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Higher Order Corrections to the Cranking Model*

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The energy levels of the ground-state bands of several deformed nuclei are calculated using a scheme whereby higher order terms in ω (nuclear angular velocity) are retained in the cranking model. Two-parameter and three-parameter fits are obtained to the absolute energies.

IN a recent publication,[1] the author suggested a scheme whereby the energies of high-spin rotational states of deformed nuclei might be obtained by an extension of the cranking model.[2] The simplicity of this scheme allows one to fit the spectra of certain nuclei (up to spin $I=16$) using only two adjustable parameters. Root-mean-square deviations for the absolute energies vary between 0.14 and 0.76% as compared to the experimental uncertainty of $\pm 0.3\%$. The purpose of this paper is to give a more detailed description of the present model and introduce certain logical extensions which result in still better agreement between theory and experiment.

In Sec. I, the usual cranking model is extended to higher order terms in ω (the nuclear angular velocity) making use of perturbation theory. In Sec. II, the essential results of the previous part are rederived using more general arguments based on self-consistency requirements. Third-order terms which seem to be required in order to fit the highest spin states considered are introduced. Sec. III contains a comparison between the numerical results of this model and experiment.

I. THE CRANKING MODEL

We begin by considering a rotating, deformed, self-consistent potential well. In the laboratory system, one has a time-dependent Hamiltonian H and state function ψ which is a solution of the equation

$$H\psi = i\partial\psi/\partial t. \tag{1}$$

If we assume that the nucleus is rotating about the x axis, we can transform (1) to the intrinsic nuclear reference frame. The wave function in the latter system is φ, where

$$\psi = U(t)\varphi. \tag{2}$$

Substituting (2) into (1), one obtains a new Schrödinger equation,

$$\tilde{H}\varphi = i(\partial\varphi/\partial t), \tag{3}$$

where H is given by

$$\tilde{H} = U^{-1}(HU - i\partial U/\partial t). \tag{4}$$

We now seek a stationary solution to (3), i.e., one for which we can write

$$\tilde{H}\varphi = \tilde{E}\varphi. \tag{5}$$

Noting that for our simple case, U is given by

$$U = \exp(-iJ_x\omega t), \tag{6}$$

(4) may be rewritten as

$$\begin{aligned}\tilde{H} &= \exp(iJ_x\omega t)H\exp(-iJ_x\omega t) - \omega J_x \\ &= H_0 - \omega J_x.\end{aligned} \tag{7}$$

The energy eigenvalues in the two systems are also simply related,

$$\begin{aligned}E &= \langle\psi|H|\psi\rangle \\ &= \tilde{E} + \omega\langle\varphi|J_x|\varphi\rangle.\end{aligned} \tag{8}$$

We now solve (5) making use of (7). For basis states, we take stationary states of the static Hamiltonian in the nuclear system, H_0. The term $H' = -\omega J_x$ is treated as a perturbation. The usual cranking model results from the use of second-order perturbation theory. We will, however, also include terms up to fourth order in H'.

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[1] S. M. Harris, Phys. Rev. Letters **13**, 663 (1964).
[2] D. R. Inglis, Phys. Rev. **96**, 1059 (1954).

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Applying fourth-order perturbation theory, we obtain for the energy eigenvalue in the nuclear reference frame,

$$\tilde{E}=E_0+\sum_m{}'\frac{\langle 0|H'|m\rangle\langle m|H'|0\rangle}{E_0-E_m}+\sum_{mnp}{}'\frac{\langle 0|H'|m\rangle\langle m|H'|n\rangle\langle n|H'|p\rangle\langle p|H'|0\rangle}{(E_0-E_m)(E_0-E_n)(E_0-E_p)}-\sum_{mn}{}'\frac{|\langle 0|H'|n\rangle|^2|\langle 0|H'|m\rangle|^2}{(E_0-E_n)^2(E_0-E_m)}. \quad (9)$$

In the above equation, $|i\rangle$ is the basis state defined by the Schrödinger equation $H_0|i\rangle=E_i|i\rangle$. All sums in (9) exclude the terms $m, n, p=0$.

The energy in the laboratory system may be calculated from (8). Since we are including terms up to fourth order in H', we must calculate φ to third order in the perturbation, paying careful attention to maintain the proper normalization. The contribution to the pertinent matrix element to fourth order is

$$\langle\varphi|H'|\varphi\rangle=-2\sum_m{}'\frac{\langle 0|H'|m\rangle\langle m|H'|0\rangle}{(E_0-E_m)}-4\sum_{mnp}{}'\frac{\langle 0|H'|m\rangle\langle m|H'|n\rangle\langle n|H'|p\rangle\langle p|H'|0\rangle}{(E_0-E_m)(E_0-E_n)(E_0-E_p)}+4\sum_{mn}{}'\frac{|\langle 0|H'|m\rangle|^2|\langle 0|H'|n\rangle|^2}{(E_0-E_m)(E_0-E_n)^2}. \quad (10)$$

Upon substituting (9) and (10) into (8), we obtain

$$E=E_0-\omega^2\sum_m{}'\frac{\langle 0|J_x|m\rangle\langle m|J_x|0\rangle}{(E_0-E_m)}-3\omega^4\sum_{mnp}{}'\frac{\langle 0|J_x|m\rangle\langle m|J_x|n\rangle\langle n|J_x|p\rangle\langle p|J_x|0\rangle}{(E_0-E_m)(E_0-E_n)(E_0-E_p)}+3\omega^4\sum_{mn}{}'\frac{|\langle 0|J_x|n\rangle|^2|\langle 0|J_x|m\rangle|^2}{(E_0-E_m)(E_0-E_n)^2}. \quad (11)$$

All terms containing ω contribute to the rotational energy. If we write the energy in the form

$$E=E_0+\tfrac{1}{2}\mathcal{I}(\omega)\omega^2, \quad (12)$$

then, upon comparing (11) and (12), we find that

$$\mathcal{I}(\omega)=\mathcal{I}_0+3C\omega^2, \quad (13)$$

where

$$\mathcal{I}_0=2\sum_m{}'\frac{|\langle m|J_x|0\rangle|^2}{E_m-E_0} \quad (14)$$

and

$$C=2\sum_{mnp}{}'\frac{\langle 0|J_x|m\rangle\langle m|J_x|n\rangle\langle n|J_x|p\rangle\langle p|J_x|0\rangle}{(E_m-E_0)(E_n-E_0)(E_p-E_0)}-\mathcal{I}_0\sum_m{}'\frac{|\langle m|J_x|0\rangle|^2}{(E_m-E_0)^2}. \quad (15)$$

The evaluation of the expectation value for the angular momentum of the state φ leads to

$$\langle\varphi|J_x|\varphi\rangle=\omega[\mathcal{I}_0+2C\omega^2]. \quad (16)$$

Upon comparing (12) and (13) with (16), one sees that a different effective moment of inertia enters into the calculations of energy and angular momentum when terms of order ω^2 are retained in $\mathcal{I}(\omega)$. The usual cranking model treatment leads to (14). We have managed to obtain a result for the moment of inertia, however, which depends on the degree of rotation. Thus, this treatment leads to a centrifugal stretching of the nucleus, reminiscent of the theory of Davydov and Chaban[3] although no interaction between rotational and vibrational modes is explicitly introduced.

II. SELF-CONSISTENCY APPROACH

It is possible to obtain the main result of the previous section without resorting to perturbation theory. The treatment of this section is perhaps more satisfactory since we will see that the large correction terms which arise from the so-called "higher order" contributions cast doubt on the rapidity of convergence of the perturbation series.

We choose to write the energy in the laboratory system in the form

$$E=E_0+\tfrac{1}{2}\omega^2\Big(\sum_{p=0}^{\infty}a_p\omega^{2p}\Big). \quad (17)$$

The angular momentum is of the form

$$\langle\varphi|J_x|\varphi\rangle=\omega\Big(\sum_{p=0}^{\infty}b_p\omega^{2p}\Big). \quad (18)$$

Using (8), we have

$$E=\tilde{E}+\omega^2\sum_p b_p\omega^{2p}, \quad (19)$$

which leads to

$$\partial E/\partial\omega=\partial\tilde{E}/\partial\omega+\sum_p b_p(2p+2)\omega^{2p+1}. \quad (20)$$

We can, however, apply a theorem due to Feynman[4] which states that for a stationary solution of

$$\tilde{H}(\omega)\varphi(\omega)=\tilde{E}(\omega)\varphi(\omega),$$

[3] A. S. Davydov and A. A. Chaban, Nucl. Phys. **20**, 499 (1960); R. M. Diamond, F. S. Stephens, and W. J. Swiatecki, Phys. Letters **11**, 315 (1964).

[4] R. P. Feynman, Phys. Rev. **56**, 340 (1939).

one has

$$\partial\tilde{E}/\partial\omega=\langle\varphi|\,\partial\tilde{H}/\partial\omega\,|\varphi\rangle.$$

Therefore, in our case

$$\partial\tilde{E}/\partial\omega=-\langle\varphi|J_x|\varphi\rangle$$
$$=-\omega\sum_p b_p\omega^{2p}. \quad (21)$$

Combining (20) and (21), we have

$$\partial E/\partial\omega=\sum_p b_p(2p+1)\omega^{2p+1}. \quad (22)$$

But from (17), we must also have

$$\partial E/\partial\omega=\tfrac{1}{2}\sum_p a_p(2p+2)\omega^{2p+1}. \quad (23)$$

Upon comparing (22) and (23), we see that both equations can only be valid if $a_p(p+1)=b_p(2p+1)$ for all p. Thus, self-consistency is achieved if we write (17) and (18) in the form

$$E=E_0+\tfrac{1}{2}\omega^2(\mathcal{I}_0+3C\omega^2+5D\omega^4+7F\omega^6+\cdots) \quad (24)$$

and

$$\langle\varphi|J_x|\varphi\rangle=\omega(\mathcal{I}_0+2C\omega^2+3D\omega^4+4F\omega^6+\cdots). \quad (25)$$

If the higher order terms (those containing D, F, etc.) are set equal to zero, (24) and (25) are identical with the results of the previous section. No use was made here of perturbation theory and, consequently, one need not make any assumptions about the relative magnitudes of the various coefficients entering into these expressions.

When describing the rotational states of deformed nuclei, we may begin with (24′) and (25′),

$$E_{\rm rot}=\tfrac{1}{2}\omega^2(\mathcal{I}_0+3C\omega^2+5D\omega^4+7F\omega^6+\cdots) \quad (24')$$

and

$$[I(I+1)]^{1/2}=\omega(\mathcal{I}_0+2C\omega^2+3D\omega^4+4F\omega^6+\cdots). \quad (25')$$

In principle, ω may be eliminated leaving one equation for $E_{\rm rot}$ as a function of nuclear spin I. The solutions depend parametrically on the coefficients $\mathcal{I}_0$, C, D, etc.

TABLE I. Constants used in two-parameter fit [Eqs. (24′) and (25′)].

Nucleus	$\mathcal{I}_0(10^{-2}$ keV$^{-1})$	$C(10^{-8}$ keV$^{-3})$
W^{172}	2.274	15.332
W^{174}	2.596	9.470
W^{176}	2.689	7.768
Hf^{166}	1.734	9.909
Hf^{168}	2.328	9.554
Hf^{170}	2.894	11.647
Hf^{172}	3.116	7.050
Yb^{164}	2.369	8.385
Yb^{166}	2.897	6.541

III. COMPARISON WITH EXPERIMENT

In the previous report on this work,[1] only the two parameters $\mathcal{I}_0$ and C were retained, and a two-parameter least-squares fit of the system of Eqs. (24′) and (25′) was obtained to the available experimental data for several nuclei.[5] Table I gives the values of $\mathcal{I}_0$ and C which resulted in the best fit to the observed spectra. Once $\mathcal{I}_0$ and C were determined, they were substituted back into (24′) and (25′) and those equations solved for E corresponding to each value of I. The results of this program appear in Table II.

The fit to the data obtained in this manner seems quite good. The rms deviations given in the last column of Table II vary from 0.14 to 0.76% (rms deviations are calculated before the theoretical energies are rounded

TABLE II. Rotational energies (keV) for two-parameter fit.

Nucleus		$J=2^+$	4^+	6^+	8^+	10^+	12^+	14^+	16^+	Rms % deviation
W^{172}	Expt.	122.9	376.9	727.2	1147	1616	2129	2677		0.69
	Theory	123.8	376.2	720.9	1137	1612	2136	2705		
W^{174}	Expt.	111.9	355.0	704.2	1137	1635	2186			0.30
	Theory	112.2	354.9	701.8	1133	1634	2196			
W^{176}	Expt.	108.7	348.5	699.4	1140	1648	2206			0.46
	Theory	109.1	348.7	696.4	1133	1645	2223			
Hf^{166}	Expt.	158.7	470.7	897.6	1407	1971	2565			0.59
	Theory	158.9	472.7	893.5	1396	1965	2591			
Hf^{168}	Expt.	123.9	385.0	756.1	1212	1734	2304			0.26
	Theory	123.8	386.2	755.0	1208	1731	2313			
Hf^{170}	Expt.	100.0	320.6	641.1	1041	1503	2013	2564	3147	0.76
	Theory	101.0	320.7	636.6	1031	1491	2008	2575	3186	
Hf^{172}	Expt.	94.5	307.9	627.0	1036	1519	2063	2651		0.46
	Theory	95.0	308.1	624.7	1030	1513	2062	2672		
Yb^{164}	Expt.	122.5	384.0	758.0	1219	1748				0.14
	Theory	122.4	384.8	757.0	1217	1750				
Yb^{166}	Expt.	101.8	329.7	667.1	1097	1604	2172			0.20
	Theory	102.0	329.7	665.9	1094	1602	2179			

[5] F. S. Stephens, N. Lark, and R. M. Diamond, Phys. Rev. Letters 12, 225 (1964); University of California Radiation Laboratory Report UCRL-11402, Berkeley, 1964, Nucl. Phys. (to be published).

TABLE III. Constants used in three-parameter fit [Eqs. (24′) and (25′)].

Nucleus	$\mathcal{I}_0(10^{-2}\ \mathrm{keV}^{-1})$	$C(10^{-8}\ \mathrm{keV}^{-3})$	$D(10^{-13}\ \mathrm{keV}^{-5})$
W^{172}	2.336	10.735	5.53
W^{174}	2.618	7.816	1.93
W^{176}	2.719	5.609	2.39
Hf^{166}	1.762	8.349	1.45
Hf^{168}	2.337	8.946	0.654
Hf^{170}	2.954	7.256	4.76
Hf^{172}	3.149	4.766	2.36
Yb^{164}	2.372	8.218	0.203
Yb^{166}	2.910	5.592	1.03

off). This should be compared with the experimental accuracy of $\pm 0.3\%$.[5] The largest deviations are usually traceable to the higher spin states. This suggests that the higher order terms (those containing D, etc.) may become significant for very large I.

In an attempt to obtain still better agreement with experiment, the above procedure was repeated for (24′) and (25′) retaining the three parameters, $\mathcal{I}_0$, C, and D. The values of these three parameters which give the best least-squares fit to the data are given in Table III. The corresponding energy levels are presented in Table IV. From Table IV, it is seen that the rms deviations have been reduced below the experimental uncertainties in all but one case by introducing the third parameter D. One may question whether this is a significant improvement in view of the generally good results of the two-parameter fits. However, a more sensitive test of the goodness of fit exists. One should also compare the transition energies which are the experimentally determined quantities. Using Tables II and IV, one finds that the rms deviations for the transition energies are usually about three times as large as the corresponding numbers for the absolute energies. It should be remembered, however, that the parameters $\mathcal{I}_0$ and C were determined so as to yield a best fit to the experimental energies. If we tried to reproduce the transition energies, larger deviations would result for the absolute energies.

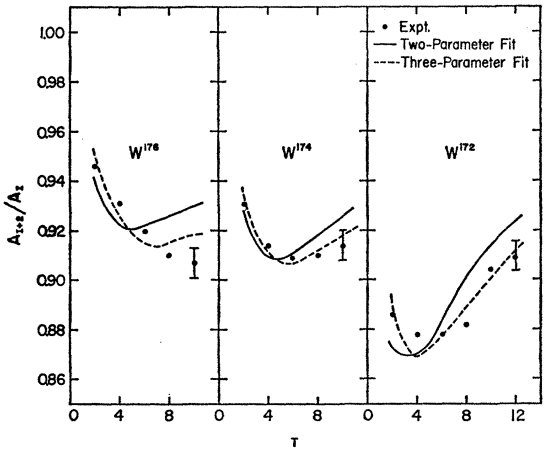

FIG. 1. A_{I+2}/A_I versus I for W isotopes.

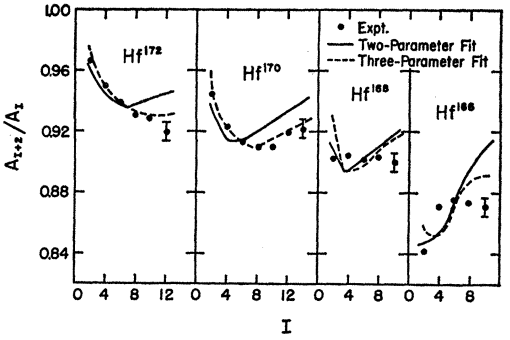

FIG. 2. A_{I+2}/A_I versus I for Hf isotopes.

In Ref. 5, graphs of weighted transition energies versus spin are presented. They introduce the parameter

$$A_I=(E_I-E_{I-2})/(4I-2),$$

and plot A_{I+2}/A_I versus I. Since the transition energies have an accuracy of $\pm 0.3\%$ associated with them, the ratios (A_{I+2}/A_I) are uncertain to $\pm 0.6\%$. The data of Tables II and IV are plotted in this manner (Figs. 1–3) so as to allow a comparison with the results of Ref. 5. In the latter work, the model of Davydov and Chaban,[3] which explicitly takes into account the interaction between rotations and β vibrations via a β-dependent moment of inertia is used to obtain good two-parameter fits to the experimental data.

IV. SUMMARY

In conclusion it may be said that the present model permits one to obtain generally good two-parameter fits to all of the rotational energy levels for the nuclei which have been investigated. In two of the cases where the deviations are significantly larger than the experimental uncertainties, excellent agreement can be obtained by including a third parameter which corresponds to retaining the third-order term in the power series expansion for the moment of inertia. If one were to observe higher spin states of rotational nuclei, it might be necessary to include still higher-order terms in this expansion. Since the worst disagreement for Hf^{166} arises for the high spin states, it may be that the next term

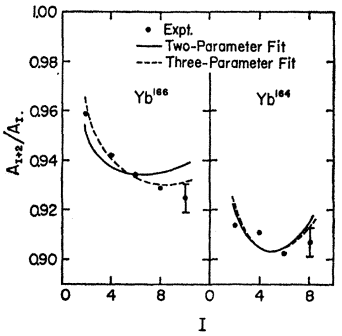

FIG. 3. A_{I+2}/A_I versus I for Yb isotopes.

TABLE IV. Rotational energies (keV) for three-parameter fit.

Nucleus		$J=2^+$	4^+	6^+	8^+	10^+	12^+	14^+	16^+	Rms % deviation
W^{172}	Expt.	122.9	376.9	727.2	1147	1616	2129	2677		0.14
	Theory	122.8	377.9	727.0	1145	1615	2129	2679		
W^{174}	Expt.	111.9	355.0	704.2	1137	1635	2186			0.08
	Theory	111.8	355.4	704.3	1136	1634	2188			
W^{176}	Expt.	108.7	348.5	699.4	1140	1648	2206			0.18
	Theory	108.5	349.4	699.9	1138	1645	2210			
Hf^{166}	Expt.	158.7	470.7	897.6	1407	1971	2565			0.48
	Theory	158.2	474.1	897.1	1399	1963	2579			
Hf^{168}	Expt.	123.9	385.0	756.1	1212	1734	2304			0.24
	Theory	123.7	386.5	756.1	1209	1731	2309			
Hf^{170}	Expt.	100.0	320.6	641.1	1041	1503	2013	2564	3147	0.11
	Theory	99.9	321.1	641.8	1041	1501	2011	2563	3151	
Hf^{172}	Expt.	94.5	307.9	627.0	1036	1519	2063	2651		0.10
	Theory	94.4	308.2	627.6	1036	1518	2060	2655		
Yb^{164}	Expt.	122.5	384.0	758.0	1219	1748				0.14
	Theory	122.4	384.9	757.3	1217	1750				
Yb^{166}	Expt.	101.8	329.7	667.1	1097	1604	2172			0.06
	Theory	101.8	329.9	667.4	1097	1602	2173			

[F in Eqs. (24), (25)] is anomalously large for this nucleus.

In principle, (14) and (15) permit one to calculate the coefficients $\mathcal{I}_0$ and C which enter here if perturbation theory is valid. $\mathcal{I}_0$ has been calculated in the quasiparticle approximation.[6] The results for rare-earth nuclei indicate that $\mathcal{I}_0$ calculated in this manner is usually about 10 to 30% smaller than the effective value determined experimentally from the $I=0\rightarrow I=2$ energy spacing. (Unfortunately, these calculations have not been performed for the specific nuclei investigated here.) In our model, however, the energy is given by

$$E=\tfrac{1}{2}\omega^2(\mathcal{I}_0+3C\omega^2),$$

whereas $\mathcal{I}_{\text{eff}}$ is determined from

$$E=\tfrac{1}{2}\omega^2\mathcal{I}_{\text{eff}}.$$

A measure of the discrepancy between $\mathcal{I}_0$ and $\mathcal{I}_{\text{eff}}$ is δ, defined by

$$\delta=\frac{\mathcal{I}_{\text{eff}}-\mathcal{I}_0}{\mathcal{I}_{\text{eff}}}=\frac{3C\omega^2}{\mathcal{I}_{\text{eff}}}=\frac{6CE}{\mathcal{I}_{\text{eff}}^2}. \tag{26}$$

Using Tables I and II, one obtains values for δ which range from about 30% for Hf^{166} to 4% for Hf^{172}. Since $C>0$ in the cases considered here, δ is always positive, indicating that $\mathcal{I}_{\text{eff}}$ is larger than $\mathcal{I}_0$ by 4 to 30%. If the nuclei considered here follow the same trend as the other rare earths, the present model would bring the value of $\mathcal{I}_0$ (calculated with pairing) into better agreement with experiment.

It would be profitable to extend the calculation of Ref. 6 to include the cases discussed above. Similar (though much more difficult) calculations could be performed to obtain the coefficient C from (15) in the quasiparticle approximation. It is only then that one could make definite statements about the applicability of perturbation theory and the extended cranking model to this problem.

ACKNOWLEDGMENTS

We would like to thank Dr. J. Weneser for pointing out the necessity for self-consistency as discussed in Sec. II. We are also indebted to Dr. R. Barrett for many valuable suggestions regarding least-squares programs and to Dr. F. Stephens for supplying his data prior to publication. The numerical calculations presented here were carried out at the Purdue University Computer Sciences Center.

[6] S. G. Nilsson and O. Prior, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. 32, No. 16 (1961); J. J. Griffin and M. Rich, Phys. Rev. Letters 3, 342 (1959).