Pushing high-spin calculation to the extreme:

Application of the Pfaffian algorithm in angular momentum projection

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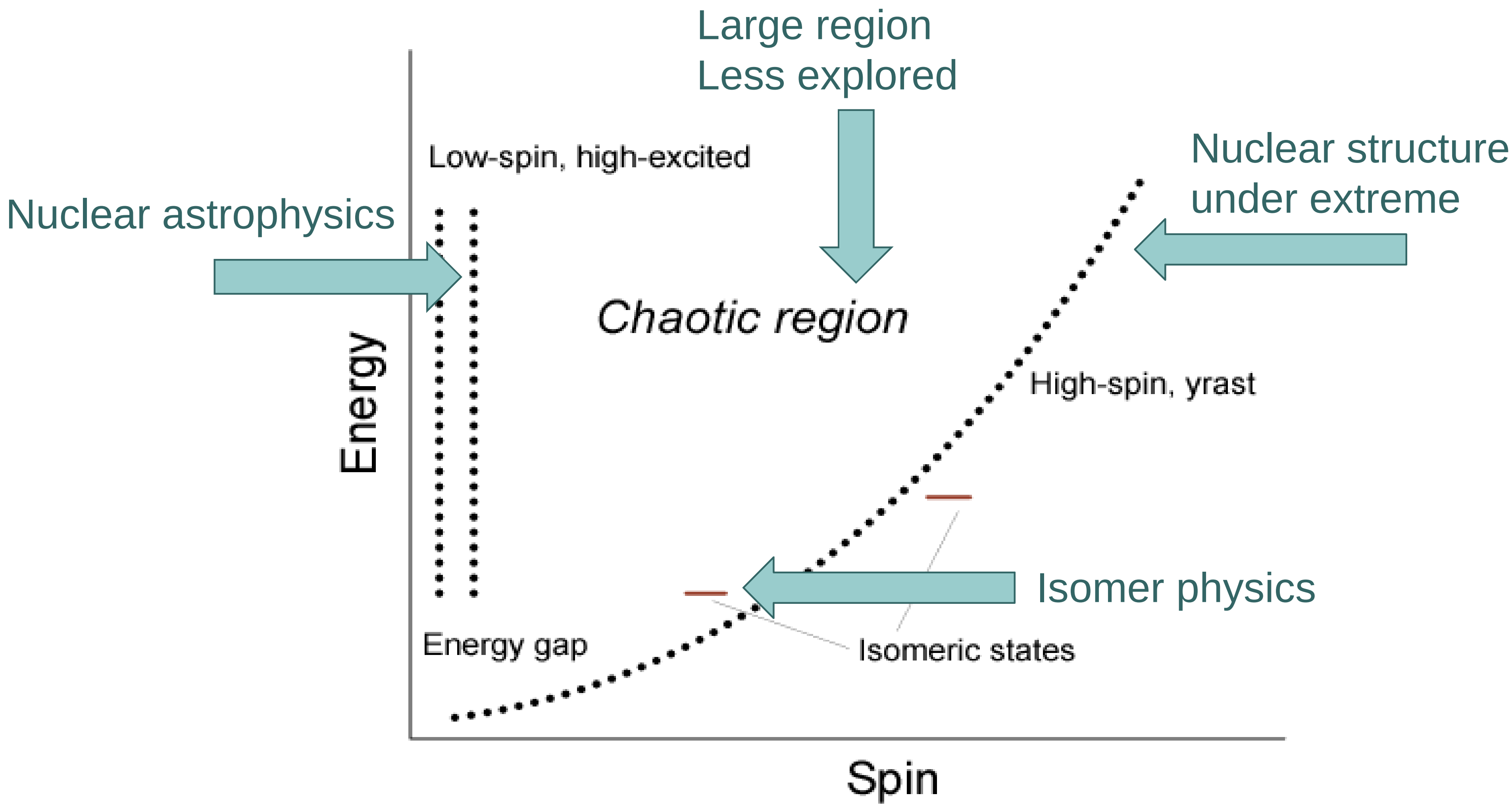
SSNET, Nov. 7-11, 2016

Nuclear states under rotation



To be discussed ...

- Along the yrast line, rotational bands can now be studied up to very high spins – extreme of angular momentum
  - Talks by M. Riley, I. Ragnarsson, A. Maj, ...
- Understanding the response of the nuclear system to fast rotation: pair-breaking (nn, pp, np), reorganization of collectivity, ...

- Multi-quasiparticle high-*K* isomers
  - Talks by Ph. Walker, A. K. Jain ...
- Understanding their formation, (unusual) decays are important for the study of superheavy elements, nuclear astrophysics, and applications

How to treat deformed nuclei with a shell-model concept

- Most nuclei in the nuclear chart are deformed. To describe a deformed nucleus, a spherical shell model has no 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 good 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

Y. Sun, *Phys. Scr.* 91 (2016) 043005

How to construct model space to describe fast rotations?

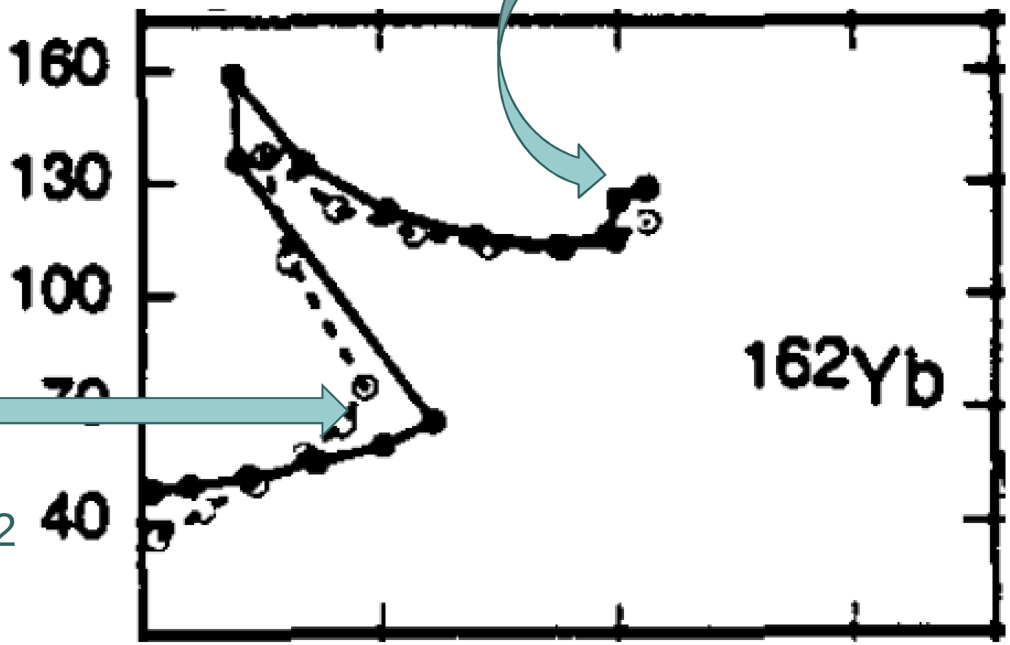
- Backbending in moment of inertia

Breaking and alignment of second high-j pair

I.-Y. Lee et al., 1977

Breaking and alignment of first high-j pair

A. Johnson, H. Ryde, 1971
F.S. Stephens, R.S. Simon, 1972



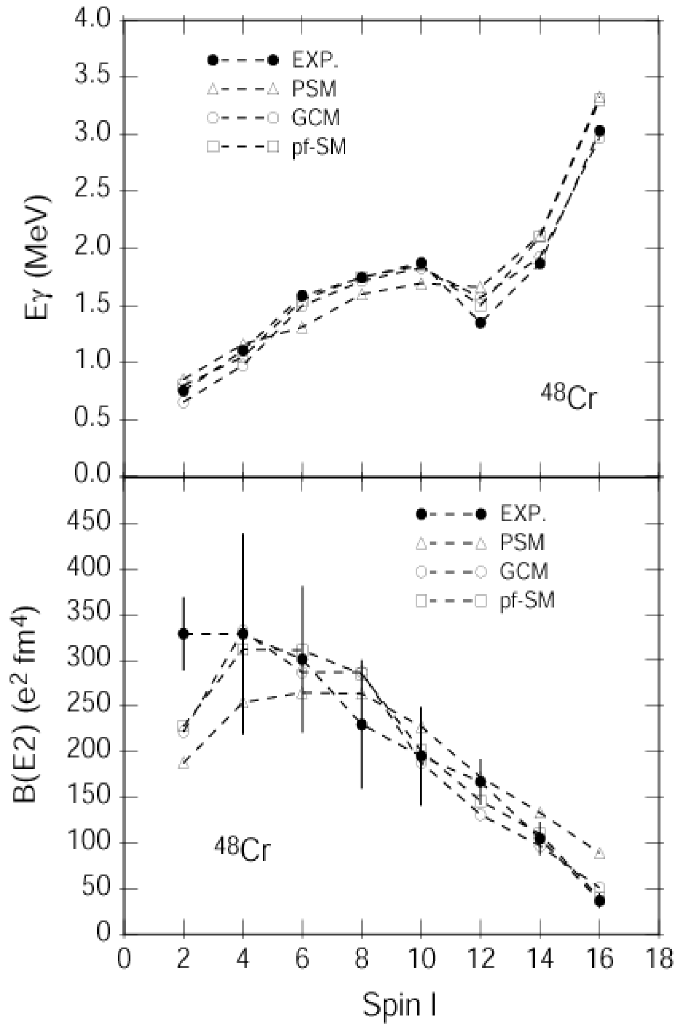
Rotation

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

- *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
- A projected intrinsic state $\hat{P}^I_{MK}\left|\phi_\kappa\right\rangle$ can be labeled by *K*
  - With axial symmetry: $\left|\phi_\kappa\right\rangle$ carries *K*
- $E^I_\kappa = H^I_{\kappa\kappa} / N^I_{\kappa\kappa}$ defines a rotational band associated with the intrinsic *K*-state $\left|\phi_\kappa\right\rangle$
- Diagonalization = mixing of various *K*-states

Deformed basis vs spherical basis

- Rotational spectrum in ^{48}Cr
  - Exp. data:
    - Brandolini et al, *NPA* 642 (1998) 387
  - PSM:
    - Hara, Sun and Mizusaki, *PRL* 83 (1999) 1922
    - Deformed basis with a.-m. projection; Basis states ~ 50
  - pf-SM:
    - Caurier *et al.*, *PRL* 75 (1995) 2466
    - Conventional M-scheme spherical shell model; Basis states ~ 2 million



Model basis in terms of quasiparticle excitations

$$
\begin{aligned}
\Big\{ & |\Phi\rangle,\ a^\dagger_{\nu_i}a^\dagger_{\nu_j}|\Phi\rangle,\ a^\dagger_{\pi_i}a^\dagger_{\pi_j}|\Phi\rangle,\ a^\dagger_{\nu_i}a^\dagger_{\nu_j}a^\dagger_{\pi_k}a^\dagger_{\pi_l}|\Phi\rangle, \\
& a^\dagger_{\nu_i}a^\dagger_{\nu_j}a^\dagger_{\nu_k}a^\dagger_{\nu_l}|\Phi\rangle,\ a^\dagger_{\pi_i}a^\dagger_{\pi_j}a^\dagger_{\pi_k}a^\dagger_{\pi_l}|\Phi\rangle, \\
& a^\dagger_{\nu_i}a^\dagger_{\nu_j}a^\dagger_{\nu_k}a^\dagger_{\nu_l}a^\dagger_{\nu_m}a^\dagger_{\nu_n}|\Phi\rangle,\ a^\dagger_{\pi_i}a^\dagger_{\pi_j}a^\dagger_{\pi_k}a^\dagger_{\pi_l}a^\dagger_{\pi_m}a^\dagger_{\pi_n}|\Phi\rangle, \\
& a^\dagger_{\pi_i}a^\dagger_{\pi_j}a^\dagger_{\nu_k}a^\dagger_{\nu_l}a^\dagger_{\nu_m}a^\dagger_{\nu_n}|\Phi\rangle,\ a^\dagger_{\nu_i}a^\dagger_{\nu_j}a^\dagger_{\pi_k}a^\dagger_{\pi_l}a^\dagger_{\pi_m}a^\dagger_{\pi_n}|\Phi\rangle, \\
& a^\dagger_{\pi_i}a^\dagger_{\pi_j}a^\dagger_{\nu_k}a^\dagger_{\nu_l}a^\dagger_{\nu_m}a^\dagger_{\nu_n}a^\dagger_{\nu_o}a^\dagger_{\nu_p}|\Phi\rangle, a^\dagger_{\pi_i}a^\dagger_{\pi_j}a^\dagger_{\pi_k}a^\dagger_{\pi_l}a^\dagger_{\nu_m}a^\dagger_{\nu_n}a^\dagger_{\nu_o}a^\dagger_{\nu_p}|\Phi\rangle, \\
& a^\dagger_{\pi_i}a^\dagger_{\pi_j}a^\dagger_{\pi_k}a^\dagger_{\pi_l}a^\dagger_{\nu_m}a^\dagger_{\nu_n}a^\dagger_{\nu_o}a^\dagger_{\nu_p}a^\dagger_{\nu_q}a^\dagger_{\nu_r}|\Phi\rangle, \\
& a^\dagger_{\nu_i}a^\dagger_{\nu_j}a^\dagger_{\nu_k}a^\dagger_{\nu_l}a^\dagger_{\pi_m}a^\dagger_{\pi_n}a^\dagger_{\pi_o}a^\dagger_{\pi_p}a^\dagger_{\pi_q}a^\dagger_{\pi_r}|\Phi\rangle \Big\}
\end{aligned}
\tag{1}
$$

L.-J. Wang *et al, Phys. Rev.* C 90 (2014) 011303(R)
L.-J. Wang *et al, Phys. Rev.* C 93 (2016) 034322

Calculation of matrix elements for multi-quasiparticle states

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

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

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

with

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

- For example, a norm matrix element

$$\mathcal{N}_{\kappa\kappa'} = \langle \Phi | a_1 \cdots a_n [\Omega] a^\dagger_{1'} \cdots a^\dagger_{n'} | \Phi \rangle$$

can be written as combinations of

$$A_{\nu\nu'}(\Omega) \equiv \langle \Phi | [\Omega] a^\dagger_\nu a^\dagger_{\nu'} | \Phi \rangle = (V^*(\Omega) U^{-1}(\Omega))_{\nu\nu'} \,,$$

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

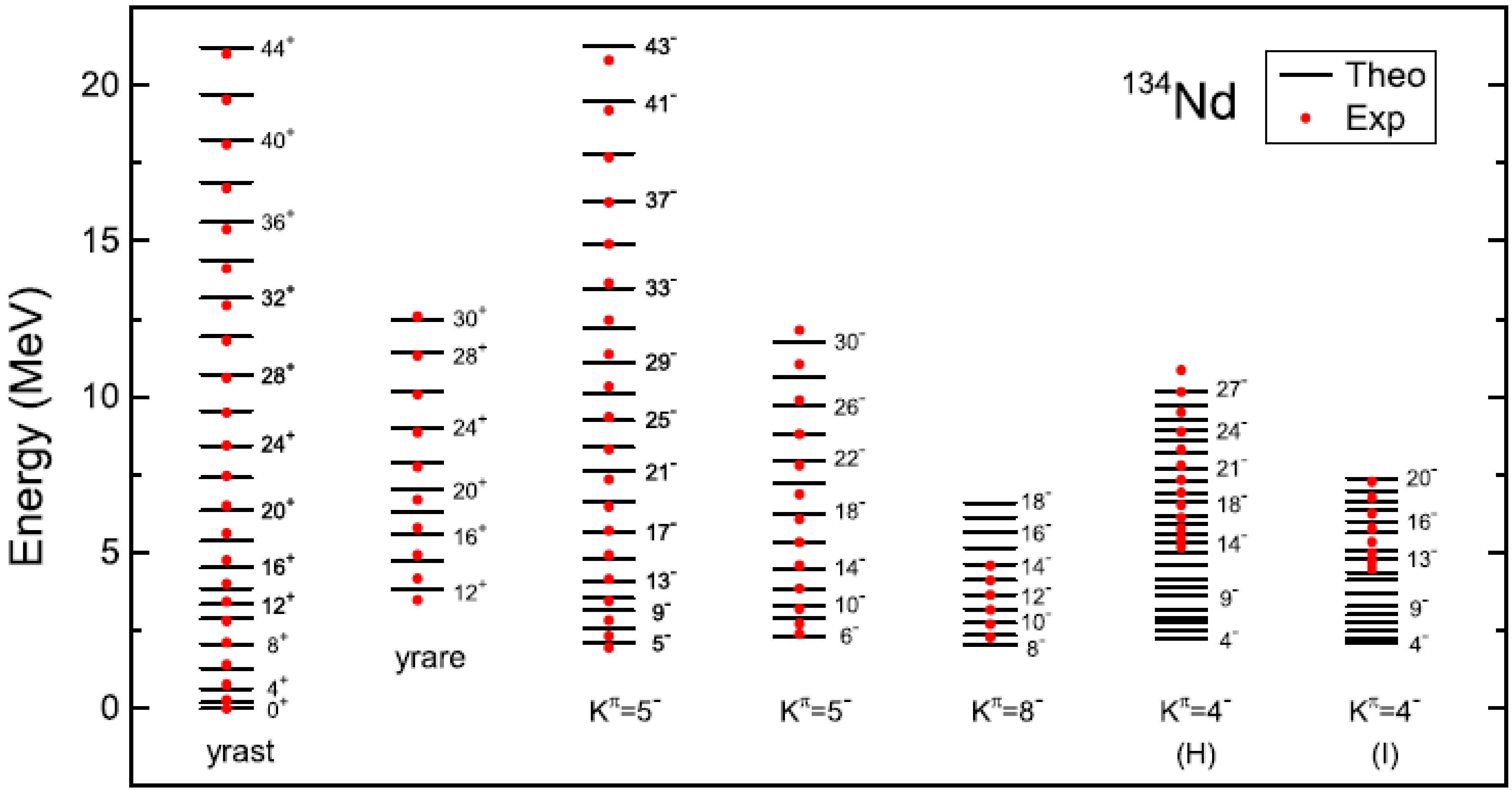
$$C_{\nu\nu'}(\Omega) \equiv \langle \Phi | a_\nu [\Omega] a^\dagger_{\nu'} | \Phi \rangle = (U^{-1}(\Omega))_{\nu\nu'} \,,$$

K. Hara, S. Iwasaki
Nucl. Phys. A
332 (1979) 61

Multi-quasiparticle computation using the Pfaffian algorithm

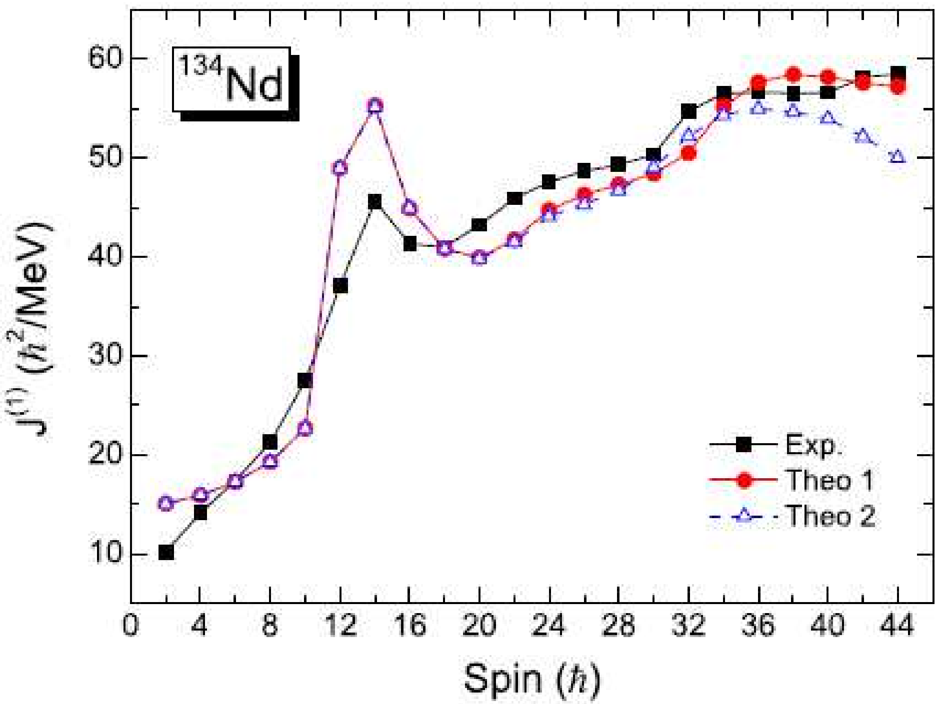
- Calculation of projected matrix elements usually uses the generalized Wick theorem
- A matrix element having n (n') qp creation or annihilation operators respectively on the left- (right-) sides of the rotation operator contains $(n + n - 1)!!$ terms in the expression – a problem of combinatorial complexity
- Use of the Pfaffian algorithm:
  - L.M. Robledo, Phys. Rev. C 79 (2009) 021302(R).
  - G. Bertsch, L.M. Robledo, Phys. Rev. Lett. 108 (2012) 042505.
  - 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
  - Q.-L. Hu, Z.-C. Gao, Y. S. Chen, Phys. Lett. B 734 (2014) 162.

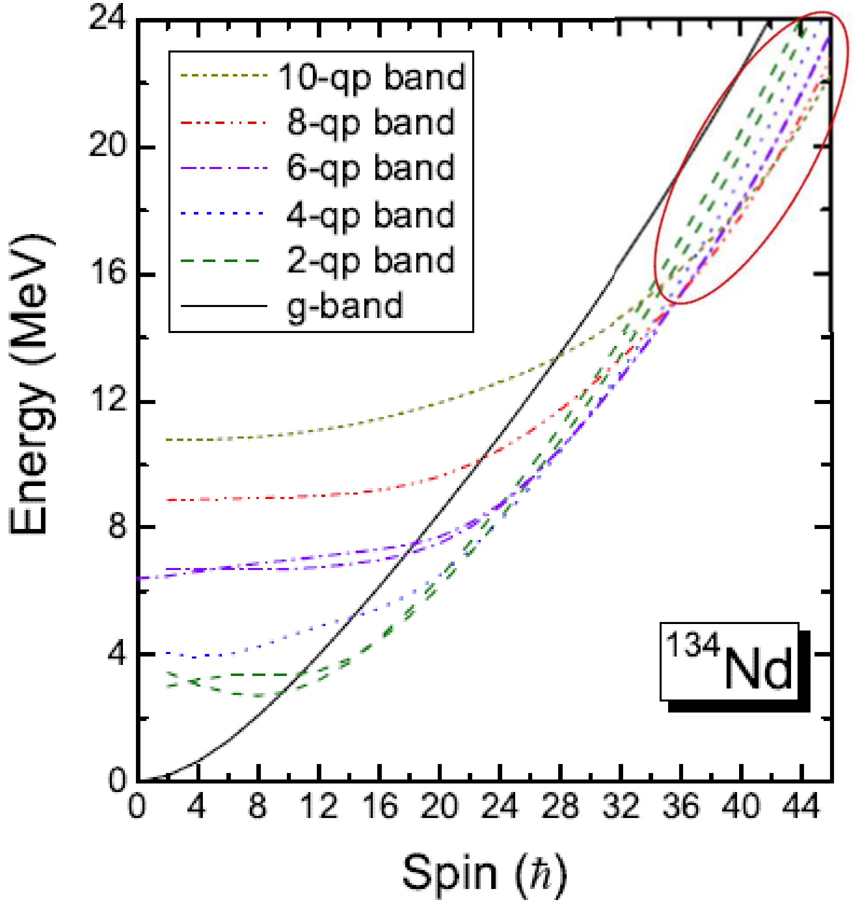
An example of ^{134}Nd



Calculated energy levels for yrast, yrare, and 2-qp K-bands in ^{134}Nd. Data: C. M. Petrache et al., Phys. Lett. B 387 (1996) 31

Going to very high-spin states





At very high spins, all states of different configurations rotate with same rotational frequency – a new collectivity?

Data: C. M. Petrache et al., Phys. Lett. B 387 (1996) 31

Major component for each configuration can be suggested

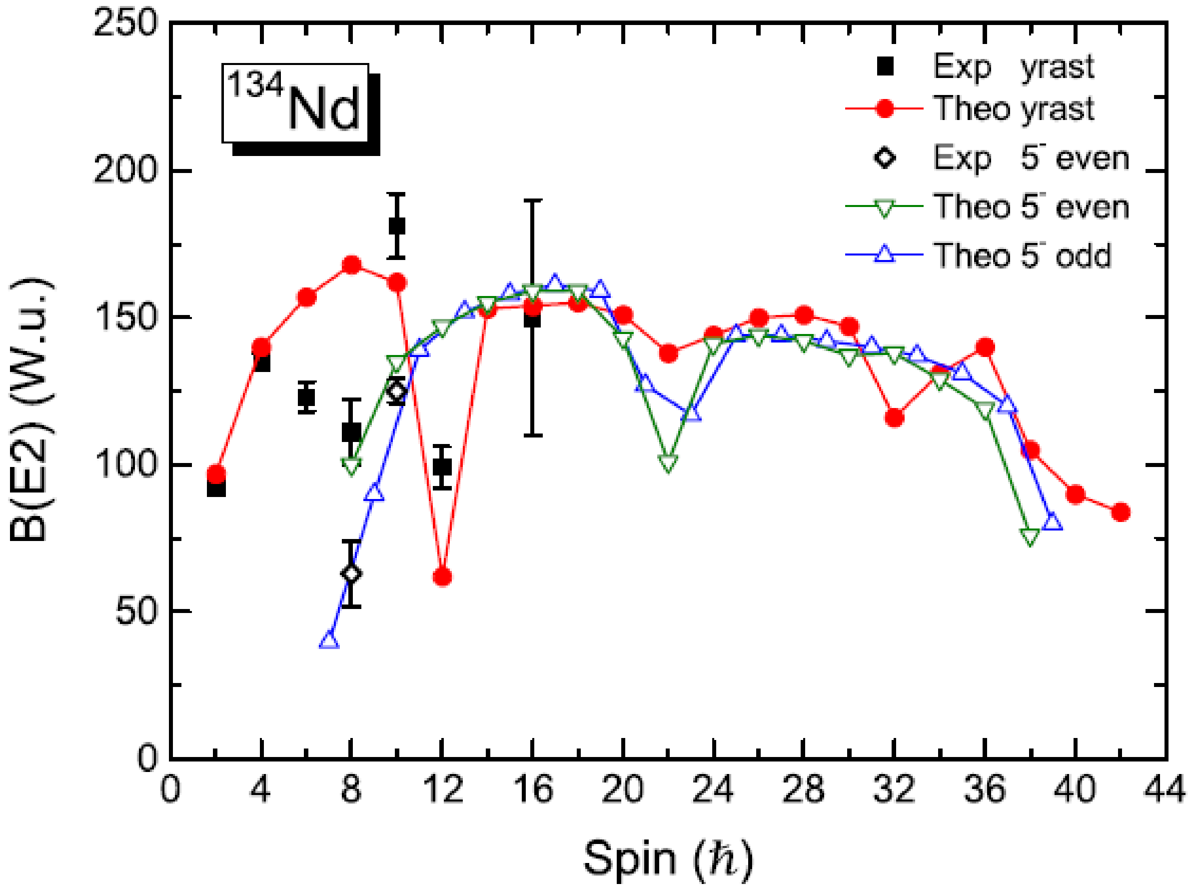
TABLE I. The K values and configurations of bands shown in the band diagram.

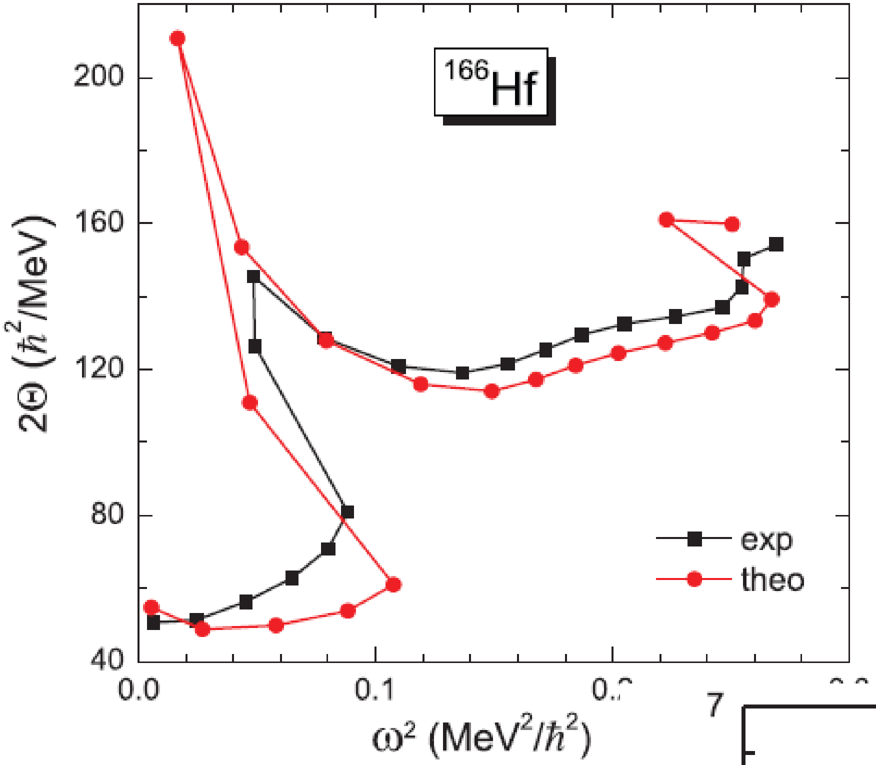
Band	K	Configuration
2-qp	1	$\pi 1/2^-[550] \otimes 3/2^-[541]$
2-qp	2	$\pi 1/2^-[550] \otimes 5/2^-[532]$
4-qp	1	$\nu 7/2^-[523]9/2^-[514] \otimes \pi 3/2^-[541]3/2^-[541]$
6-qp	0, 2	$\nu 7/2^-[523]9/2^-[514] \otimes \pi 1/2^-[550]3/2^-[541]5/2^-[532]5/2^-[532]$
8-qp	2	$\nu 5/2^-[532]7/2^-[523]1/2^-[541]1/2^-[541] \otimes \pi 1/2^-[550]3/2^-[541]5/2^-[532]5/2^-[532]$
10-qp	1	$\nu 5/2^-[532]7/2^-[523]1/2^-[541]1/2^-[541] \otimes \pi 1/2^-[550]3/2^-[541]5/2^-[532]5/2^-[532] \otimes \pi 3/2^+[411]5/2^+[413]$

Each basis state represents a real observable band !

Reduction of collectivity at very high spins

- While MoI keeps constant, B(E2) gradually decreases at high spins
- Successive band crossings among different quasiparticle states
- Structure changes in wave functions reduce B(E2) values



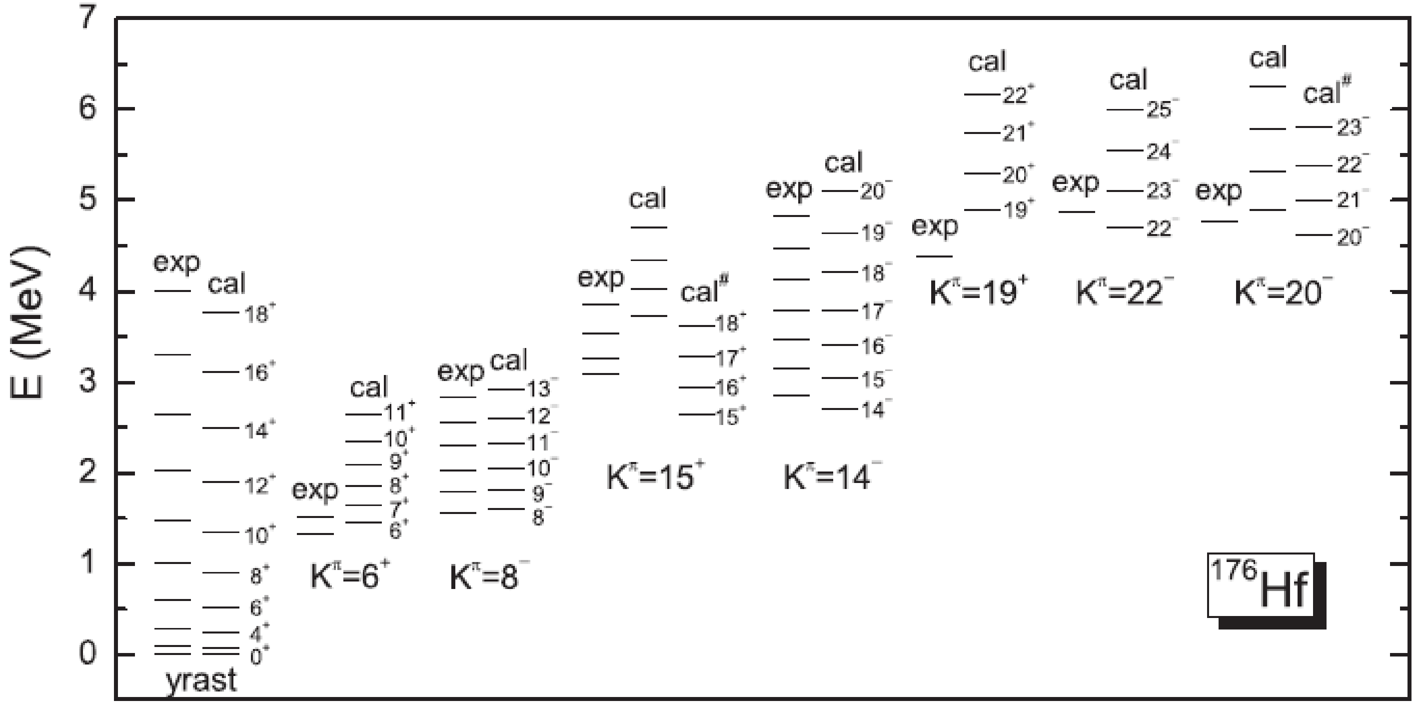


A third band-crossing is described.

$$\{|\Phi\rangle,\ a^\dagger_{\nu_i}a^\dagger_{\nu_j}|\Phi\rangle,\ a^\dagger_{\pi_i}a^\dagger_{\pi_j}|\Phi\rangle,\ a^\dagger_{\nu_i}a^\dagger_{\nu_j}a^\dagger_{\pi_k}a^\dagger_{\pi_l}|\Phi\rangle,$$
$$\times\ a^\dagger_{\nu_i}a^\dagger_{\nu_j}a^\dagger_{\nu_k}a^\dagger_{\nu_l}|\Phi\rangle,\ a^\dagger_{\pi_i}a^\dagger_{\pi_j}a^\dagger_{\pi_k}a^\dagger_{\pi_l}|\Phi\rangle,$$
$$\times\ a^\dagger_{\nu_i}a^\dagger_{\nu_j}a^\dagger_{\nu_k}a^\dagger_{\nu_l}a^\dagger_{\nu_m}a^\dagger_{\nu_n}|\Phi\rangle,\ a^\dagger_{\pi_i}a^\dagger_{\pi_j}a^\dagger_{\pi_k}a^\dagger_{\pi_l}a^\dagger_{\pi_m}a^\dagger_{\pi_n}|\Phi\rangle,$$
$$\times\ a^\dagger_{\pi_i}a^\dagger_{\pi_j}a^\dagger_{\nu_k}a^\dagger_{\nu_l}a^\dagger_{\nu_m}a^\dagger_{\nu_n}|\Phi\rangle,\ a^\dagger_{\nu_i}a^\dagger_{\nu_j}a^\dagger_{\pi_k}a^\dagger_{\pi_l}a^\dagger_{\pi_m}a^\dagger_{\pi_n}|\Phi\rangle\}$$

Example of some 2-, 4-, and 6-qps *K*-isomer bands in ^{176}Hf.

Data:
G. Mukherjee et al. Phys. Rev. C 82 (2010) 054316



L.-J. Wang, F-Q Chen, T. Mizusaki, M. Oi, Y. Sun, *Phys. Rev.* C90 (2014) 011303(R)

Isomer transition rates

TABLE I. Comparison of calculated $B(E2)$ values (in W.u.) for the isomeric states in ^{176}Hf with the available data taken from [40,42].

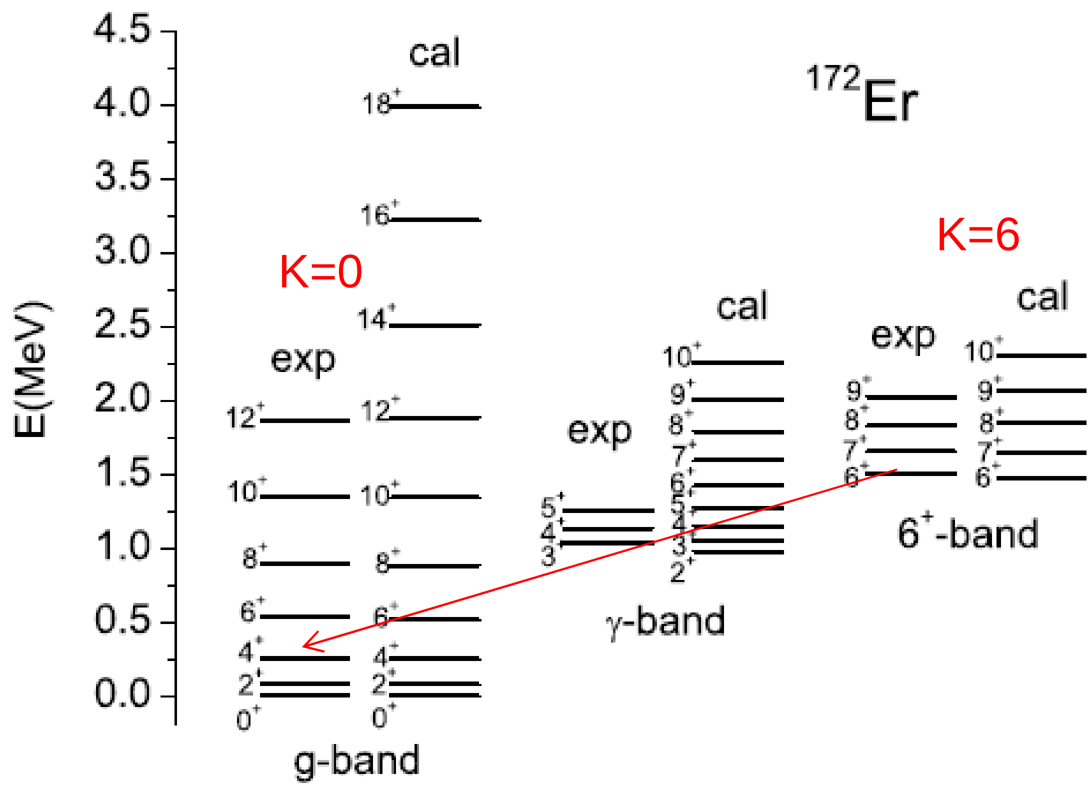
K_i^π	I_i	K_f^π	I_f	$B(E2; I_i \to I_f)$	
				Expt.	Calc.
6^+	6	0^+	6	2.82×10^{-6}	1.93×10^{-9}
6^+	6	0^+	4	3.16×10^{-7}	2.21×10^{-9}
14^-	14	8^-	12	5.33×10^{-7}	5.55×10^{-8}
22^-	22	20^-	20	4.8×10^{-3}	3.7×10^{-2}

Calculations for isomer transition rates including *K*-mixing can qualitatively distinguish allowed and *K*-forbidden transitions, but quantitative description leads to exploration of specific abnormal decays.

K-forbidden transition from 6^+ isomers in N = 104 isotones

- Very different *E2* decay rates from the two-quasineutron $K^\pi = 6^+$ isomers in N = 104 isotones ^{172}Er, ^{174}Yb, ^{176}Hf, and ^{178}W.
- Calculation assuming axially deformed basis cannot describe them.

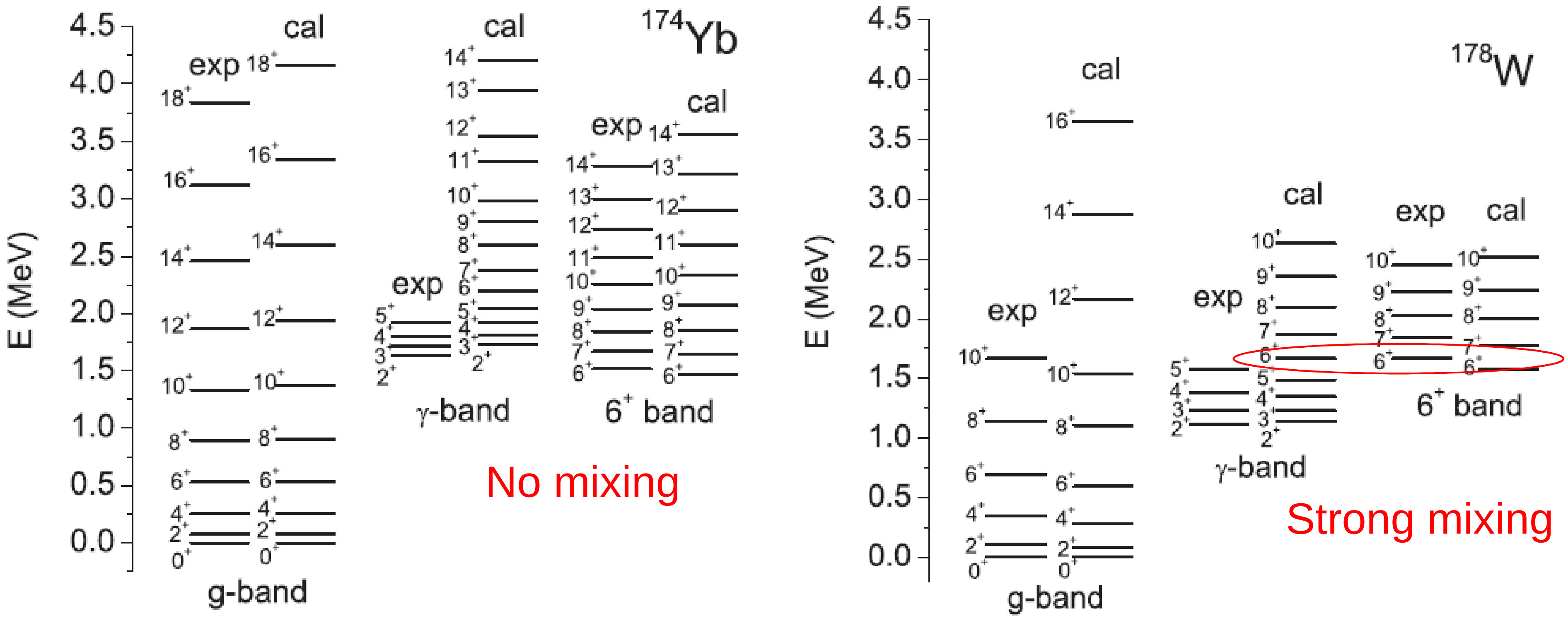
	Exp.	Cal.
^{172}Er	—[a]	6.72×10^{-11}
^{174}Yb	7.2×10^{-11}[b]	4.10×10^{-11}
^{176}Hf	3.16×10^{-7}[c]	4.36×10^{-11}
^{178}W	4.67×10^{-4}[d]	5.64×10^{-11}



Chen, Sun, Walker, Dracoulis, Shimizu, Sheikh, *J. Phys. G* 40 (2013) 015101

K-forbidden transition from 6^+ isomers in N = 104 isotones

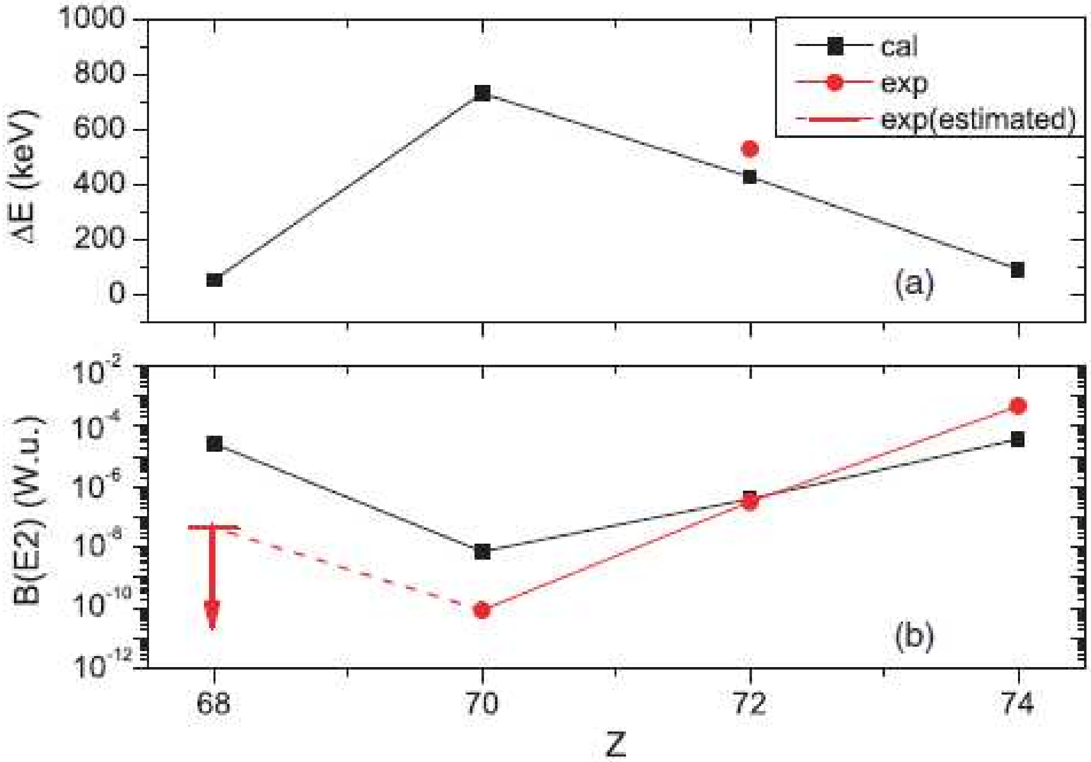
- Two-quasineutron $K^\pi = 6^+$ isomer in all N = 104 isotones has same configuration { $5/2^-[512]+7/2^-[514]$ }.



Chen, Sun, Walker, Dracoulis, Shimizu, Sheikh, *J. Phys. G* 40 (2013) 015101

K-forbidden transition from 6^+ isomers in N = 104 isotones

- Large variation of $K^\pi = 6^+$ isomer decay rate in N = 104 isotones originates from mixing with the γ-vibrational state.



- Three basic excitation modes (rotational, vibrational, single-particle) coexist and interact in the low-spin region!

Chen, Sun, Walker, Dracoulis, Shimizu, Sheikh, *J. Phys. G* 40 (2013) 015101

Stellar enhancement of decay rate

- A stellar enhancement can result from the thermal population of excited states

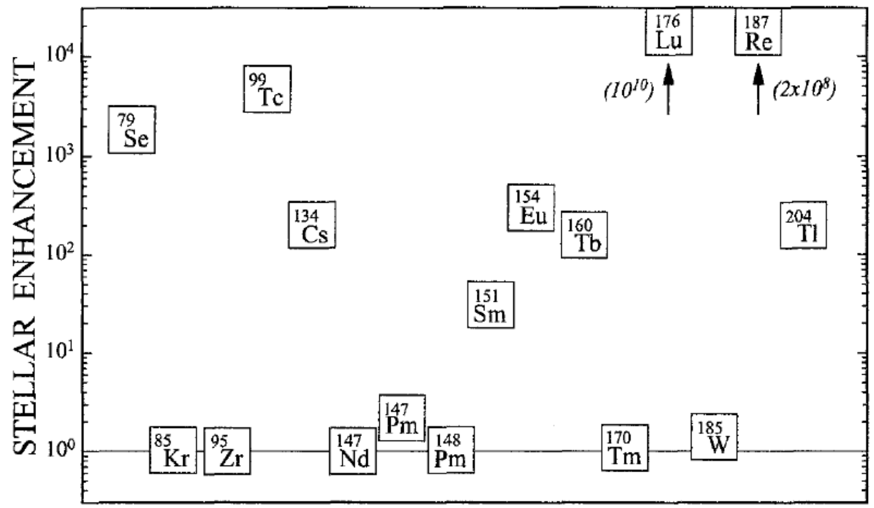
$$\lambda_\beta = \sum_i \left(p_i \times \sum_j \lambda_{\beta ij} \right)$$

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

- Examples in the s-process

F. Kaeppeler,
Prog. Part. Nucl. Phys. 43 (1999) 419

Also talk by A. Petrovici



Features of GT calculation by PSM

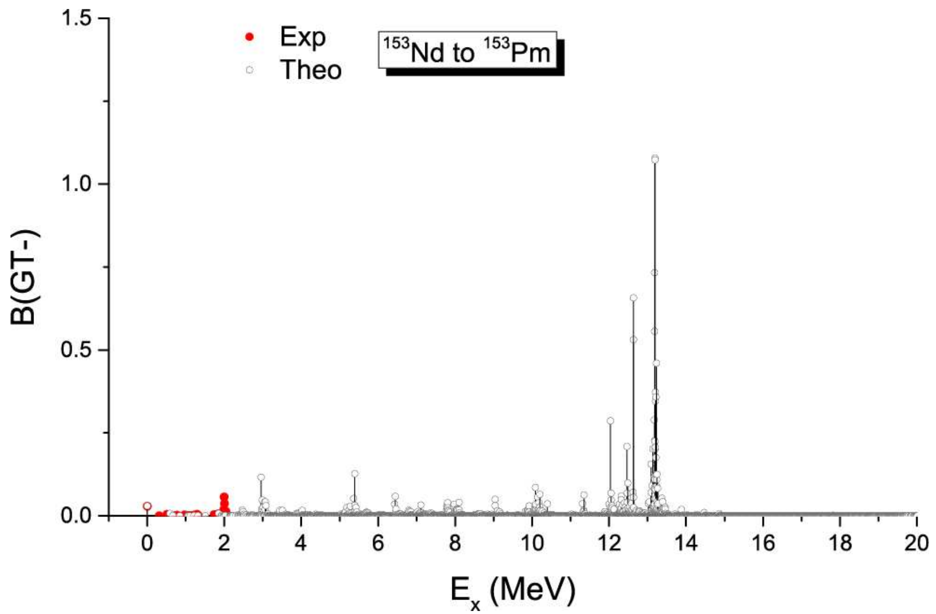
- As a shell model, PSM can be applied to any heavy, deformed nuclei without a size limitation.
- Its wavefunctions contain correlations beyond mean-field and are written in laboratory frame having definite good quantum numbers (angular-momentum and parity).
- A state-by-state evaluation of GT transition rates is computationally feasible, which enables calculations of GT transitions of excited states in a parent nucleus connecting to many states in a daughter.

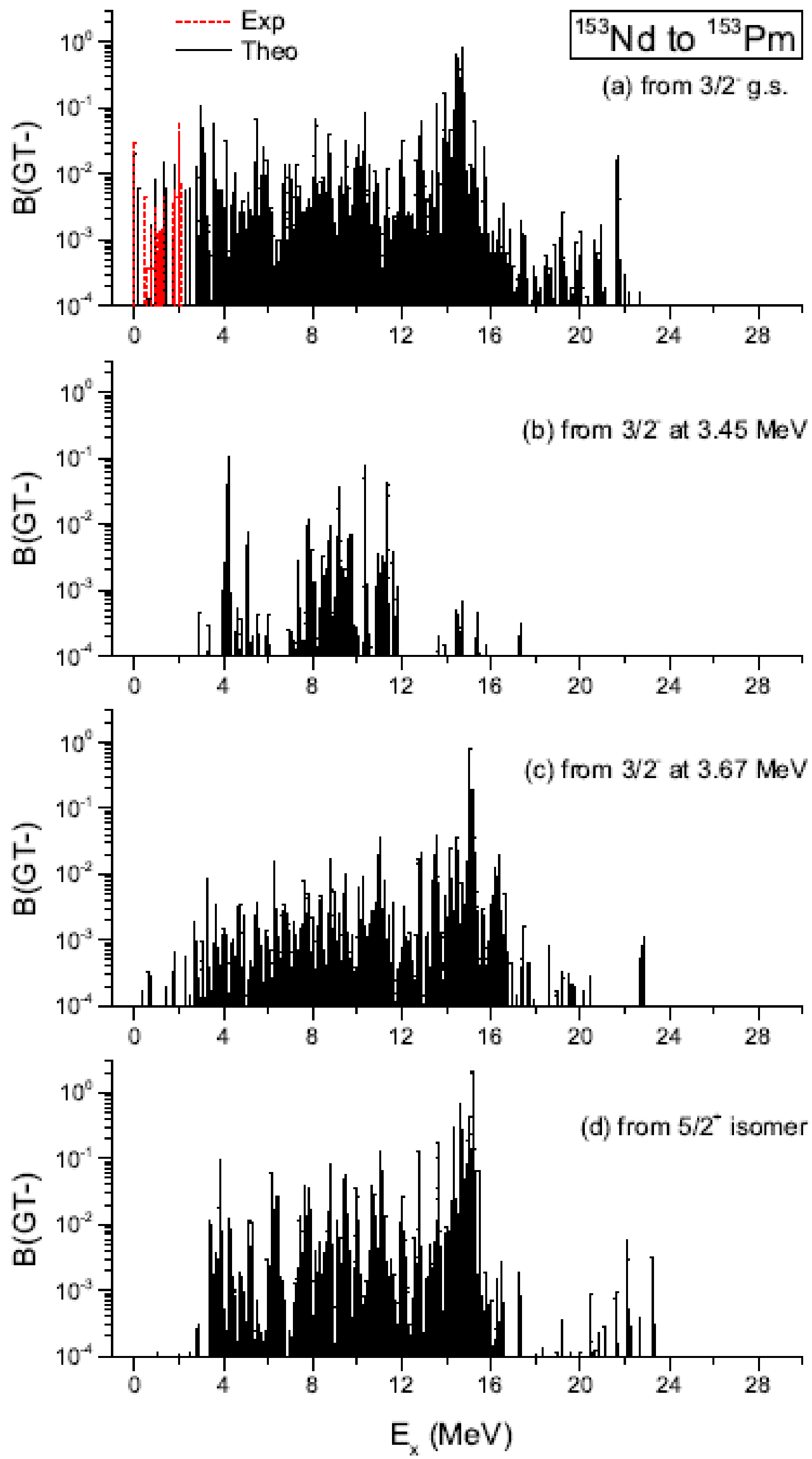
Features of GT calculation by PSM

- Calculations of forbidden transitions require multishell model spaces, not possible for most of conventional shell models working in one-major shell bases. PSM is a multishell shell model, and can treat situations when forbidden transitions are dominated.
- Isomeric states belong to a special group of nuclear states because of their long half-lives, which could alter significantly the elemental abundances produced in nucleosynthesis. PSM is capable of describing the detailed structure of isomeric states.
  - A. Aprahamian and Y. Sun, Nature Phys. 1, 81 (2005)

B(GT) of ^{153}Nd → ^{153}Pm

By using Pfaffian method, B(GT) of odd-mass nuclei can be calculated in a basis up to 6-qps



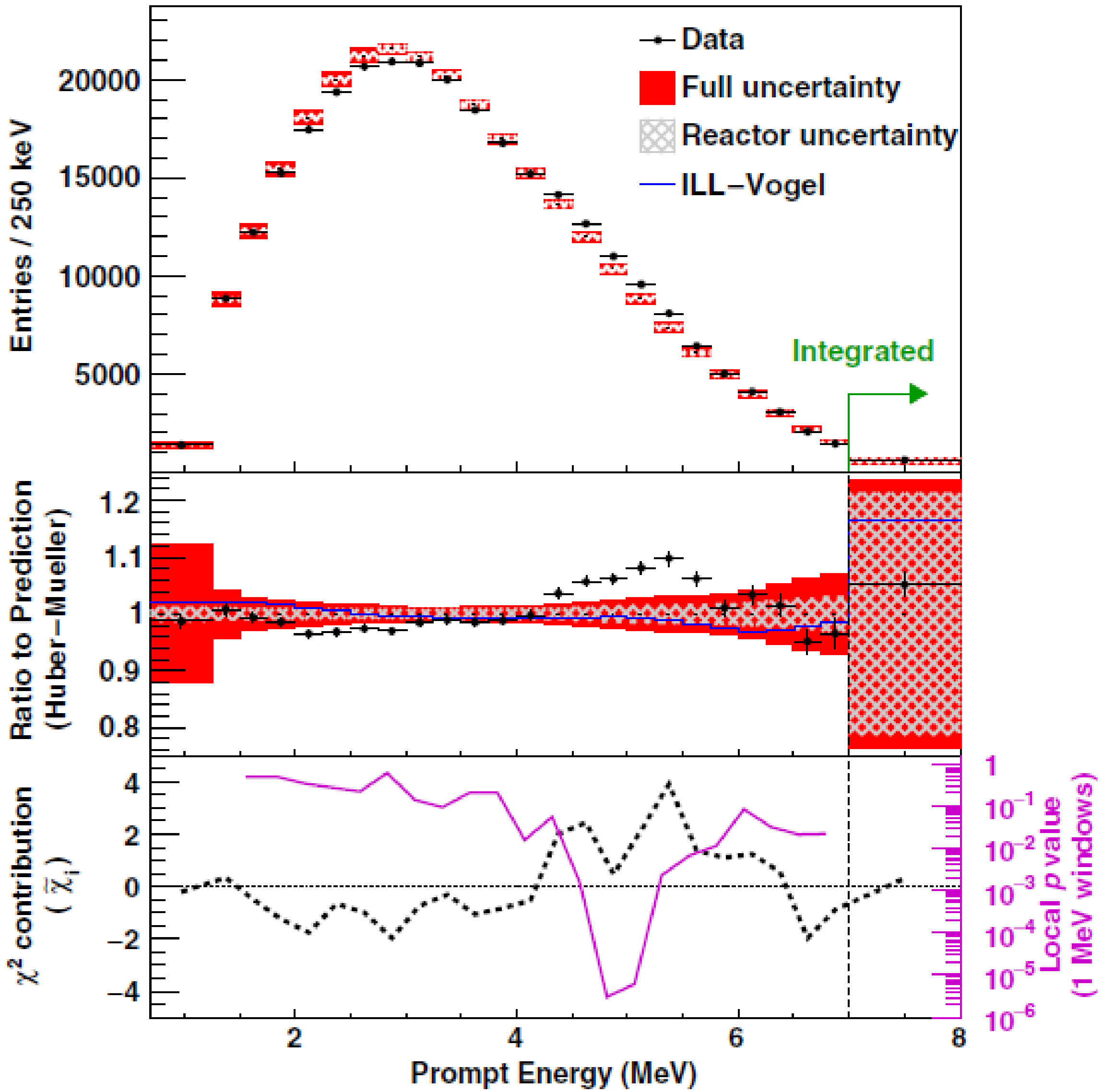


Z.-C. Gao, Y. Sun, Y.-S. Chen, *PRC 74* (2006) 054303

L.-J. Wang, Y. Sun, et al., to be published

Application in fundamental and nuclear astro-physics

- Energy spectrum of electron anti-neutrinos from nuclear reactors at Daya Bay, China
- An excess of ~10% of events within the 4-6 MeV region
- Tentative explanation: nuclear physics uncertainties in β-decays and fission yields



PRL 116 (2016) 061801

Anomaly in reactor neutrinos

- β-decays from about 10 neutron-rich fission products are important.
- Forbidden transitions are important.
- Current knowledge of β spectra from fission products is poor.
- Odd-mass nuclides are the main contributors.

A.A. Sonzogni et al., Phys. Rev. C 91 (2015) 011301(R)

CGS16
Shanghai, 2017

The 16th International Symposium on Capture Gamma-Ray Spectroscopy and Related Topics

18-22September, 2017

Shanghai Jiaotong University, Shanghai, China

The interactions

- Total Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_{QP} + \hat{H}_{GT}$
- Quadrupole + monopole-pairing + quadrupole-pairing

$$\hat{H}_{QP} = -\frac{1}{2}\chi_{QQ}\sum_{\mu}\hat{Q}^{\dagger}_{2\mu}\hat{Q}_{2\mu} - G_M\hat{P}^{\dagger}\hat{P} - G_Q\sum_{\mu}\hat{P}^{\dagger}_{2\mu}\hat{P}_{2\mu}$$

- Charge-exchange (Gamow-Teller)

$$\hat{H}_{GT} = +2\chi_{GT}\sum_{\mu}\hat{\beta}^{-}_{1\mu}(-1)^{\mu}\hat{\beta}^{+}_{1-\mu} - 2\kappa_{GT}\sum_{\mu}\hat{\Gamma}^{-}_{1\mu}(-1)^{\mu}\hat{\Gamma}^{+}_{1-\mu}$$

$$\hat{\beta}^{-}_{1\mu} = \sum_{\pi,\nu}\langle\pi|\sigma_{\mu}\tau_{-}|\nu\rangle c^{\dagger}_{\pi}c_{\nu}, \quad \hat{\beta}^{+}_{1\mu} = (-)^{\mu}(\beta^{-}_{1-\mu})^{\dagger}$$

$$\hat{\Gamma}^{-}_{1\mu} = \sum_{\pi,\nu}\langle\pi|\sigma_{\mu}\tau_{-}|\nu\rangle c^{\dagger}_{\pi}c^{\dagger}_{\bar{\nu}}, \quad \hat{\Gamma}^{+}_{1\mu} = (-)^{\mu}(\Gamma^{-}_{1-\mu})^{\dagger}$$

  - Kuz'min & Soloviev, *Nucl. Phys*. A 486 (1988) 118

An example: ^{164}Ho – ^{164}Dy

- Parameters:
  - $\varepsilon_2 = 0.28$
  - $G_{M,n} = 17.5/A = 0.107$ MeV
  - $G_{M,p} = 22.7/A = 0.138$ MeV
  - $G_Q = 0.18\ G_M$

  Hara & Sun, IJMP E4 (1995) 637

  - $\chi_{GT} = 23/A = 0.14$ MeV
  - $\kappa_{GT} = 7.5/A = 0.046$ MeV

  Kuz'min & Soloviev,

  NPA 486 (1988) 118