Iterative relationship in two-parameter formulas for rotational spectra and a universal equation

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(Received 15 September 1997)

An iterative relationship connecting a series of two-parameter formulas for rotational spectra is revealed. It is also pointed out that various two-parameter formulas are merely solutions of a universal equation with different powers. [S0556-2813(98)03104-5]

PACS number(s): 21.10.Re, 21.60.Ev, 27.70.+q, 27.90.+b

Phenomenological analysis of energy levels of well-deformed even-even nuclei has gone on for more than four decades since Bohr and Mottelson described the ground-state rotational bands with a rigid rotor expression [1]

$$E=\frac{\hbar^2}{2\mathcal{J}}I(I+1)\equiv AI(I+1). \tag{1}$$

Up to now a variety of empirical formulas have been developed to correct the systematic deviation between Eq. (1) and experiment. Among these formulas two-parameter ones have been used more generally for their less parameters. A brief summation is as follows.

(1) *AB formula*: In principle, the rotational energy may be expanded as an infinite power series of $I(I+1)$ [1]. The first-order approximation is of the form

$$E=AI(I+1)-BI^2(I+1)^2, \tag{2}$$

where the second term represents the vibrational correction.

(2) *A variant of AB formula (Warke-Khadikikar formula)* [2]: If the magnitude of the second term in Eq. (2) is small enough compared with the first one, one can rewrite the equation as

$$E=AI(I+1)\left[1-\frac{B}{A}I(I+1)\right]\approx\frac{AI(I+1)}{1+\frac{B}{A}I(I+1)}. \tag{3}$$

The difference between Eqs. (2) and (3) is that the latter is convergent as I increases. Using such a simple formula, Bonatsos [3] has accounted for the gradual increase of the moment of inertia with angular momentum below band crossing in the actinide and rare-earth regions.

(3) *Harris ω^2 expansion* [4]:

$$E=\alpha\omega^2+\beta\omega^4, \tag{4}$$

with ω denoting rotational angular frequency. This expansion converges faster than the angular-momentum expansion and can give a good fit to the data in many cases.

(4) *Variable moment of inertia (VMI) model*:

$$E=\frac{\hbar^2}{2\mathcal{J}}I(I+1)+\frac{1}{2}C(\mathcal{J}-\mathcal{J}_0)^2, \tag{5}$$

where $\mathcal{J}(I)$ is determined from the variational condition $\partial E(I)/\partial\mathcal{J}|_I=0$. It has been proved [5] that the VMI model is equivalent to the $\alpha\beta$ formula.

(5) *ab formula*: From experimental level systematics and, alternatively, from nuclear hydrodynamics, Holmberg and Lipas [6] deduced a closed formula

$$E=a[\sqrt{1+bI(I+1)}-1]. \tag{6}$$

Previous to them, Najakov and Mikhailov already derived the same formula from a generation of the Inglis cranking model [7].

(6) *pq formula*: Recently, following the way of Ref. [4], we derived another formula

$$E=p\left\{\sqrt[3]{\left(\frac{x}{2}\right)^2+\sqrt{\left(\frac{x}{2}\right)^4+\left(\frac{x}{3}\right)^3}}+\sqrt[3]{\left(\frac{x}{2}\right)^2-\sqrt{\left(\frac{x}{2}\right)^4+\left(\frac{x}{3}\right)^3}}\right\}, \tag{7}$$

where $x=qI(I+1)$. Various comparisons show that our formula is the best one among all two-parameter formulas we we have known until now in fitting ground rotational bands of even-even nuclei in rare-earth and actinide regions [8]. There are also some other two-parameter formulas, which are omitted here for their either complicated forms or not being designed especially for rotational spectra. Up to now, there have been many references to discuss various formulas for rotational spectra [9–14].

The formulas enumerated above are all successful in varying degrees in fitting experimental data. This fact is by no means accidental and suggests that there must be some intrinsic relationships among them. Many years ago, Mantri and Sood gave an excellent unified summary of various formulas advanced up to that time and proposed a basic set of equations from which one can obtain various energy expressions. However, their set of equations is too complicated for practical application and there are some formulas which, pro-

posed later, have not been discussed in their paper. This motivates us to try to give a new discussion of the problem.

Recalling the derivation of Eq. (7), we practically take the following steps (see Ref. [8]): (i) assuming that the deviation between Eq. (1) and experiment is caused by the variation of the moment of inertia $\mathcal{J}$, with E. That is, $\mathcal{J}$ is the function of E. Thus we have

$$E=\frac{\hbar^2}{2\mathcal{J}(E)}I(I+1); \tag{8}$$

(ii) rewriting the ab formula as the form of $E=(\hbar^2/2\mathcal{J}[bI(I+1)])I(I+1)$ and then replacing $bI(I+1)$ in the expression of $\mathcal{J}[bI(I+1)]$ with $2E/a$ by using the pure-rotor limit of the ab formula, $E=\frac{1}{2}abI(I+1)$, to get an expression similar to Eq. (8) and then yield a cubic equation of E

$$E^3+a^2bI(I+1)E-\frac{a^3[bI(I+1)]^2}{2}=0; \tag{9}$$

(iii) solving the above equation, one can obtain the pq formula, where p and q, corresponding to a and b, respectively, are introduced to avoid confusion with the ab formula. Obviously, these steps make an iterative process in essence. Enlightened by this, we may perform the same process to other two-parameter formulas. Let us start from the simplest one, Eq. (2), which, according to steps (i) and (ii), can be rewritten as

$$E=AI(I+1)\left[1-\frac{B}{A^2}E\right]. \tag{10}$$

With a slight rearrangement, one obtains the expression of E just the same as Eq. (3).

Now we deal with Eq. (3) in turn. Its variant in analogue with Eq. (8) is

$$E=\frac{AI(I+1)}{1+\frac{B}{A^2}E}, \tag{11}$$

namely,

$$E^2+\frac{A^2}{B}E-\frac{A^3}{B}I(I+1)=0. \tag{12}$$

Its physical root is just the ab formula with $a=A^2/2B$ and $b=4B/A$. Thus we see that Eqs. (2), (3), (5), and (6) are connected by an iterative relationship. The ab formula is a starting point of the iteration. We are now interested in what the limitation of the iteration is and how to get it. To this end, we denote the E in Eqs. (1), (2), (3), (4), and (5) as E_A, E_0, E_1, E_2, and E_3, respectively, and rearrange the last four equations into the following forms:

$$E_0^0+\frac{A^2}{B}E_A^{-2}(E_0-E_A)=0, \tag{13}$$

$$E_1^1+\frac{A^2}{B}E_A^{-1}(E_1-E_A)=0, \tag{14}$$

$$E_2^2+\frac{A^2}{B}E_A^{0}(E_2-E_A)=0, \tag{15}$$

$$E_3^3+\frac{A^2}{B}E_A^{1}(E_3-E_A)=0. \tag{16}$$

An obvious regulation shows up from these equations, i.e., they constitute an organic series and have a common form:

$$E_n^n+\frac{A^2}{B}E_A^{n-2}(E_n-E_A)=0, \tag{17}$$

or, equivalently,

$$E_n^n+2aE_A^{n-2}(E_n-E_A)=0. \tag{18}$$

Naturally we expect that this equation is valid for any integer n. In other words, E_n in Eq. (18) is just the result of nth iteration. To show this, we offer a demonstration instead of a strict proof by applying the iteration procedure to the pq formula. First, making use of the relation $u+v=(u^3+v^3)/(u^2-uv+v^2)$, one can change Eq. (8) into

$$E=p\frac{2\left(\frac{x}{2}\right)^2}{\sqrt[3]{\left[\left(\frac{x}{2}\right)^2+\sqrt{\left(\frac{x}{2}\right)^4+\left(\frac{x}{3}\right)^3}\right]^2}+\frac{x}{3}+\sqrt[3]{\left[\left(\frac{x}{2}\right)^2-\sqrt{\left(\frac{x}{2}\right)^4+\left(\frac{x}{3}\right)^3}\right]^2}}. \tag{19}$$

Then replacing each x by $2E/a$, except the one in the numerator which is recovered into $bI(I+1)$, one obtains

$$E=p\frac{2\left(\frac{E}{a}\right)\frac{bI(I+1)}{2}}{\sqrt[3]{\left[\left(\frac{E}{a}\right)^2+\sqrt{\left(\frac{E}{a}\right)^4+\left(\frac{2E}{3a}\right)^3}\right]^2}+\frac{2E}{3A}+\sqrt[3]{\left[\left(\frac{E}{a}\right)^2-\sqrt{\left(\frac{E}{a}\right)^4+\left(\frac{2E}{3a}\right)^3}\right]^2}}. \tag{20}$$

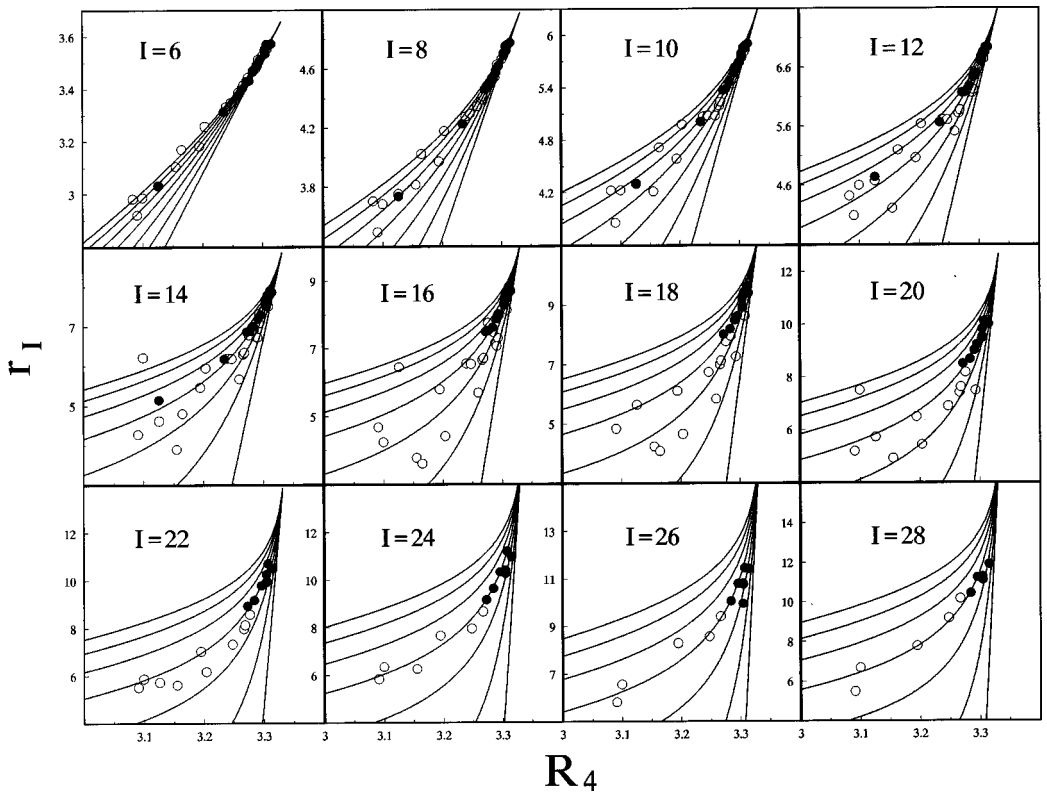

FIG. 1. The Mallmann plots for Eq. (18) by solid lines for integers $n=0$, 1, 2, 3, 4, 5, and 6 from right to left. The experimental data are denoted by closed circles for the actinide nuclei and open circles for the rare-earth nuclei.

After a tedious but straightforward derivation, one can simplify the equation into

$$E^4+2aE_A^2(E-E_A)=0, \tag{21}$$

which is just the same as Eq. (18) in the case of taking $n=4$.

Using the Mallmann plot [15], i.e., the plot of $R_I\equiv(E_I-E_0)/(E_2-E_0)$ (or $r_I\equiv R_I-R_{I-2}$) versus R_4, we may assess which value of n in Eq. (18) will lead to the best fitting to the experiment. Figure 1 shows the plots of r_I vs R_4, for $I=6, 8, \ldots, 28$, for $n=0, 1, \ldots, 6$, respectively, by solid lines from right to left with the values of R_4 spanning from 3.0 to 3.33. All the experimental data available now for the ground-state bands of even-even rare-earth and actinide nuclei [8] (with band-crossing spin $I_c\geqslant 16$) are displayed in the figure by open and solid circles, respectively. It can be apparently seen that the curve corresponding to $n=3$ (i.e., the pq formula) passes through the most experimental points for almost each spin, apart from the first two small ones. In other words, when taking $n=3$, Eq. (18) gives the best fitting in systematical meaning. This conclusion is consistent with Ref. [8]. It should be noticed that the band-crossing spins of ground bands of most rare-earth nuclei are about $I_c=16$, therefore the experimental points of $I>16$ for these nuclei in Fig. 1 are plotted for reference only.

We now discuss the relation between the $\alpha\beta$ formula and Eq. (18). If n is limited to taking the integer only, the $\alpha\beta$ formula does not belong to the series given by Eq. (18). But if we expand the value field of n to any positive real number, it might become an approximate solution of Eq. (18), at least in the typical rotational range of $3.2<R_4\leqslant 3.33$. To see this, we have also given the Mallmann plots of the $\alpha\beta$ formula in Fig. 2 by dashed lines. One can see that the dashed line for each of the spins is located between two solid ones with $n=3$ and 4, respectively. In fact, it almost overlaps with the curve, shown in Fig. 2 by solid lines, plotted by taking $n\simeq 3.4$ in Eq. (18). Thus we may take n as a free parameter and regard it as a mark of the stretching effect because the larger n is, the more down-bent of the curve of $\mathcal{J}$ vs E is. After extending the value range of n, and regarding it as a fitting parameter to be determined for each rotational band, Eq. (18) essentially becomes a three-parameter equation and its solutions can cover the entire distribution of the experimental data.

We have also accomplished least-square fits of Eq. (18), for $n=0, 1, \ldots, 6$, to each of the ground-state bands of well-deformed nuclei, respectively. Since Eq. (18) has no analytical solutions when n takes integers larger than 5 or real numbers, one must solve the equation in value in these cases. Table I lists the root-mean-square (r.m.s.) errors, calculated by

$$\sigma_n=\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\frac{E_n^{\rm cal}(i)-E^{\rm exp}(i)}{E^{\rm exp}(i)}\right)^2}, \tag{22}$$

with N denoting the number of data points considered, which allows us to see to what extent the experimental data can be described by Eq. (18) with varying n. It can be seen from the table that the best n values range from 0 to 5. However, $n=3$ generates the best agreement for most nuclei, while n

TABLE I. The r.m.s. deviation defined by Eq. (22) for $n=0, 1, 2, 3, 4, 5$, and 6. The minimum of the r.m.s. is denoted by italic. The experimental data are taken from recent Nuclear Data Sheets (see Ref. [8]).

		$\sigma\times10^2$						
Nuclei	$AI(I+1)$	$n=0$	1	2	3	4	5	6
^{154}Sm	7.499	1.406	0.973	0.577	0.227	*0.170*	0.452	0.727
^{156}Gd	7.735	1.240	0.785	0.384	*0.161*	0.407	0.706	0.984
^{162}Dy	6.066	0.761	0.469	0.206	*0.085*	0.288	0.495	0.688
^{164}Dy	3.935	0.305	0.179	0.062	*0.051*	0.155	0.254	0.347
^{160}Er	11.859	4.333	3.283	2.341	1.571	1.088	*1.055*	1.337
^{162}Er	11.112	1.271	*0.635*	0.826	1.370	1.906	2.388	2.815
^{164}Er	5.737	0.647	0.391	0.164	*0.112*	0.293	0.477	0.649
^{166}Er	7.052	0.552	*0.150*	0.212	0.533	0.823	1.084	1.320
^{168}Er	2.270	0.106	0.070	0.042	*0.041*	0.066	0.098	0.130
^{164}Yb	13.991	4.314	2.831	1.631	*0.982*	1.288	1.941	2.553
^{166}Yb	9.664	2.066	1.336	0.708	*0.318*	0.577	1.001	1.400
^{168}Yb	8.707	1.052	0.449	*0.115*	0.566	0.982	1.353	1.684
^{170}Yb	4.507	0.247	*0.120*	0.131	0.243	0.364	0.480	0.590
^{172}Yb	3.696	0.391	0.281	0.179	0.085	*0.045*	0.116	0.197
^{174}Yb	4.981	0.547	0.344	0.157	*0.037*	0.187	0.338	0.479
^{176}Yb	4.371	*0.078*	0.084	0.226	0.358	0.481	0.596	0.702
^{168}Hf	14.259	4.373	2.845	1.485	*0.354*	0.792	1.638	2.331
^{170}Hf	12.332	2.791	1.613	0.586	*0.348*	1.113	1.782	2.351
^{172}Hf	9.204	1.450	0.795	*0.250*	0.366	0.808	1.215	1.580
^{174}Hf	8.471	0.943	0.376	*0.165*	0.592	0.985	1.337	1.651
^{176}Hf	5.318	0.519	0.295	*0.095*	0.119	0.292	0.456	0.609
^{178}Hf	6.970	0.314	*0.105*	0.434	0.740	1.014	1.261	1.485
^{182}W	4.003	0.446	0.323	0.210	*0.113*	0.082	0.147	0.233
^{178}Os	17.572	6.373	4.100	2.040	*0.277*	1.208	2.327	3.095
^{184}Os	6.852	1.454	1.111	0.791	0.498	0.249	*0.176*	0.349
^{186}Os	8.368	1.813	1.322	0.879	0.512	*0.338*	0.493	0.756
^{226}Ra	12.396	3.275	2.129	1.107	*0.271*	0.649	1.311	1.873
^{228}Th	8.002	1.440	0.947	0.499	*0.123*	0.310	0.640	0.942
^{230}Th	9.775	2.029	1.282	0.616	*0.087*	0.528	1.003	1.430
^{232}Th	11.888	2.837	1.717	0.734	*0.141*	0.888	1.553	2.139
^{230}U	6.730	1.082	0.722	0.391	*0.091*	0.196	0.451	0.687
^{232}U	7.454	1.151	0.705	0.302	*0.074*	0.399	0.700	0.975
^{234}U	10.287	2.263	1.419	0.668	*0.061*	0.600	1.128	1.601
^{236}U	9.736	1.549	0.780	*0.119*	0.483	1.000	1.459	1.870
^{238}U	9.638	1.499	0.758	*0.145*	0.478	0.976	1.423	1.823
^{236}Pu	4.197	0.350	0.209	0.081	*0.063*	0.173	0.282	0.385
^{238}Pu	3.828	0.419	0.300	0.189	0.084	*0.033*	0.118	0.208
^{240}Pu	2.941	0.225	0.154	0.087	*0.024*	0.039	0.098	0.154
^{242}Pu	6.405	0.817	0.485	0.187	*0.108*	0.352	0.583	0.796
^{244}Pu	5.429	0.641	0.407	0.196	*0.076*	0.219	0.387	0.546
^{248}Cm	8.232	0.877	0.326	*0.187*	0.603	0.981	1.320	1.625

$=2$ gives the smallest discrepancies for most of the remaining nuclei. There are only a few nuclei which can be best fitted by taking $n=0, 1, 4$, and 5.

In this paper, we have revealed an intrinsic iterative relationship present in some elementary two-parameter formulas for rotational energy spectra and then obtained a universal equation [Eq. (18)] satisfied by these formulas, which has in turn established definite correspondences among the parameters in different formulas proposed before and, therefore, allows us to give them consistent physical explanations. In fact, this work implies that various successful formulas undoubtedly have a common microscopic basis. In other words, Eq. (18) can certainly be derived from a microscopic model. There only remains the task of performing it. We firmly believe this point also in view of the fact that Eq. (2) ($n=0$) is obtained under symmetric consideration whereas Eq. (3) ($n=1$) can be obtained from a microscopic approach [2], or from combining the Bohr-Mottelson model and the interacting boson model (IBM) [16,17]. Moreover, Eqs. (5) ($n=2$) and (6) ($n=3$) have backgrounds of nuclear hydrodynamics and the former can also be obtained from the Bohr and Mottelson model under certain approximation [18].

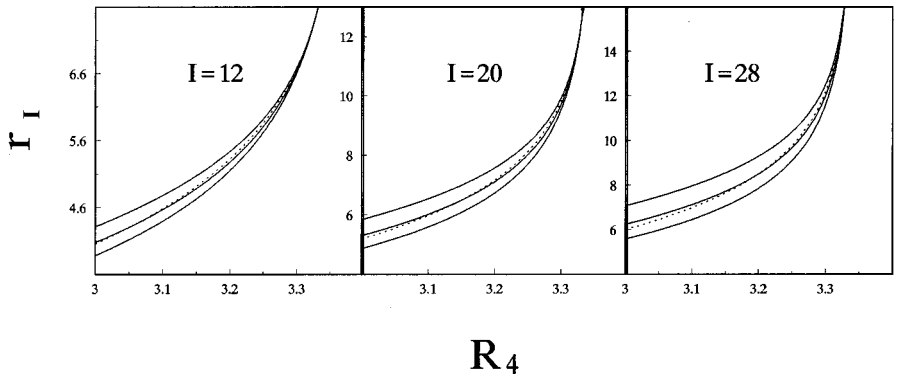

FIG. 2. The Mallmann plots, for three representative spins $I=12$, 20, and 28, for Eq. (18) by solid lines for $n=3$, 3.4, and 4 from right to left and by dashed line for the $\alpha\beta$ formula (VMI model).

We have also accomplished the comparisons between Eq. (18) and experiment and obtained the fitting results with high accuracy. From this equation we can easily derive some useful quantities, such as the softness parameter and the functional dependences of kinematic and dynamical moments of inertia, $\mathcal{J}^{(1)}$ and $\mathcal{J}^{(2)}$, on angular momentum. Moreover, if we replace E in Eq. (18) with $E-E_0$, this equation can be used to analyze excited rotational bands and superdeformed bands. Another intriguing problem is to investigate if it can be applied to transitional and γ unstable regions; in view of that we have expanded the range of the value of n to any positive real number. It is also an open question, how to get the universal equations for $B(E2)$ and quadruple moments, corresponding to Eq. (18).

This work is supported by the National Natural Science Foundation of China.

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