New yrast energy formula for soft rotors

P. von Brentano,[1,2] N. V. Zamfir,[1] R. F. Casten,[1,2] W. G. Rellergert,[1] and E. A. McCutchan[1]
[1]*Wright Nuclear Structure Laboratory, Yale University, New Haven, Connecticut 06520-8124, USA*
[2]*Insitiut für Kernphysik, Universiät zu Köln, Köln, Germany*
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A new two parameter formula for yrast energies, which works best for soft rotors or transitional nuclei, is proposed and compared with existing data.

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Our understanding of nuclear structure is framed within the context of a number of idealized benchmarks. These include the axial rotor [1], the harmonic vibrator [2], γ-soft deformed nuclei [3,4] and, very recently, the new critical point symmetries [5–8] for phase transitional regions. These models generally predict sequences of energies and either a subset or all of the $B(E2)$ values within the model space. For example, for the pure rotor, the yrast energies go as $I(I+1)$.

No nucleus need obey these paradigms exactly and, historically, their proposal has been rather quickly followed by schemes that embody perturbations to the idealized structures they envision. Examples are the energy expansions in powers of $I(I+1)$, or the Harris formula [9], the variable moment of inertia (VMI) [10], the Ejiri formula [11], and the Holmberg-Lipas formula [12] for rotor-like nuclei, or the anharmonic vibrator (AHV) formula which actually describes a range of nuclei from spherical to deformed [13,14]. In the framework of the interacting boson model, to describe the increase of the moment of inertia at high spin states in deformed nuclei, a spin-dependent term $1/(1+f\mathbf{L}\cdot\mathbf{L})$ was included in the Hamiltonian [15]. These perturbation schemes embody expected physical effects, such as centrifugal stretching and rotation-vibration coupling for the rotor or phonon-phonon interactions for the vibrator.

Of course, the further a nucleus is in structure from one of the paradigms, the larger the perturbations to the predictions of that paradigm will have to be, and, generally, the worse or less applicable, it will be. This is preeminently the case for transitional nuclei between spherical and deformed limits where neither the vibrator or rotor limits is very apt [16].

The value of any of the paradigms is that they provide an expected pattern that, once identified in an actual nucleus, helps establish its structure, and that deviations from them reveal additional degrees of freedom that would be difficult or impossible to spot without the prior existence of ideal guidelines. Therefore, the development of optimized benchmarks is a valuable effort.

With the high spin data often available for transitional and well-deformed nuclei, perturbations to the rotor expansion for yrast (or other rotational band) energies, become quite important. Effects such as centrifugal stretching, pairing collapse, and bandmixing are at work and numerous perturbations to idealized models have attempted to take these into account.

It is the purpose of this work to offer a new formula, simple in practical usage, which works as well as or nearly as well as existing expressions for well-deformed nuclei and better than any in the transitional region.

The basis of this expression is utterly simple: it is the ideal rotor expression

$$E = \frac{1}{\mathcal{J}(I,E)} I(I+1), \tag{1}$$

but where the moment of inertia depends linearly on spin I and excitation energy E. That is,

$$\mathcal{J} = \mathcal{J}_0(1 + \alpha I + \beta E), \tag{2}$$

where α and β are parameters and $\mathcal{J}_0$ sets the overall scale. In this paper we will work almost solely with a simplification of Eq. (2), dropping the energy-dependent term, since test fits show that it is very small in the transitional region of most interest here. Henceforth, therefore, unless otherwise specified, we use

$$E = \frac{1}{\mathcal{J}_0(1 + \alpha I)} I(I+1). \tag{3}$$

For reasons that will become obvious, we call Eq. (3) the "soft-rotor formula" (SRF). Fits to yrast data can be done either by using the 2^+ and 4^+ energies to fix the parameters, in which case Eq. (3) predicts all the higher spin levels, or by doing a least squares fit to the entire (pre-backbending or alignment portion of the) band or quasiband. To show the quality of the energy expression in Eq. (3), we first follow the latter approach. After inspecting the results, an application of the first approach will be discussed.

To stringently test Eq. (3) for all kinds of collective nuclei in a broad region of the nuclear chart, we carried out least squares two-parameter $(\mathcal{J}_0, \alpha)$ fits of Eq. (3) to all collective [i.e., $R_{4/2} \equiv E(4_1^+)/E(2_1^+) \geqslant 2.0$] even-even nuclei with $Z > 52$ (164 nuclei) and yrast band known at least up to 8^+ [17]. The maximum spin included in the analysis is 20^+, except for 22 cases where an irregularity in E vs I plot occurs earlier (e.g., backbend, upbend, etc.), then the yrast sequence is included up to that spin value. In carrying out the least squares fits great care must be taken in assigning the uncertainties. It is incorrect to simply take the experimental values since they vary, in some cases, from electron volts for the 2^+ level to keV for higher spins and this would weight the 2^+ and 4^+ state energies by orders of magnitude. Rather, one must ask what is the theoretical "uncertainty," that is, the expected

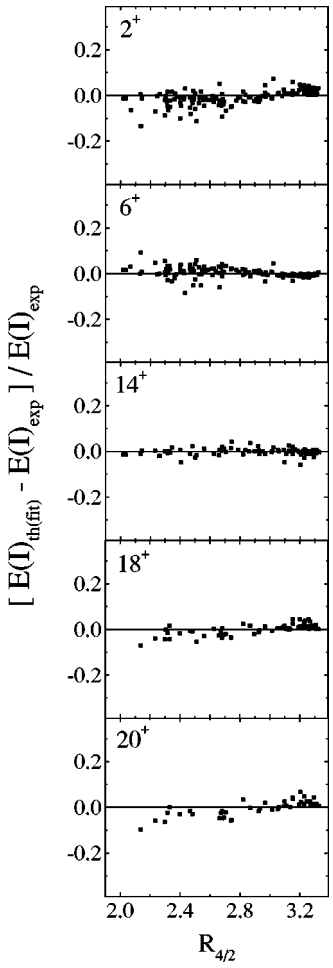

FIG. 1. Relative differences between experimental and calculated yrast energies [Eq. (4)] as a function of $R_{4/2}$ for different spin values. Calculated energies were found through a least squares fit of Eq. (3) to the yrast bands of collective nuclei with $Z=54-102$ (see text).

accuracy of any model. We used a constant relative uncertainty of 0.5%. Typically, this is about $\lesssim 1$ keV for the 2^+ level and a few keV in the range 16^+-20^+.

We summarize the results in Fig. 1 in terms of the differences between the experimental and calculated energies,

$$\frac{dE(I)}{E(I)} \equiv [E(I)_{th(fit)} - E(I)_{exp}]/E(I)_{exp}. \qquad (4)$$

Each panel is for a given spin and each point is a specific nucleus, plotted according to its $R_{4/2}$ value so that the dependence of the fit quality on structure can be seen at a glance.

Figure 2 gives the values of the fitted parameters $\mathcal{J}_0$ and α, again plotted against $R_{4/2}$. The positive values of α reflect the well known fact that $\mathcal{J}$ increases with spin, due to centrifugal stretching, pairing, or other effects.

Our survey of nuclei includes a wide range of species. To show how different classes of nuclei behave, Fig. 2 uses different symbols for the main bulk of nuclei (with $Z=54-76$), Pt, Hg, and the actinides. Particularly for $\mathcal{J}_0$, the behavior of these classes is interesting. The actinides have

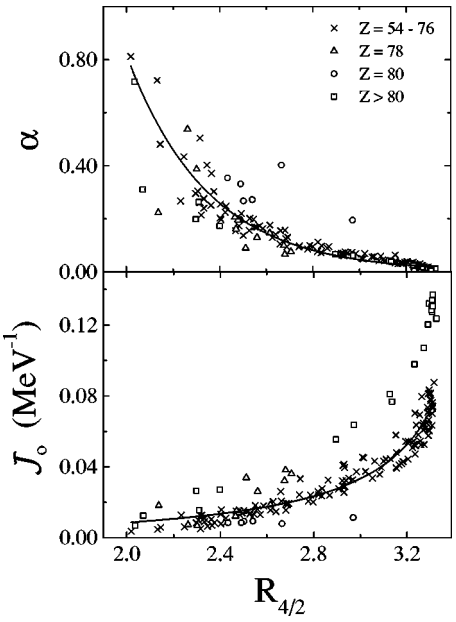

FIG. 2. Values of the fitted parameters $\mathcal{J}_0$ and α as a function of $R_{4/2}$ from the least squares fit shown in Fig. 1. The continuous curves are fits to the data with $\mathcal{J}_0=260e^{-x/0.35}$ and $\alpha=x/(530-150x)$, where $x\equiv R_{4/2}$.

systematically larger $\mathcal{J}_0$ values, reflecting the smaller energy spacings both for deformed and spherical nuclei. The Pt nuclei near the O(6) limit ($R_{4/2}\sim 2.6$) also have relatively large $\mathcal{J}_0$ values. In contrast, the Hg isotopes, where coexisting sets of levels descend into and mix with the yrast levels, show anomalous behavior. For $R_{4/2}>2.4$, the main trajectories of parameter values in Fig. 2 have a smooth and relatively compact trend. As a guide to these trends, $\mathcal{J}_0$ and α are parametrized in terms of $R_{4/2}$ and the resulting curves, fitting the data, are shown in Fig. 2. We caution that the $\mathcal{J}_0$ and α values given by these expressions are not meant to be used for fits in new nuclei but just as rough guidelines that may be of some use in nuclei off stability where only the lowest yrast levels are known.

The results in Fig. 1 are interesting and clearly confirm that Eq. (3) provides an useful expression for yrast energies in *all* structural regions. The deviations from experiment are small throughout the range of nuclei, $R_{4/2}$ values, and spins (and especially from $R_{4/2}\sim 2.8-3.2$, see below). Several nuclei are almost perfectly reproduced: more or less random examples spanning a range of $R_{4/2}$ values are ^{244}Pu($R_{4/2}=3.32$), ^{172}W($R_{4/2}=3.06$), ^{152}Sm($R_{4/2}=3.01$), and ^{158}Yb($R_{4/2}=2.33$).

Any good quality method of correlating large amounts of data can often also serve to highlight cases where relatively large deviations occur. In the present case, these appear in two forms—either as nuclei with relatively poor fits or nuclei whose fit parameters stray from the smooth trends. Examples of the former in Fig. 1 are ^{182}Os($R_{4/2}=3.15$) and several Hg isotopes ($2.4<R_{4/2}<2.9$) at $I=6^+$. These exceptions are not unexpected since they are probably related to the presence of deformed intruder states in the low lying spectrum. In Fig. 2, the α values for the same Hg isotopes again stand out above

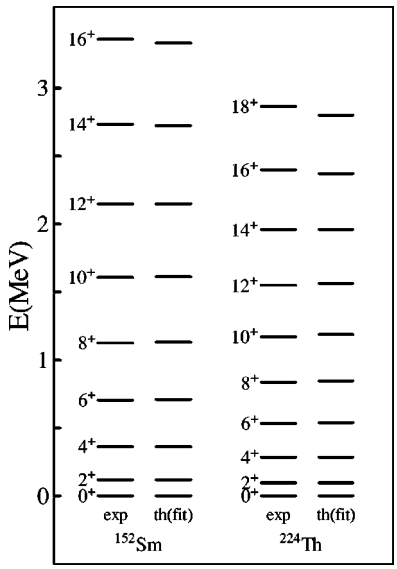

FIG. 3. Comparison of experimental level energies with fits of Eq. (3) for ^{152}Sm and ^{224}Th. Fits with the VMI [10] are comparable but Eq. (3) is simpler, more intuitive, and works well over a broader range of $R_{4/2}$ values.

the general trend. In the plot of the $\mathcal{J}_0$ values the Pt isotopes stand out at $R_{4/2}\sim 2.5$, and the entire region of transitional actinide nuclei ($2.3\lesssim R_{4/2}\lesssim 3.2$) follow a trajectory well above the main trend.

The results for the highest spins $(18^+, 20^+)$ in Fig. 1 point to an interesting aspect of the energy expression. Note the trend in the deviations for these spins. There is a slight slope from negative values near $R_{4/2}=2.7$ to positive for rotor nuclei. The origin of this should be pursued. We only note here that, if the βE term is kept in Eq. (2), this trend flattens out. We stress that with either formula for $\mathcal{J}$, the deviations nearly vanish near $R_{4/2}\sim 3.0$, which is a value typical of soft or transitional nuclei and of phase transitional structures such as X(5) [6]. This suggests that Eq. (3) is particularly suited for such nuclei, which tend to be less well adapted to other energy expressions whose starting point is the pure rotor or vibrator.

To illustrate the quality of the fits for soft rotors, we show in Fig. 3 the data and fits for two such nuclei, namely ^{152}Sm, which has been of much interest lately as a critical point nucleus [8], and ^{224}Th, with $R_{4/2}=3.1$. The fits are, indeed, almost perfect. Other energy formulas, such as the VMI [10], also produce good fits, but we feel Eq. (3) is simpler and more intuitive.

This suggests a specific use of Eq. (3), applicable especially in exotic nuclei. In such nuclei, data will be sparse and, especially after first experiments on new nuclei, only a couple of levels (e.g., 2_1^+, 4_1^+) may be known. In such cases, if $R_{4/2}$ is in the range $\sim$2.8 to $\sim$3.2, one can use Eq. (3) in "predictive" mode by fitting the 2^+ and 4^+ states exactly and predicting the higher spin levels.

This approach can provide useful guides in designing further experiments to identify higher levels by their γ-ray decays. Such predictions, if they turn out to be incorrect, can be of use in identifying nuclei with exotic structures. Given that

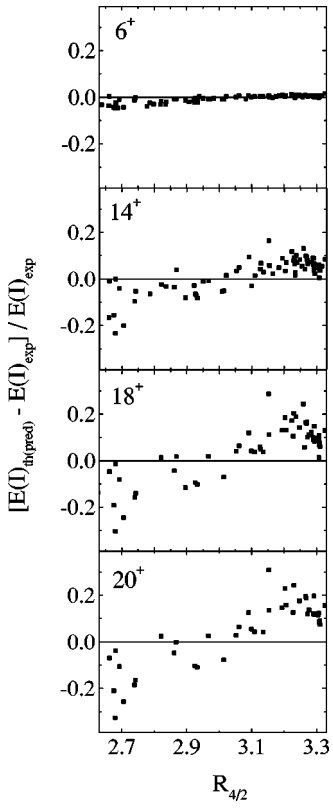

FIG. 4. Similar to Fig. 1, but the theoretical values were obtained by fixing the parameters using the 2^+ and 4^+ energies.

one expects unfamiliar behavior to be a more common feature of nuclei far off stability, Eq. (3) could provide a very useful guide.

To illustrate the predictive power of Eq. (3) for soft nuclei, we show the predictions for $I=6^+-20^+$, for $R_{4/2}$ values above 2.6 in Fig. 4. Naturally, the deviations are larger than with the least squares fit to all the energies. They grow with spin, and they show the same systematic trend as seen in Fig. 1 of underpredicting the energies near $R_{4/2}\sim 2.7$ and overpredicting them for $R_{4/2}\sim 3.2$. As before, the results are excellent near $R_{4/2}\sim 3.0$.

To summarize, we have proposed a new two-parameter energy formula, which is applicable for all collective even-even nuclei, regardless of structure, and which gives excellent fits to the data up to the highest yrast spins known (or up to a backbend/upbend if such effects exist). The formula is particularly successful in soft rotors with $2.8\lesssim R_{4/2}\lesssim 3.2$ which, historically, have been the most difficult to treat.

By providing a tight correlation with the data, the expression provides a means of identifying anomalous nuclei. The energy expression may be particularly useful in exotic nuclei far from stability where it can be used in conjunction with initial data on the lowest yrast energies to provide predictions for higher spin levels, thereby both guiding further experiments and helping to spot the anomalies that are widely expected in exotic nuclei, especially in regions of weak binding.

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