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ROTATIONAL ENERGY EXPRESSIONS AND LEAST-SQUARES FITTING OF BACKBENDERS AND SIMILAR NUCLEI †

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Abstract: The backbending or irregularities of band spacings of states near the yrast line were fit using simple rotational energy expressions which include band mixing of the yrast and yrare states. In our model the sharp backbending requires two large mixing terms, a spin-independent term arising from the pairing interaction and a Coriolis coupling term. Least-squares fitting of backbenders in the deformed even-even nuclei indicate a near cancellation of the mixing matrix elements near the virtual band crossing. Although the idealized and simplified expressions for the backbending spin in terms of the pairing gap Δ, high-j orbital spacing, high-j Coriolis matrix element $J_\perp$, and moment of inertia $\mathcal{I}$ may not be quantitatively correct, they do indicate the general conditions required for backbending.

1. Introduction

With the increasing knowledge of states near the yrast line in deformed even-even nuclei, it appears that irregularities in spacings (backbending or upbending) may be

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associated with band crossing. The band that crosses the ground band (g-band) at some critical spin I_c will here be referred to as the S-band (for "superband" or "Stockholm band"). The band-mixing picture has been invoked in numerous studies. Broglia, Regge and Molinari [1]) have adjusted matrix elements in semiempirical three- and four-band mixing calculations to fit the yrast levels. El Masri [2]) *et al.* have analyzed ground and higher bands by mixing. Sheline [3]) early made systematics assuming an S-band with rigid-body moment of inertia, band-head energy at the pairing condensation energy, and band-head spin zero or small. There has been some thought inspired by the early Mottelson-Valatin [4]) work that the yrast levels beyond I_c, hence the S-band, represent "normal" matter after a pairing collapse.

Stephens *et al.* [5]) especially have advanced the picture that the S-band involves the decoupling of a pair of particles in a high-j orbital to a resultant $J_P = 2j-1$ angular momentum, to which the core angular momentum adds in stretched fashion to yield the resultant spin I. In its purest form the decoupled S-band should show a a band-head spin of $J_P(= 2j-1)$ and energies of

$$E_S(I) = E_0 + \frac{\hbar^2}{2\mathscr{J}_s} R(R+1), \tag{1}$$

with

$$R = |I - J_P|. \tag{2}$$

2. Graphical determination of band-head spins

Can we determine in a simple graphical way the approximate value of the band-head spin? Bohr and Mottelson [6]) have plotted angular momentum $I(\omega)$ versus rotational frequency ω. The angular momentum difference $i_\alpha(\omega)$ between the curves for ground and S-band is associated with the aligned angular momentum. When $i_\alpha(\omega)$ is extrapolated to $\omega = 0$, one can obtain an estimate of band-head spin J_P for the S-band. An even simpler approach is to plot the first difference of the band energies, i.e., the $\Delta E_{I\to I-2}$ transition energies, versus spin I for the S-band members. From eqs. (1) and (2) we get that

$$\Delta E_{I\to I-2} = 4\frac{\hbar^2}{2\mathscr{J}}(|I - J_P| - \tfrac{1}{2}). \tag{3}$$

That is, the x-intercept is $I_x = J_P + \frac{1}{2}$, and the slope is four times the rotational constant $\hbar^2/2\mathscr{J}$. The practical difficulty of determining J_P is that usually only a few states beyond the crossing are known, a long extrapolation is involved, and band mixing perturbs levels near the virtual crossing.

We can also apply this plotting method to odd-A rotational bands [7]). Due to the alternating energy shift terms, the plots for $I+\frac{1}{2}$ even and $I+\frac{1}{2}$ odd are usually displaced. In particular, the high-spin members of bands with an odd $i_{13/2}$ neutron often

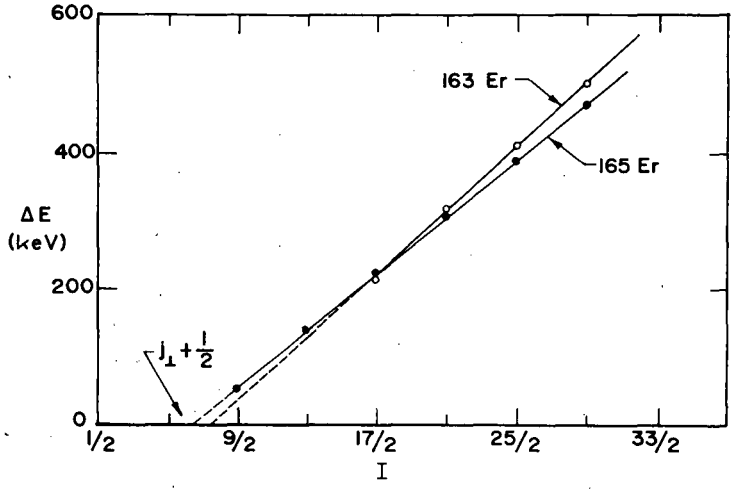

Fig. 1. Simple $\Delta E_{I \to I-2}$ versus I analysis for odd $i_{13/2}$ rotational bands in ^{163}Er and ^{165}Er. The extrapolated value of aligned angular momentum is $j_\perp \approx 3$. Data are from ref. [10]).

extrapolate to non-zero values of J_p, as can be seen in fig. 1. Indeed, it appears that the J_p values for odd-A $i_{13/2}$ bands are around half those for S-bands of neighboring even-even nuclei. This point was discussed by Bohr and Mottelson [4]) in their analysis.

Because in so many cases we only have the yrast levels known near the band-crossing region, it is difficult to extrapolate with confidence to determine an apparent band-head spin for the S-band either by our method or by that of ref. [6]). It is not clear whether one should make a straight-line extrapolation on the plots of transition energy versus initial spin (such as fig. 1) or whether to make a curving extrapolation parallel to the ground band plot and reflecting the changing moment of inertia of the ground band. Thus, we seek some simple limiting models from which we can derive analytical energy formulas with few enough parameters to use least squares fitting of experimental energies.

In the region of 90 neutrons and somewhat above there are low-lying collective bands of β- and γ-vibrational character and pairing is strong. Perhaps Sheline's approach using two bands with zero-spin band heads is valid in this region. A more detailed understanding in this region may require the three- or four-band approaches.

In the region of 100 neutrons a different limiting case may be approached, where pairing is weak and collective shape-vibrational strength lies higher. In this region the ground and S-band properties may be defined largely by the nearest high-j Nilsson orbitals just above and below the neutron chemical potential. That is, the S-band, or at least its strength function, is a band generated by operating twice with j_+ on the ground band.

3. Coriolis band-mixing models

The perturbation theory treatment of Coriolis band mixing between well-separated bands was shown long ago [8,9]). The lowest order effect is to renormalize the apparent moment of inertia but to leave the $I(I+1)$ energy dependence. The opposite limiting case of two bands, degenerate in the absence of Coriolis interaction, also has a simple analytical solution.

Consider the case of a deformed even-even nucleus with neutron chemical potential between Ω and $\Omega+1$ orbitals of high j. We suppose that the $i_{\frac{13}{2}}$ neutrons play the major role in the backbending phenomenon and that essential features are dominated by the two nearest-lying $i_{\frac{13}{2}}$ orbitals. From these orbitals we can generate an excited 1^+ band and an excited 0^+ band that involve, respectively, promotion of one and two nucleons across the Fermi surface from $|j\Omega\rangle$ to $|j\Omega+1\rangle$. To avoid spurious 0^+ states we treat the problem in a particle, not quasiparticle, representation. The three bands (including ground 0^+) will interact via pairing and Coriolis interactions, and one could do three-band mixing, as did Broglia *et al.* [1]). However, the physical nature we postulate for the important bands allows us to treat them by successive 2×2 diagonalizations. If we approximate the upper $K = 0^{+\prime}$ and $K = 1^+$ bands as degenerate † before Coriolis interaction, we get simple energy solutions with maximal 50 : 50 state mixing,

$$W_1 = E_0 + AI(I+1) \pm H_{\text{cor.}}, \tag{4}$$

where $A = \hbar^2/2\mathcal{J}$, the rotational constant, and the Coriolis matrix element is $H_{\text{cor.}} = 2A[j(j+1)-\Omega(\Omega+1)]^{\frac{1}{2}}[I(I+1)-\Omega(\Omega+1)]^{\frac{1}{2}}$. Taking the lower (minus) sign we have our approximate expression for the superband energies in the absence of mixing with the ground band.

In the limit of low Ω we get the "decoupled band" expression of eq. (2). This is the idealized Stephens decoupling limit. In our case the spin for minimum energy will in general not be $2j-1$ but more nearly $2j_\perp$ $(= 2\sqrt{j(j+1)-\Omega(\Omega+1)}$, decreasing as the heavier deformed lanthanides are reached, where $\Omega = \frac{7}{2}$ or $\frac{9}{2}$ orbitals lie nearest the Fermi energy. Neglecting Ω compared to I, we get approximately $W_1 \approx E_0' + AI^*(I^*+1)$ with $I^* = I-2j$.

Thus, before considering ground-band mixing we have parabolic bands with the same constant A, but the upper two bands are displaced upward by E_0', the Nilsson orbital spacing, and horizontally by $\pm 2j_\perp$.

4. Least squares fitting of yrast and yrare levels

Having derived a simple analytical expression for the S-band energies, we now wish to introduce mixing with the ground band. The character of the S-band in our

† It may be rationalized that retention in the zeroth order Hamiltonian of the diagonal matrix elements of pairing could make the $0^{+\prime}$ band degenerate with the 1^+.

model is a 50 : 50 mixture of the $K = 1$, $|\Omega+1, \Omega^{-1}\rangle$ particle-hole state and the $K = 0'$, $|(\Omega+1)^2, (\Omega)^{-2}\rangle$ two-particle two-hole state. The mixing matrix elements with the ground band should consist of (a) spin-independent terms coupling the 0^+ components and coming from pairing force and $\boldsymbol{j}_1 \cdot \boldsymbol{j}_2$ recoil and (b) of Coriolis terms with the $K = 1$ component having the spin dependence $\sqrt{I(I+1)}$. We shall constrain the Coriolis term to have the same $\langle\Omega+1|j_+|\Omega\rangle$ matrix element as in the unmixed S-band expression. The spin-independent term will be a variable to be determined by fitting.

It is to be expected that the rotation of the core excluding the $i_{\frac{13}{2}}$ neutron orbitals will need a correction to the moment of inertia, such as $\mathscr{J}(I) = \mathscr{J}_0[1+\lambda I(I+1)]$.

In general, the energies were assumed to have the form

$$E_g = A\hat{I}^2/V_1, \tag{5}$$

$$E_s = A[D+F(\hat{I}-2j_\perp)^2/V_2], \tag{6}$$

where

$$A = \frac{\hbar^2}{2\mathscr{J}_0}, \qquad \hat{I}^2 = I(I+1),$$

The two different classes of calculations correspond to different forms for the non-rotational curvature terms V_1 and V_2:

(i) no λ in S-band,

$$V_1 = 1+\lambda\hat{I}^2, \qquad V_2 = 1,$$

(ii) λ_s in S-band,

$$V_1 = 1+\lambda\hat{I}^2, \qquad V_2 = 1+\lambda_s(\hat{I}-2j_\perp)^2.$$

In addition, for some cases $j_\perp$ was fixed at various values and one of the above formulations was used. As discussed below all calculations reported here used either $\lambda_s = 0$, or $\lambda_s = \lambda$ due to insufficient data to allow a free parameter λ_s. The energies for the states were taken from two-band mixing as

$$W_\pm = \tfrac{1}{2}(X+Y) \pm \tfrac{1}{2}\sqrt{(X-Y)^2+4Z^2} + E_0, \tag{8}$$

where

$$X = E_g, \qquad Y = E_s,$$

and where the Coriolis mixing term was assumed to be

$$Z = A(B_0 + j\sqrt{2\hat{I}})/V_1. \tag{9}$$

The constant E_0 renormalizes the $W_\pm$ solution such that $W_-(I = 0) = 0$ and is given by

$$E_0 = \tfrac{1}{2}\{\sqrt{[Y(0)]^2+4[Z(0)]^2} - Y(0)\}. \tag{10}$$

TABLE 1

Best-fit parameters for the case $\lambda_s = 0$*

Nucleus	A (MeV)	AD (MeV)	AF (MeV)	$j_\perp$	λ	AB_0 (MeV)	X^2	ref.
$^{130}_{58}Ce_{72}$	0.02652	2.397	0.01962	2.95	0.00114	−0.992	8.8×10^{-4}	a)
$^{132}_{58}Ce_{74}$	0.02930	3.255	0.03575	4.51	0.00196	−1.828	1.9×10^{-3}	a)
$^{134}_{58}Ce_{76}$	0.03850	2.487	0.02502	2.73	0.00310	−1.521	4.0×10^{-3}	a)
$^{158}_{68}Er_{90}$	0.01803	3.372	0.02037	5.00*	0.00090	−1.260	2.8×10^{-3}	
	0.01820	2.794	0.01853	4.00*	0.00091	−1.025	2.4×10^{-3}	b, m)
	0.01985	2.052	0.01066	2.00*	0.00110	−0.500	5.0×10^{-3}	
$^{158}_{66}Dy_{92}$	0.01260	2.705	0.02155	4.50*	0.00053	−1.072	6.2×10^{-4}	
	0.01580	3.135	0.01027	3.00*	0.00048	−0.171	1.5×10^{-4}	c, h)
	0.01517	2.253	0.00971	2.00*	0.00067	−0.193	1.7×10^{-4}	
$^{160}_{68}Er_{92}$	0.01878	4.526	0.01070	4.50*	0.00012	−0.336	1.1×10^{-3}	
	0.01547	1.626	0.01655	3.00*	0.00117	−0.920	6.2×10^{-4}	d)
	0.01667	1.099	0.01448	2.00*	0.00145	−0.656	3.2×10^{-4}	
$^{162}_{68}Er_{94}$	0.01340	1.968	0.01970	4.00*	0.00072	−1.057	7.4×10^{-4}	
	0.01378	1.680	0.01433	3.00*	0.00076	−0.812	9.3×10^{-4}	d)
	0.01453	2.109	0.00696	2.00*	0.00101	−1.551	6.4×10^{-3}	
$^{164}_{70}Yb_{94}$	0.01493	2.125	0.01284	3.18	0.00060	−0.772	1.7×10^{-3}	e, g, i, n)
$\underline{^{164}_{68}Er_{96}}$	0.01358	1.655	0.00964	1.94	0.00050	−0.536	8.2×10^{-4}	f, o)
$\underline{^{166}_{70}Yb_{96}}$	0.01467	1.556	0.00924	1.58	0.00070	−0.455	8.7×10^{-4}	e, g)
$\underline{^{168}_{72}Hf_{96}}$	0.01553	1.669	0.01118	2.39	0.00100	−0.677	1.1×10^{-3}	b)
$^{168}_{70}Yb_{98}$	0.01247	1.217	0.02220	2.26	0.00060	−0.542	1.5×10^{-4}	j, k)
$^{170}_{74}W_{96}$	0.01631	2.334	0.01810	4.30	0.00100	−1.089	1.5×10^{-3}	e)
$^{182}_{76}Os_{106}$	0.01993	3.470	0.01276	3.95	−0.00044	−0.269	8.2×10^{-4}	l)

* $j_\perp$ held constant at this value.

Underlined cases are more reliable, since these are the only cases where at least one pair of levels with the same spin is known.

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where

$$Y(0) = A(D + 4Fj_\perp^2), \qquad Z(0) = AB_0.$$

Fitting was done for the transition energies $\Delta E_{I \to I-2}$ rather than for the level energies, with a minimization with respect to A, D, F, B_0, λ, and in some cases, $j_\perp$.

Results are summarized in table 1. The general philosophy has been to calculate nuclei for which several states are known above the backbend and/or for which non-yrast states in the crossing bands are known. We have also included several cases where these conditions were not adequately fulfilled, but for which there existed another isotone fulfilling the conditions, thereby allowing $j_\perp$ to be fixed and stabilize the calculation. In addition to rare-earth nuclei, we have included ^{132}C, ^{134}Ce ($h_{\frac{11}{2}}$ protons), and ^{182}Os as cases fulfilling the above conditions.

5. Discussion

In figs. 2 and 3 are plotted the fitted curves with experimental data points are plotted. The nuclei shown are the three with best data, i.e., having at least two levels of the same spin identified, and one case ^{170}W, where only the yrast levels are

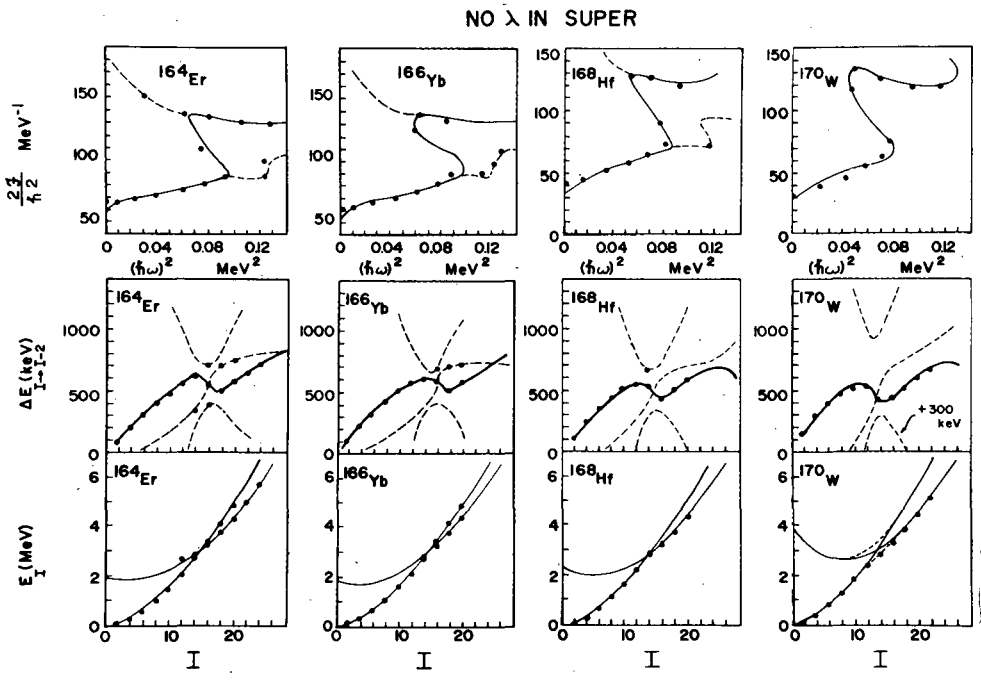

Fig. 2. Examples from the "no λ_s" fits (fixed S-band moment-of-inertia) of table 1. The dots are for the experimental data and curves for the least-squares fit and its extrapolations. In the ΔE versus I plots there are four branches corresponding to the four possible values of $\Delta E_{I \to I-2}$ for the case of two crossing bands. The yrast branch is shown by the solid line in each case.

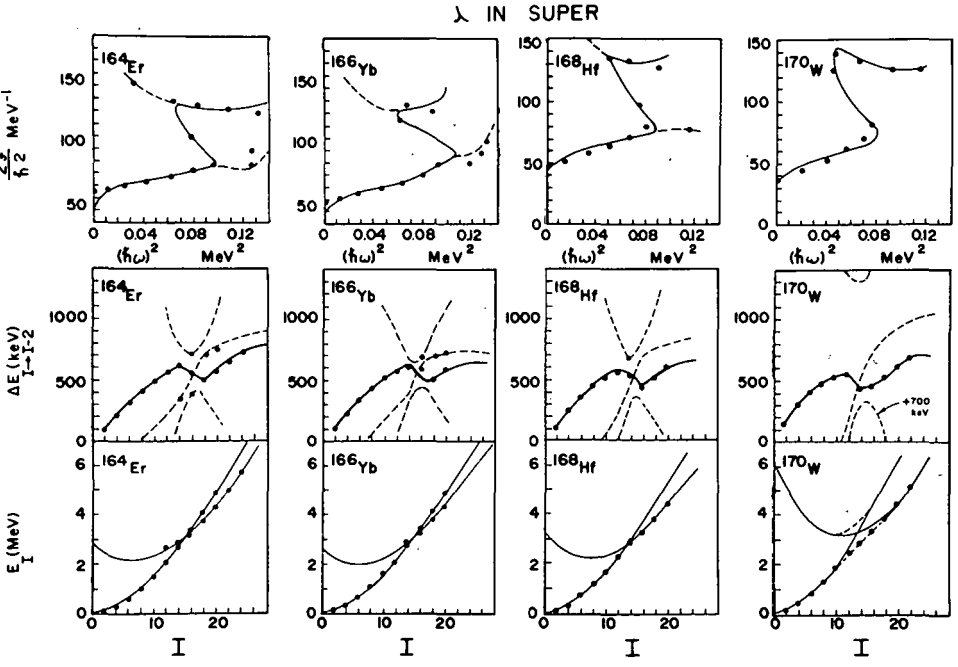

Fig. 3. Examples from the "with λ_s" fits of table 2, where the S-band is given the same moment-of-inertia variation as the ground band ($\lambda_s = \lambda$). See the caption to fig. 2 for further explanation.

known. Fig. 2 shows fits with fixed moment of inertia in the S-band ($\lambda_s = 0$) with corresponding parameters and χ^2 values in table 1. Fig. 3 shows fits with the same moment-of-inertia change factor in both ground and S-bands ($\lambda_s = \lambda$) with parameters and χ^2 values in table 2. The "a" sections of the figures are backbending plots calculated in the Copenhagen convention. The "b" sections show $\Delta E_{I \to I-2}$ versus I and E_I versus I plots. Table 3 gives numerical values for the experimental transition energies and the best-fit λ_s values for ^{164}Er, ^{166}Yb, and ^{168}Hf.

Let us examine results in table 3 for ^{164}Er, the experimentally best-determined case. Except for the $2^+ \to 0^+$ transition, the transition energies are fit to within ± 10 keV. The fits to ^{166}Yb and ^{168}Hf are somewhat poorer.

Which form of the fitting expression is preferred? Ideally, we would like to give each band the freedom to adjust its moment-of-inertia variation constants (λ and λ_s). However, the attempts to fit with the extra parameter were not satisfactory. There are insufficient data points known in both bands, except possibly for ^{164}Er, to justify an additional variational parameter of this type.

A comparison of figs. 2 and 3 shows little difference in quality of fits between the two forms. The "no λ_s" form gives a rather straight extrapolation of the S-band on the ΔE versus I plot of fig. 2b, as contrasted with the curved extrapolation of the "with λ_s" form of fig. 3b. Hence, the band-head spin of the S-band, i_α ($\omega = 0$), inferred

is quite different for the two forms. The "no λ_s" table 1 lists $j_\perp$, which is approximately half the intercept value, i.e., band-head spin of the S-band, as 1.94, 1.58, and 2.38, respectively, for the best data cases, the 96-neutron isotones $^{164}_{68}$Er, $^{166}_{70}$Yb, and $^{168}_{72}$Hf. By contrast, the "with λ_s" form of table 2 gives $j_\perp$ of 3.2, 3.07, and 4.42, respectively. These two forms correspond to alternative ways of extrapolating Bohr and Mottelson's aligned angular momentum $i_\alpha(\omega)$ for the S-band to $\omega = 0$ (cf. the top curve of fig. 11, ref. [6])); the "with λ_s" alternative would be an extrapolation observing the curvature and the "no λ_s" would be approximately a flat extrapolation. The principle that the aligned angular momentum ($2j_\perp$) in the S-band is approximately twice that of the $i_{\frac{13}{2}}$ band in the neighboring even-odd nuclei (fig. 1) would seem to favor the "with λ_s" form. However, it is generally observed that the even-even ground bands appear softer than neighboring odd mass. We can rationalize this observation microscopically; in the odd-mass cases it can be shown that fourth-order Coriolis band-mixing gives a positive $I^2(I+1)^2$ energy correction term that can nearly cancel the negative term from the rotor (even-even core). Thus, the S-band, with its odd $i_{\frac{13}{2}}$ nucleons should appear to have a stiffer rotor than the ground band. Thus, we favour the "no λ_s" analysis of table 1 and fig. 2 though the choice is by no means clear-cut.

Now compare in table 1 the ground rotational constant A and the S-band rotational constant AF. The favorable $N = 96$ cases all show $\sim 30\%$ smaller AF value. Stephens has emphasized that the analysis for aligned angular momentum should take into account that the effective rotor moment of inertia will not be the same in ground band and S-band. Our least squares calculation, by varying the parameter F, allows for this difference. However, the "no λ_s" and "with λ_s" fittings lead to qualitatively different interpretations. In the purest form of the Stephens-Simon model for a pair of neutrons in $i_{\frac{13}{2}}$, the full-alignment to $12\hbar$ units of angular momentum removes any $i_{\frac{13}{2}}$ neutron contribution from the rotor in the S-band, whereas the $i_{\frac{13}{2}}$ neutrons contributed 20–30% of the moment of inertia in the ground band. In table 2 the F values for "with λ_s" analysis are indeed greater than unity. In our microscopic picture this limit is reached where the $K = 1^+$ and $K = 0^{+\prime}$ states are really degenerate at zero rotational velocity. On the other hand, the "no λ_s" analysis gives a better two-band approximation where the $K = 1^+, 0^{+\prime}$ zeroth order band head separations may be larger than or comparable to the Coriolis interaction matrix elements. In this case the mixing of $K = 1^+$ and $0^{+\prime}$ in the S-band is not as complete. Cranking a multiparticle $(i_{\frac{13}{2}})^n$ configuration with two promoted particles will give a larger effective moment of inertia than for the ground band; thus may we rationalize the observations from table 1 for the "no λ_s" analysis.

By either analysis the energy of the band-head of the S-band for the good cases ($N = 96$) is around 1.5–1.8 MeV. The band intercepts near zero spin will be somewhat greater, namely, $E_s(I = 0) \approx AD + AF(2j_\perp)^2/V_2$. These values are near the band gap of 2Δ, as expected.

The spin-independent part of the ground-S-band mixing matrix elements AB_0 is around -0.5 MeV for the good cases in the "no λ_s" analysis of table 1 and around

twice this value for the "with λ_s" analysis of table 2. In the limit of weak pairing and maximal $K = 1^+$, $0^{+\prime}$ mixing in the S-band, the AB_0 term should have a value $\sqrt{\frac{1}{2}G}$, where G is the pairing matrix element, usually of order $24/A$ MeV. The fitted

TABLE 2

Best fit parameters for same λ in the ground and super bands ($\lambda = \lambda_s$)

Nucleus	A (MeV)	AD (MeV)	AF (MeV)	$J_\perp$	λ	AB_0 (MeV)	X_2	Ref.
$^{162}_{68}Er_{94}$	0.01345	1.857	0.0163	3.38	0.00060	−0.844	8.2×10^{-4}	[d]
	0.01331	2.000	0.0202	4.00*	0.00063	−1.025	8.2×10^{-4}	
$\underline{^{164}_{68}Er_{96}}$	0.01241	1.655	0.0140	3.18	0.00040	−0.836	3.3×10^{-3}	[f, o]
$\underline{^{166}_{70}Yb_{96}}$	0.01374	1.443	0.0150	2.81	0.00072	−0.784	1.4×10^{-3}	[e, g]
$\underline{^{168}_{72}Hf_{96}}$	0.01428	1.715	0.0182	3.70	0.00078	−1.004	2.5×10^{-3}	[b]
$^{170}_{74}W_{96}$	0.01622	2.880	0.0283	5.45	0.00091	−1.340	1.8×10^{-3}	[i]
	0.01645	2.062	0.0128	3.00*	0.00028	−0.626	4.5×10^{-4}	

See table 1 for references.

* $J_\perp$ held constant at this value.

Underlined cases are more reliable, since these are the cases where at least one pair of levels with the same spin is known.

TABLE 3

Some experimental and fitted transition energies for cases where data exist in both crossing bands on either side of the crossing point [a]

I_i	I_f	^{164}Er		^{166}Yb		^{168}Hf	
		ΔE_{exp} (keV)	ΔE_{fit} (keV)	ΔE_{exp} (keV)	ΔE_{fit} (keV)	ΔE_{exp}	ΔE_{fit} (keV)
2	0	91.4	113.5	102.3	116.0	124.0	141.6
4	2	208.1	212.2	228.1	222.3	261.7	250.7
6	4	315.9	311.9	337.5	327.2	371.3	358.3
8	6	410.0	405.0	430.3	422.5	456.7	452.0
10	8	493.5	489.4	507.6	505.7	522.2	529.0
12	10	564.5	563.2	569.5	574.7	570.1	584.1
14	12	619.8	621.0	603.5	617.9	551.5	547.8
16	14	560.5	565.1	494.5	491.8	453.0	462.2
18	16	505.5	512.4	509.1	515.3	522.2	525.9
20	18	577.1	579.4	588.8	584.9	607.7	595.5
22	20	654.4	650.7				
24	22	729.0	719.3				
16′	14	708.6	711.1	689.0	696.4		
14′	12′	355.7	359.0				
18′	16′	710.0	715.9	712.0	701.2		
14′	12	792.0	787.3			684.6	682.8
20′	18′			724.0	721.4		

[a] The convention above is that the lowest level of a given spin (yrast) is unprimed and the next level of a given spin is primed.

values are more of the order $\sqrt{\frac{1}{2}\Delta}$, and we can perhaps rationalize this for pairing correlation not small, though a detailed microscopic analysis is complicated.

In our model sharp backbending requires that the two large mixing terms nearly cancel at the virtual band crossing. The spin-independent term we believe arises from the pairing interaction coupling to the $K = 0^{+\prime}$ component of the S-band wave function, and the other term is Coriolis coupling to the $K = 1^+$ component.

For those nuclei where only yrast (and no yrare) levels are known, the least squares analysis with all parameters gives an ambiguous determination of parameters. The fits with j fixed near values extracted from the good cases ($N = 96$) with known yrare levels can perhaps give reliable estimates of bandhead energies AD, and spin independent mixing AB_0. The values are similar to those for the good cases.

There is obviously a great need for more experimental data about the S-band, especially the location of lower-spin members. A useful spectroscopic probe might be $(\alpha, {}^3\mathrm{He})$ and $({}^3\mathrm{He}, \alpha)$ reactions on even-odd nuclei with an odd $i_{13/2}$ neutron state in ground. The target nuclei of choice would be ${}^{161}_{66}\mathrm{Dy}$ $(\frac{5}{2}^+)$, ${}^{167}_{68}\mathrm{Er}$ $(\frac{7}{2}^+)$, or ${}^{179}_{72}\mathrm{Hf}$ $(\frac{9}{2}^+)$. There have been studies of some of these nuclei by (d, p) or (d, t) reactions, but these are not as effective as the $(\alpha, {}^3\mathrm{He})$ and inverse for transferring high-j neutrons.

As more data become available, it may be appropriate to go beyond the two-band to a multiband analysis. At present the two-band fitting we have done seems a reasonable approach in those regions where collective β-vibrational ($K = 0^+$) and γ-vibrational ($K = 2^+$) strength lies rather higher than the strength function generated by twice operating with j_+. In the region near $N = 90$, where this vibrational strength comes low in energy, a multi-band approach may be necessary from the outset.

By idealizing and simplifying we derive in the appendix an expression (A.3) for the backbending spin in terms of pairing gap Δ, high-j orbital spacing, high-j Coriolis matrix element $j_\perp$, and moment of inertia $\mathcal{J}$. While this relationship may not be quantitatively correct in real nuclei, it may indicate the general conditions for backbending. It seems appropriate to characterize the S-band as a strong admixture of the $K = 1^+$ excitation generated by j_+ and the $K = 0^{+\prime}$ excitation generated by the double application of the j_+ operator to the highest-j configuration in the ground band. Although we do not literally contend that only the nearest two $i_{13/2}$ orbitals are involved at high spin, we hope that our simple picture retains a validity even in a more sophisticated approach, where the basis states would be dressed with admixture of high-j orbitals beyond the closest two.

We have enjoyed discussions on the backbending problem especially with Frank Stephens, Jerry Garrett, Lee Riedinger, and Ikuko Hamamoto. One of us (J.O.R.) expresses appreciation for the hospitality and support of Nordita at Copenhagen and Lund during completion of this paper.

Appendix

APPROXIMATE ALGEBRAIC RELATIONS FOR BAND CROSSING

After all this least squares analysis what can we say about the systematics of backbending? Is it accidental or not that the mixing matrix elements between ground and S-band are so small near the virtual band crossing in sharp backbenders? And what is it that determines the degree of backbending? To get simple algebraic relations we shall simplify and idealize the least squares expressions by setting the curvature correction λ to zero, F to unity for equal moments of inertia in the bands. Let us assume that the band separation is equal to the gap 2Δ and that the mixing term AB_0 is $-\sqrt{\frac{1}{2}}\Delta$. Then the virtual band crossing will be found for spin values satisfying the following equation:

$$\frac{\hbar^2}{2J}\hat{I}^2_{\text{cross}} = 2\Delta - 4Aj_\perp^2 \frac{\hbar^2}{2\mathscr{J}}(\hat{I}_{\text{cross}} - 2j_\perp)^2,$$
$$\hat{I}_{\text{cross}} = \mathscr{J}\Delta/\hbar j_\perp^2. \tag{A.1}$$

The spin at which the mixing matrix element vanishes will be

$$Z = 0 = -2^{-\frac{1}{2}}\Delta + \frac{\hbar^2}{2\mathscr{J}} j_\perp \sqrt{2}\hat{I}_{\text{no mix}},$$

or

$$\hat{I}_{nm} = \mathscr{J}\Delta/\hbar^2 j_\perp. \tag{A.2}$$

The expressions (A.1) and (A.2) are identical, saying that super band mixing to ground vanishes at the crossing point in this idealized model with the S-band a maximal 50 : 50 mixture of $K = 1^+$ and $K = 0^{+\prime}$ configurations, zero-spin band separation of 2Δ, and identical rotor moments of inertia in both bands. Thus, sharp backbending should be the rule where real nuclear conditions approach this ideal. The expressions break down for very weak pairing because the $K = 1^+$ excitation is always at greater energy than 2Δ, actually $\sqrt{(\varepsilon_\Omega - \lambda)^2 + \Delta^2} + \sqrt{(\varepsilon_{\perp+1} - \lambda)^2 + \Delta^2}$ in the quasiparticle approximation. If the chemical potential is halfway between the Ω and $\Omega+1$ Nilsson orbitals, we may make a better approximation replacing (A.1), namely:

$$I_{\text{cross}} = [(\tfrac{1}{2}(\varepsilon_{\Omega+1} - \varepsilon_\Omega))^2 + \Delta^2]^{\frac{1}{2}}(\mathscr{J}/\hbar)\langle \Omega+1|j_+|\Omega\rangle, \tag{A.3}$$

where we have rewritten $j_\perp$ explicitly as the Coriolis matrix element.

The relation of the above analysis to the backbending conditions derived by Bengtssson, Hamamoto, and Mottelson [11]) may go as follows: Our simple model implicitly puts the chemical potential halfway between two high-j ($i_{\frac{13}{2}}$) orbitals Ω and $\Omega+1$. On fig. 2 of Bengtsson *et al.* [11]) there is some tendency to have sharpest backbending when the chemical potential is between these orbitals, though closer to the lower one.

The simplest way we could simulate in a particle representation a system with chemical potential at one of the high-j orbitals is as follows: take three high-j orbitals and one opposite parity orbital degenerate with the middle of the three. Put four neutrons into this system. The j_+ operator can then generate two 1^+ configurations by operating on the ground state and a second operation generates two 2^+ configurations. It is unlikely that the band crossing and the mixing element cancellation occurs at the same spin value in this complicated system.

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