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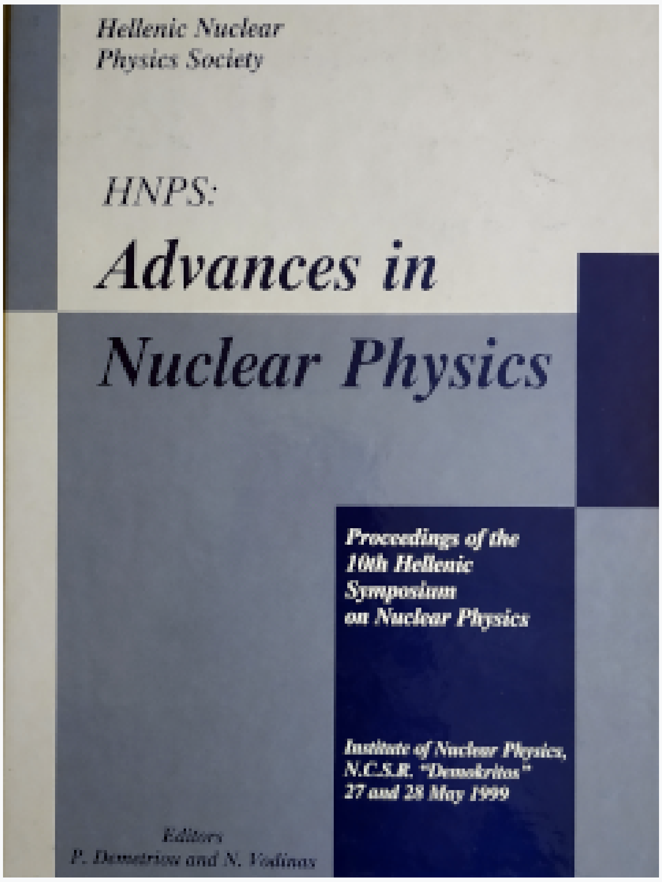

## Staggering Effects in Nuclear and Molecular Spectra

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# Staggering Effects in Nuclear and Molecular Spectra

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## Abstract

It is shown that the recently observed $\Delta I = 2$ staggering seen in superdeformed nuclear bands is also occurring in certain electronically excited rotational bands of diatomic molecules, in which it is attributed to interband interactions (bandcrossings). In addition, a $\Delta I = 1$ staggering effect (i.e. a relative displacement of the levels with even angular momentum $I$ with respect to the levels of the same band with odd $I$) is seen in molecular bands free from $\Delta I = 2$ staggering (i.e. free from interband interactions/bandcrossings). The magnitude of the $\Delta I = 1$ staggering is found to be constant as a function of $I$, in agreement with the predictions of algebraic models (u(11) model, u(16) model, Vector Boson Model) used for the description of octupole nuclear bands, i.e. bands corresponding to pear-like shapes, suggesting that the presence of $\Delta I = 1$ staggering in rotational bands of diatomic molecules could be attributed in general to the inequality of the masses of the two atoms of which the molecule is composed. The existence of the $\Delta I = 1$ staggering effect is corroborated by the fact that separate Dunham expansions for the even levels and the odd levels of such bands give similar but different parameter sets.

## 1 Introduction

Several *staggering* effects are known in nuclear spectroscopy [1]:

1) In rotational $\gamma$ bands of even nuclei the energy levels with odd angular momentum $I$ ($I$=3, 5, 7, 9, ...) are slightly displaced relatively to the levels with even $I$ ($I$=2, 4, 6, 8, ...), i.e. the odd levels do not lie at the energies predicted by an $E(I) = AI(I+1)$ fit to the even levels, but all of them lie systematically above or all of them lie systematically below the predicted energies [2].

2) In octupole bands of even nuclei the levels with odd $I$ and negative parity ($I^\pi$=$1^-$, $3^-$, $5^-$, $7^-$, ...) are displaced relatively to the levels with even $I$ and positive parity ($I^\pi$=$0^+$, $2^+$, $4^+$, $6^+$, ...) [3].

3) In odd nuclei, rotational bands (with $K = 1/2$) separate into signature partners, i.e. the levels with $I$=3/2, 7/2, 11/2, 15/2, ... are displaced relatively to the levels with $I$=1/2, 5/2, 9/2, 13/2, ... [4].

In all of the above mentioned cases each level with angular momentum $I$ is displaced relatively to its neighbours with angular momentum $I \pm 1$. The effect is then called $\Delta I = 1$ *staggering*. In all cases the effect has been seen in several nuclei and its magnitude is clearly larger than the experimental errors. In cases 1) and 3) the relative displacement of the neighbours increases in general as a function of the angular momentum $I$ [2,4], while in case 2) (octupole bands), the relevant models [5–9] predict constant displacement of the odd levels with respect to the even levels as a function of $I$, i.e. all the odd levels are raised (or lowered) by the same amount of energy.

A new kind of staggering ($\Delta I = 2$ *staggering*) has been recently observed [10,11] in superdeformed nuclear bands [12–14]. In the case in which $\Delta I = 2$ staggering is present, the levels with $I$=2, 6, 10, 14, ..., for example, are displaced relatively to the levels with $I$=0, 4, 8, 12, ..., i.e. the level with angular momentum $I$ is displaced relatively to its neighbours with angular momentum $I \pm 2$.

Although $\Delta I = 1$ staggering of the types mentioned above has been observed in several nuclei and certainly is an effect larger than the relevant experimental uncertainties, $\Delta I = 2$ staggering has been seen in only a few cases [10,11,15,16] and, in addition, the effect is not clearly larger than the relevant experimental errors.

There have been by now several theoretical works related to the possible physical origin of the $\Delta I = 2$ staggering effect [17–23], some of them [24–29] using symmetry arguments which could be of applicability to other physical systems as well.

On the other hand, rotational spectra of diatomic molecules [30] are known to show great similarities to nuclear rotational spectra, having in addition the advantage that observed rotational bands in several diatomic molecules [31–34] are much longer than the usual rotational nuclear bands. We have been therefore motivated to make a search for $\Delta I = 1$ and $\Delta I = 2$ staggering in rotational bands of diatomic molecules. The questions to which we have hoped to provide answers are:

1) Is there $\Delta I = 1$ and/or $\Delta I = 2$ staggering in rotational bands of diatomic molecules?

2) If there are staggering effects, what are their possible physical origins?

In Section 2 of the present work the $\Delta I = 2$ staggering in superdeformed nuclear bands will be briefly reviewed. In Section 3 the formalism of the $\Delta I = 2$ staggering in molecular spectra will be given (in Subsection 3.1) and the interpretation of the relevant empirical observations will be discussed (in Subsection 3.2). In Section 4 the formalism of the $\Delta I = 1$ staggering in nuclear and molecular spectra will be given (in Subsection 4.1) and the relevant empirical information will be shown (in Subsection 4.2). In addition, relevant algebraic models will be discussed (in Subsection 4.3) and an interpretation of the empirical observations will be given (in Subsection 4.4). Finally, Section 5 will contain the conclusions of the present study and plans for further work.

## 2 $\Delta I = 2$ staggering in superdeformed nuclear bands

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

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

is used, where $E(I)$ denotes the energy of the level with angular momentum $I$. The deviation of the $\gamma$-ray transition energies from the rigid rotator behavior can be measured by the quantity [11]

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

Using the rigid rotator expression $E(I) = AI(I+1)$, one can easily see that in this case $\Delta E_{2,\gamma}(I)$ vanishes. In addition the perturbed rigid rotator expression $E(I) = AI(I+1) + B(I(I+1))^2$, gives vanishing $\Delta E_{2,\gamma}(I)$. These properties are due to the fact that Eq. (2) is a (normalized) discrete approximation of the fourth derivative of the function $E_{2,\gamma}(I)$, i.e. essentially the fifth derivative of the function $E(I)$.

In superdeformed nuclear bands the angular momentum of the observed states is in most cases unknown. To avoid this difficulty, the quantity $\Delta E_{2,\gamma}$ is usually plotted not versus the angular momentum $I$, but versus the angular frequency

$$\omega = \frac{dE(I)}{dI}, \tag{3}$$

which for discrete states takes the approximate form

$$\omega = \frac{E(I+2)-E(I)}{\sqrt{(I+2)(I+3)}-\sqrt{I(I+1)}}. \tag{4}$$

For large $I$ one can take the Taylor expansions of the square roots in the denominator, thus obtaining

$$\omega = \frac{E(I+2)-E(I)}{2} = \frac{E_{2,\gamma}(I)}{2}. \tag{5}$$

Superdeformed nuclear bands exhibiting $\Delta I = 2$ staggering have been seen in $^{149}$Gd [10] and $^{194}$Hg [11]. Related $\Delta I = 2$ staggering plots can be seen in Figs 1–2 of Ref. [35]. We say that $\Delta I = 2$ staggering is observed if the quantity $\Delta E_2(I)$ exhibits alternating signs with increasing $\omega$ (i.e. with increasing $I$, according to Eq. (5)). The following observations have been made:

1) The magnitude of $\Delta E_2(I)$ is of the order of $10^{-4}$–$10^{-5}$ times the size of the gamma transition energies.

2) The best example of $\Delta I = 2$ staggering is given by the first superdeformed band of $^{149}$Gd, shown in Fig. 1a of Ref. [35]. In this case the effect is almost larger than the experimental error.

3) In most cases the $\Delta I = 2$ staggering is smaller than the experimental error (see Figs 1b, 2a, 2b of Ref. [35]), with the exception of a few points in Fig. 1b of Ref. [35].

## 3 $\Delta I = 2$ staggering in rotational bands of diatomic molecules

### 3.1 Formalism

In the case of molecules [36] the experimentally determined quantities regard the R branch $((v_{lower}, I) \rightarrow (v_{upper}, I+1))$ and the P branch $((v_{lower}, I) \rightarrow (v_{upper}, I-1))$, where $v_{lower}$ is the vibrational quantum number of the initial state, while $v_{upper}$ is the vibrational quantum number of the final state. They are related to transition energies through the equations [36]

$$E^R(I) - E^P(I) = E_{v_{upper}}(I+1) - E_{v_{upper}}(I-1) = DE_{2,v_{upper}}(I), \tag{6}$$

$$\begin{aligned} E^R(I-1) - E^P(I+1) = E_{v_{lower}}(I+1) - E_{v_{lower}}(I-1) \\ = DE_{2,v_{lower}}(I), \end{aligned} \tag{7}$$

where in general

$$DE_{2,v}(I) = E_v(I+1) - E_v(I-1). \tag{8}$$

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

$$\Delta E_{2,v}(I) = \frac{1}{16}(6DE_{2,v}(I) - 4DE_{2,v}(I-2) - 4DE_{2,v}(I+2) \\ +DE_{2,v}(I-4) + DE_{2,v}(I+4)). \tag{9}$$

### *3.2 Interpretation of observations*

Results for several rotational bands in different electronic and vibrational states of various diatomic molecules have been given in Figs 3–9 of Ref. [35]. We say that $\Delta I = 2$ staggering is observed if the quantity $\Delta E_2(I)$ exhibits alternating signs with increasing $I$ ($I$ is increased by 2 units each time). The magnitude of $\Delta E_2(I)$ is usually of the order of $10^{-3}$–$10^{-5}$ times the size of the interlevel separation energy.

The staggering patterns appearing in Figs 3–9 of Ref. [35] can be explained by the assumption that the staggering observed is due to the presence of one or more bandcrossings [37,38]. The following points support this assumption:

1) It is known [39] that bandcrossing occurs in cases in which the interband interaction is weak. In such cases only the one or two levels closest to the crossing point are affected [40]. However, if one level is influenced by the crossing, in the corresponding staggering figure six points get influenced. For example, if E(16) is influenced by the crossing, the quantities $DE_2(15)$ and $DE_2(17)$ are influenced (see Eq. (8) ), so that in the corresponding figure the points $\Delta E_2(I)$ with $I = 11$, 13, 15, 17, 19, 21 are influenced, as seen from Eq. (9). This fact explains why points showing appreciable staggering appear in the figures of Ref. [35] in groups of 6 at a time.

2) It is clear that if bandcrossing occurs, large staggering should appear in approximately the same angular momentum regions of both even levels and odd levels. In the figures of Ref. [35] this is indeed the case.

3) It is clear that when two bands cross each other, maximum staggering will appear at the angular momentum for which the energies of the relevant levels of each band are approximately equal [40]. If this angular momentum value happens to be odd, then $\Delta E_2(I)$ for even values of $I$ in this region (the group of 6 points centered at this $I$) will show larger staggering than the $\Delta E_2(I)$ for odd values of $I$ in the corresponding region, and vice versa. For example, if the closest approach of two

bands occurs for $I = 31$, then $\Delta E_2(I)$ for even values of $I$ in the $I = 26$–$36$ region will show larger staggering than $\Delta E_2(I)$ for odd values of $I$ in the same region. This is in agreement with the empirical observation in the figures of Ref. [35] that in some cases the odd levels show larger staggering than the even levels, while in other cases the opposite holds.

4) The presence of staggering in the "upper" (electronically excited) bands and the lack of staggering in the "lower" (electronic ground state) bands, observed in the figures of Ref. [35], can be attributed to the fact that the electronically excited bands have several neighbours with which they can interact, while the bands built on the electronic ground state are relatively isolated, and therefore no bandcrossings occur in this case. In the case of the CrD molecule, in particular, it is known [32] that there are many strong Cr atomic lines present, which frequently overlap the relatively weaker (electronically excited) molecular lines. In addition, Ne atomic lines are present [32]. Similarly, in the case of the YD molecule the observed spectra are influenced by Y and Ne atomic lines [31], while in the case of the CrH molecule there are Ne and Cr atomic lines influencing the molecular spectra [33].

5) The fact that consistency between results for the same band calculated from two different sets of data is observed in the figures of Ref. [35] only in the cases in which the staggering is much larger than the experimental error, corroborates the bandcrossing explanation. The fact that the results obtained in areas in which the staggering is of the order of the experimental error, or even smaller, appear in the figures of Ref. [35] to be random, points towards the absence of any real effect in these regions.

It should be noticed that bandcrossing has been proposed [41–43] as a possible explanation for the appearance of $\Delta I = 2$ staggering effects in normally deformed nuclear bands [23,41,43] and superdeformed nuclear bands [42].

The presence of two subsequent bandcrossings can also provide an explanation for the effect of mid-band disappearance of $\Delta I = 2$ staggering observed in superdeformed bands of some Ce isotopes [15]. The effect seen in the Ce isotopes is very similar to the mid-band disappearance of staggering seen, for example, in Fig. 3a of Ref. [35].

In conclusion, several examples of $\Delta I = 2$ staggering in electronically excited bands of diatomic molecules have been found. The details of the observed effect are in agreement with the assumption that it is due to one or more bandcrossings. In these cases the magnitude of the effect is clearly larger than the experimental error. In cases in which an effect of the order of the experimental error appears, it has been seen that this is an artifact of the method used, since different sets of data from the same experiment and for the same molecule lead to different staggering results for the same rotational band. The present work emphasizes the need to ensure in all cases (including staggering candidates in nuclear physics) that the effect is larger than the experimental error and, in order to make assumptions about any new symmetry, that it is not due to a series of bandcrossings.

## 4 $\Delta I = 1$ staggering in rotational bands of diatomic molecules

### 4.1 *Formalism*

We have seen that $\Delta I = 2$ staggering appears in several rotational bands of diatomic molecules, and that this effect can be attributed to interband interactions (bandcrossings). In what follows we are going to look for $\Delta I = 1$ staggering in molecular bands free from $\Delta I = 2$ staggering, in order to make sure that $\Delta I = 1$ staggering is not an effect due to the same cause as $\Delta I = 2$ staggering.

In analogy with Eq. (2), $\Delta I = 1$ staggering in nuclei can be measured by the quantity

$$\Delta E_{1,\gamma}(I) = \frac{1}{16}(6E_{1,\gamma}(I) - 4E_{1,\gamma}(I-1) - 4E_{1,\gamma}(I+1) \\ + E_{1,\gamma}(I-2) + E_{1,\gamma}(I+2)), \tag{10}$$

where

$$E_{1,\gamma}(I) = E(I+1) - E(I). \tag{11}$$

The transition energies $E_{1,\gamma}(I)$ are determined directly from experiment.

As we have already seen, in the case of molecules [36] the experimentally determined quantities regard the R branch $((v_{lower}, I) \rightarrow (v_{upper}, I+1))$ and the P branch $((v_{lower}, I) \rightarrow (v_{upper}, I-1))$, which are related to transition energies through Eqs (6) and (7). In order to be able to use an expression similar to that of Eq. (10) for the study of $\Delta I = 1$ staggering in molecular bands we need transition energies similar to those of Eq. (11), i.e. transition energies between levels differing by one unit of angular momentum. However, Eqs (6) and (7) can provide us only with transition energies between levels differing by two units of angular momentum. Assuming for a band $E(0) = 0$ we can determine from Eqs (6) or (7) all of its levels with even $I$

$$E_{v_{upper}}(2) = E^R(1) - E^P(1), \tag{12}$$

$$E_{v_{upper}}(4) = E_{v_{upper}}(2) + E^R(3) - E^P(3), \ldots \tag{13}$$

$$E_{v_{lower}}(2) = E^R(0) - E^P(2), \tag{14}$$

$$E_{v_{lower}}(4) = E_{v_{lower}}(2) + E^R(2) - E^P(4), \ldots \tag{15}$$

In order to be able to determine the levels with odd $I$ from Eqs (6) and (7) in an analogous way, one needs $E(1)$. Then

$$E_{v_{upper}}(3) = E_{v_{upper}}(1) + E^R(2) - E^P(2), \tag{16}$$

$$E_{v_{upper}}(5) = E_{v_{upper}}(3) + E^R(4) - E^P(4), \ldots \tag{17}$$

$$E_{v_{lower}}(3) = E_{v_{lower}}(1) + E^R(1) - E^P(3), \tag{18}$$

$$E_{v_{lower}}(5) = E_{v_{lower}}(3) + E^R(3) - E^P(5), \ldots \tag{19}$$

For the determination of $E(1)$ one could use the overall fit of the experimental data (for the R and P branches) by a Dunham expansion [44]

$$\begin{aligned} E(I) = T_v + B_v I(I+1) - D_v[I(I+1)]^2 \\ +H_v[I(I+1)]^3 + L_v[I(I+1)]^4, \end{aligned} \tag{20}$$

which is usually given in the experimental papers. We found, however, that it is more accurate to fit by a Dunham expansion separately the transition energies for the even levels, as they are obtained from the experimental data through Eqs (6) and (7), and separately the transition energies for the odd levels, obtained from the same equations. The two sets of parameters (one for the even levels and one for the odd levels) obtained in this way are slightly different, as we shall see below, a fact that is an additional indication of some kind of relative displacement between the even and the odd levels, i.e. a fingerprint of $\Delta I = 1$ staggering. We then determine $E(1)$ from the Dunham expansion obtained for the odd levels.

The separate Dunham expansions just mentioned are also useful from another viewpoint. In several cases the experimental data for the R and P branches are "broken", i.e. for certain values of the angular momentum the relevant measurements are missing. Then the Dunham expansions can be used for "mending" the sequence of experimental data, as shown in the following example. Suppose that in some experiment $E^R(18)$ is missing. The energies $E_{v_{lower}}(I)$ with $I = 2$–$18$ can be determined in the way described by Eqs (18), (19), ... In the next step, however, which is

$$E_{v_{lower}}(20) = E_{v_{lower}}(18) + E^R(18) - E^P(20), \tag{21}$$

the problem shows up, since $E^R(18)$ is unknown. In this case we have made the following choice: We determine $E_{v_{lower}}(20)$ from the Dunham expansion for the even levels of this band and then use Eq. (21) in order to determine the "missing" value $E^R(18)$.

After determining the energy levels by the procedure described above, we estimate $\Delta I = 1$ staggering by using the following analogue of Eq. (10),

$$\begin{aligned} \Delta E_{1,v}(I) = \frac{1}{16}(6DE_{1,v}(I) - 4DE_{1,v}(I-1) - 4DE_{1,v}(I+1) \\ +DE_{1,v}(I-2) + DE_{1,v}(I+2)), \end{aligned} \tag{22}$$

where

$$DE_{1,v} = E_v(I) - E_v(I-1). \tag{23}$$

Table 1
Dunham coefficients (Eq. 20) in cm$^{-1}$ for various $v = 0$ bands in the ground $X^6\Sigma^+$ state of CrD. In the first column the source of the data (taken from Ref. [32]), which regard the 0–0 band of the $A^6\Sigma^+$–$X^6\Sigma^+$ system of CrD, is given, while in the last column the angular momentum $I_{max}$ up to which the fitting has been performed is indicated. In the last line of the table the parameters resulting from the overall fit performed in Ref. [32] are shown for comparison.

| | $B_v$ | $10^{-5}D_v$ | $10^{-9}H_v$ | $I_{max}$ |
|---|---|---|---|---|
| R1,P1 even | 3.14377 | 8.28450 | −15.2168 | 18 |
| R1,P1 odd | 3.14537 | 9.21941 | 0.416427 | 19 |
| R2,P2 even | 3.14332 | 9.10426 | 15.9856 | 40 |
| R2,P2 odd | 3.14344 | 9.11832 | 1.64908 | 41 |
| R3,P3 even | 3.14312 | 9.14380 | 1.75501 | 36 |
| R3,P3 odd | 3.14326 | 9.16420 | 1.88112 | 35 |
| Ref. [32] | 3.14249 | 9.08803 | 1.5934 | |

### *4.2 Observations*

The formalism described above has been applied [45] to the 0–0 bands of the $A^6\Sigma^+$–$X^6\Sigma^+$ system of CrD [32]. Attention has been focused on the ground $X^6\Sigma^+$ state, which is known to be free from $\Delta I = 2$ staggering effects [35], while the $A^6\Sigma^+$ state is known to exhibit $\Delta I = 2$ staggering effects, which are fingerprints of interband interactions (bandcrossings) [35]. The Dunham coefficients obtained from the (R1, P1), (R2, P2), (R3, P3) branches for the even levels and for the odd levels of the corresponding bands are given in Table 1, while in Fig. 1 of Ref. [45] the corresponding $\Delta I = 1$ staggering patterns, calculated through Eq. (22) have been given. The following comments apply:

1) The Dunham coefficients obtained in each case for the even levels are very similar but not identical to the coefficients obtained for the odd levels, indicating that a relative displacement of the even levels with respect to the odd levels is present.

2) In Figs 1a, 1c, 1d of Ref. [45] almost constant $\Delta I = 1$ staggering (of different magnitude in each case) is seen. No interpolations of missing experimental data have been used in these figures. $E(1)$ in all figures (and $E(2)$ in Figs 1c, 1d, for which the experimental value of $E^R(0)$ is missing) have been calculated using the Dunham expansion (Eq. (20)). The experimental errors are very small (of the order of 0.001 cm$^{-1}$ for the R and P branches) and thus cannot be seen in the figures. It is clear that $\Delta I = 1$ staggering is an effect much larger than the experimental errors.

3) Concerning the error in the determination of $E(1)$, the following observations can be made: From the numerical values of the Dunham coefficients reported in Table 1

and the form of Eq. (20) it is clear that for $I = 1$ most of the error will come from the $B_v I(I+1)$ term, which in this case is $2B_v$. From the differences between the values of $B_v$ reported in Table 1 we see that the error of $B_v$ will be of the order of $0.002\ \mathrm{cm}^{-1}$. Therefore the error of $E(1)$ will be of the order of $0.004\ \mathrm{cm}^{-1}$, which is much smaller than the $\Delta I = 1$ staggering seen in Figs 1a, 1c, 1d of Ref. [45].

4) Fig. 1b of Ref. [45] is an extension of Fig. 1a, in which the missing experimental value of R(18) has been determined in the way indicated by Eq. (21). The observed "jump" in the staggering at the point corresponding to the interpolation shows the sensitivity of the staggering to small errors in the transition energies. In fact, as we see from Eq. (21), the "jump" is due to the fact that $E(20)$ has been determined from the relevant Dunham expansion. It is easily seen that an error of the order of $0.002\ \mathrm{cm}^{-1}$ in $B_v$ (as estimated in 3) ) can cause an error of the order of $0.84\ \mathrm{cm}^{-1}$ in $E(20)$, for which the first term in the Dunham expansion is $420B_v$. Indeed, the "jump" in Fig. 1b is of the order of $1\ \mathrm{cm}^{-1}$.

### *4.3 Algebraic models*

As we have seen in the previous subsection, there is evidence for $\Delta I = 1$ staggering of constant magnitude in the $v = 0$ bands of the ground $\mathrm{X}^6\Sigma^+$ state of the molecule CrD. It is useful at this point to recall algebraic models used in nuclear structure, which predict constant $\Delta I = 1$ staggering. As we have already mentioned, these models are related to the description of octupole degrees of freedom, which are responsible for the presence of octupole bands, i.e. bands with a sequence of levels with $I^\pi = 0^+, 1^-, 2^+, 3^-, 4^+, 5^-, \ldots$ [46]. These bands are thought to be present in cases in which the nucleus acquires a shape with octupole deformation, i.e. a pear-like shape [47].

#### *4.3.1 The u(11) model*

In the u(11) model [5], $s$, $p$ and $f$ bosons are used. Octupole bands are described in the su(3) limit, which corresponds to the chain

$$\mathrm{u}(11) \supset \mathrm{u}(10) \supset \mathrm{su}(3) \supset \mathrm{o}(3) \supset \mathrm{o}(2). \tag{24}$$

The relevant basis is

$$|N, N_b, \omega_b, (\lambda_b, \mu_b), K_b, I, M>, \tag{25}$$

where $N$ is the total number of bosons labelling the irreps of u(11), $N_b$ is the total number of negative parity bosons ($p$ and $f$) labelling the irreps of u(10), $\omega_b$ is the "missing" quantum number in the decomposition u(10)$\supset$su(3), $(\lambda_b, \mu_b)$ are the Elliott quantum numbers [48] labelling the irreps of su(3), $K_b$ is the "missing" quantum number in the decomposition su(3)$\supset$o(3), $I$ is the angular momentum quantum number labelling the irreps of o(3), $M$ is the $z$-component of the angular momentum labelling the irreps of o(2). The energy eigenvalues are given by

$$E(N_b, \lambda_b, \mu_b, I) = \alpha + \beta N_b + \gamma N_b^2 + \kappa C(\lambda_b, \mu_b) + \kappa' I(I+1), \tag{26}$$

where

$$C(\lambda, \mu) = \lambda^2 + \mu^2 + \lambda\mu + 3\lambda + 3\mu. \tag{27}$$

It is clear that positive parity states occur when $N_b$ is even, while negative parity states occur when $N_b$ is odd. In the case of $N$ being even, the ground state band is sitting in the $(3N, 0)$ irrep, while the odd levels of negative parity are sitting in the $(3N-3, 0)$ irrep. Then from Eq. (22) one obtains

$$\Delta E(I) = \begin{cases} +(\beta + \gamma(2N-1) + 18\kappa N), & \text{for } I = \text{even}, \\ -(\beta + \gamma(2N-1) + 18\kappa N), & \text{for } I = \text{odd}. \end{cases} \tag{28}$$

In the case of $N$ being odd, the ground state band is sitting in the $(3N-3, 0)$ irrep, while the odd levels of negative parity are sitting in the $(3N, 0)$ irrep. Then from Eq. (22) one has

$$\Delta E(I) = \begin{cases} -(\beta + \gamma(2N-1) + 18\kappa N), & \text{for } I = \text{even}, \\ +(\beta + \gamma(2N-1) + 18\kappa N), & \text{for } I = \text{odd}. \end{cases} \tag{29}$$

Since $N$ is a constant for a given nucleus, expressing the number of valence nucleon pairs counted from the nearest closed shells, we see that $\Delta I = 1$ staggering of constant amplitude is predicted.

This model could be used in molecular physics as an extension of the molecular vibron model [49,50], in which rovibrational spectra of diatomic molecules are described in terms of $s$ and $p$ bosons, the latter representing the degree of freedom corresponding to the distance between the two atoms of which the molecule is composed, while the boson number $N$ indicates the number of excitation quanta. The $f$ boson will then correspond to the octupole degree of freedom, which could be due to the fact that the diatomic molecule consists of two unequal atoms, therefore it possesses a pear-like shape, which is a fingerprint of octupole deformation [47].

### *4.3.2 The u(16) model*

In the u(16) model [5,6], $s$, $p$, $d$ and $f$ bosons are taken into account. Octupole bands are described in the su(3) limit, which corresponds to the chain

$$\mathrm{u}(16) \supset \mathrm{u_a}(6) \otimes \mathrm{u_b}(10) \supset \mathrm{su_a}(3) \otimes \mathrm{su_b}(3) \supset \mathrm{su}(3) \supset \mathrm{o}(3) \supset \mathrm{o}(2). \tag{30}$$

The relevant basis is

$$|N, N_a, N_b, \omega_b, (\lambda_a, \mu_a), (\lambda_b, \mu_b), (\lambda, \mu), K, I, M >, \tag{31}$$

where $N$ is the total number of bosons labelling the irreps of u(16), $N_a$ is the number of positive parity bosons labelling the irreps of $\mathrm{u}_a(6)$, and $N_b$ is the number of negative parity bosons labelling the irreps of $\mathrm{u}_b(10)$. The rest of the quantum numbers are analogous to those appearing in the basis of the u(11) model, described above. su(3) is the algebra obtained by adding the corresponding generators of $\mathrm{su}_a(3)$ and $\mathrm{su}_b(3)$. The energy eigenvalues are given by

$$\begin{aligned} E(N_b, \lambda_a, \mu_a, \lambda_b, \mu_b, \lambda, \mu, I) = \alpha + \beta N_b + \gamma N_b^2 \\ +\kappa_a C(\lambda_a, \mu_a) + \kappa_b C(\lambda_b, \mu_b) + \kappa C(\lambda, \mu) + \kappa' I(I+1). \end{aligned} \tag{32}$$

The ground state band is sitting in the $(2N, 0)_a$ irrep (which contains $N$ bosons of positive parity and no bosons of negative parity), while the odd levels of negative parity are sitting in the $(2N-2, 0)_a$ $(3, 0)_b$ $(2N+1, 0)$ band (which contains $N-1$ bosons of positive parity and one boson of negative parity). Then from Eq. (22) one has

$$\Delta E(I) = \begin{cases} -(\beta + \gamma - 2k_a(4N+1) + 18k_b + 4k(N+1)), & I = \text{even}, \\ +(\beta + \gamma - 2k_a(4N+1) + 18k_b + 4k(N+1)), & I = \text{odd}. \end{cases} \tag{33}$$

Therefore $\Delta I = 1$ staggering of constant amplitude is predicted.

In comparison with the molecular vibron model [49], which uses the bosons $s$ and $p$, the u(16) model contains in addition the bosons $d$ and $f$, corresponding to quadrupole and octupole deformations respectively. The constant $\Delta I = 1$ staggering in rotational bands can be used as an argument in favour of the use of the $f$ boson, as we have already seen. The $d$ boson could be added if an argument in favour of its use is found. For the present needs the $f$ boson suffices, i.e. one can remain within the framework of the u(11) model.

### *4.3.3 The Vector Boson Model*

In the Vector Boson Model (VBM) [7–9], the collective states are described in terms of two distinct kinds of vector bosons, whose creation operators $\boldsymbol{\xi}^+$ and $\boldsymbol{\eta}^+$ are o(3) vectors and in addition transform according to two independent su(3) irreducible representations (irreps) of the type $(\lambda, \mu) = (1, 0)$. Octupole bands are described in the su(3) limit of the VBM, which corresponds to the chain

$$\mathrm{u}(6) \supset \mathrm{su}(3) \otimes \mathrm{u}(2) \supset \mathrm{so}(3) \otimes \mathrm{u}(1). \tag{34}$$

The relevant basis is

$$|N, (\lambda, \mu), (N, T), K, I, T_0 >, \tag{35}$$

where $N$ is the total number of bosons labelling the irreps of u(6), $(\lambda, \mu)$ are the Elliott quantum numbers [48] labelling the irreps of su(3), $N$ and $T$ are the quantum numbers labelling the irreps of u(2), $K$ is the "missing" quantum number in the su(3)⊃so(3) decomposition, $I$ is the angular momentum quantum number labelling the irreps of so(3), and $T_0$ is the pseudospin projection quantum number labelling the irreps of u(1). The algebras su(3) and u(2) are mutually complementary [51], their irreps $(\lambda, \mu)$ and $(N, T)$ being related by

$$N = \lambda + 2\mu, \qquad T = \lambda/2. \tag{36}$$

The energy eigenvalues are given by

$$\begin{aligned} E(N, \lambda, \mu, K, I, T_0 = T) &= aN + a_6 N(N+5) \\ &+ a_3 C(\lambda, \mu) + b_3 I(I+1) + a_1 \frac{\lambda^2}{4}. \end{aligned} \tag{37}$$

The ground state band is sitting in the $(0, \mu) = \left(0, \frac{N}{2}\right)$ irrep of su(3), while the odd levels of negative parity are sitting in the $(2, \mu - 1) = \left(2, \frac{N}{2} - 1\right)$ irrep. Then from Eq. (22) one obtains

$$\Delta E(I) = \begin{cases} -(6a_3 + a_1), & \text{for } I = \text{even}, \\ +(6a_3 + a_1), & \text{for } I = \text{odd}. \end{cases} \tag{38}$$

Therefore $\Delta I = 1$ staggering of constant amplitude is predicted.

The vector bosons of the VBM are interpreted as quanta of elementary collective excitations, the boson number $N$ counting the number of excitation quanta. Therefore vector bosons are equally suitable for the description of collective effects both in nuclei and in molecules.

### *4.4 Interpretation*

We have shown evidence for a $\Delta I = 1$ staggering effect (i.e. a relative displacement of the odd levels with respect to the even levels) in rotational bands of diatomic molecules (like the $v = 0$ bands of the ground $X^6\Sigma^+$ state of CrD) which are known to be free from $\Delta I = 2$ staggering (i.e. free from interband interactions/bandcrossings). The magnitude of the $\Delta I = 1$ staggering has been found to be constant as a function of the angular momentum $I$, in agreement with the predictions of algebraic models including octupole degrees of freedom, suggesting a possible explanation of the effect in terms of pear-like shapes, occuring in diatomic molecules in general because of the inequality of the masses of the two atoms of which the molecule is composed. The existence of the effect is corroborated by the fact that Dunham fits of the even levels separately and the odd levels separately for the same rotational band lead to similar but different parameter sets.

$\Delta I = 1$ staggering of constant magnitude has also been seen in several bands of AgH [52]. If the explanation of the effect in terms of octupole (pear-like) shapes due to the inequality of the masses of the two atoms composing the molecule is correct, the effect should be detectable in several cases of bands of diatomic molecules free from bandcrossing effects, while it should be absent in diatomic molecules consisting of two identical atoms. A search for more examples of molecular bands exhibiting constant $\Delta I = 1$ staggering is clearly needed, before final conclusions could be made. A starting point for this search can be these of the bands of the molecules YD, CrH, CoH, which have been found [35] to be free from $\Delta I = 2$ staggering.

In the case of the AgH molecule, in addition to the bands showing constant $\Delta I = 1$ staggering, there are also bands showing $\Delta I = 1$ staggering of varying amplitude [52]. The physical origins of such variations are an interesting problem.

## 5 Conclusions

We have seen that the $\Delta I = 2$ staggering observed in superdeformed nuclear bands is also occuring in certain electronically excited rotational bands of diatomic molecules, in which it is attributed to interband interactions (bandcrossings). (A preliminary version of this work has been given in [53], while a complete version has appeared in [35].) In addition, we have seen that a $\Delta I = 1$ staggering effect (i.e. a relative displacement of the levels with even angular momentum $I$ with respect to the levels of the same band with odd $I$) is observed in molecular bands free from $\Delta I = 2$ staggering (i.e. free from interband interactions/bandcrossings). The magnitude of the $\Delta I = 1$ staggering is found to be constant as a function of $I$, in agreement with the predictions of algebraic models (u(11) model, u(16) model, Vector Boson Model) used for the description of octupole nuclear bands, i.e. bands corresponding to pear-like shapes, suggesting that the presence of $\Delta I = 1$ staggering in rotational bands of diatomic molecules could be attributed in general to the inequality of the masses of the two atoms of which the molecule is composed. The existence of the $\Delta I = 1$ staggering effect is corroborated by the fact that separate Dunham expansions for the even levels and the odd levels of such bands give similar but different parameter sets.

However, further work is called for on the following point: Non-constant $\Delta I = 1$ staggering has been seen in some bands of AgH [52]. The physical reasons behind the variations of the staggering amplitude should be clarified and possible improvements of the relevant algebraic models, which will make them able to incorporate this effect, should be searched for.

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