

## Calculation of rotational spectra of well-deformed nuclei up to very high spins

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A new three-parameter formula is presented and is used to analyze systematically the rotational spectra up to very high spins (below band crossing). An overall and excellent agreement between the calculated and the observed spectra is obtained for all the actinide and the rare-earth deformed nuclei. In the derivation of this formula from the phenomenological Bohr Hamiltonian, a small axial asymmetry and vibrational effects (including anharmonic vibration) have been taken into account.

### I. INTRODUCTION

In recent years, Coulomb excitation experiments with very heavy-ion beams (e.g.,  $^{208}\text{Pb}$  ions) provided abundant information about the high-spin levels of ground rotational bands (GRB's) in actinide nuclei. Because the moments of inertia of actinide nuclei are about twice those of the rare-earth nuclei, the two-quasiparticle  $S$  bands do not compete with the GRB until much higher spins.<sup>1</sup> Therefore, the yrast levels with even spin and parity in actinide nuclei may belong to the GRB to higher spins than those in rare-earth nuclei. Thus, the recent data provide an ideal opportunity to test the applicability of various formula for rotational spectra.

Usually, it is believed that the Harris<sup>2</sup> two-parameter  $\omega^2$  expansion  $E = \alpha\omega^2 + \beta\omega^4$  is better than the two-parameter  $I(I+1)$  expansion

$$E = AI(I+1) + BI^2(I+1)^2.$$

However, analysis of the new data on rotational bands to higher spins clearly shows that<sup>1</sup> the Harris parameter  $\alpha$  is by no means constant, but varies, sometimes violently, with increasing  $\omega^2$  [or  $I(I+1)$ ]. In Ref. 3 the Mallmann plots<sup>4</sup> were used to display how well the various variable moment of inertia (VMI) models (distinguished by an additional parameter  $n$ , see Ref. 3) can be fitted to the experimental data. The results show that for rotational nuclei

$$[R_4 = E(4)/E(2) \gtrsim 3.20],$$

the best value for the model appears to be  $n \approx 1$  (which is equivalent to the two-parameter Harris formula) at low spins ( $I < 10$ ), increasing towards  $\infty$  for high-spin states ( $I > 16$ ). Recently, the three-parameter Sood<sup>5,6</sup> semiempirical formula (SSEF) was used to fit the GRB in  $^{232}\text{Th}$ ,  $^{232-238}\text{U}$ . By choosing appropriate values of the parameters, fair agreement was obtained with the experimental data.

In this paper a new three-parameter formula for rotational spectra is presented and is used to analyze systematically the rotational spectra of well-deformed nuclei up to very high spins (below bandcrossing). Comparison between the calculation using this formula and a large number of observed rotational spectra is carried out. An

overall and excellent agreement is obtained. The theoretical argument for this formula is briefly sketched.

### II. FORMALISM AND CALCULATION

#### A. Two-parameter expression for rotational spectra

In Ref. 7 the collective spectrum of a well-deformed nucleus with small axial asymmetry ( $\sin^2 3\gamma \ll 1$ ) was investigated in the framework of the phenomenological Bohr Hamiltonian with a  $\beta$  separable potential

$$V = \frac{1}{2}C\beta^2 + \frac{1}{2B\beta^2}\chi(\cos 3\gamma), \quad (1)$$

where the first term is the usual harmonic potential with surface rigidity  $C$  and the second one is due to the centrifugal stretching effect.  $B$  is the inertia parameter. In a simple estimation, the function  $\chi(\cos 3\gamma)$  is assumed to be

$$\chi(\cos 3\gamma) = \chi_0 + \frac{9\nu(\nu-1)}{\cos^2 3\gamma}, \quad (2)$$

with parameters  $\chi_0$  and  $\nu$ . Expanding the rotational energy of the Bohr Hamiltonian in powers of  $\sin^2 3\gamma$  and omitting the contribution of  $\mathcal{O}(\sin^4 3\gamma)$  to the energy eigenvalues, we obtain a simple closed form expression for individual rotational bands in well-deformed nuclei. For the GRB of an even-even nucleus it reads<sup>8</sup>

$$E(I) = a[\sqrt{1 + bI(I+1)} - 1], \quad (3)$$

where only two parameters,  $a$  and  $b$ , are involved and

$$a = \hbar\omega[\chi_0 + 9(\nu + \frac{1}{2})^2]^{1/2}, \quad \omega = \sqrt{C/B}. \quad (4)$$

$$b = \frac{1}{3} \frac{1 + \frac{2}{9} \frac{2}{2\nu+3}}{\chi_0 + 9(\nu + \frac{1}{2})^2}. \quad (5)$$

It was shown<sup>7</sup> that Eq. (3) is equivalent to the VMI model<sup>9</sup> except that a smoothly varying stiffness parameter is introduced. The parameters  $a$  and  $b$  are found to be related to the nuclear moment of inertia at  $I=0$ ,  $\mathcal{J}_0$ , and nuclear softness,  $\sigma$ ,

$$\mathcal{J}_0 = \frac{\hbar^2}{ab}, \quad (6)$$

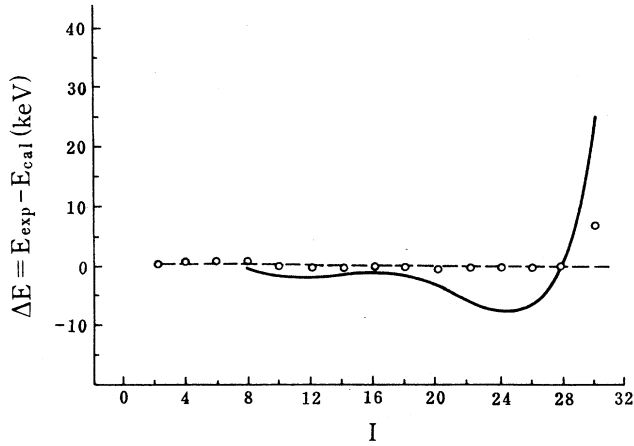


FIG. 1.  $\Delta E = E(I)_{\text{exp}} - E(I)_{\text{cal}}$  vs  $I$  for  $^{238}\text{U}$ . The open circle gives the results calculated using the two-parameter Eq. (3) and the thick line shows the result by the three-parameter SSEF (Refs. 5 and 6).

$$\sigma = \frac{b}{2}. \quad (7)$$

From Eq. (3) the radius of convergence  $I_r$  for the energy expansion in powers of  $I(I+1)$  can be estimated

$$I_r \sim \frac{1}{\sqrt{b}}. \quad (8)$$

From Eq. (3), and definition  $I_x = [I(I+1) - K^2]^{1/2}$ , it can be shown that the kinematical moment of inertia is given by

$$\mathcal{J}^{(1)} = \hbar^2 I_x \left[ \frac{dE}{dI_x} \right]^{-1} = \mathcal{J}_0 \sqrt{1 + bI(I+1)}, \quad (9)$$

which increases with increasing  $I$ . Equation (3) can also be rewritten as

$$E(\omega_I) = a \left\{ \left[ 1 - \frac{(\hbar\omega_I)^2}{a^2 b} \right]^{-1/2} - 1 \right\} \\ = \frac{1}{2} \mathcal{J}_0 \omega_I^2 + \frac{3}{4} \mathcal{J}_1 \omega_I^4 + \frac{5}{6} \mathcal{J}_2 \omega_I^6 + \dots, \quad (10)$$

$$\frac{\mathcal{J}_1}{\mathcal{J}_0} = \frac{1}{2} \frac{\hbar^2}{a^2 b}, \quad \frac{\mathcal{J}_2}{\mathcal{J}_0} = \frac{3}{8} \left[ \frac{\hbar^2}{a^2 b} \right]^2, \dots, \quad (11)$$

in terms of the rotational frequency

$$\omega_I = \frac{1}{\hbar} \frac{dE}{dI_x}.$$

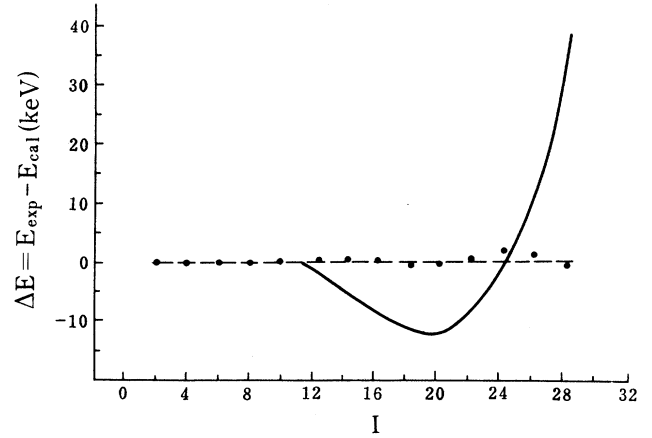


FIG. 2.  $\Delta E = E(I)_{\text{exp}} - E(I)_{\text{cal}}$  vs  $I$  for  $^{234}\text{U}$ . The filled circle gives the result calculated using the three-parameter Eq. (4) and the thick line shows the result obtained by the three-parameter SSEF (Refs. 5 and 6).

Therefore, the puzzling fact that  $\omega_I^2$  expansion converges much more rapidly than the  $I(I+1)$  expansion is understandable because the inequality

$$\frac{(\hbar\omega_I)^2}{a^2 b} = \frac{b[(I + \frac{1}{2})^2 - K^2]}{1 + bI(I+1)} < 1 \quad (12)$$

always holds.

In a previous paper<sup>10</sup> preliminary analyses on the GRB's in even-even actinide nuclei show that the two-parameter expression (3) can fit the observed data very well up to very high spins (below bandcrossing). As an illustrative example, the differences between the observed rotational spectra in  $^{238}\text{U}$  and the results obtained using the two-parameter formula, Eq. (3), as well as those by the SSEF three-parameter formula for comparison, are given in Fig. 1. Moreover, from Eq. (3) the observed fact that the dynamical moment of inertia  $\mathcal{J}^{(2)}$  is always larger than the kinematical moment of inertia  $\mathcal{J}^{(1)}$  (except in the bandcrossing region) can be reproduced naturally.<sup>10</sup>

### B. Modification. Three parameter expression for rotational spectra

For most actinide nuclei the results calculated using Eq. (3) agree very well with the observed data. However, for a few lighter actinide nuclei (e.g.,  $^{232}\text{Th}$ ), the agreement is less satisfactory. Analysis shows that for  $^{232}\text{Th}$

TABLE I. Experimental and calculated energies (in keV) of  $^{232}\text{U}$ . The calculated values correspond to the three-parameter description explained in the text and SSEF is from Abzouzi *et al.* (Refs. 5 and 6).

	2	4	6	8	10	12	14	16	18	20
Exp <sup>a</sup>	47.57	156.17	322.3	540.7	805.5	1111.2	1453.5	1828.0	2231.5	2658.4
Cal	47.34	156.01	322.1	540.5	805.5	1111.6	1453.8	1828.1	2230.7	2658.8
SSEF	47.3	155.9	321.6	539.7	803.8	1109.4	1451.7	1826.5	2230.0	2658.0

<sup>a</sup>Reference 6.

TABLE II. Experimental and calculated energies (in keV) of even actinide nuclei. The calculated values correspond to the three-parameter description explained in the text.

Nucleus	2	4	6	8	10	12	14	16	18	20	22	24	26	28
<sup>248</sup> Cm Exp <sup>a</sup>	43.4	144.2	299.5	506.9	763.0	1064.0	1405.4	1782.8	2190.7	2624.6	3080.6	3556.0	4051.0	4567.3
Cal	43.6	144.3	300.2	508.2	764.6	1065.2	1405.6	1781.4	2188.4	2622.6	3080.5	3558.7	4054.2	4564.5
<sup>244</sup> Pu Exp <sup>b</sup>	46	153	315.4	531.8	798.3	1110.7	1464.4	1855.4	2279.2	2730.7				
Cal	45.8	151.5	314.6	531.8	798.8	1111.3	1464.8	1855.1	2278.4	2731.2				
<sup>242</sup> Pu Exp <sup>c</sup>	44.54	147.3	306.4	518.1	778.7	1084.0	1431.3	1816.3	2235.6	2686.0	3163	3662		
Cal	44.34	146.9	305.5	517.1	778.1	1084.5	1432.2	1817.2	2236.0	2685.1	3161.6	3663.0		
<sup>240</sup> Pu Exp <sup>d</sup>	42.83	141.69	294.32	497.50	747.8	1041.8	1375.6							
Cal	42.80	141.64	294.27	497.54	747.9	1041.7	1375.6							
<sup>238</sup> Pu Exp <sup>d</sup>	44.08	145.98	303.4	513.4	772.8	1078.5	1427.2	1816.2	2240.5					
Cal	43.96	145.65	303.0	513.3	773.0	1078.9	1427.4	1815.5	2240.8					
<sup>236</sup> Pu Exp <sup>d</sup>	44.63	145	303.5	513.4	771.2	1072.0	1411.3	1783.7						
Cal	44.08	145.98	303.4	513.2	771.0	1072.1	1411.4	1783.6						
<sup>238</sup> U Exp <sup>e</sup>	44.91	148.41	307.21	517.8	775.7	1076.5	1415.3	1788.2	2190.7	2618.7	3067.2	3534.5	4017.3	4516.5
Cal	44.61	147.57	306.30	517.1	775.6	1076.9	1416.2	1788.9	2190.8	2617.8	3066.7	3534.3	4018.3	4516.2
<sup>236</sup> U Exp <sup>f</sup>	45.24	149.48	309.79	522.25	782.8	1086.2	1425	1800	2203	2630	3080	3549	4038	4548
Cal	45.32	149.78	310.45	523.26	783.4	1086.0	1426.0	1799.1	2201.3	2629.1	3079.7	3550.7	4040.0	4546.2
<sup>234</sup> U Exp <sup>g</sup>	43.48	143.34	296.04	497.02	741.2	1024.0	1340.8	1688.0	2063.0	2464.2	2889.7	3339	3808	4297
Cal	43.57	143.55	296.34	497.22	741.2	1023.6	1340.3	1687.8	2063.4	2464.8	2890.2	3338.1	3807.5	4297.5
<sup>230</sup> U Exp <sup>d</sup>	51.72	169.5	347.0	578.3	856.5	1175.8	1531.7	1921.3						
Cal	51.56	169.1	347.1	578.5	856.6	1175.7	1531.6	1921.4						
<sup>232</sup> Th Exp <sup>e</sup>	49.37	162.12	333.2	556.9	827.0	1137.4	1482.8	1858.9	2262.9	2691.9	3144.9	3619.0	4116.9	4632.9
Cal	49.39	162.31	333.8	557.6	827.4	1137.2	1482.2	1858.3	2262.4	2692.0	3145.2	3620.4	4116.5	4632.5
<sup>230</sup> Th Exp <sup>e</sup>	53.20	174.08	356.6	594.1	879.7	1207.8	1572.9	1971.5	2397.8	2850	3325			
Cal	52.69	173.07	355.7	593.8	880.2	1208.6	1573.7	1971.1	2397.2	2849.4	3325.6			
<sup>228</sup> Th Exp <sup>h</sup>	57.76	186.82	378.17	622.2	911.5	1238.7	1595.9							
Cal	57.26	186.27	378.11	622.9	911.8	1237.9	1596.2							

<sup>a</sup>References 11 and 12.<sup>b</sup>Reference 13.<sup>c</sup>Reference 14.<sup>d</sup>Reference 15.<sup>e</sup>Reference 16.<sup>f</sup>Reference 17.<sup>g</sup>Reference 18.<sup>h</sup>Reference 19.

TABLE III. Experimental and calculated energies (in keV) of the GRB's of rare-earth even nuclei. The calculated value corresponds to the three-parameter description explained in the text.

Nucleus	2	4	6	8	10	12	14	16	18	20
<sup>178</sup> Hf Exp <sup>a</sup>	93.17	306.61	632.2	1058.6	1571.0	2150.7	2777.6	3436.2		
Cal	93.00	306.53	632.5	1059.0	1570.7	2150.1	2778.4	3436.0		
<sup>176</sup> Hf Exp <sup>b</sup>	83.36	290.19	597.08	998.1	1481.4	2034.0	2646.7			
Cal	88.21	290.09	597.17	998.2	1481.1	2034.1	2646.7			
<sup>174</sup> Hf Exp <sup>c</sup>	90.99	297.38	608.3	1009.6	1485.9	2020.5	2597.5	3208.9		
Cal	90.65	297.14	608.5	1010.0	1485.7	2019.8	2598.2	3208.7		
<sup>172</sup> Hf Exp <sup>d</sup>	95.24	309.26	628.1	1037.3	1521.1	2064.6	2654.0	3277.2		
Cal	94.20	307.83	627.9	1038.1	1521.9	2064.4	2653.0	3277.7		
<sup>170</sup> Hf Exp <sup>e</sup>	100.80	321.99	642.9	1043.3	1505.5	2016.4	2567.2	3151.6		
Cal	99.90	321.39	643.2	1043.7	1505.6	2016.2	2566.9	3151.8		
<sup>176</sup> Yb Exp <sup>a</sup>	82.13	271.69	564.8	954.1	1431.2	1984.8	2602	3270		
Cal	82.11	271.84	564.8	954.2	1431.1	1984.6	2602.2	3269.9		
<sup>174</sup> Yb Exp <sup>c</sup>	76.47	253.12	526.04	889.9	1336	1861	2457	3117	3836	4610
Cal	76.47	253.10	525.90	889.3	1336.7	1861.4	2456.7	3116.8	3836.1	4610.0
<sup>172</sup> Yb Exp <sup>d</sup>	78.75	260.29	540.00	912.2	1370.1	1907.2	2518.4	3198.1		
Cal	78.69	260.22	540.05	912.2	1370.0	1907.3	2518.3	3198.1		
<sup>170</sup> Yb Exp <sup>e</sup>	84.26	277.45	573.54	963.7	1438.0	1983.8	2580.9			
Cal	83.73	276.68	573.11	964.3	1438.7	1982.9	2581.2			
<sup>168</sup> Yb Exp <sup>a</sup>	87.73	286.55	585.30	970.1	1424	1936	2489	3073		
Cal	87.37	286.11	585.13	969.9	1425.0	1935.6	2488.7	3073.2		
<sup>166</sup> Er Exp <sup>f</sup>	80.57	264.99	545.44	911.2	1349.6	1846.6	2389.4	2968.6		
Cal	80.59	265.12	545.68	911.3	1349.2	1846.3	2389.9	2968.4		
<sup>164</sup> Er Exp <sup>g</sup>	91.39	299.46	614.4	1024.6	1518.0	2082.7	2702.5			
Cal	90.87	298.66	614.2	1025.3	1518.7	2081.7	2702.8			
<sup>164</sup> Dy Exp <sup>g</sup>	73.39	242.23	501.32	843.7	1261.3	1745.8	2290			
Cal	73.37	242.21	501.35	843.7	1261.2	1745.9	2290.0			
<sup>162</sup> Dy Exp <sup>h</sup>	80.66	265.66	548.52	920.9	1374.9	1901.4	2492.4	3138.4	3837.0	
Cal	80.39	265.16	548.19	921.3	1375.3	1901.5	2491.7	3138.8	3837.0	
<sup>156</sup> Gd Exp <sup>i</sup>	88.97	288.18	584.71	965.1	1416.0	1924.4	2475.4			
Cal	87.94	287.03	584.79	966.1	1416.5	1923.2	2476.2			

<sup>a</sup>Reference 16.

<sup>b</sup>Reference 20.

<sup>c</sup>Reference 21.

<sup>d</sup>Reference 22.

<sup>e</sup>Reference 23.

<sup>f</sup>Reference 24.

<sup>g</sup>Reference 25.

<sup>h</sup>Reference 26.

<sup>i</sup>Reference 27.

the value of the parameter  $a$  in Eq. (3) increases slowly with  $I$  (within 8%). It is expected that a better expression may be obtained if a weak  $I$  dependence of the parameter  $a$  is taken into account. So, Eq. (3) is tentatively modified as follows:

$$E(I) = a[I + cI(I+1)][\sqrt{1 + bI(I+1)} - 1], \quad (13)$$

with an additional parameter  $c$ . A possible argument for such a modification will be given herein. Now let us analyze the GRB's of well-deformed nuclei in terms of Eq. (13). Table I lists the calculated and experimental results of  $^{232}\text{U}$  and Fig. 2 gives

$$\Delta E(I) = E(I)_{\text{exp}} - E(I)_{\text{cal}}$$

of  $^{234}\text{U}$ . For comparison, the SSEF results<sup>6</sup> are also shown in Table I and Fig. 2, respectively. It can be seen that the present results are better than those of the SSEF. The overall comparisons between the results calculated using Eq. (13) and the experimental data for all the actinide nuclei are listed in Table II. It is well known that, for the most rare-earth nuclei, the bandcrossing occurs at  $I_c \sim 10-12$ , so only four to five yrast levels belong to the GRB. This clearly limits the conclusions that can be drawn about the general applicability of a formula for rotational spectra. Therefore, only those rare-earth nuclei with  $I_c > 16$  are considered, and the results are given in Table III. Obviously, from Tables II and III, it can be seen that an overall excellent agreement between the calculation with Eq. (13) and observed data is obtained.

Now we give a possible argument for the modified Eq. (13). For the high-spin states it seems more reasonable to add an anharmonic term into the potential (1), i.e.,

$$V = \frac{1}{2}C\beta^2 + \frac{1}{2B\beta^2}\chi(\cos 3\gamma) + k\beta^4, \quad (14)$$

where  $k$  is a new adjustable parameter. Indeed, to the first order of perturbation, the energies of the GRB can be written in a three-parameter form, namely,

$$\begin{aligned} E(I) &= a[\sqrt{1 + bI(I+1)} - 1] + k[\langle \beta^4 \rangle_I - \langle \beta^4 \rangle_0] \\ &= a'[\sqrt{1 + bI(I+1)} - 1][1 + k'\sqrt{1 + bI(I+1)}], \end{aligned} \quad (15)$$

in which the original parameters  $a$  and  $k$  have been replaced by two equivalent parameters  $a'$  and  $k'$ . Obviously, because the  $k'$  term is a small correction, Eq. (15) can be rewritten as a simpler and more convenient form, Eq. (13). In fact, the results calculated by Eq. (15) are almost the same as, and in some cases better than, those obtained by Eq. (13).

### III. DISCUSSION AND SUMMARY

A new three-parameter formula for the rotational band of a well-deformed nucleus is suggested on the basis of the phenomenological Bohr Hamiltonian. In the derivation of this formula a small axial asymmetry and vibrational effects (including anharmonicity) have been taken into account. The agreement between the calculation using this formula and the observed ground bands (below bandcrossing) of all the actinide and the rare-earth deformed nuclei is astonishingly excellent, which perhaps implies that the formalism described earlier may have some truth.

The physical meaning of the parameters involved in this formula and their relation with the VMI model are discussed. (1) The value of  $b$  may be considered as a measure of nuclear softness. The relative spacing of a rotational spectrum

$$R(I) = E(I)/E(2),$$

is mainly determined by  $b$ , and the radius of convergence of the  $I(I+1)$  expansion of  $E(I)$  can be estimated from the value of  $b$ . (2)  $\hbar^2/ab = \mathcal{J}_0$  represents the nuclear moment of inertia at spin  $I=0$ . The moment of inertia increases with increasing  $I$  (or  $\omega_I$ ) which reflects the influence of the centrifugal stretching and vibrational effects. (3) Parameter  $c$  describes the effect of anharmonicity, and analysis shows that for most well-deformed nuclei the value of  $c$  is very small. (4) Finally, when  $b$  and  $c$  tend to zero we get a strict  $I(I+1)$  rule characterizing the spectrum of a rigid rotor with axial symmetry.

As pointed out by Hamamoto<sup>28</sup> although around the ground state of medium or heavy nuclei there is no clear-cut evidence for the deviation of nuclear shape from axial symmetry, the deviation is expected for high-spin states. Nuclear axial asymmetry (the  $\gamma$  dependence of the Bohr Hamiltonian) may be considered as, at least partly, a macroscopic manifestation of the Coriolis interaction in a rotating nucleus. According to the cranked shell model (CSM), axial symmetry cannot remain when an axially symmetric nucleus is cranked around an axis (e.g.,  $x$  axis) perpendicular to the symmetry axis ( $z$  axis), and the projection of angular momentum along the symmetry axis,  $K$ , is no longer a good quantum number. A particle-number-conserving treatment for the CSM Hamiltonian shows<sup>29</sup> that the  $K$  structure and the seniority structure of the ground band, and the low-lying excited bands, will become rather complicated due to the Coriolis antipairing effect in the high-spin states. Details will be published subsequently.

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