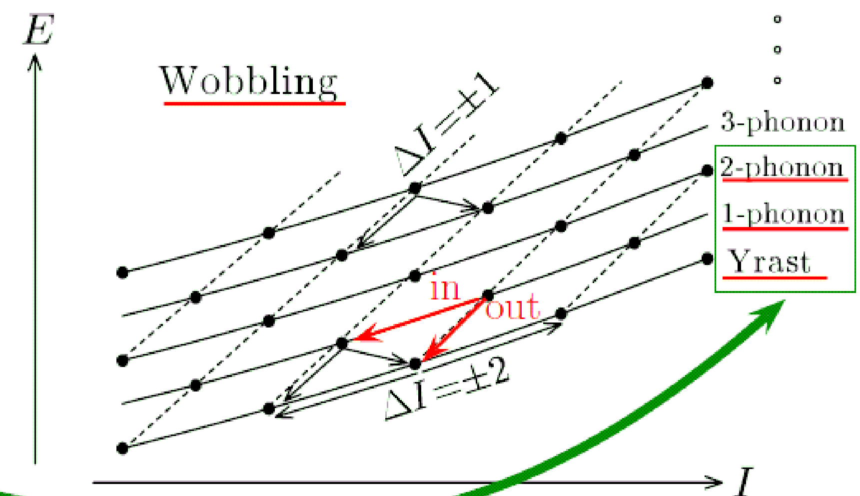
TSD bands

Wobbling Spectra

(Triaxial Superdeformed Band)

D. R. Jensen at al., Eur. Phys. J. **A19** (2004), 173.

First identified by Ødegård et al. (2001)



Very large $B(E2)_{\mathrm{in}}$ and $B(E2)_{\mathrm{out}}$ are observed !!

$B(E2)_{\mathrm{in}} \approx 500$W.u., $B(E2)_{\mathrm{out}} \approx 100$W.u.

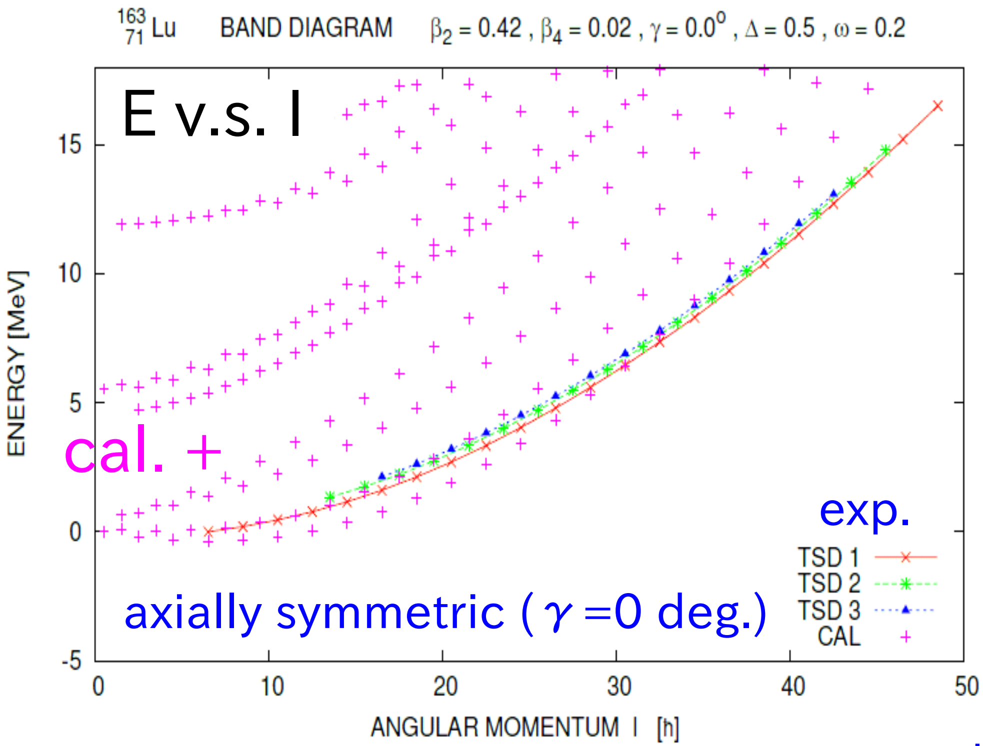
observed in $^{161,163,165,167}\mathrm{Lu}$

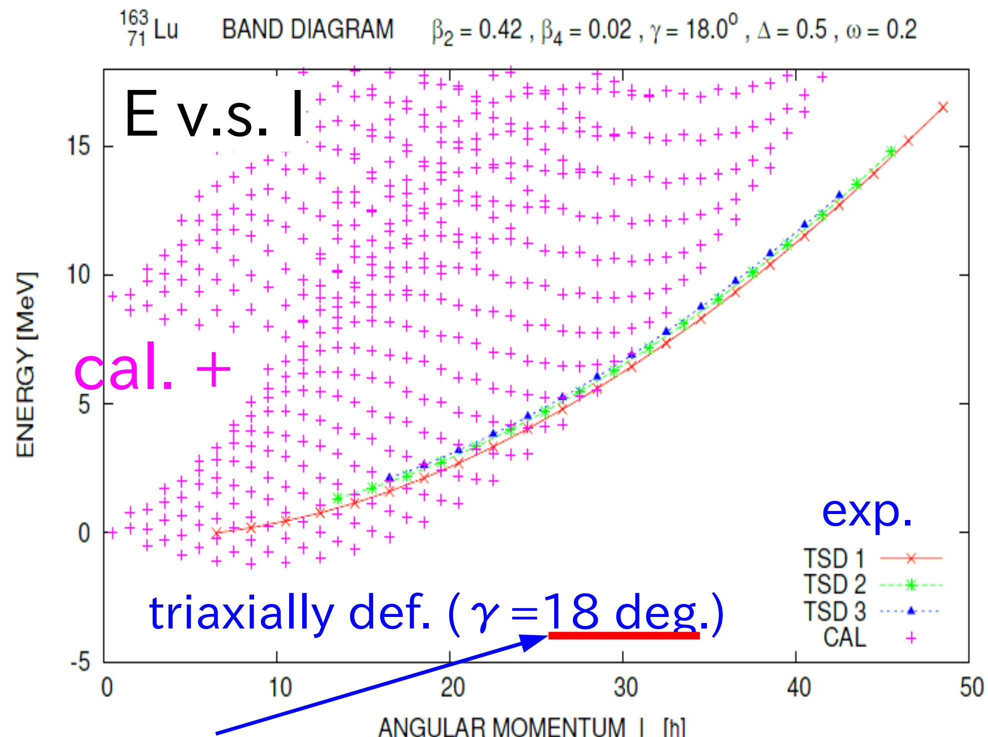
Result of angular momentum projection for wobbling rotational bands (1)

projection from one intrinsic state

$^{163}\mathrm{Lu}_{92}$

$\omega_{\mathrm{rot}} = 0.2\mathrm{MeV}$





predicted by Strutinsky cal.

no wobbling bands

wobbling bands appear!!
(although moment of inertia is too small)

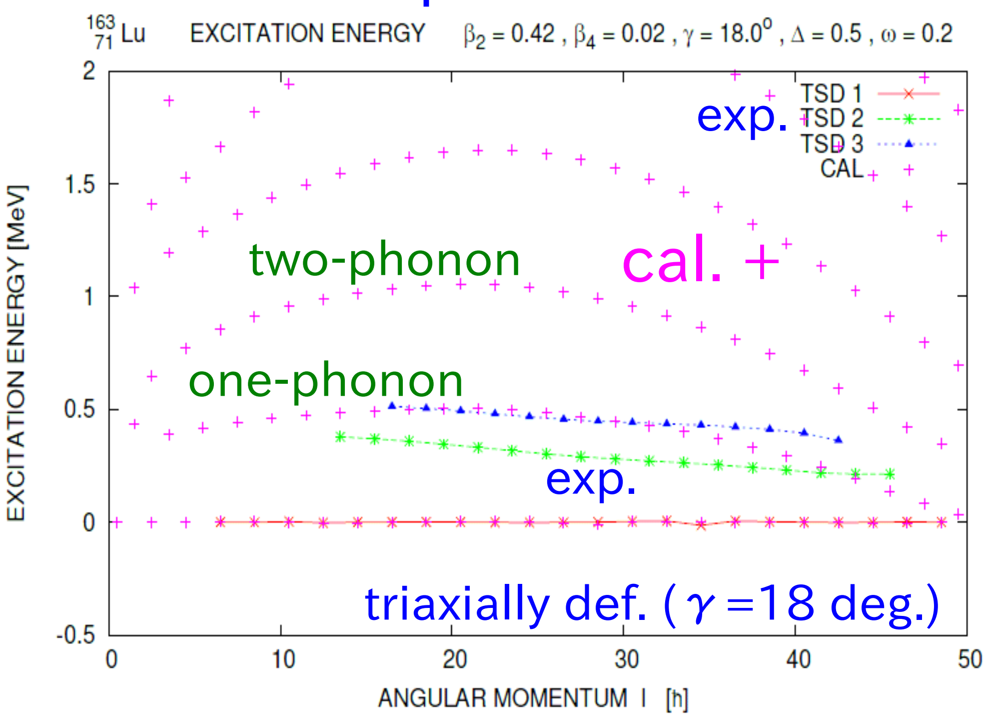
Result of angular momentum projection for wobbling rotational bands (2)

$^{163}\mathrm{Lu}_{92}$

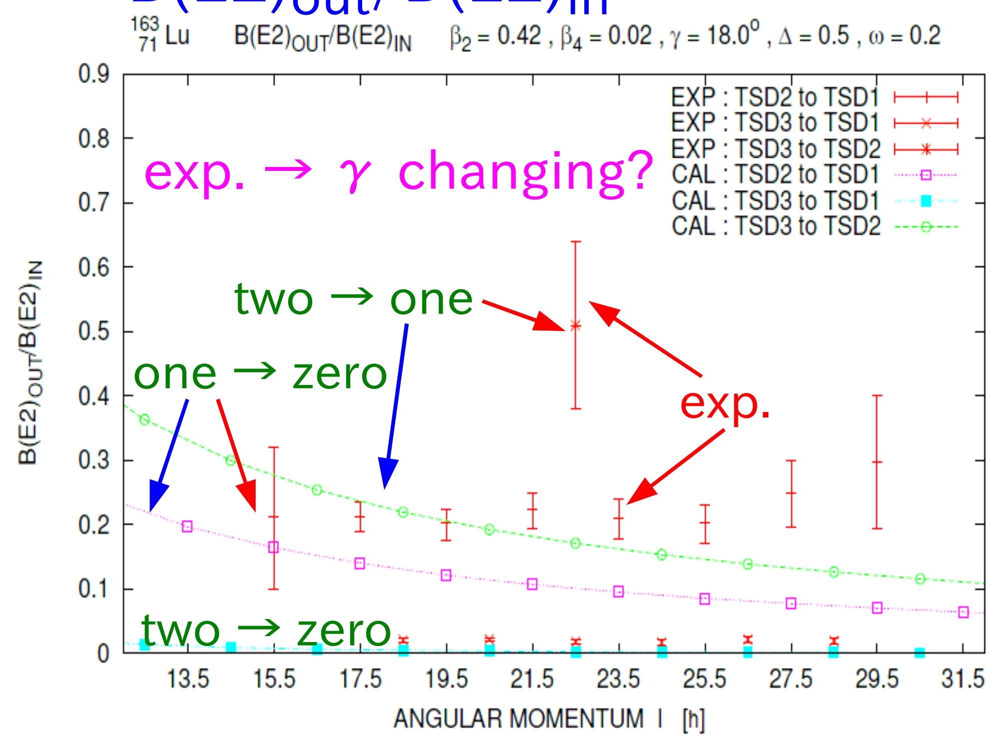
projection from one intrinsic state

$\omega_{\mathrm{rot}} = 0.2\mathrm{MeV}$

relative spactra



$B(E2)_{out}/B(E2)_{in}$



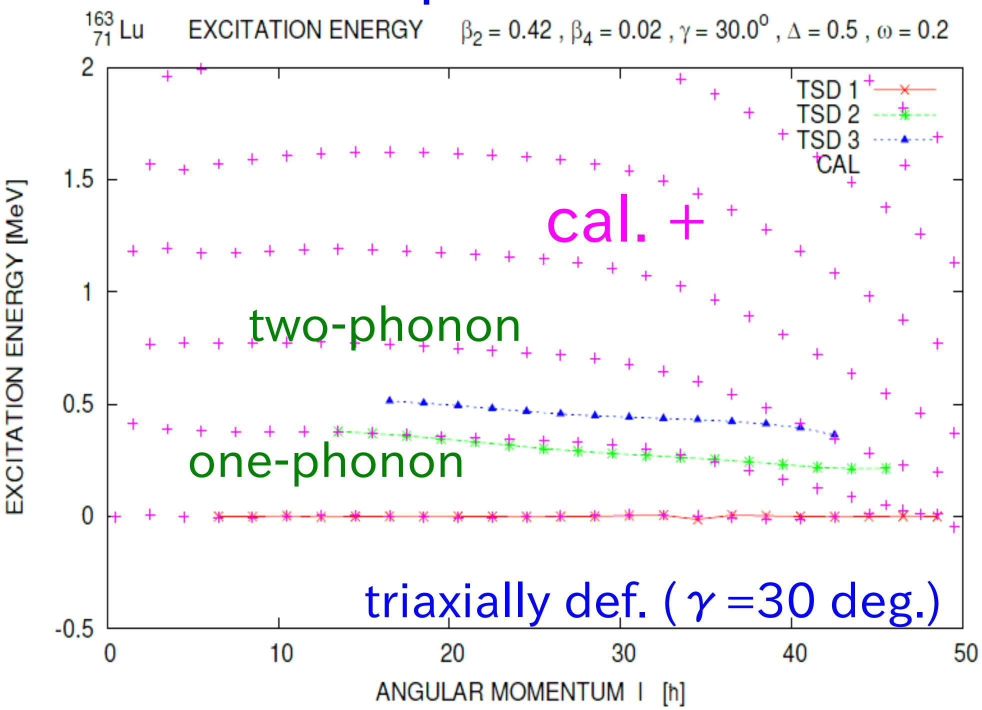
rotor-model-like results obtained by the microscopic projection

Result of angular momentum projection for wobbling rotational bands (3)

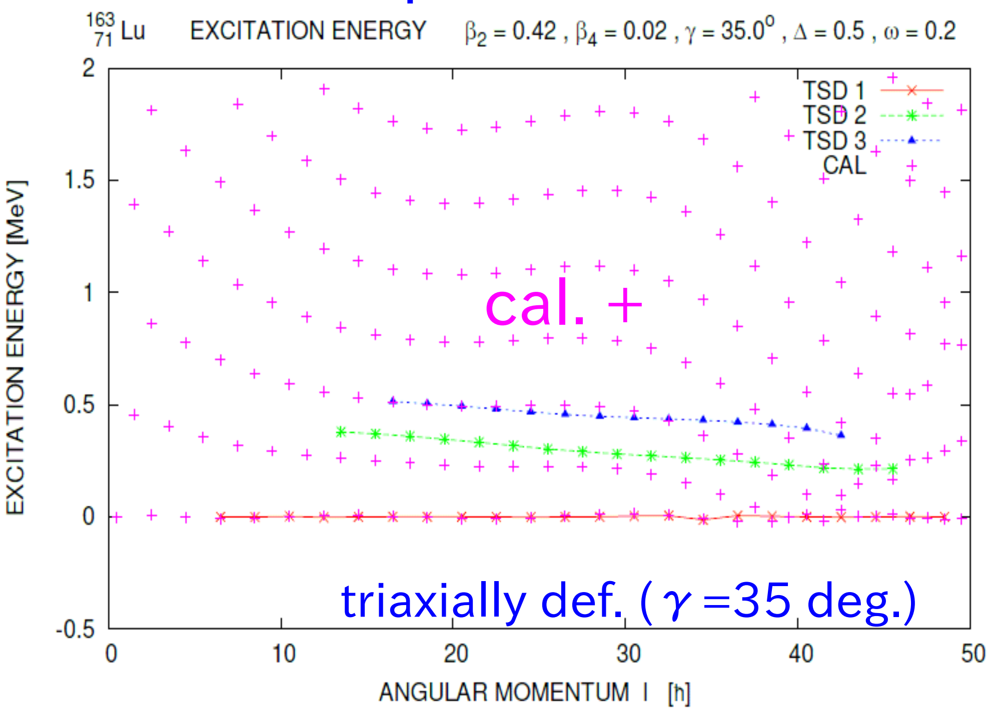
$^{163}\mathrm{Lu}_{92}$

projection from one intrinsic state

relative spactra



relative spactra



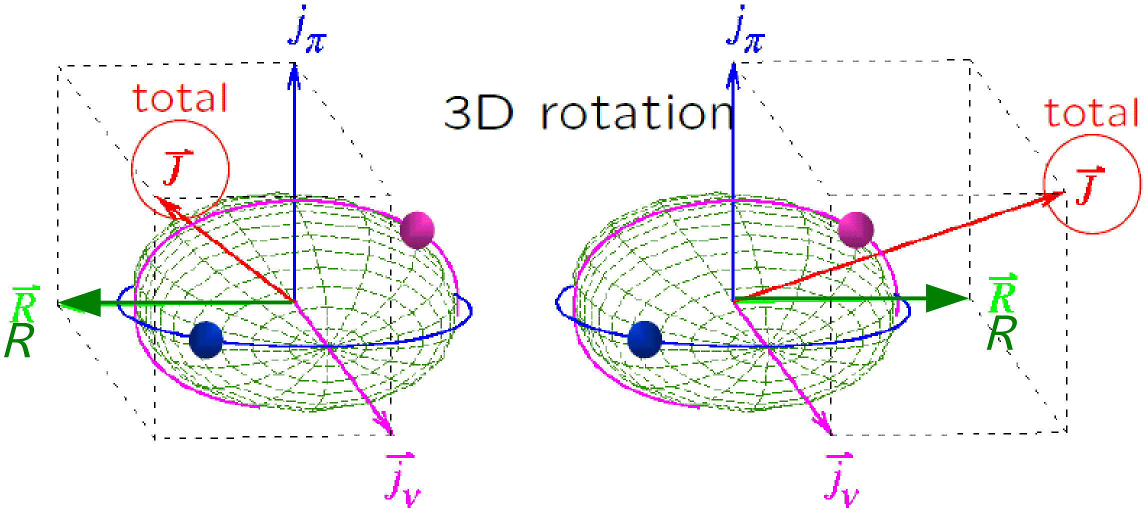
difficult to simultaneously reproduce both one- and two-phonon energies

Chiral doublet band

Importance of triaxial deformation

Breaking right-/left-handed symmetry ⇒ two degenerate bands

(c.f. Parity breaking → Parity doublet) Frauendorf-Meng, NPA617(1997),131.



$\boxed{\text{triaxial def.} \Rightarrow \text{short, inter, long}}$

j_π: high-j particle → short-axis

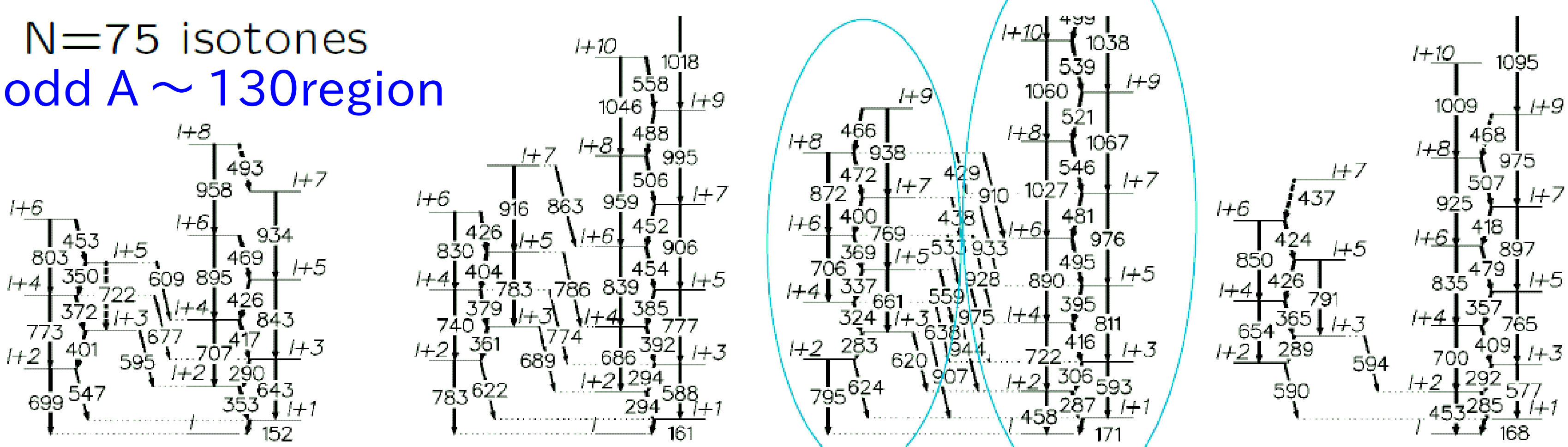
j_ν: high-j hole → long-axis

R: irrotatinal inertia → inter-axis

c.f. $R \approx 0 \Rightarrow$ magnetic rotation in the Pb region

N=75 isotones

odd-odd A ∼ 130region



^{130}Cs ^{132}La ^{134}Pr ^{136}Pm

Starosta et al., PRL86(2001),971.

questioned?

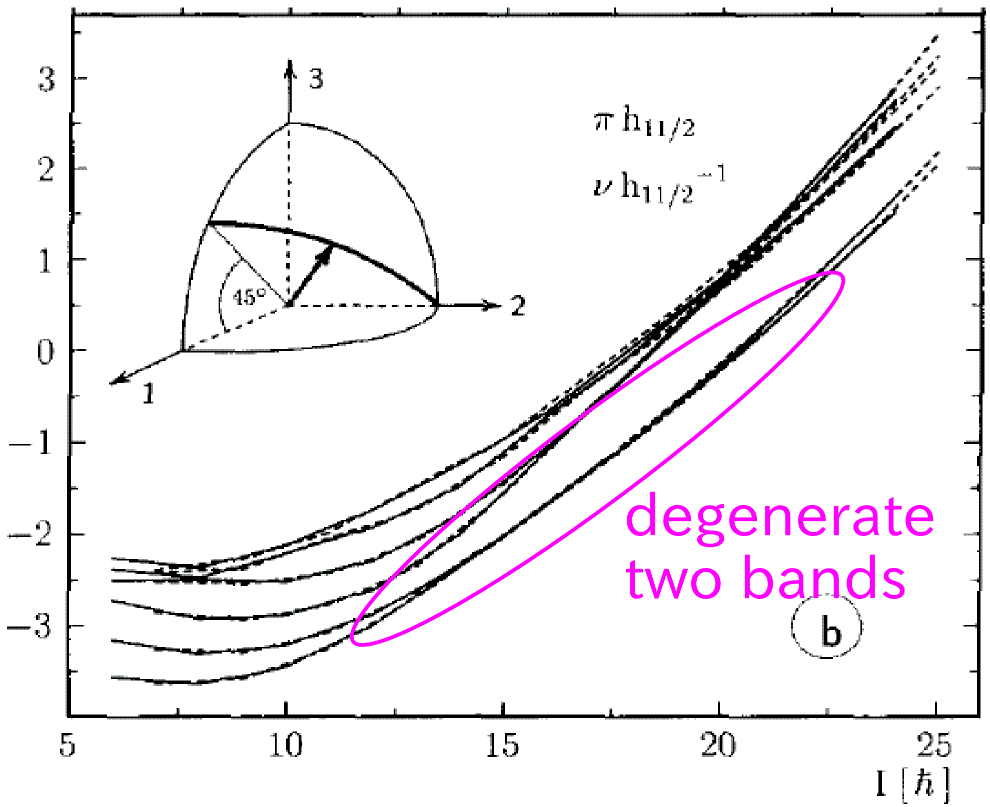
Tonev et al., PRL96(2006),052501.

Result of two-particle rotor coupling model

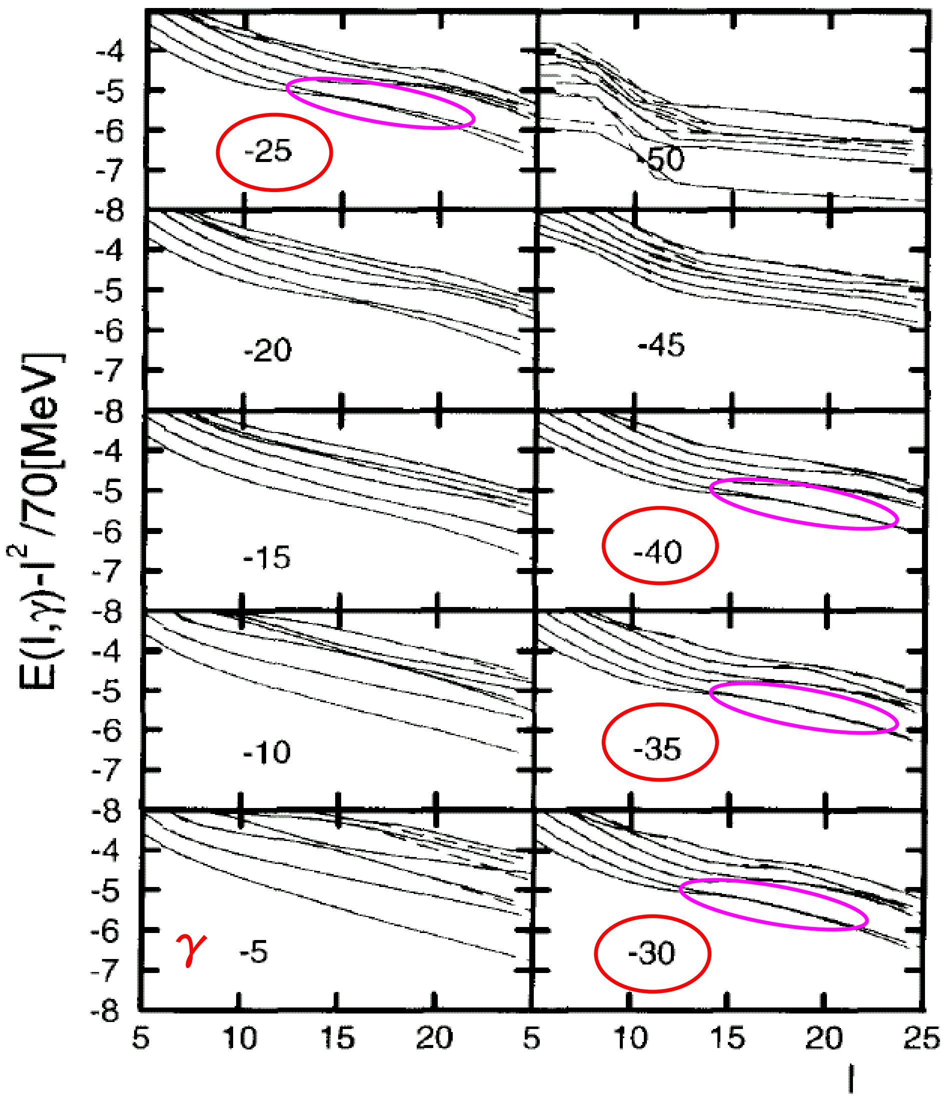
Macroscopic model analysis: the original paper

S.Frauendorf and J.Meng, NPA617(1997),131.

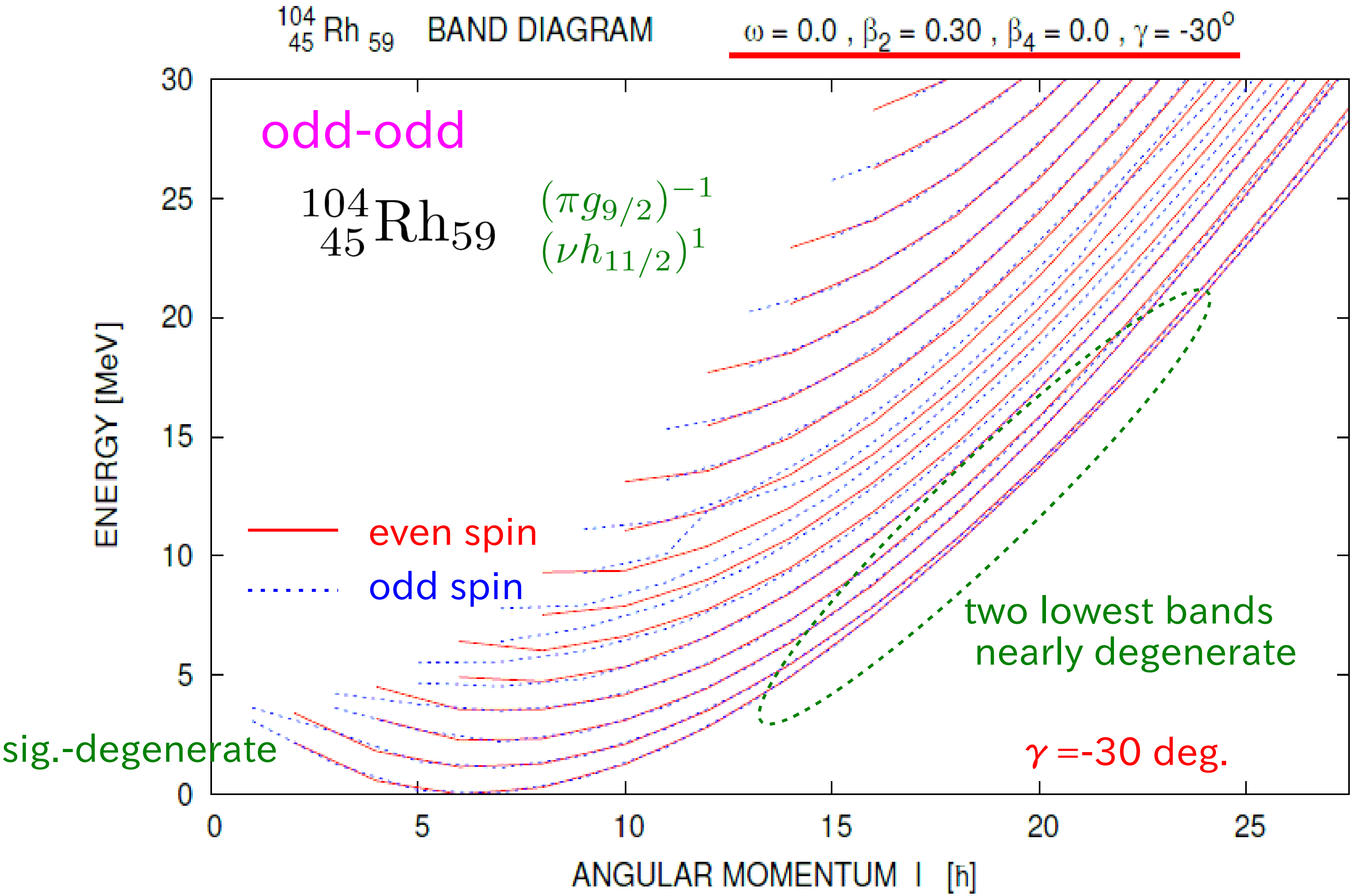
Rotor + particle-hole



$\gamma = -30$ deg.

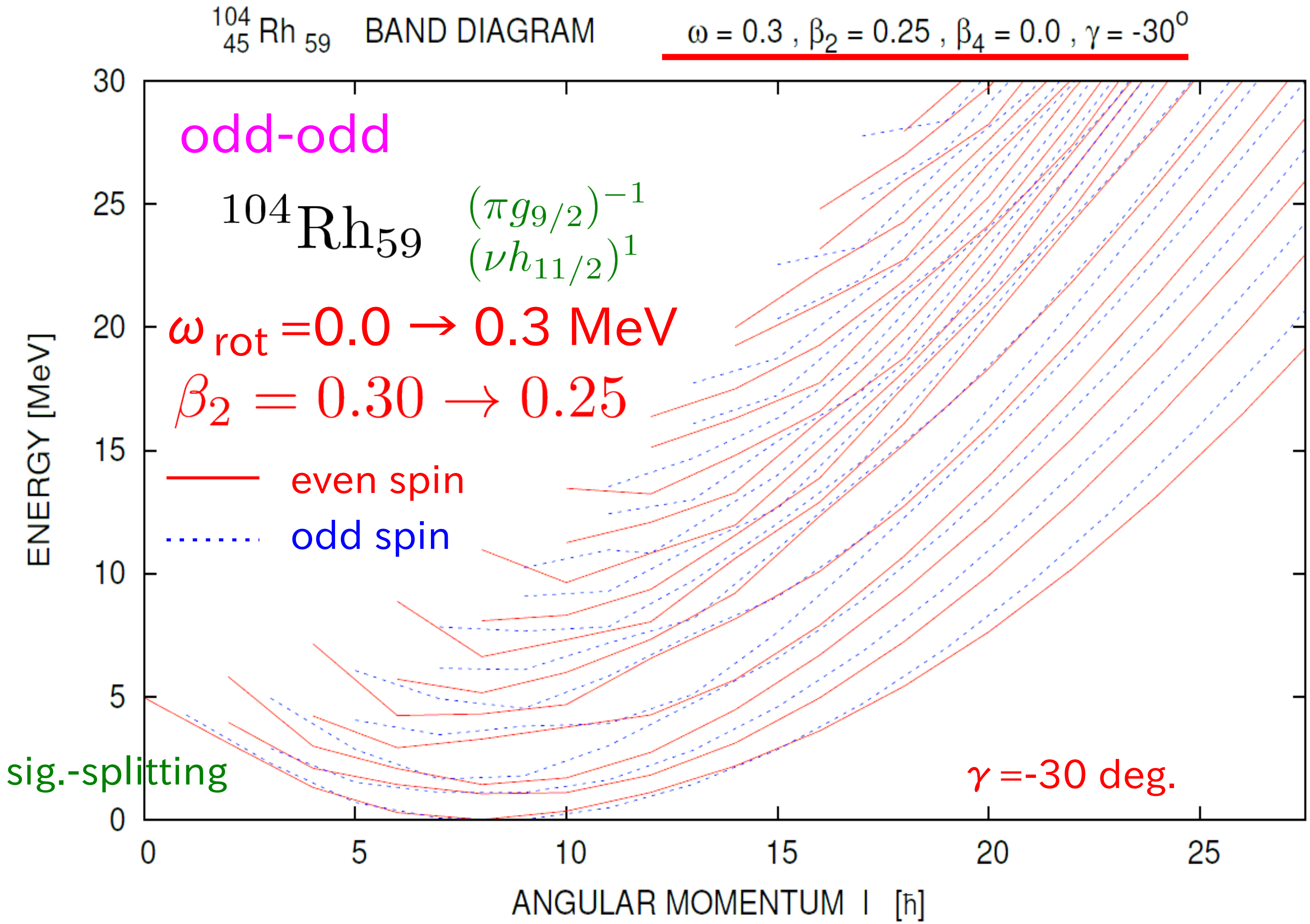


Result of angular momentum projection for chiral doublet band



Only spectra, BE2・BM1 not yet calculated!!

No doublet bands, e.g. if ω_{rot} increased!



Summary

- Effective method for projection

  1) canonical-basis truncation
  2) full use of Thouless amplitude

  from most general HFB-type states!

- Application to nuclei with tetrahedral shape

  Td-symmetry → specific spin-parity combinations
  Expected spectra not only for closed-shell but also for one-particle and two-particle systems
  However, there are considerble splittings

- Application to high-spin states

  Wobbling bands: confirmed full-microscopically, but not easy for quantitative description

  Chiral doublet bands: seems to be existing in full-microscopic calculations, need more study, e.g., electromagnetic transitions etc.