Analysis of $\Delta I = 2$ Staggering
in Nuclear Rotational Spectra

K. Hara
Physik-Department, Technische Universität München
D-85747 Garching bei München, Germany

and

G. A. Lalazissis
Department of Theoretical Physics, Aristotle University of Thessaloniki
GR-54006 Thessaloniki, Greece

Abstract

A method is proposed and tested for the analysis of $\Delta I = 2$ staggering observed in nuclear rotational bands. We examine six super- and hyper-deformed bands, among which that of $^{149}$Gd and possibly of $^{147}$Gd seem to exhibit real staggering. However, we emphasize that the presence of staggering may not necessarily imply the occurrence of bifurcation. It is also shown that a similar staggering seen in normally deformed bands is a manifestation of band crossings. A more extensive analysis is planned.
Recently, a striking feature of $\Delta I = 2$ staggering in rotational spectra has been reported for several super- and hyper-deformed bands [1-7] attracting much attention and interest in the nuclear physics community. As a result, it has become a most frequently debated subject and a considerable amount of effort has been spent on understanding its physical implication based on various theoretical ideas [8-14]. Nevertheless, definite conclusions have not yet been reached until present time. On the other hand, a similar staggering can also be observed in molecular rotational spectra, whose underlying mechanism is not known either. In particular, for diatomic molecules [15-22], the occurrence of staggering is definitely not due to the presence of $C_4$ type symmetry of the system because of their dumb-bell structure. In both nuclear and molecular cases, one presents the experimental data in terms of a 5-point formula (which is denoted as $\Delta E_7$ in Ref.[2])

$$\Delta^{(5)}E_2(I) \equiv \frac{1}{16}[6E_2(I) - 4E_2(I + 2) - 4E_2(I - 2) + E_2(I + 4) + E_2(I - 4)]$$  \hspace{1cm} (1)$$

where we have introduced the notation for an n-point formula $\Delta^{(n)}E_{\Delta I}(I)$ with respect to $E_{\Delta I}(I) \equiv E(I) - E(I - \Delta I).$  \hspace{1cm} (2)

It is the regularity of the result obtained by this formula that one is interested in. It may be instructive to note that, although there is a close similarity between the observation in nuclear and molecular systems, their dynamical laws and the energy scales are totally different except for the kinematical aspect that both of them are “rotating”. This seems to suggest that the phenomenon of staggering is rather independent of characteristic properties of actual systems. The purpose of the present work is to gain more information and insight about the nature of staggering by analyzing experimental data.

A typical example of the $\Delta I = 2$ staggering in nuclear rotational spectra is presented in Fig. 1 for a super-deformed band of the nucleus $^{149}$Gd [1].

![Fig. 1](image-url)

It is usual to interpret such a $\Delta I = 2$ staggering as the occurrence of a $\Delta I = 4$ bifurcation in the corresponding spectrum. However, we stress that it may not necessarily be true. In
fact, one notices a remarkable fact that the same spectrum shows also a $\Delta I = 4$ staggering if one applies the 5-point formula with $\Delta I = 4$ \cite{23}.

$$\Delta^{(5)} E_4(I) \equiv \frac{1}{16}[6E_4(I) - 4E_4(I + 4) - 4E_4(I - 4) + E_4(I + 8) + E_4(I - 8)]. \quad (3)$$

Note that $E_4(I)$ is obtained from the $\Delta I = 2$ transition energy $E_2(I)$ using the relation

$$E_4(I) = E(I) - E(I - 4) = E_2(I) + E_2(I - 2).$$

Figs. 2 shows the 5-point formula (3) resulting from the same data as Figs. 1.

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Fig. 2

According to the usual interpretation, one would conclude from Figs. 2 that there exists a $\Delta I = 8$ bifurcation. Similarly, for a spectrum measured over a sufficiently wide range of spins as in the case of many molecular bands, one can observe a $\Delta I = 6$ staggering in the quantity $\Delta^{(5)} E_6(I)$, from which one might conclude the existence of a $\Delta I = 12$ bifurcation \cite{23}. We would consider it rather questionable to regard such a result as a finger print of bifurcations. In the same token, the $\Delta I = 2$ staggering might not necessarily imply the presence of a $\Delta I = 4$ bifurcation. Although the bifurcation may be a possible interpretation, it has to be proved (or disproved) by further theoretical investigations. Accordingly, it seems necessary to gain more information and insight about the nature of the staggering from the existing data and this is what we aim at in the present work.

A large number of similar staggering can be found also in the yrast spectra of normally deformed doubly even rare-earth nuclei. Let us take the nucleus $^{160}$Yb \cite{24} as an example. Figs. 3 and 4 show the results of 5-point formulas (1) and (3), respectively.

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Fig. 3     Fig. 4

Although one sees both $\Delta I = 2$ and $\Delta I = 4$ staggering in these figures, no one would believe that the yrast spectrum of $^{160}$Yb possesses any kind of bifurcation. On the one hand, the formulas (1) and (3) are proportional roughly to the “fifth” order derivative of
the energy $E(I)$ in finite differences. On the other hand, it is known that there are crossings between the g- and s-band around $I = 12$ and between the s- and a 4-quasiparticle band around $I = 26$ in this nucleus [25]. This fact gives us a hint about a possible origin of the staggering at least for the present case. Indeed, if there occurs a band crossing, the spectrum will have a kink at the crossing point so that its derivatives become discontinuous. Because of the use of finite differences, however, this discontinuity propagates over other spin values and appears as a staggering over a certain spin range around the crossing point. Obviously, this is a localized phenomenon centered at the crossing point but, if more than one band crossing takes place sequentially, the staggering can extend over a wider spin region. This is what we actually see in Figs. 3 and 4.

In order to make the mechanism qualitatively described above more quantitative and clearly visible, let us tailor a simple schematic model in which two band crossings take place among three unperturbed bands, which is essentially an extension of a two-band crossing model discussed in [28]. Their rotational energies will be assumed as

$$
E_0 = A_0 I(I + 1) \\
E_1 = A_1 [I(I + 1) - 2B_1 (I - I_1)] + C_1 \\
E_2 = A_2 [I(I + 1) - 2B_2 (I - I_2)] + C_2
$$

(4)

with $A_0 > A_1 > A_2$. The band 0 and 1 are assumed to cross each other at $I = I_1$ and band 1 and 2 at $I = I_2$ ($I_1 < I_2$). The quantity $B_1$ ($B_2$) controls the crossing angle between band 0 and 1 (1 and 2) while $C_1$ and $C_2$ are determined by the crossing conditions such that $E_0 = E_1$ at $I = I_1$ and $E_1 = E_2$ at $I = I_2$, so that they are given by

$$
C_1 = (A_0 - A_1)I_1(I_1 + 1), \quad C_2 = (A_1 - A_2)I_2(I_2 + 1) - 2A_1B_1(I_2 - I_1) + C_1.
$$

(5)

For simplicity, we assume that only the lowest two bands couple with each other as the band higher than the lowest two is unimportant for the yrast energy in the crossing region. The coupling strength will be taken to be spin independent. The yrast energy of the system thus becomes

$$
E(I) = E - \sqrt{D^2 + V^2}
$$

(6)
where the quantities $E$, $D$ and $V$ are defined by

$$E = \frac{1}{2}(E_0 + E_1), \quad D = \frac{1}{2}(E_0 - E_1) \quad \text{and} \quad V = V_{01} \text{ if } E_0 \leq E_2$$

and

$$E = \frac{1}{2}(E_1 + E_2), \quad D = \frac{1}{2}(E_1 - E_2) \quad \text{and} \quad V = V_{12} \text{ if } E_0 > E_2.$$ (8)

To visualize the situation clearly, we present a diagram for the rotational energies of these bands (lines) together with the yrast energy (dots) in Fig. 5.

The yrast spectrum has a kink at a crossing point. We note that the sharpness of a kink determines the amplitude of the resulting staggering. Obviously, the larger the crossing angle and/or the weaker the coupling strength, the sharper the kink making the amplitude of the staggering larger. In fact, if the band coupling is switched off, the yrast energy (6) becomes $E(I) = E - |D|$ which leads to the sharpest possible kink for a given crossing angle. In this limiting case, the discontinuity of derivatives of $E(I)$ at a crossing point arises from the term $|D|$ because $D$ changes sign at each crossing point.

Figs. 6 and 7 show respectively the case of vanishing and non-vanishing coupling strength for the yrast energy (6) using the formula (1), which produces a $\Delta I = 2$ staggering. Needless to say, the formula (3) will produce a $\Delta I = 4$ staggering if one uses it in place of the formula (1). The feature of a staggering depends sensitively on the crossing angle, the relative position of the crossing points and the strength of the coupling. One can simulate and study possible features of staggering by changing the parameters of the model. It should be clearly stated that the staggering in question is caused by the use of a 5-point formula and is not due to a physical effect. It is merely a manifestation of band crossings which produce kinks in the spectrum. For the analysis of data, one should avoid using
formulas such as Eqs. (1) and (3) which are not free from the effect of band crossings. Such an effect has to be first removed if one wants to see the presence of real (physical) staggering. On the one hand, what we are ultimately interested in is the actual behavior of the $\Delta I = 2$ transition energy $E_2(I)$. On the other hand, this quantity is a globally increasing function of spin extending from some 100 keV to a value well beyond 1 MeV, so that its fine variations of less than 1 keV are invisible in the plot of $E_2(I)$. However, this is only a matter of proper scaling. We can circumvent it by subtracting a smoothly increasing part from the measured transition energy $E_2(I)$.

For this purpose, let us define a 1-point formula by the expression

$$\Delta^{(1)}E_2(I) \equiv E_2(I) - a - bI - cI^2 - dI^3. \quad (9)$$

The coefficients $a$, $b$, $c$ and $d$ are determined by minimizing the function

$$f(a, b, c, d) = \sum_{I}^{|\Delta I = 2|} [\Delta^{(1)}E_2(I)]^2 \quad (10)$$

with respect to $a$, $b$, $c$ and $d$. The summation over spin $I$ in Eq. (10) is taken in step of $\Delta I = 2$. If the absolute spins are not known as in the case of a super- or hyper-deformed band, we may measure them with respect to a (unknown) reference spin $I_{\text{ref}}$, which means that we simply take $I = 2, 4, \cdots$. The minimization conditions

$$\frac{\partial f(a, b, c, d)}{\partial a} = \frac{\partial f(a, b, c, d)}{\partial b} = \frac{\partial f(a, b, c, d)}{\partial c} = \frac{\partial f(a, b, c, d)}{\partial d} = 0$$

lead to a set of linear equations for $a$, $b$, $c$ and $d$

$$S_0a + S_1b + S_2c + S_3d = F_0$$
$$S_1a + S_2b + S_3c + S_4d = F_1$$
$$S_2a + S_3b + S_4c + S_5d = F_2$$
$$S_3a + S_4b + S_5c + S_6d = F_3 \quad (11)$$

where the coefficients in these equations are defined by

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1 The determinant of Eq. (11) is ill-conditioned. First eliminate $d$ by using the fourth equation and then solve the resulting linear equations for $a$, $b$ and $c$ for the sake of numerical stability.
\[ S_n = \sum_{I} \Delta I^n, \quad F_n = \sum_{I} I^n E_2(I). \] (12)

The subtracting part \( a + bI + cI^2 + dI^3 \) is thus nothing other than the \( \chi \)-square fit of \( E_2(I) \). For the schematic model presented above as well as for a normally deformed band, subtracting a linear term \( a + bI \) is sufficient. However, for a super-/hyper-deformed and molecular band, the spectrum will behave globally as

\[ E(I) \approx AI(I + 1) + B[I(I + 1)]^2, \] (13)

so that inclusion of higher order terms of \( I \) may be significant. We note that, depending on the sign of the quantity \( B \) in Eq. (13), the effective moment of inertia will decrease \((B > 0, \) a stretched rotational spectrum\) or increase \((B < 0, \) a compressed rotational spectrum\) as a function of spin. Both cases are possible for super-/hyper-deformed bands while molecular bands belong to the latter. We will come back to this point later.

The 1-point formula (9) would not change the staggering feature of \( E_2(I) \), if any. The quantity \( \Delta^{(1)}E_2(I) \) represents a deviation from the mean (smooth) behavior of \( E_2(I) \) and changes its sign by construction which should not be confused with regular oscillations. In particular, a sudden decrease of the value of \( \Delta^{(1)}E_2(I) \) implies that there is a band crossing. If the regular oscillations which are present in \( \Delta^{(5)}E_2(I) \) disappear in \( \Delta^{(1)}E_2(I) \), it means that this staggering is produced by band crossings or more generally by kinks in \( \Delta^{(1)}E_2(I) \). It should be stressed that even a weak kink in \( \Delta^{(1)}E_2(I) \) will cause a discontinuity of its derivatives and this will produce a staggering in \( \Delta^{(5)}E_2(I) \). In other words, the 5-point formula (1) is so fragile that it may well happen that the same band measured at different laboratories might exhibit different staggering features due to different experimental uncertainties. In contrast, the 1-point formula (9) is robust and reliable.

On the other hand, if the quantity \( \Delta^{(1)}E_2(I) \) exhibits regular oscillations, there can be two possible reasons, the occurrence of either a real (physical) staggering or successive band crossings that take place closely one after the other. One cannot distinguish these two cases from each other without going into a detailed theoretical analysis of the system. We now present results of the 1-point formula (9).
Figs. 8 and 9 show the results of the 1-point formula (9) applied to the schematic model (cf. Fig. 7) and the nucleus $^{160}$Yb (cf. Fig. 4), respectively. These figures exhibit no regular oscillation and thus indicate correctly that the staggering seen in Figs. 7 and 4 stem from band crossings. A weak (third) band crossing is seen in the nucleus $^{160}$Yb in the highest spin region. In general, we can state that the mechanism leading to the staggering in normally deformed bands can be attributed to such band crossings. These examples are however just to show how the 1-point formula works. In what follows, we turn to the analysis of super-/hyper-deformed bands.

Fig. 10 shows the 1-point formula (9) applied to the super-deformed band of the nucleus $^{149}$Gd (cf. Fig. 1). In this figure, one sees regular oscillations in the spin region 16 – 36 (relative to an unknown reference spin $I_{ref}$). It is most likely that they do not stem from band crossings. The reason will be given below in connection with the (dynamic) moment of inertia.

The dynamic moment of inertia (a 2-point formula)

$$\Theta^{(2)} = \frac{4}{\Delta^{(2)}E_2(I)},$$

$$\Delta^{(2)}E_2(I) \equiv E_2(I + 2) - E_2(I)$$

(14)

can provide us with some information about the staggering depending on the situation. As mentioned before, the quantity $B$ in Eq. (13) can be positive (a stretched rotational spectrum) or negative (a compressed rotational spectrum) in super- and hyper-deformed bands corresponding to globally decreasing (e.g. $^{149}$Gd and $^{154}$Er) or globally increasing (e.g. $^{191}$Hg and $^{194}$Hg) moment of inertia, although there is the third case in which the moment of inertia oscillates about a certain value (e.g. $^{147}$Gd and $^{195}$Pb). If the moment of inertia decreases, one may exclude the occurrence of band crossing. In fact, it should increase if there occurs a band crossing because the moment of inertia of the crossing band
has to be larger than that of the crossed band. Figs. 11 and 12 compare the dynamic moments of inertia for $^{149}$Gd and $^{194}$Hg, respectively.

One can exclude band crossing in the case of the nucleus $^{149}$Gd as its moment of inertia decreases (globally) with spin. One may thus conclude that the staggering in this nucleus is most likely a real (physical) one. However, for the nucleus $^{194}$Hg, one cannot exclude possible band crossing as its moment of inertia increases. Under such a circumstance, it is most interesting to compare the 5-point formula (1) with the 1-point formula (9). This is done in Figs. 13 and 14.

Although one may regard the 5-point formula for $^{194}$Hg practically as zero because of large error bars, it shows a staggering if one takes the most probable values of data. On the other hand, the 1-point formula for this nucleus is outside the error bars and clearly shows irregular kinks. It is clear that the staggering of $\Delta^{(5)}E_2(I)$ for $^{194}$Hg stems from irregular kinks which lead to discontinuities in the derivative of $\Delta^{(1)}E_2(I)$. Therefore, the staggering in question is not a real one. The result for the nucleus $^{191}$Hg is similar.

On the other hand, the moment of inertia of $^{147}$Gd and $^{195}$Pb oscillate about some values. The 1-point formula for $^{147}$Gd shows a staggering which is not so regular as in the case of $^{149}$Gd while that of $^{195}$Pb shows mostly irregular kinks although a very short oscillation can be seen if one discards error bars. Finally, the moment of inertia of the nucleus $^{154}$Er decreases as in the case of $^{149}$Gd. However, the 1-point formula shows only irregular kinks so that the staggering in this nucleus is not a real one either. Fig. 15 summarizes the results of the 1-point formula quoted in these discussions.

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$^2$We note in passing that a staggering can be regarded as a series of “regular kinks” due to large and small function values that occur alternatingly.
In Fig. 15, all error bars are removed for the sake of clarity but we remark that one may not conclude the presence of oscillations if the amplitude of the staggering is small because of large error bars. This applies in particular to the nucleus $^{191}$Hg and $^{195}$Pb. Among six nuclei studied in the present work, the nucleus $^{149}$Gd and possibly $^{147}$Gd remain as candidates of exhibiting real staggering, although a possibility of band crossings cannot be excluded in the latter. However, as we stressed before, whether a staggering implies bifurcation of the corresponding spectrum or not has to be investigated in future studies. On the other hand, kinks that occur in the 1-point formula inherently produce oscillations in the 5-point formula, so that a staggering of such an origin should not be accepted as a real (physical) one, although there may still be a room for debating whether or not random kinks in measured transition energies have physical significance to be studied in more detail. In any case, irregular kinks should be understood differently from a regular staggering. We mention in this connection that, theoretically, an irregularity would be more difficult to understand than a regularity.

To summarize, we have attempted to obtain as much information as possible from (some) existing data to gain more insight to the nature of observed staggering. In the first place, we called attention to the fact that the use of 5-point formulas (1) and (3) always produce a $\Delta I = 2$ and $\Delta I = 4$ staggering, respectively. This fact warns of the danger of concluding the existence of bifurcations simply from the presence of staggering patterns. We emphasize that, even if a staggering turns out to be a real one, it may or may not imply a bifurcation. At present, its physical interpretation is not well established and thus has to be still sought in future theoretical studies. We also called attention to the fact that band crossings can lead to a staggering if one uses a multi-point formula. For normally deformed bands, this is the origin of the staggering.

Most generally speaking, the feature of a staggering depends on the multi-point formula one uses for the presentation of data as it originates from (regular as well as irregular)
kinks that occur in measured transition energies. In fact, a 3-point formula

\[ \Delta^{(3)} E_2(I) \equiv E_2(I) - \frac{1}{2}[E_2(I + 2) + E_2(I - 2)] \]

will produce less number of oscillations than the 5-point formula [28]. To avoid such a formula-dependence as well as the effect of band crossings, we proposed to use the 1-point formula (9) which measures a deviation from the smooth behavior. It provides us with more direct information of the transition energy than multi-point formulas.

The following table summarizes the result of six super- and hyper-deformed bands studied in the present work. The question mark in the last column for the nucleus \(^{147}\text{Gd}\) is to indicate that the item is not certain but probable.

| Nucleus | 5-Point Formula | Dyn. Mom. Inertia | 1-Point Formula |
|---------|----------------|------------------|----------------|
| \(^{147}\text{Gd}\) | staggering | oscillating | staggering? |
| \(^{149}\text{Gd}\) | staggering | decreasing | staggering |
| \(^{154}\text{Er}\) | staggering | decreasing | irreg. kinks |
| \(^{191}\text{Hg}\) | staggering | increasing | irreg. kinks |
| \(^{194}\text{Hg}\) | staggering | increasing | irreg. kinks |
| \(^{195}\text{Pb}\) | staggering | oscillating | irreg. kinks |

We stress that, before attempting a theoretical analysis of an observed staggering, one should make sure whether the staggering in question is a real one or simply due to irregular kinks. Otherwise, there is a danger that one may be dealing with an object which does not exist in reality and this may lead theoretical investigations in a wrong direction. The proposed 1-point formula is proved to be a useful tool for filtering out such cases, although it is quite possible that the present method of analysis may still have to be improved. For example, one could further subtract a fourth order term in the 1-point formula. In fact, Fig. 15 suggests the presence of such a global behavior. We shall study
this in the future when we carry out a more extensive analysis of the existing data on
super- and hyper-deformed bands.

We have done a similar analysis for molecular rotational bands and confirmed also that
staggering does not necessarily imply bifurcation. The conclusion has been quite similar
to the nuclear case presented here. The result will be reported elsewhere.

Finally, we should like to mention that, with minor modifications (taking $\Delta I = 1$
instead of 2 and subtracting only a first order polynomial $a + bI$ instead of the third
order one), the proposed 1-point formula is applicable to the usual signature dependent
spectrum of a normally deformed band exhibiting a genuine $\Delta I = 1$ staggering (signature
dependence) which leads to the signature splitting (a $\Delta I = 2$ bifurcation). In fact, it
might be quite practical for the analysis of odd proton nuclei and in particular of doubly
odd nuclei in which the signature dependence is in most cases extremely delicate and is
not distinctly discernible if one plots the $\Delta I = 1$ transition energy $E(I) - E(I-1)$ itself.
We remark that, in these nuclei, a bifurcation (signature splitting) and a band crossing
(which may cause a signature inversion) often occur simultaneously [26, 27].

In the meantime, we have noticed that a (two-) band crossing model similar to our
(three-) band crossing model Eq. (4) is used in a recently published work [29], in which
the authors investigate the $\Delta I = 2$ staggering (mainly of the normally deformed bands)
in terms of various multi-point formulas.

One of the authors (G. A. L.) acknowledges a support from the European Union under
the contract TMB-EU/ERB FMBCICT-950216.
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FIGURE CAPTIONS

Fig. 1: $\Delta I = 2$ staggering obtained by the 5-point formula Eq. (1) for a super-deformed band of the nucleus $^{149}$Gd

Fig. 2: $\Delta I = 4$ staggering obtained by the 5-point formula Eq. (3) for a super-deformed band of the nucleus $^{149}$Gd

Fig. 3: $\Delta I = 2$ staggering obtained by the 5-point formula Eq. (1) for the normally deformed band of the nucleus $^{160}$Yb

Fig. 4: $\Delta I = 4$ staggering obtained by the 5-point formula Eq. (3) for the normally deformed band of the nucleus $^{160}$Yb

Fig. 5: Band energies in a schematic band crossing model with three bands 0, 1 and 2 in which the bands 0 and 1 (1 and 2) cross at $I = 12$ (26)

Fig. 6: $\Delta I = 2$ staggering obtained by the 5-point formula Eq. (1) for the schematic band crossing model (band coupling switched off)

Fig. 7: $\Delta I = 2$ staggering obtained by the 5-point formula Eq. (1) for the schematic band crossing model (band coupling switched on)

Fig. 8: The 1-point formula Eq. (9) for the schematic model, cf. Fig. 7

Fig. 9: The 1-point formula Eq. (9) for the nucleus $^{160}$Yb, cf. Fig. 4

Fig. 10: The 1-point formula Eq. (9) for the nucleus $^{149}$Gd, cf. Fig. 1

Fig. 11: The dynamic moment of inertia Eq. (14) for the nucleus $^{149}$Gd

Fig. 12: The dynamic moment of inertia Eq. (14) for the nucleus $^{194}$Hg

Fig. 13: The 5-point formula Eq. (1) for the nucleus $^{194}$Hg, cf. Fig. 14

Fig. 14: The 1-point formula Eq. (9) for the nucleus $^{194}$Hg, cf. Fig. 13

Fig. 15: Results of the 1-point formula Eq. (9) for six super-/hyper-deformed bands
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