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# An angular momentum expansion of energy and structure of high spin states*

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**Abstract.** A new angular momentum expansion of level energies of ground-state band of even-even nuclei has been obtained which is found to converge rapidly even for the most back-bending nuclei. Attempts have been made to interpret the parameters and calculate them microscopically. It is found that nuclear structure in the forward bending region is quite different compared to that in the back-bending region.

**Keywords.** Back-bending phenomena; angular momentum; energy expansion; microscopic calculation of parameters in rare earth nuclei.

## 1. Introduction

Understanding the underlying mechanism of back-bending phenomena and the consequent description of high spin states has been a quite challenging problem. During the last few years, attempts have been made at both the microscopic (Faessler *et al* 1974; Warke and Gunye 1976; Nair and Ansari 1973; Beck *et al* 1970; Banerjee *et al* 1973; Mang 1975) and phenomenological (Molinari and Regge 1972; Saethre *et al* 1973; Wahlborn and Gupta 1972) levels to find a successful explanation of this effect. The situation is quite far from satisfactory. The expansion of energy in terms of $J(J+1)$ has long been recognized to have very poor convergence. The angular velocity expansion of energy has been found to converge comparatively faster (Bohr 1970). However, the attempt of Saethre *et al* (1973) to fit the back-bending $S$-curve using this series has not been successful. In this paper, following the spirit of microscopic theories usually adopted to describe high spin states, we have tried to obtain a new expansion which would fit the $S$-curve.

## 2. Theory

In the variation after angular momentum projection (VAP) approach, the expectation value of the Hamiltonian $H$ is obtained with a good angular momentum state projected from an intrinsic wave-function $\Phi_k$ and then minimized

$$\delta\left\{\frac{\langle \Phi_k \mid HP^J \mid \Phi_k \rangle}{\langle \Phi_k \mid P^J \mid \Phi_k \rangle}\right\}=0 \tag{1}$$

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where $P^J$ is the usual projection operator. This determines the intrinsic wavefunction $\Phi_k$ which is now $J$ dependent. Then the energy of the state $J$ is calculated with this $\Phi_k(J)$ as

$$E^J = \frac{\langle \Phi_k | HP^J | \Phi_k \rangle}{\langle \Phi_k | P^J | \Phi_k \rangle}. \tag{2}$$

We restrict ourselves to even-even nuclei and drop the subscript $k$ which is zero. Equation (2) has been shown (Villars 1966) in an approximate way to be equivalent to

$$E^J = E + BJ(J+1) \tag{3}$$

where $E = \langle \Phi(J) | H | \Phi(J) \rangle$ is the intrinsic energy and $B$ is inverse of twice the moment of inertia appropriate to the $J$ state. $E$ and $B$ are functions of $\Phi(J)$. Equation (3) is also valid for any type of intrinsic state, not necessarily $HF$ type, as has been shown by Lamme and Boeker (1968), who derived the same without using any $HF$ condition on $\Phi$. Making Taylor's expansion of $\Phi(J)$ at $J = 0$, and retaining only first two terms in the expansion, one obtains from eq. (3) as

$$E^J = E\left\{\Phi(J=0) + J\frac{\delta\Phi}{\delta J}\bigg|_{J=0}\right\} + B\left\{\Phi(J=0) + J\frac{\delta\Phi}{\delta J}\bigg|_{J=0}\right\}(J+1) \tag{4}$$

Again performing Taylor's expansion of $E$ and $B$ at $\Phi(J=0)$ one may write eq. (4) as

$$\begin{aligned} E^J &= E\{\Phi(J=0)\} + J\frac{\delta\Phi}{\delta J}\bigg|_{J=0}\frac{\delta E}{\delta\Phi}\bigg|_{\Phi=\Phi(J=0)} + \ldots \\ &\quad + \left[B\{\Phi(J=0)\} + J\frac{\delta\Phi}{\delta J}\bigg|_{J=0}\frac{\delta B}{\delta\Phi}\bigg|_{\Phi=\Phi(J=0)} + \ldots\right]J(J+1) \\ &= E_0 + (J\Phi'E' + \ldots) + (B_0 + J\Phi'B' + \ldots)J(J+1). \end{aligned} \tag{5}$$

Keeping only the first order correction term in $\Phi(J)$, the above can be written as

$$E^J = E_0 + B_0J(J+1) + J\Phi'E' + J\Phi'B'J(J+1). \tag{6}$$

We would like to mention here that $\frac{\delta E}{\delta\Phi}\Big|_{\Phi=\Phi(J=0)}$ is not zero, since $E$ and $B$ do not correspond to results of self-consistent Hartree-Fock calculation.

In a model termed as shape-fluctuation (SF) model proposed by Satpathy and Satpathy (1971) before the discovery of back-bending, eq. (6) was derived starting from a somewhat different viewpoint. The parameters $B_0$, $\Phi'B'$ and $\Phi'E'$ can be put into a more meaningful form. From eq. (5) we can write the moment of inertia parameter $B_J$ of the state $J$ as

$$\begin{aligned} B_J &= B_0 + J\Phi'B' = B_0 + J\left(\frac{\delta B}{\delta J}\right)_{J=0} \\ &= B_0 + JB'_0. \end{aligned} \tag{7}$$

Thus, $\Phi'B'$ is essentially the rate of change of moment of inertia parameter, $B$. Similarly $\Phi'E'$ would denote the rate of change of the intrinsic energy $\frac{\delta E}{\delta J}\Big|_{J=0} = E$.

Thus $B'_0$ and $E'_0$ arise out of the fluctuations of the intrinsic shape due to rotation. Of course $B_0$ corresponds to the ground state moment of inertia parameter. Fixing the ground state as the zero energy, $E_0$ can be set equal to zero, and then eq. (6) can be written as

$$E^J = aJ + bJ^2 + cJ^3 \tag{8}$$

where $a$, $b$, $c$ are identified as $B_0 + E'_0$, $B_0 + B'_0$ and $B'_0$ respectively. The parameters $B_0$, $B'_0$ and $E'_0$ can be extracted once $a$, $b$, $c$ are known by fitting the experimental spectrum with the above expression (8). It is interesting to note that these three parameters can be calculated microscopically. It would be shown in the following that such calculated values compare quite well with those determined from the fit. When expression (8) is applied to the study of backbending phenomena, it would be shown *aposteriori* that, it can describe the sudden rise of moment of inertia with angular frequency, and as such, can fit all data pertaining to the back-bending region of $S$-curve, but fails to fit its forward bending portion.

To describe the data of both the forward bending and back-bending, we could extend the model in a very natural way by taking into account the higher order terms, in the expansions given by eqs (4) and (5). If we retain terms up to all orders in the Taylor's expansion of $E^J$ in eq. (4), then it reduces to

$$E^J = E\left\{\Phi(J=0) + J\frac{\delta\Phi}{\delta J}\bigg|_{J=0} + \frac{J^2}{2!}\frac{\delta^2\Phi}{\delta J^2}\bigg|_{J=0} + \ldots\right\}$$

$$+ B\left\{\Phi(J=0) + J\frac{\delta\Phi}{\delta J}\bigg|_{J=0} + \frac{J^2}{2!}\frac{\delta^2\Phi}{\delta J^2}\bigg|_{J=0} + \ldots\right\} J(J+1). \tag{9}$$

By making Taylor's expansion of $E$ and $B$ and retaining terms up to all orders one obtains the expression for energy as a series

$$E^J = \sum_{n\geqslant 1} a_n J^n \tag{10}$$

which would in principle have an infinite number of terms. This series in powers of $J$ though appears to be in contrast to the original Böhr-Mottelson series in powers of $J(J+1)$, the former could be obtained from the latter by rearrangement. This new series eq. (10) appears to converge faster compared to Böhr-Mottelson series. Equation (10) cannot be of much practical use in fitting the level energies as it contains a very large number of parameters. We attempt to rewrite eq. (10) under the following criteria:

(a) The series converges for all values of angular momentum observed in ground-state band of even-even nuclei. Obviously the maximum value of $J$ would be less than 30.

(b) The formula should have few parameters and should be capable of simulating the series given by (10).

(c) The formula should have as leading terms the shape fluctuation expression for energy like (8).

To fulfil the above condition, a possible form of $E^J$ is

$$E^J = \frac{aJ + bJ^2 + cJ^3}{1+dJ^3}. \tag{11}$$

Taking the four parameter form of shape fluctuation expression as leading terms, one arrives at the five parameter formula.

$$E^J = \frac{aJ + bJ^2 + cJ^3 + dJ^4}{1+eJ^4}. \tag{12}$$

A general $(n+1)$ parameter formula would be

$$E^J = \frac{\Sigma_{i=1}^{n} a_i J^i}{1+bJ^n}. \tag{13}$$

## 3. Results

It would be shown in the following that the expansion given by (12) is quite adequate to describe the data of nuclei with full $S$ shape back-bending curve. We would like to stress here that to our knowledge, for the first time an expansion (eq. (13)) for energy in terms of the angular momentum is found which converges rapidly even for the high spin states.

First we have applied eq. (8) to fit the level energies of about hundred nuclei, and we find that it can provide good fit to known level energies of all nuclei like $^{164}$Yb, $^{182}$Os, etc. which show only back-bending. However, this fails in the case of nuclei like $^{158}$Er, $^{162}$Er, etc. which show both back-bending and forward bending i.e. full $S$-shape curve. The seven nuclei $^{132}$Ce, $^{158}$Er, $^{160}$Er, $^{162}$Er, $^{156}$Dy, $^{158}$Dy and $^{166}$Yb belong to this group. We have studied the convergence of the series (13) by fitting the experimental level energies of these seven nuclei with four parameter (eq. (11)), five parameter (eq. (12)) and also the six parameter formulas. This series is found to converge rapidly. We find that the $S$-curves could be fitted with four parameter expression, however, the fit obtained with the five parameter expression, is much better, which we have chosen for presentation in table 1. Unlike in Wahlborn and Gupta (1972), we have treated all the five parameters on equal footing and their values have been determined by a least square fit to the experimental energies. These values are presented in table 2. From an analysis of table 1, it is clear that the five parameterexpression (eq. (12)) is good enough to describe the data of most back-bending nuclei.

To further test the goodness of the series we have chosen the two most difficult nuclei $^{132}$Ce and $^{158}$Er as representatives for drawing the $\mathcal{I}_J \propto \omega_J^2$ curve. We have used the standard relations

$$\hbar\omega_J = 2\sqrt{J(J+1)}\,\frac{dE^J}{dJ(J+1)} \tag{14}$$

$$\frac{\hbar^2}{2\mathcal{I}_J} = \frac{dE^J}{dJ\,(J+1)} \tag{15}$$

Table 1. Excitation energies

| $J$ / Nucleus | 2 | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | 22 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $^{132}$Ce | 325·4 | 857·6 | 1540·0 | 2326·8 | 3154·5 | 3724·2 | 4236·4 | 4935·0 | 5758·4 | | |
| | 280·0 | 861·3 | 1590·3 | 2352·0 | 3071·6 | 3717·1 | 4301.9 | 4904·2 | 5761·7 | | |
| $^{156}$Dy | 137·8 | 404·1 | 770·3 | 1215·5 | 1724·9 | 2286·0 | 2887·8 | 3498·8 | 4026·2 | 4636·1 | 5320·8 |
| | 144·1 | 400·2 | 762·6 | 1214·9 | 1734·6 | 2297·6 | 2881·9 | 3470·0 | 4051·6 | 4631·1 | 5320·7 |
| $^{158}$Dy | 98·9 | 317·3 | 637·9 | 1044·0 | 1519·9 | 2049·2 | 2612·5 | 3190·5 | 3781·3 | 4407·1 | 5085·2 |
| | 100·9 | 316·5 | 636·3 | 1044·3 | 1521·7 | 2049·3 | 2609·7 | 3190·4 | 3785·7 | 4403·4 | 5086·0 |
| $^{158}$Er | 192·0 | 527·1 | 970·2 | 1493·2 | 2072·1 | 2680·2 | 3190·2 | 3663·0 | 4229·3 | | |
| | 197·4 | 522·4 | 967·8 | 1499·5 | 2074·7 | 2655·9 | 3215·3 | 3662·3 | 4223·3 | | |
| $^{160}$Er | 125·6 | 389·4 | 764·7 | 1228·4 | 1760·1 | 2339·3 | 2931·5 | 3465·4 | 4019·8 | | |
| | 132·2 | 384·7 | 758·5 | 1231·2 | 1769·8 | 2340·6 | 2915·3 | 3474·0 | 4019·4 | | |
| $^{162}$Er | 102·1 | 329·6 | 666·8 | 1096·8 | 1602·9 | 2165·1 | 2745·7 | 3292·3 | 3846·5 | 4462·8 | |
| | 106·9 | 326·5 | 662·5 | 1099·1 | 1609·5 | 2163·8 | 2735·0 | 3301·1 | 3844·4 | 4462·7 | |
| $^{166}$Yb | 102·3 | 330·3 | 667·6 | 1098·0 | 1605·5 | 2174·8 | 2778·1 | 3272·6 | 3781·7 | 4370·5 | |
| | 105·0 | 323·6 | 662·7 | 1104·9 | 1620.2 | 2175·7 | 2742·4 | 3295·9 | 3779·9 | 4370·2 | |

The calculated energies are obtained from the fit with five parameter expression eq. (12). The first and second rows represent the experimental and calculated energies respectively.

**Table 2.** Value of the parameters corresponding to the fit with expression (12)

| Nucleus | $a$ (keV) | $b$ (keV) | $c$ (keV) | $d$ (keV) | $e$ ($10^5$) |
|---|---|---|---|---|---|
| $^{132}$Ce | 35·229 | 60·376 | −4·1301 | 0·068901 | −0·4 |
| $^{156}$Dy | 44·864 | 13·071 | 0·3474 | −0·042919 | −0·35 |
| $^{158}$Dy | 21·012 | 14·773 | 0·0248 | −0·022082 | −0·2 |
| $^{158}$Er | 70·915 | 11·806 | 1·3296 | −0·145586 | −1·5 |
| $^{160}$Er | 40·033 | 11·260 | 1·0783 | −0·099410 | −0·9 |
| $^{162}$Er | 29·138 | 10·601 | 0·9321 | −0·077864 | −0·65 |
| $^{166}$Yb | 29·279 | 9·588 | 1·2111 | −0·098917 | −0·85 |

The $\mathcal{J}_J \propto \omega_J^2$ curves for $^{132}$Ce and $^{158}$Er are presented in figure 1a. The dotted and full line curves refer to the calculated and experimental ones respectively. The agreement is indeed very satisfactory. Wahlborn and Gupta (1972) in their description of high spin states have written down a five parameter expression of moment of inertia. The corresponding energy expression does not have a series structure like ours. They have got excellent fit by determining three parameters through the least squares method and adjusting the remaining two to reproduce asymptotic behaviour.

In view of the above, it is now desirable to attempt at an understanding of the physics that is conveyed by the good fit with expression (12). The parameters of the expression (11) or (12) are not amenable to such clear interpretation as the three

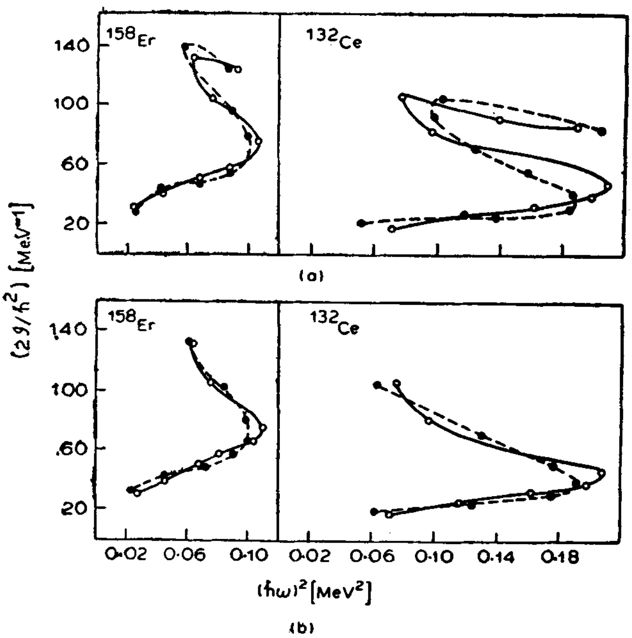


**Figure 1.** Plot of moment of inertia vs the square of angular velocity for $^{158}$Er and $^{132}$Ce: **a.** all the known levels including forward bending region fitted with eq. (12). **b.** levels excluding the forward bending region fitted with eq. (8)

parameters of expression (8). However, it would be shown that use of (8) in conjugation with (11) or (12) would lead to meaningful exploration of nuclear structure of the high spin states. As mentioned before, eq. (8) could fit the level energies of the back-bending region. We have used this expression to fit all the levels covering the back-bending region only for two nuclei $^{158}$Er and $^{132}$Ce. For $^{158}$Er the levels up to $J = 16$, and in the case of $^{132}$Ce, the levels up to $J = 14$ were taken to fit with expression (8). The parameters so determined are (all in keV):

$$^{158}\text{Er} : a = 46{\cdot}32 \qquad b = 24{\cdot}08 \qquad c = 0{\cdot}79$$
$$^{132}\text{Ce} : a = 77{\cdot}72 \qquad b = 41{\cdot}29 \qquad c = -1{\cdot}80$$

The corresponding $\mathcal{I}_J \propto \omega_J^2$ curves are presented in figure 1b. The calculated ones (dotted) agree quite well with the experimental ones (full curve). We can interpret these results since the three parameters $B_0$, $B'_0$ and $E'_0$, as mentioned earlier, have definite physical meaning. $^{132}$Ce is a much softer nucleus compared to $^{158}$Er and hence the magnitude of $B'_0$ and $E'_0$ should be comparatively much larger. These values (in keV) calculated from above parameters are 1·80, 34·63 and 0·79, 21·45 respectively which bear out this expectation. To further increase our confidence in the interpretation of these parameters we have calculated them microscopically for $^{158}$Er. Using the pairing + quadrupole interaction of Baranger and Kumar (1968) and Hartree-BCS intrinsic wavefunction we have performed a VAP calculation. In this calculation, the deformation parameter $\beta$, and the pairing parameter $\triangle$ have been varied and the total projected energy, the intrinsic energy and the intrinsic wave function $\Phi$ for each angular momentum state $J$ have been determined. Then the moment of inertia for each state has been calculated using the cranking formula. The details would appear elsewhere (Ansari and Nair 1977). Thus the calculated moments of inertia parameters $B_J$ $(=1/2\ \mathcal{I}_J)$ for different states are presented in the first line of table 3.

Also using eq. (7) and the parameters $B_0$ and $B'_0$ determined from our fit we have calculated $B_J$'s which are presented in the second line. In the third, line, the value of $B_J$ extracted from experimental energies using the prescription of Böhr and Mottelson (eq. (15)) are presented. The three sets of $B_J$ compare reasonably well. The value of $E'_0$, i.e., the rate of change of the intrinsic energy determined from our fit is 21·5 keV. This is an average quantity as it is found from least squares fit. The corresponding quantity is obtained from the microscopic calculation as follows. If

**Table 3.** Values of the moment of inertia parameter, $B_J$ for $^{158}$Er.

| $J$ | 0 | 2 | 4 | 6 | 8 | 10 | 12 | 14 | 16 |
|---|---|---|---|---|---|---|---|---|---|
| (i) | 28·3 | 28·3 | 28·1 | 26·1 | 22·9 | 14·7 | 7·7 | 7·1 | 7·7 |
| (ii) | 24·9 | 23·3 | 21·7 | 20·1 | 18·5 | 17·0 | 15·4 | 13·8 | 12·2 |
| (iii) | | 32·0 | 23·9 | 20·1 | 17·4 | 15·2 | 13·2 | 9·4 | 7·6 |

(i) Results of the microscopic calculation
(ii) Values determined using eq. (8) of the text. Levels fitted up to $J=16$
(iii) Extracted from expriment using eq. (15)

$E^J_{\mathrm{int}}$ is the intrinsic energy of the $J$ state, then $E'_0 = \left(E^J_{\mathrm{int}} - E^0_{\mathrm{int}}\right)/J$. We have taken the mean over all the $J$ states and $E'_0$ thus determined is 23 keV. This compares quite well with the fitted result (21·5 keV).

## 4. Conclusion

We have now full confidence in the meaning of the parameters $B_0$, $B'_0$ and $E'_0$ and since they contain only first order change in $\Phi$, we can conclude that the intrinsic structure smoothly changes from one state to the other in the region of back-bending that is e.g. up to $J = 16$ in case of $^{158}$Er. We would like to stress here that when we include $J = 18$ for $^{158}$Er which is the only point in the forward bending part, we find that it cannot be fitted with three parameter expression (8) or its extension to four or more number of parameters (10). Further we find that when we applied expression (11) to fit the back-bending portion i.e. up to $J = 16$, the value of $d$ is found to be zero. Expression (8) could be considered as a special case of the more general expression (11) or (12), as the latter goes over to former in the case of smooth variation (first order change in $\Phi$). It is interesting to note that the values of $a$, $b$, $c$ given above which describe only the back-bending region are quite different compared to the corresponding ones presented in table 2, which describe the full $S$-curve. From this, we can infer that nuclear structure in the forward bending region is rather different compared to that in the back-bending region. This is suggestive of the existence of two different bands.

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