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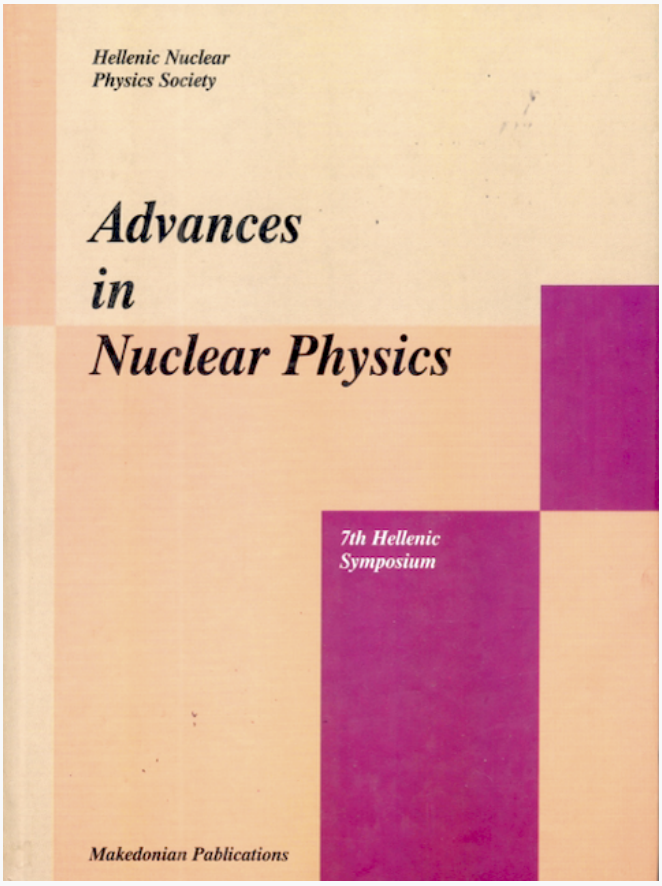

ΔJ = 2 Staggering in Rotational Bands of Diatomic Molecules

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$\Delta J = 2$ Staggering in Rotational Bands of Diatomic Molecules

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Abstract

It is shown that the recently observed $\Delta J = 2$ staggering seen in superdeformed nuclear bands is also occurring in rotational bands of diatomic molecules.

Rotational bands of diatomic molecules [1] and rotational bands of deformed nuclei [2] have many features in common, despite the different energy scales involved in each case. Molecular rotational bands are in general closer to the behavior of the rigid rotator than their nuclear counterparts. In the last decade much interest has been attracted by superdeformed nuclear bands [3-5], which are characterized by relatively high angular momenta and behavior closer to the rigid rotator limit in comparison to normal deformed nuclear bands.

A rather surprising feature has been recently discovered [6-9] in superdeformed nuclear bands: Sequences of states differing by four units of angular momentum are displaced relative to each other, the relative shift being of order of 10^{-4} of the energies separating the levels of these bands. A few theoretical proposals for the possible explanation of this $\Delta J = 4$ bifurcation, which is also called $\Delta J = 2$ staggering, have already been made [10-14].

A reasonable question is therefore whether $\Delta J = 4$ bifurcations (i.e. $\Delta J = 2$ staggering) also occur in rotational spectra of diatomic molecules. We are

going to show in this work that this is indeed the case.

In nuclear physics the experimentally determined quantities are the γ-ray transition energies between levels differing by two units of angular momentum ($\Delta J = 2$). For these the symbol

$$E_{2,\gamma}(J) = E(J+2) - E(J) \tag{1}$$

is used, where $E(J)$ denotes the energy of the level with angular momentum J. The deviation of the γ-ray transition energies from the rigid rotator behavior can be measured by the quantity [7]

$$\begin{aligned}\Delta E_{2,\gamma}(J) = \tfrac{1}{16}(6E_{2,\gamma}(J) - 4E_{2,\gamma}(J-2) - 4E_{2,\gamma}(J+2) \\ +E_{2,\gamma}(J-4) + E_{2,\gamma}(J+4)).\end{aligned} \tag{2}$$

Using the rigid rotator expression $E(J) = AJ(J+1)$ one can easily see that in this case $\Delta E_{2,\gamma}(J)$ vanishes. This is due to the fact that Eq. (2) is the discrete approximation of the fourth derivative of the function $E_{2,\gamma}(J)$.

Several nuclear superdeformed rotational bands such as (a) to (e) for ^{149}Gd [6] and the bands (1) to (3) for ^{194}Hg [7] were analyzed. The corresponding tables are not included in this short presentation, being reserved for a forthcoming longer publication. The analysis shows that the $\Delta E_{2,\gamma}(J)$ values exhibit an anomalous staggering. It should be noted, however, that only for the band (a) of ^{149}Gd [6], the amplitude of the oscillations (see for example fig. 3 of ref. [7]) is definitely outside the experimental errorbars. The following observations can be made:

i) $\Delta E_{2,\gamma}(J)$ obtains alternating positive and negative values. This is why this effect has also been called "$\Delta J = 2$ staggering".

ii) The magnitude of $\Delta E_{2,\gamma}(J)$ is of order 10^{-4}–10^{-5} of that of the γ-ray transition energies.

iii) The staggering oscillation width is an increasing function of the angular momentum J.

In the case of molecules the experimentally determined quantities regard the R branch ($(v_i, J) \rightarrow (v_f, J+1)$) and the P branch ($(v_i, J) \rightarrow (v_f, J-1)$), where v is the vibrational quantum number, and the subscripts i and f indicate the initial and the final band respectively. They are related to transition energies through the equations [15]

$$E^R(J) - E^P(J) = E(v_f, J+1) - E(v_f, J-1) = DE_2(v_f, J-1), \tag{3}$$

$$E^R(J) - E^P(J+2) = E(v_i, J+2) - E(v_i, J) = DE_2(v_i, J), \tag{4}$$

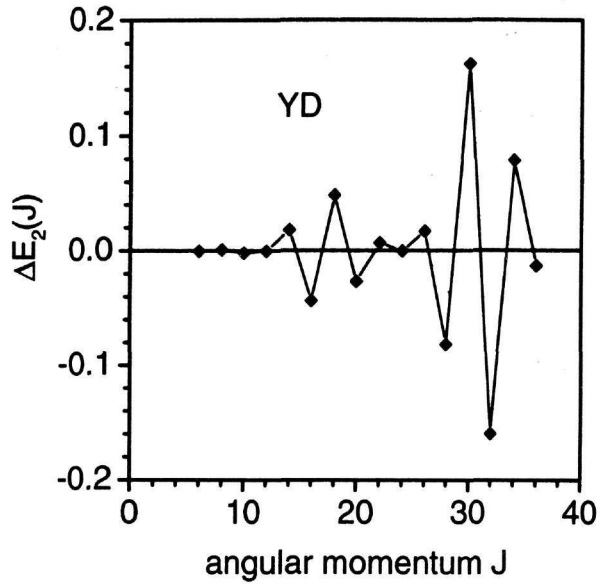

Fig. 1. $\Delta J = 2$ staggering for the rotational band (1-1) $v_f = 1$ of the $C^1\Sigma^+$–$X^1\Sigma^+$ system of the molecule YD. Even values of J are used (data from [16]). The error bars are of the size of the symbols representing the experimental points.

where in general

$$DE_2(v, J) = E(v, J+2) - E(v, J). \tag{5}$$

$\Delta J = 2$ staggering can then be estimated by using Eq. (2), with $E_{2,\gamma}(J)$ replaced by $DE_2(v, J)$:

$$\begin{aligned}\Delta E_2(v, J) = \tfrac{1}{16}\big(&6DE_2(v, J) - 4DE_2(v, J-2) - 4DE_2(v, J+2) \\ &+DE_2(v, J-4) + DE_2(v, J+4)\big).\end{aligned} \tag{6}$$

It is noted that for the sake of simplicity a normalized form of the discrete fourth derivative is used in (6) as well as in the subsequent equations (7), (9), and (12).

We have analyzed quite a few molecular rotational bands for several diatomic molecules. Some of them, revealing a staggering effect, are shown in Figs 1, 2 and 3. In Fig. 1 a typical example of the $\Delta J = 2$ staggering in molecular rotational spectra is shown. The (1-1) $v_f = 1$ rotational band of the $C^1\Sigma^+$–$X^1\Sigma^+$ system of YD (data from [16]) has been used. (The notation means the rotational band built on the $v_f = 1$ vibrational state, as obtained from the R and P branches of the (1-1) transition using Eq. (3).) In Fig. 2 the (2-2) $v_f = 2$ rotational band of the $A^1\Sigma^+$–$X^1\Sigma^+$ system of YN (data from [17]) is drawn. In Fig. 3 the (4-3) $v_f = 4$ band for the CS is given (data from [18]). Similar results

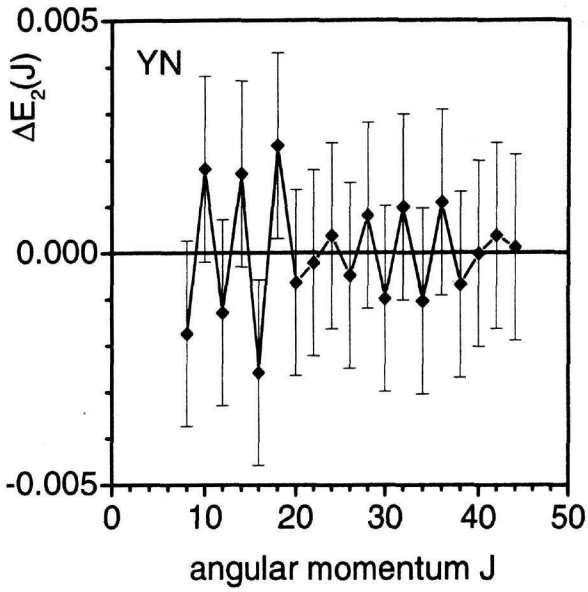

Fig. 2. $\Delta J = 2$ staggering for the rotational band (2-2) $v_f = 2$ of the $A^1\Sigma^+$–$X^1\Sigma^+$ system of YN. Even values of J are used (data from [17]).

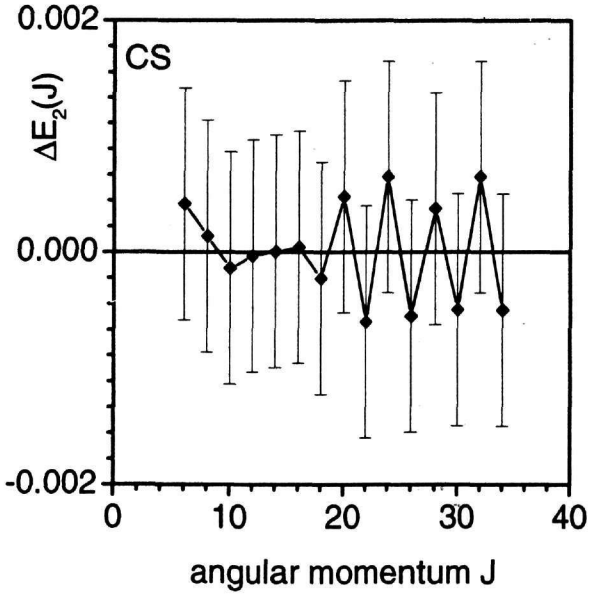

Fig. 3. $\Delta J = 2$ staggering for the rotational band (4-3) $v_f = 4$ for the molecule CS. Even values of J are used (data from [18]).

can be obtained from the other available bands of these molecules and from the $A^6\Sigma^+$–$X^6\Sigma^+$ system of CrD (data from [19]). The following comments are in place:

i) $\Delta E_2(v,J)$ exhibits alternating signs with increasing J, a fingerprint of $\Delta J = 2$ staggering for the v_f band, while the v_i band data (which are not shown) do not permit a clear cut identification of the staggering effect. Even for the v_f bands, only in the case of YD is the magnitude of the effect clearly larger than the experimental uncertainties.

ii) The magnitude of the perturbation, $\Delta E_2(v,J)$, is of order 10^{-3}–10^{-5} of that of the interlevel separation energy.

iii) The staggering oscillation width is not a monotonically increasing function of the angular momentum J. The irregularities in the magnitude of $\Delta E_2(v,J)$ might indicate the presence of subsequent bandcrossings [20]. It is known that the bandcrossing effect is seeing only when the interaction between the two bands which cross each other is relatively weak [21]. Therefore only the levels neighboring the crossing are affected by the interaction. From Eq. (6) it is then clear that perturbing an energy level results in perturbing 5 consequent values of $\Delta E_2(v,J)$. In view of this, Fig. 1 looks very much like depicting two subsequent bandcrossings. Figures 2 and 3, however, do not immediately accept such an interpretation. Bandcrossing has been recently suggested as a possible source of the $\Delta J = 4$ bifurcation in nuclei [22,23].

iv) The staggering effect is more prominent in the case of even angular momentum data than in the case of odd angular momentum data (which are not shown).

One might further wonder if staggering with $\Delta J > 2$ can also occur. In the nuclear case, the existence of $\Delta J = 4$ staggering can be checked by using the quantity

$$\begin{aligned}\Delta E_{4,\gamma}(J) = \tfrac{1}{16}\big(&6E_{4,\gamma}(J) - 4E_{4,\gamma}(J-4) - 4E_{4,\gamma}(J+4) \\ &+E_{4,\gamma}(J-8) + E_{4,\gamma}(J+8)\big),\end{aligned} \tag{7}$$

where

$$E_{4,\gamma}(J) = E(J+4) - E(J). \tag{8}$$

Results for several superdeformed nuclear bands have been calculated. In Fig. 4 the $\Delta J = 8$ bifurcation for the superdeformed band (a) of ^{149}Gd [6] is shown. Note that no angular momentum assignments are shown, since they are still uncertain. The following remarks apply:

i) $\Delta E_{4,\gamma}(J)$ acquires alternating signs with increasing J, indicating the exis-

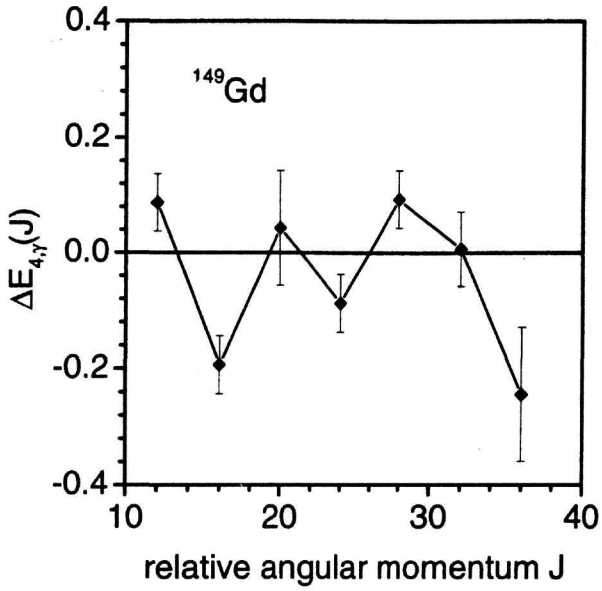

Fig. 4. $\Delta J = 4$ staggering for the superdeformed band (a) of the ^{149}Gd nucleus. (Data from [6].) Since no final angular momentum assignments have been made for this spectrum, angular momentum is measured relative to the lowest observed level of the superdeformed band.

tence of a $\Delta J = 4$ staggering.

ii) The order of magnitude of the $\Delta J = 4$ staggering is the same as that of the $\Delta J = 2$ staggering.

In the case of diatomic molecules one can search for $\Delta J = 4$ staggering by using the quantity

$$\begin{aligned}\Delta E_4(v,J) = \tfrac{1}{16}\big(&6DE_4(v,J) - 4DE_4(v,J-4) - 4DE_4(v,J+4)\\ &+DE_4(v,J-8) + DE_4(v,J+8)\big),\end{aligned} \tag{9}$$

where

$$DE_4(v,J) = E(v,J+4) - E(v,J). \tag{10}$$

In our study we have analyzed the larger known bands of the molecule CS, i.e. the bands (1-0) $v_f = 1$, (2-1) $v_i = 1$, (4-3) $v_i = 3$ [18]. The results for the rotational bands of the $A^6\Sigma^+$-$X^6\Sigma^+$ system of CrD (data from [19]), the $C^1\Sigma^+$-$X^1\Sigma^+$ system of YD (data from [16]), and the $A^1\Sigma^+$-$X^1\Sigma^+$ system of YN (data from [17]) were also considered. For these molecules experimental data of long enough bands exist, permitting the calculations. In Fig. 5 the $\Delta J = 4$ staggering ($\Delta J = 8$ bifurcation) for the (1-1) $v_f = 1$ band of the

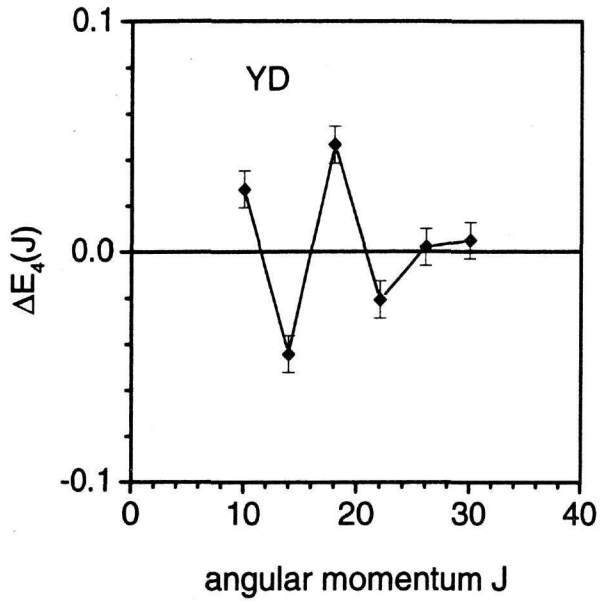

Fig. 5. $\Delta J = 4$ staggering for the rotational band (1-1) $v_f = 1$ of the $C^1\Sigma^+$–$X^1\Sigma^+$ system of the molecule YD. Even values of J are used (data from [16]).

molecule YD is shown. The following comments can be made:

i) Alternating signs of $\Delta E_4(v, J)$, a fingerprint of $\Delta J = 4$ staggering, is shown.

ii) The magnitude of the $\Delta J = 4$ staggering appears to be the same as that of the $\Delta J = 2$ staggering.

$\Delta J = 6$ staggering can be searched for through use of the quantity

$$\begin{aligned}\Delta E_6(v, J) = \tfrac{1}{16}\big(&6DE_6(v, J) - 4DE_6(v, J-6) - 4DE_6(v, J+6) \\ &+DE_6(v, J-12) + DE_6(v, J+12)\big),\end{aligned} \tag{11}$$

where

$$DE_6(v, J) = E(v, J+6) - E(v, J). \tag{12}$$

Calculations have been carried out for a few cases of rotational bands of CS (data from [18]), and for the $B^1\Sigma_u^+$–$X^1\Sigma_g^+$ system of $^{63}Cu^{65}Cu$ (data from [24]), in which bands long enough for such a calculation are known. These results look like being in favor of the existence of $\Delta J = 6$ staggering of the same order of magnitude as $\Delta J = 4$ and $\Delta J = 2$ staggering, but they are not enough for drawing any final conclusions.

The observation of $\Delta J = 2$ and $\Delta J = 4$ staggering in rotational spectra of

diatomic molecules offers a corroboration of the existence of the same effect in nuclei, since the experimental techniques used in each case are quite different, so that the occurrence of the same systematic errors in both cases is improbable. Furthermore, the energy scales involved in nuclei and molecules are very different (the separation of energy levels in molecules is of the order of 10^{-2}eV, while in nuclei of the order of 10^{5}eV), but the staggering effects are in both cases of the same order of magnitude relative to the separation of the energy levels, indicating that the same basic mechanism, possibly related to some perturbations of given symmetry, might be responsible for these effects in both cases.

In conclusion, we have shown that:

i) $\Delta J = 2$ staggering, first observed in superdeformed nuclear bands [6,7], occurs as well in rotational bands of diatomic molecules.

ii) In all cases the magnitude of the $\Delta J = 2$ staggering is 10^{-3}–10^{-5} of that of the separation of the energy levels.

iii) Furthermore $\Delta J = 4$ staggering appears to be present both in superdeformed nuclear bands as well as in rotational bands of diatomic molecules, its order of magnitude being the same as that of the $\Delta J = 2$ staggering in the same physical system.

iv) In most cases the magnitude of the staggering does not show any simple dependence on angular momentum. In several cases one sees about 5 points deviating very much from the smooth rotational behavior, then several points much closer to the pure rotational behavior, then again about 5 points deviating very much from the smooth rotational behavior, and so on. Such a picture raises suspicions about the presence of bandcrossings at the points at which the large deviations occur [22,23].

Concerning the theoretical explanation of the $\Delta J = 2$ staggering effect, some proposals in the nuclear physics framework already exist [10-14]. However, one cannot draw any firm conclusions up to now. In view of the present results, further efforts, in investigating other molecular and nuclear data, are necessary.

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