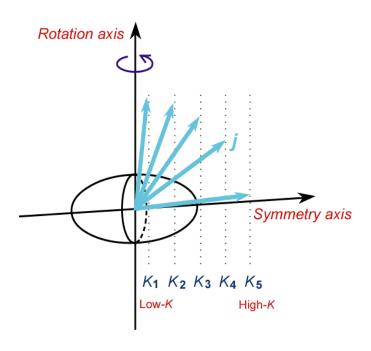
Projected shell model description of K-isomers

Yang Sun

K quantum number

- K is the projection of total angular momentum of a nucleon state on the symmetry axis. It can be used to label nuclear states
- K is a conserved quantum number, if
 - nucleus is axially deformed
 - the system is non-rotating
- Electromagnetic transitions from a state K_1 to a state K_2 change Kby $\Delta K = K_2 - K_1$
- Electromagnetic transitions of multipolarity λ are forbidden if ΔK > λ



• • K violation

- K-forbidden transitions violate the usual K-selection rules – observed in many examples
 - A nucleus changes from having its angular momentum generated by individual nucleons rotating around the symmetry axis (large K) to collective rotation perpendicular to the symmetry axis (small K)
- Classical explanation: shape change involving quantum tunneling through a potential barrier in the axially asymmetric γ-degree of freedom
- More general microscopic explanation: K-mixing

• • Nuclear structure models

Shell-model diagonalization method

- Most fundamental, quantum mechanical
- 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, no correlations beyond mean-field
- States with broken symmetry, cannot be used to calculate electromagnetic transitions and decay rates

Bridge between shell-model and mean-field method

- Projected shell model
 - Use more physical states (e.g. solutions of a deformed meanfield) and angular momentum projection technique to build shell model basis
 - Perform configuration mixing (shell-model concept)
 - K. Hara, Y. Sun, Int. J. Mod. Phys. E 4 (1995) 637
 - Y. Sun, K. Hara, Comp. Phys. Commun. 104 (1997) 245
 - Y. Sun, C.-L. Wu, Phys. Rev. C 68 (2003) 024315
- The method works in between conventional shell model and mean field method, can take advantages of both

• • Deformed HFB solutions

- A general HFB solution gives quasiparticle vacuum $|0\rangle$, with quasiparticle operators α_i^+,α_i^-
- |0⟩ can be obtained from deformed HFB or Nilsson (Woods-Saxon)+BCS calculations, associated with a deformation
- i labels a set of quantum numbers, e.g. K=7/2 of $i_{13/2}$ or 7/2+[613]
- A two-quasiparticle state $|\phi_K\rangle = \alpha_{K1}^+ \alpha_{K2}^+ |0\rangle$ with $K = K_1 \pm K_2$

• • • What do we need for *K*-isomer description?

- To describe K-mixing It is preferable
 - to construct basis states with good angular momentum I and parity π, classified by K
 - to mix these K-states by residual interactions at given I and π
 - to use resulting wavefunctions to calculate electromagnetic transitions in shell-model framework
- ullet A projected intrinsic state $|\hat{P}_{\scriptscriptstyle MK}^{\scriptscriptstyle I}|\phi_{\scriptscriptstyle \kappa}\rangle$ can be labeled by K
- $E_{\kappa}^{I} = H_{\kappa\kappa}^{I}/N_{\kappa\kappa}^{I}$ defines a rotational band associated with the intrinsic *K*-state $|\phi_{\kappa}\rangle$
- Diagonalization = mixing of various K-states

Model space constructed by angular-momentum projected states

• Wavefunction:
$$\psi_{M}^{I} = \sum_{\kappa} f_{\kappa} \hat{P}_{MK_{\kappa}}^{I} |\phi_{\kappa}\rangle$$

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

• Eigenvalue equation:
$$\sum_{\kappa} \left(H_{\kappa\kappa'}^{I} - E N_{\kappa\kappa'}^{I} \right) f_{\kappa'} = 0$$

with matrix elements:
$$H_{\kappa\kappa'}^{I} = \left\langle \phi_{\kappa} \middle| \widehat{H} \widehat{P}_{KK'}^{I} \middle| \phi_{\kappa} \right\rangle$$
 $N_{\kappa\kappa'}^{I} = \left\langle \phi_{\kappa} \middle| \widehat{P}_{KK'}^{I} \middle| \phi_{\kappa} \right\rangle$

Hamiltonian is diagonalized in the projected basis

$$\left\{ \widehat{P}_{\scriptscriptstyle MK}^{\scriptscriptstyle I} \middle| \phi_{\scriptscriptstyle \kappa}
ight
angle
ight\}$$

Building blocks: a.-m.-projected multi-quasi-particle states

• Even-even nuclei:

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

Odd-odd nuclei:

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

Odd-neutron nuclei:

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

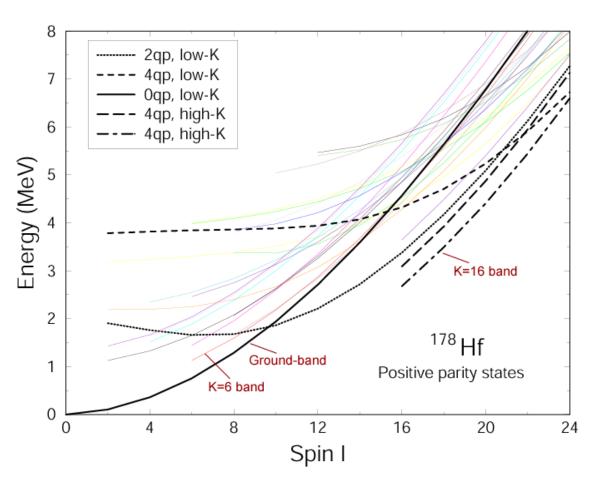
Odd-proton nuclei:

$$\left\{\hat{P}_{MK}^{I}lpha_{\pi}^{+}\middle|0
ight>,\hat{P}_{MK}^{I}lpha_{
u}^{+}lpha_{
u}^{+}lpha_{
u}^{+}lpha_{\pi}^{+}\middle|0
ight>,\hat{P}_{MK}^{I}lpha_{
u}^{+}lpha_{\pi}^{+}lp$$

Hamiltonian and single particle space

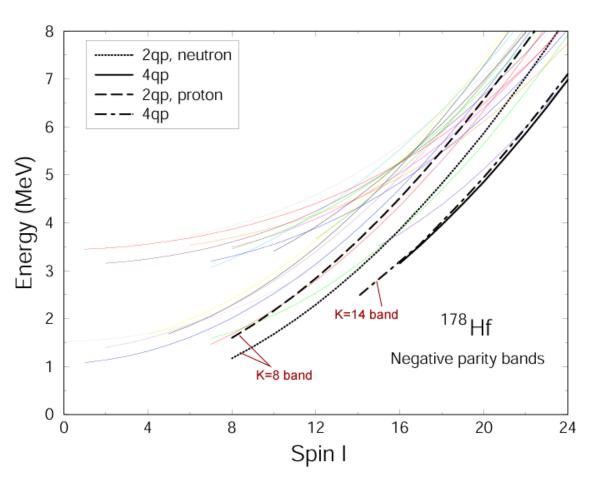
- The Hamiltonian $H = H_0 \sum_{\lambda} \frac{\chi_{\lambda}}{2} \sum_{\mu} Q_{\lambda\mu}^+ Q_{\lambda\mu} G_M P^+ P G_Q \sum_{\mu} P_{\mu}^+ P_{\mu}$ Interaction strengths
 χ is related to deformation ε by $\chi_{\tau\tau'} = \frac{2/3 \ \varepsilon \hbar \omega_{\tau} \hbar \omega_{\tau'}}{\hbar \omega_n \langle Q_0 \rangle_n + \hbar \omega_p \langle Q_0 \rangle_p}$
- - $G_{\rm M}$ is determined by observed even-odd mass difference
 - $G_{\rm O}$ is assumed to be proportional to $G_{\rm M}$ with a ratio ~ 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

¹⁷⁸Hf example: Theoretical bands of positive parity



Band diagram before K-mixing

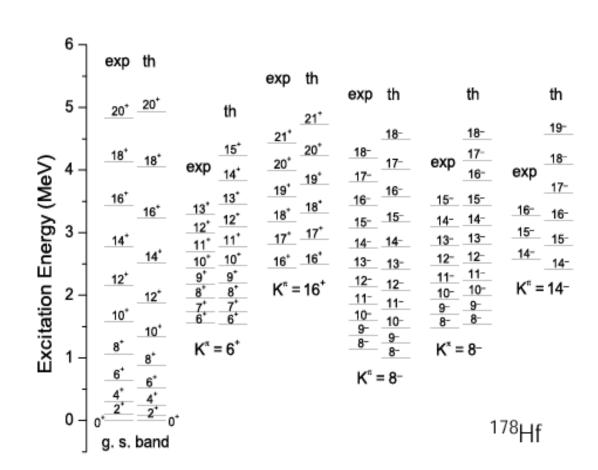
¹⁷⁸Hf example: Theoretical bands of negative parity



Band diagram before K-mixing

K-isomers:¹⁷⁸Hf example

- PSM caclulation for ¹⁷⁸Hf
 - Sun, Zhou, Long, Zhao, Walker, Phys. Lett. B 589 (2004) 83
- Data
 - S.M. Mullins *et al*,
 Phys. Lett. B 393 (1997) 279

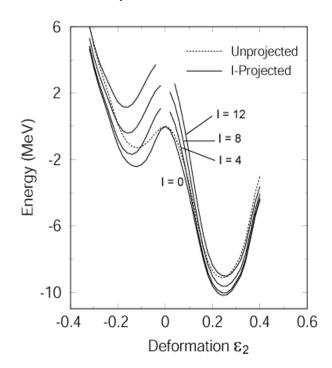


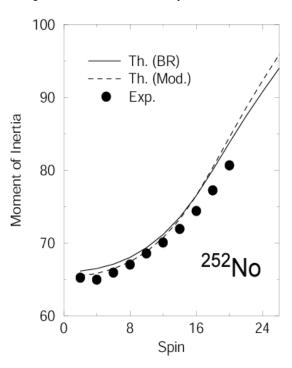
• • • K-isomers in transfermium nuclei

- K-isomer contains important information on single quasi-particles
 - e.g. for the proton $2f_{7/2}$ – $2f_{5/2}$ spin–orbit partners, strength of the spin–orbit interaction determines the size of the Z=114 gap
 - Information on the position of $\pi 1/2[521]$ is useful
 - Herzberg et al., Nature 442 (2006) 896
 - Tandel et al., Phys. Rev. Lett. 97 (2006) 082502
- K-isomer in superheavy nuclei may lead to increased survival probabilities of these nuclei
 - Xu et al., Phys. Rev. Lett. 92 (2004) 252501

Superheavy nuclei: general features

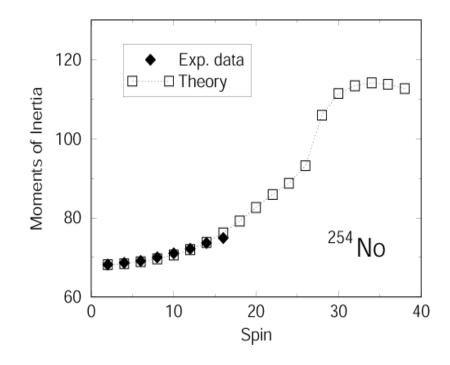
- Potential energy calculation shows deep prolate minimum
 - A very good rotor, quadrupole + pairing interaction dominant
 - Low-spin rotational feature of even-even nuclei can be easily described (relativistic mean field, Skyrme HF, ...)





Structure in ²⁵⁴No - Rotational behavior

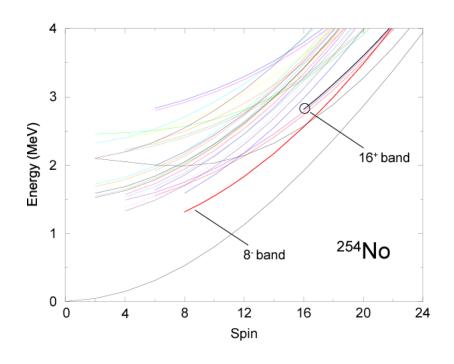
- Current yrast state data stop at spin-16 – rotational alignment of the first nucleon-pair
 - Reiter *et al.*, Phys. Rev. Lett.
 82 (1999) 509
- A up-bending in Mol predicted at spin-28, due to a simultaneous alignment of a neutron and a proton pair
 - Al-Khudair, Long, Sun, Phys.
 Rev. C 79 (2009) 034320



K-isomers in ²⁵⁴No

- A high-K band with $K^{\pi} = 8^{-1}$ starts at ~1.3 MeV
 - A neutron 2-qp state:
 (7/2+ [613] + 9/2- [734])
- A high-K band with $K^{\pi} = 16^{+}$ at 2.7 MeV
 - A 4-qp state coupled by two neutrons and two protons:

$$v (7/2^{+} [613] + 9/2^{-} [734]) + \pi (7/2^{-} [514] + 9/2^{+} [624])$$



K-isomers in ²⁵⁴No

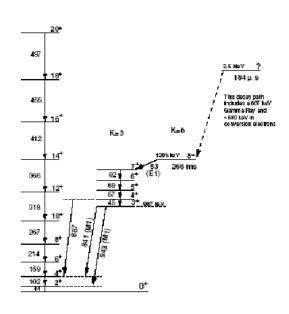
nature

Vol 442|24 August 2006|doi:10.1038/nature05069

LETTERS

Nuclear isomers in superheavy elements as stepping stones towards the island of stability

- An experimental team in Europe found two isomers in 254 No : $T_{1/2}$ = 266 \pm 2 ms and 184 \pm 3 μ s
- Study of structure and decay path of the isomers can gain information on singleparticle states for superheavy elements
- o Herzberg et al., Nature 442 (2006) 896



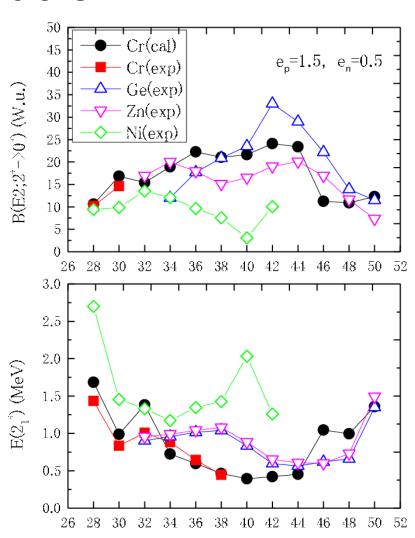
Shell structure changes in neutron-rich nuclei

 Experimental data for Ni (Z=28), Zn (Z=30), Ge (Z=32), Cr (Z=24)

• Upper: B(E2, $I=2\rightarrow 0$)

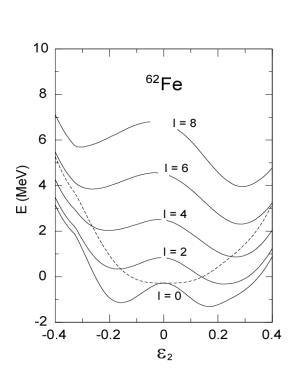
Lower: first 2+ energy

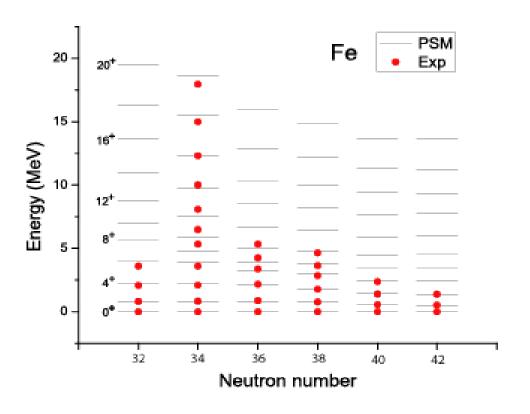
 K. Kaneko, et al. Phys. Rev. C 78 (2008) 064312



Neutron-rich Fe isotopes: Projected shell model calculations

o Sun et al., Phys. Rev. C80 (2009) 054306





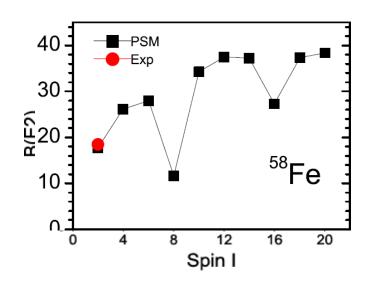
Rotational properties of neutronrich Fe isotopes

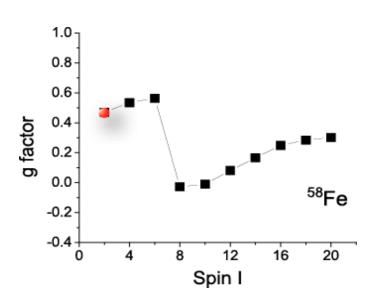
- Comparison of calculated moments of inertia with data
 - Irregularity at I ~ 8: alignment of $g_{9/2}$ neutrons

at I ~ 16: alignment of $f_{7/2}$ protons 0 24 20 16 12 Moment of Inertia 24 20 16 12 Spin I

Transition properties of neutronrich Fe isotopes

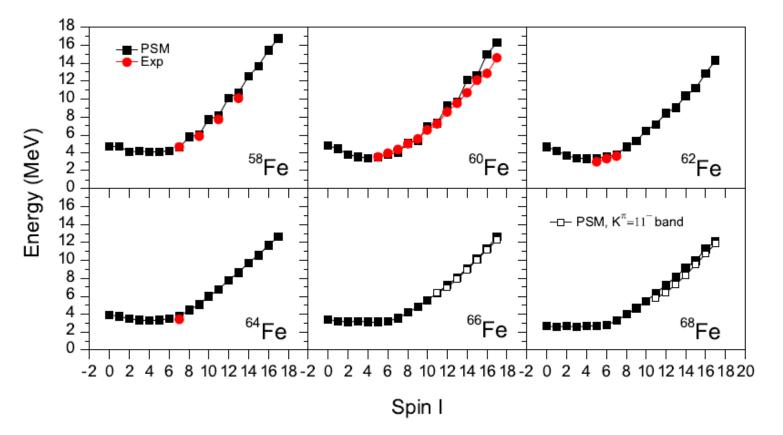
- B(E2) reflects band-crossings at I = 8 and 16
- g-factor shows a sudden drop at I = 8: neutron alignment
 - o g-factor data: East, Stuchbery et al., PRC 79 (2009) 024304





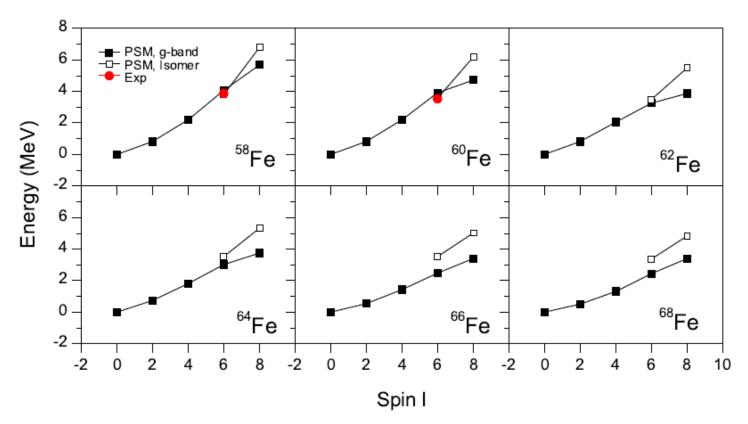
Negative-parity states in neutronrich Fe isotopes

- Experimental bandheads start at I = 5 (60,62 Fe) or 7 (58,64 Fe)
- Predicted 2-qp states are low K-states ($f_{5/2}$ coupled to $g_{9/2}$ +)

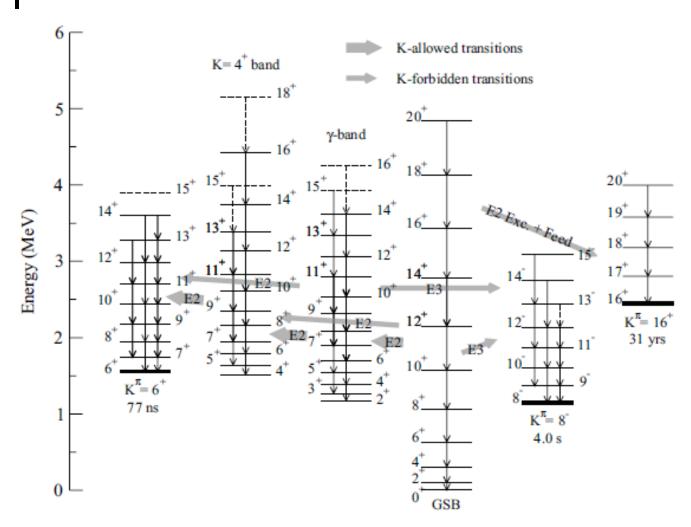


K-isomers in neutron-rich Fe isotopes

• K = 6 isomer states have a structure of 2-qp states of $f_{7/2}$ protons



Coulomb excitation experiment



Hayes et al, PRC 75, 034308 (2007)

Puzzle of the 6+ state transition

 6+ K isomers in N=104 Hf, W, Os isotones showed direct branches to the low-K rotational bands with unexpectedly large transition probabilities.

Measured hindrance factors questioned the validity of

K quantum number.

γ-tunneling calculations can
 reproduce the large E2 transition

Narimatsu, Shimizu, Shizuma,Nucl. Phys. A 601 (1996) 69.

 It failed to describe the very small E2 transition of their immediate neighboring isotone ¹⁷⁴Yb

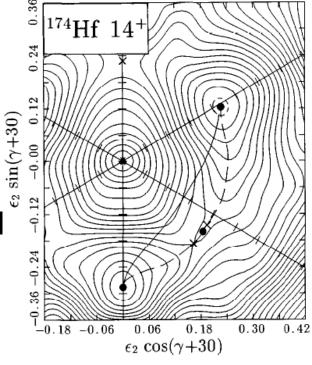


TABLE I: Comparison of calculated ¹⁷⁴Yb ground band with data. E(I) are in keV and $B(E2, I \rightarrow I - 2)$ in W.u..

| Spin $I \mid E(I)$, Exp $\mid E(I)$, PSM $\mid B(E2)$, Exp $\mid B(E2)$, PSM | | | | | | |
|--|-------|--------|---------|--------|--|--|
| 2 | 76.5 | 71.1 | 201(7) | 195.18 | | |
| 4 | 253.1 | 236.7 | 280(9) | 279.01 | | |
| 6 | 526.0 | 496.1 | 370(50) | 307.59 | | |
| 8 | 889.9 | 848.0 | 388(21) | 322.31 | | |
| 10 | 1336 | 1290.3 | 325(22) | 331.28 | | |
| 12 | 1861 | 1820 | 369(23) | 337.13 | | |
| 14 | 2457 | 2433 | 320 | 340.91 | | |

TABLE II: Comparison of calculated ¹⁷⁴Yb 6⁺ isomer band with data. E(I) are in keV and $B(E2, I \rightarrow I - 2)$ in W.u..

| $\overline{\operatorname{Spin} I E(I), \operatorname{Exp} E(I), \operatorname{PSM} B(E2), \operatorname{PSM}}$ | | | | | | |
|--|--------|------|--------|--|--|--|
| 6 | 1518.0 | 1503 | | | | |
| 7 | 1671.1 | 1683 | | | | |
| 8 | 1844.7 | 1886 | 36.76 | | | |
| 9 | 2038.3 | 2117 | 78.18 | | | |
| 10 | 2251.5 | 2372 | 115.81 | | | |
| 11 | 2483.7 | 2652 | 147.96 | | | |
| 12 | 2734.4 | 2956 | 174.91 | | | |
| 13 | 3003.1 | 3283 | 197.41 | | | |
| | ' | ı | ı | | | |

TABLE III: Comparison of calculated inter-band transition of 174 Yb $^{6+}$ isomer to ground band. B(E2) is in e^2fm^4

Data: Dracoulis *et al*, PRC 71, 044326 (2005)

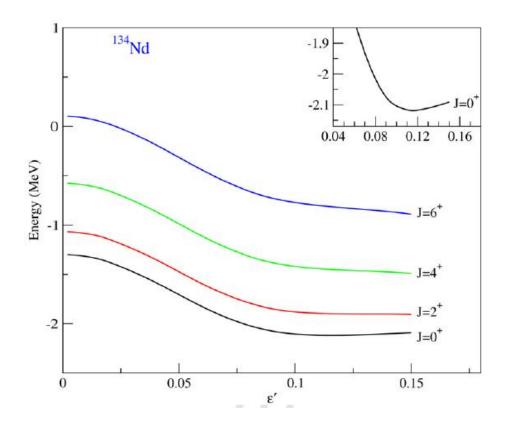
Transition |
$$B(E2)$$
, Exp | $B(E2)$, PSM
 $6_i \rightarrow 4_g | 4.3(8) \times 10^{-9} | 8.49 \times 10^{-8}$

Triaxial projected shell model

- Break axial symmetry in single particle states use triaxial Nilsson states as basis
- K is no longer a good quantum number each Nilsson state is a combination of all possible K-states
- Angular-momentum-projection calculation on trlaxially deformed qp states – rotational bands
- o K-mixing occurs at two levels:
 - Within all possible K-states in each Nilsson state
 - Among all qp configurations

A.-m.-projected energy surfaces

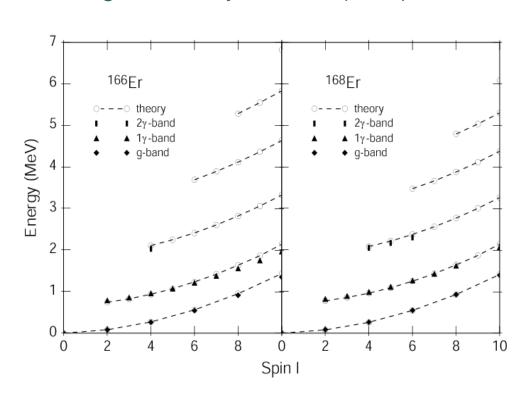
• It shows considerable γ -softness in A~130 nuclei.



Triaxially deformed 0-qp state and γ -vibration

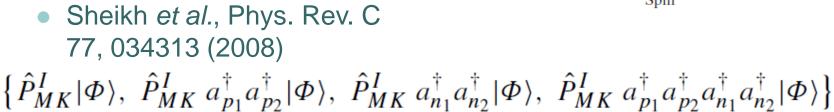
- \circ γ -vibration states: triaxial basis with 3-dimentional angular momentum projection
 - o Sun, Hara, Sheikh, Hirsch, Velazguez, Guidry, PRC 61 (2000) 064323
- Projection onto triaxial 0-qp state

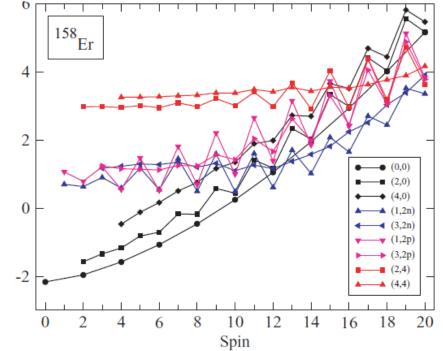
$$\{\hat{P}_{MK}^{I}|\Phi\rangle,\ 0\leq K\leq I\}$$



Triaxially deformed multi-qp excitations

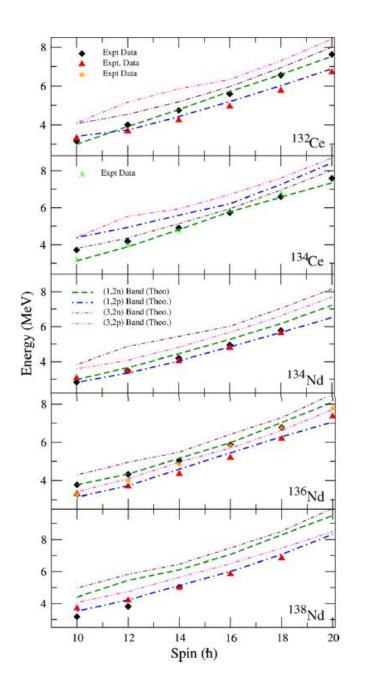
- 0-phonon (K=0), 1-phonon (K=2), 2-phonon (K=4) γ -vibrational bands
 - Sun et al, Phys. Rev. C61 (2000) 064323
- Each phonon γ-vibrational mode can have qp states on top of them – enriched basis, introduce more mixing





Triaxially deformed multi-qp excitations

- 0-phonon (K=0), 1-phonon (K=2), 2-phonon (K=4) γ -vibrational bands
 - Sun et al, Phys. Rev. C61 (2000) 064323
- Each phonon γ-vibrational mode can couple with qp states – generalization of the usual concept of γvibration
 - Sheikh et al., Nucl. Phys. A 824 (2009) 58



• • Summary

- Angular momentum projection is an efficient way of truncating shell model space to perform shell model calculations for heavy, deformed nuclei.
- The projection technique is well developed. Projected shell model is a practical example.
- Using the familiar Nilsson basis to construct *K*-states, but going further by (1) projecting them onto good angular momentum and (2) mixing them by residual interactions.
- Can discuss various K-bands, inter-transitions, and electromagnetic properties.