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ODD–EVEN STAGGERING EFFECTS IN ROTATIONAL SPECTRA OF NUCLEI AND MOLECULES

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Abstract

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1) In octupole bands of light actinides the odd–even staggering is found to exhibit a "beat" behaviour as a function of the angular momentum I, forcing us to revise the traditional belief that this staggering decreases gradually to zero and then remains at this zero value. Various algebraic models (spf-Interacting Boson Model, spdf-IBM, Vector Boson Model, Nuclear Vibron Model) predict in their su(3) limits constant staggering for this case, being thus unable to describe the "beat" behaviour. An explanation of the "beat" behaviour is given in terms of two Dunham expansions (expansions in terms of powers of $I(I+1)$) with slightly different sets of coefficients for the ground state band and the negative parity band, the difference in the values of the coefficients being attributed to Coriolis couplings to other negative parity bands.

2) The existence of 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 examined in molecular bands free from $\Delta I = 2$ staggering (i.e. free from interband interactions/bandcrossings). Bands of YD offer evidence for the absence of any $\Delta I = 1$ staggering effect due to the disparity of nuclear masses, while bands of sextet electronic states of CrD demonstrate that $\Delta I = 1$ staggering is a sensitive probe of deviations from rotational behaviour, due in this particular case to the spin–rotation and spin–spin interactions.

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1 Introduction

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

1) In rotational γ 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,

[1]Deceased.

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^π=1^-, 3^-, 5^-, 7^-, ...) are displaced relatively to the levels with even I and positive parity (I^π=0^+, 2^+, 4^+, 6^+, ...) [3, 4, 5, 6].

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, ...[7].

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*.

A new kind of staggering ($\Delta I = 2$ *staggering*) has been recently observed [8, 9, 10] in superdeformed nuclear bands [11, 12, 13]. If $\Delta I = 2$ staggering is present, then, for example, the levels with I=2, 6, 10, 14, ... 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 (see Ref. [14] for relevant references) 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, some of them using symmetry arguments which could be of applicability to other physical systems as well (see Ref. [14] for relevant references).

In the present work we are going to focus attention on the $\Delta I = 1$ staggering in octupole bands of even nuclei. Such bands are found in the light actinides [3], as well as in the A$\approx$150 mass region [4]. They have been attributed to the existence of octupole deformation, i.e. to the assumption that the nucleus acquires a pear-like shape [5, 6, 15], although alternative interpretations in terms of alpha clustering have been proposed [16, 17].

In particular we are going to examine the dependence of the amplitude of the $\Delta I = 1$ staggering effect on the angular momentum I in octupole bands. The situation up to now has as follows:

1) Algebraic models of nuclear structure appropriate for the description of octupole bands, like the spf-Interacting Boson Model (spf-IBM) with u(11) symmetry [18], the spdf-IBM with u(16) symmetry [18, 19], and the Vector Boson Model (VBM) with u(6) symmetry [20], predict in their su(3) limits $\Delta I = 1$ staggering of constant amplitude, i.e. all the odd levels are raised (or lowered) by the same amount of energy with respect to the even levels [21, 22]. In other words, $\Delta I = 1$ staggering takes alternatively positive and negative values of equal absolute value as I increases.

2) Algebraic models of nuclear structure suitable for the description of alpha clustering effects, like the Nuclear Vibron Model (NVM) with u(6)$\otimes$u(4) symmetry [16], also predict in the su(3) limit $\Delta I = 1$ staggering of constant amplitude [22].

3) Older experimental work [3, 4] on octupole nuclear bands suggests that $\Delta I = 1$ staggering starts from large values and its amplitude decreases with increasing I. These

findings are in agreement with the interpretation that an octupole band is gradually formed as angular momentum increases [15].

Motivated by these recent findings, we make in the present work a systematic study in the light actinide region of all octupole bands for which at least 12 energy levels are known [23, 24, 25, 26, 27, 28, 29], taking advantage of recent detailed experimental work in this region. The questions to which we have hoped to provide answers are:

1) What patterns of behaviour of the amplitude of the $\Delta I = 1$ staggering appear?

2) Can these patterns be interpreted in terms of the existing models [16, 18, 19, 20], or in terms of any other theoretical description?

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, 32, 33, 34] are much longer than the usual rotational nuclear bands. We have been therefore motivated to make a search for $\Delta I = 1$ staggering in rotational bands of diatomic molecules. The questions to which we have hoped to provide answers are:

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

2) If there is, what are its possible physical origins?

It should be noticed that in addition the $\Delta I = 2$ staggering effect has been seen [35] in rotational bands of various molecules (YD, CrD, CrH, CoH), and has been attributed [14] 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 Section 2 of the present paper the formalism of staggering in nuclei is discussed, and is subsequently applied to the experimental data for octupole bands of light actinides in Section 3. Section 4 contains an interpretation of the nuclear experimental observations, while in Section 5 the formalism concerning molecular spectra is developed and is subsequently applied to experimental molecular spectra in Section 6. Finally, in Section 7 the conclusions reached, as well as plans for future work are given.

2 Formalism for nuclei

Traditionally the odd–even staggering ($\Delta I = 1$ staggering) in octupole bands has been estimated quantitatively through use of the expression [36]

$$\delta E(I) = E(I) - \frac{(I+1)E(I-1) + IE(I+1)}{2I+1}, \tag{1}$$

where $E(I)$ denotes the energy of the level with angular momentum I. This quantity vanishes if the first two terms of the expression

$$E(I) = E_0 + AI(I+1) + B(I(I+1))^2 \tag{2}$$

are plugged into it, but it does not vanish if the third term of the above expression is substituted into it. Therefore it is suitable for measuring deviations from the pure rotational behaviour.

Recently, however, a new measure of the magnitude of staggering effects has been introduced [10] in the study of $\Delta I = 2$ staggering of nuclear superdeformed bands. In this case the experimentally determined quantities are the γ-ray transition energies between levels differing by two units of angular momentum ($\Delta I = 2$). For these the symbol

$$E_{2,\gamma}(I) = E(I+2) - E(I) \tag{3}$$

is used. The deviation of the γ-ray transition energies from the rigid rotator behavior is then measured by the quantity [10]

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

Using the perturbed rigid rotator expression of Eq. (2) one can easily see that $\Delta E_{2,\gamma}(I)$ vanishes. This property is due to the fact that Eq. (4) 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 $E(I)$. Therefore we conclude that Eq. (4) is a more sensitive probe of deviations from rotational behaviour than Eq. (1).

By analogy, $\Delta I = 1$ staggering in nuclei can be measured by the quantity

$$\Delta E_{1,\gamma}(I) = \frac{1}{16}(6E_{1,\gamma}(I) - 4E_{1,\gamma}(I-1) - 4E_{1,\gamma}(I+1) + E_{1,\gamma}(I-2) + E_{1,\gamma}(I+2)), \tag{5}$$

where

$$E_{1,\gamma}(I) = E(I+1) - E(I). \tag{6}$$

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

3 Analysis of nuclear experimental data

We have applied the formalism described above to all octupole bands of light actinides for which at least 12 energy levels are known [23, 24, 25, 26, 27, 28, 29] and which show no backbending (i.e. bandcrossing) [37] behaviour. Several of these nuclei ($^{222-226}$Ra, $^{224-228}$Th) are rotational or near-rotational (having $10/3 \geq R_4 \geq 2.7$), while others ($^{218-222}$Rn, ^{220}Ra, $^{220-222}$Th) are vibrational or near-vibrational (having $2.4 \geq R_4 \geq 2$), where the ratio $R_4 = \frac{E(4)}{E(2)}$ is a well known characteristic of collective behaviour. A special case is ^{218}Ra, for which it has been argued [24] that it is an example of a new type of transitional nuclei, in which the octupole deformation dominates over all other types of deformation.

The staggering results for $^{218-222}$Rn, $^{218-226}$Ra, and $^{220-228}$Th, have been given in Fig. 1, Fig. 2, and Fig. 3 of Ref. [22] respectively, which are not reproduced here because of space limitations. In all cases the experimental errors are of the size of the symbol used for the experimental point and therefore are not visible. The following observations can be made:

1) In all cases the shapes appearing are consistent with the following pattern: $\Delta I = 1$ staggering starts from large values at low I, it gradually decreases down to zero, then it starts increasing again, then it decreases down to zero and starts raising again. In other

words, figures resembling beats appear. The most complete "beat" figures appear in the cases of ^{220}Ra, ^{224}Ra, ^{222}Th, as well as in the cases of ^{218}Ra, ^{222}Ra, ^{226}Ra.

2) In all cases within the first "beat" (from the beginning up to the first zero of $\Delta E_{1,\gamma}(I)$) the minima appear at odd I, indicating that in this region the odd levels are slightly raised in comparison to the even levels. Within the second "beat" (i.e. between the first and the second zero of $\Delta E_{1,\gamma}(I)$), the opposite holds: the minima appear at even I, indicating that in this region the odd levels are slightly lowered in comparison to the even levels. Within the third "beat" (after the second zero of $\Delta E_{1,\gamma}(I)$) the situation occuring within the first "beat" is repeated. (Notice that ^{220}Th is not an exception, since what is seen in the figure is the second "beat", starting from $I = 6$.)

3) In the case of ^{222}Rn the decrease of the staggering with increasing I, in the region for which experimental data exist, is very slow, giving the impression of almost constant staggering. One can get a similar impression from parts of the patterns shown, as, for example, in the cases of ^{220}Ra (in the region $I = 12 - 20$), ^{222}Ra (for $I = 9 - 17$), ^{224}Ra (for $I = 10 - 16$), ^{226}Ra (for $I = 14 - 20$), ^{222}Th (for $I = 10 - 18$).

The following comments are also in place:

1) The same "beat" pattern appears in both rotational and vibrational nuclei. The only slight difference which can be observed, is that the first vanishing of the staggering amplitude seems to occur at higher I for the rotational isotopes than for their vibrational counterparts. Indeed, within the Ra and Th series of isotopes under study, the I at which the first vanishing of the staggering amplitude occurs seems to be an increasing function of R_4, i.e. an increasing function of the quadrupole collectivity.

2) The present findings are partially consistent with older work [3, 4]. The limited sets of data of that time were reaching only up to the I at which the first vanishing of the staggering amplitude occurs. It was then reasonable to assume that the staggering amplitude decreases down to zero and remains zero afterwards, since no experimental evidence for "beat" patterns existed at that time.

4 Interpretation of the experimental observations in nuclei

Although the su(3) limits of the various algebraic models mentioned in the introduction are sufficient for providing an explanation for $\Delta I = 1$ staggering in the cases in which this appears as having almost constant amplitude [21, 22], it is clear that some additional thinking is required for the many cases in which the experimental results show a "beat" pattern, as in Section 3 has been seen.

A simple explanation for the appearance of "beat" patterns can be given if one describes the ground state band by

$$E_+(I) = AI(I+1) - B(I(I+1))^2 + C(I(I+1))^3 + \cdots \tag{7}$$

where the subscript + reminds us of the positive parity of these levels, and the negative parity levels by

$$E_-(I) = E_0 + A'I(I+1) - B'(I(I+1))^2 + C'(I(I+1))^3 + \ldots, \tag{8}$$

where the subscript $-$ reminds us of the negative parity of these levels and E_0 is the bandhead energy of the negative parity band. Such expansions in terms of powers of $I(I+1)$ have been long used for the description of nuclear collective bands [38]. They also occur if one considers [39] Taylor expansions of the energy expressions provided by the Variable Moment of Inertia (VMI) model [40] and the $su_q(2)$ model [41]. Notice that fits to experimental data [38] indicate that one always has $A > 0$, $B > 0$, $C > 0$, ..., while A is usually 3 orders of magnitude larger than B, B is 3 orders of magnitude larger than C, etc. A', B', C', ... are assumed to follow a similar pattern. Eq. (7) has been long used in molecular spectroscopy as well, under the name of Dunham expansion [42].

In the above expansions it is reasonable to assume that $A > A'$, $B > B'$, $C > C'$, ... This assumption is in agreement with earlier work [43, 44], in which the Coriolis couplings between the lowest $K = 0$ negative parity band and higher negative parity bands with $K \neq 0$ are taken into account, resulting in an increase of the monent of inertia of the lowest $K = 0$ negative parity band [45]. This argument means that the coefficient A' in Eq. (8), which is inversely proportional to the moment of inertia of the negative parity band, should be smaller than the coefficient A in Eq. (7), which is inversely proportional to the moment of inertia of the positive parity band. In analogy to the relation $A > A'$, which we just justified, one can assume $B > B'$, $C > C'$, ... This last argument is admitedly a weak one, which is however driving to interesting results, as one can easily see.

The details of the explanation of the "beat" patterns in octupole bands in terms of the simple model exposed above have been given in Ref. [22] and are not going to be repeated here, because of space limitations. The conclusion is that the "beat" patterns can be explained in terms of two Dunham expansions with slightly different sets of coefficients, one for the ground state band with quadrupole deformation and another for the negative parity band in which in addition the octupole deformation appears. This is, however, a phenomenological finding, the microscopic origins of which should be searched for.

5 Formalism for molecules

In the case of molecules, the $\Delta I = 1$ staggering will again be estimated through the use of Eq. (5). In the present case, however, 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 I denotes the total angular momentum of the molecule and v_{lower} is the vibrational quantum number of the initial state, while v_{upper} is the vibrational quantum number of the final state [46]. They are related to transition energies through the equations [46]

$$E^R(I) - E^P(I) = E_{v_{upper}}(I+1) - E_{v_{upper}}(I-1) = DE_{2,v_{upper}}(I), \tag{9}$$

$$E^R(I-1) - E^P(I+1) = E_{v_{lower}}(I+1) - E_{v_{lower}}(I-1) = DE_{2,v_{lower}}(I), \tag{10}$$

where in general

$$DE_{2,v}(I) = E_v(I+1) - E_v(I-1). \tag{11}$$

In order to be able to use an expression similar to that of Eq. (5) for the study of $\Delta I = 1$ staggering in molecular bands we need transition energies similar to those of Eq. (6), i.e.

transition energies between levels differing by one unit of angular momentum. However, Eqs (9) and (10) can provide us only with transition energies between levels differing by two units of angular momentum. In order to be able to determine the levels with even I from Eqs (9) or (10), one needs the bandhead energy $E(0)$. Then one has

$$E_{v_{upper}}(2) = E_{v_{upper}}(0) + E^R(1) - E^P(1), \tag{12}$$

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

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

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

In order to be able to determine the levels with odd J from Eqs (9) and (10) 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 $E(0)$ and $E(1)$ one can use the overall fit of the experimental data (for the R and P branches) by a Dunham expansion [42]

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

which is usually given in the experimental papers.

After determining the energy levels by the procedure described above, we estimate $\Delta I = 1$ staggering by using the following analogue of Eq. (5),

$$\Delta E_{1,v}(I) = \frac{1}{16}(6DE_{1,v}(I) - 4DE_{1,v}(I-1) - 4DE_{1,v}(I+1) + DE_{1,v}(I-2) + DE_{1,v}(I+2)), \tag{21}$$

where

$$DE_{1,v}(I) = E_v(I) - E_v(I-1). \tag{22}$$

Using Eq. (22) one can put Eq. (21) in the sometimes more convenient form

$$\Delta E_{1,v}(I) = \frac{1}{16}(10E_v(I) - 10E_v(I-1) + 5E_v(I-2) - 5E_v(I+1) + E_v(I+2) - E_v(I-3)). \tag{23}$$

In realistic cases the first few values of $E^R(I)$ and $E^P(I)$ might be experimentally unknown. In this case one is forced to determine the first few values of $E(I)$ using the Dunham expansion of Eq. (20) and then continue by using the Eqs (12)-(19) from the appropriate point on. Denoting by I_{io} the "initial" value of odd I, on which we are building through the series of equations starting with Eqs (16)-(19) the energy levels of odd I, and by I_{ie} the "initial" value of even I, on which we are building through the series of equations

starting with Eqs (12)–(15) the energy levels of even I, we find that the error for the levels with odd I is

$$Err(E(I)) = D(I_{io}) + (I - I_{io})\epsilon, \tag{24}$$

while the error for the levels with even I is

$$Err(E(I)) = D(I_{ie}) + (I - I_{ie})\epsilon, \tag{25}$$

where $D(I_{io})$ and $D(I_{ie})$ are the uncertainties of the levels $E(I_{io})$ and $E(I_{ie})$ respectively, which are determined through the Dunham expansion of Eq. (20), while ϵ is the error accompanying each $E^R(I)$ or $E^P(I)$ level, which in most experimental works has a constant value for all levels.

Using Eqs (24) and (25) in Eq. (23) one easily sees that the uncertainty of the $\Delta I = 1$ staggering measure $\Delta E_{1,v}(I)$ is

$$Err(\Delta E_{1,v}(I)) = D(I_{io}) + D(I_{ie}) + (2I - I_{io} - I_{ie} - 1)\epsilon. \tag{26}$$

This equation is valid for $I \geq \max\{I_{io}, I_{ie}\} + 3$. For smaller values of J one has to calculate the uncertainty directly from Eq. (23).

6 Analysis of molecular experimental data

6.1 YD

We have applied the formalism described above to the 0–1, 1–1, 1–2, 2–2 transitions of the $C^1\Sigma^+$–$X^1\Sigma^+$ system of YD [31]. We have focused attention on the ground state $X^1\Sigma^+$, which is known to be free from $\Delta I = 2$ staggering effects [14], while the $C^1\Sigma^+$ state is known to exhibit $\Delta I = 2$ staggering effects, which are fingerprints of interband interactions (bandcrossings) [14]. No staggering has been found in the $v = 1$ and $v = 2$ bands of the $X^1\Sigma^+$ state of YD. The relevant details have been given in Ref. [47] and are not reproduced here because of space limitations.

This negative result has the following physical implications. It is known in nuclear spectroscopy that reflection asymmetric (pear-like) shapes give rise to octupole bands, in which the positive parity states ($I^\pi = 0^+, 2^+, 4^+, \dots$) are displaced reletively to the negative parity states ($I_\pi = 1^-, 3^-, 5^-, \dots$) [3, 4, 5, 6, 15, 48]. Since a diatomic molecule consisting of two different atoms possesses the same reflection asymmetry, one might think that $\Delta I = 1$ staggering might be present in the rotational bands of such molecules. Then YD, because of its large mass asymmetry, is a good testing ground for this effect. The negative result obtained above can, however, be readily explained. Nuclei with octupole deformation are supposed to be described by double well potentials, the relative displacement of the negative parity levels and the positive parity levels being attributed to the tunneling through the barrier separating the wells [15, 48]. (The relative displacement vanishes in the limit in which the barrier separating the two wells becomes infinitely high.) In the case of diatomic molecules the relevant potential is well known [30] to consist of a single well. Therefore no tunneling effect is possible and, as a result, no relative displacement of the positive parity levels and the negative parity levels is seen.

6.2 CrD

The formalism of Section 5 has in addition been applied to a more complicated case, the one of the 0–0 and 1–0 transitions of the $A^6\Sigma^+$–$X^6\Sigma^+$ system of CrD [32]. We have focused our attention on the ground state $X^6\Sigma^+$, which is known to be free from $\Delta I = 2$ staggering effects [14], while the $A^6\Sigma^+$ state is known to exhibit $\Delta I = 2$ staggering effects, which are fingerprints of interband interactions (bandcrossings) [14]. The CrD system considered here has several differences from the the YD system considered in the previous subsection, which are briefly listed here:

1) The present system of CrD involves sextet electronic states. As a result, each band of the $A^6\Sigma^+$–$X^6\Sigma^+$ transition consists of six R- and six P-branches, labelled as R1, R2, ..., R6 and P1, P2, ..., P6 respectively [32]. In the present study we use the R3 and P3 branches, but similar results are obtained for the other branches as well.

2) Because of the presence of spin–rotation interactions and spin–spin interactions, the energy levels cannot be fitted by a Dunham expansion in terms of the total angular momentum I, but by a more complicated Hamiltonian, the N^2 Hamiltonian for a $^6\Sigma$ state [49, 50]. This Hamiltonian, in addition to a Dunham expansion in terms of N (the rotational angular momentum, which in this case is different from the total angular momentum $\mathbf{I} = \mathbf{N}+\mathbf{S}$, where S the spin), contains terms describing the spin–rotation interactions (preceded by three γ coefficients), as well as terms describing the spin–spin interactions (preceded by two λ coefficients [32, 49]).

In the present study we have calculated the staggering measure of Eq. (21) for the $v = 0$ band of the $X^6\Sigma^+$ state of CrD, using the R3 and P3 branches of the 0–0 and 1–0 transitions of the $A^6\Sigma^+$–$X^6\Sigma^+$ system. Since in this case the Dunham expansion involves the rotational angular momentum N, and not the total angular momentum I, the formalism of Section 5 has been used with I replaced by N everywhere. This is why the calculated staggering measure of Eq. (21) should in this case be denoted by $\Delta E_1(N)$ and not by $\Delta E_1(I)$, the relevant effect being called $\Delta N = 1$ staggering instead of $\Delta I = 1$ staggering. The details have been given in Ref. [47] and are not going to be repeated here because of space limitations.

The conclusion is that in the $v = 0$ band of the $X^6\Sigma^+$ state of CrD two different calculations give consistent results, despite the error accumulation. The result looks like $\Delta N = 1$ staggering of almost constant amplitude. The reason behind the appearance of this staggering is, however clear: It is due to the omission of the spin-rotation and spin-spin terms of the N^2 Hamiltonian mentioned above [32, 49, 50]. As a result, we have not discovered any new physical effect. What we have demonstated, is that Eq. (21) is a very sensitive probe, which can uncover small deviations from the pure rotational behaviour. However, special care should be taken when using it, because of the accumulation of errors, which is inherent in this method. This problem is avoided by producing results for the same band from two different sets of data, as done in Ref. [47]. If both sets lead to consistent results, some effect is present. If the two sets give randomly different results, it is clear that no effect is present.

It should be pointed out at this point that the appearance of $\Delta I = 1$ staggering (or $\Delta N = 1$ staggering) does *not* mean that an effect with oscillatory behaviour is present.

Indeed, suppose that the energy levels of a band follow the $E(I) = AI(I+1)$ rule, but to the odd levels a constant term c is added. It is then clear from Eq. (23) that we are going to obtain $\Delta E_1(I) = +c$ for odd values of I, and $\Delta E_1(I) = -c$ for even values of I, obtaining in this way perfect $\Delta I = 1$ staggering of constant amplitude c, without the presence of any oscillatory effect. This comment directly applies to the results obtained in Ref. [47] for the $v = 0$ band of the $X^6\Sigma^+$ state of CrD. The presence of $\Delta N = 1$ staggering of almost constant amplitude is essentially due to the omission of the rotation–spin and spin–spin interactions in the calculation of the $E(3)$ and $E(4)$ levels. The difference of the omitted terms in the $N = 3$ and $N = 4$ cases plays the role of c in this case.

7 Discussion

In the present work we have considered $\Delta I = 1$ (odd–even) staggering effects in rotational spectra of nuclei and molecules.

As far as nuclei are concerned, we have demonstrated that octupole bands in the light actinides exhibit $\Delta I = 1$ staggering (odd–even staggering), the amplitude of which shows a "beat" behaviour. The same pattern appears in both vibrational and rotational nuclei, forcing us to modify the traditional belief that in octupole bands the staggering pattern is gradually falling down to zero as a function of the angular momentum I and then remains there.

The su(3) limits of various algebraic models, including octupole degrees of freedom [18, 19, 20] or based on the assumption that alpha clustering is important in this region [16], predict $\Delta I = 1$ staggering of amplitude constant as a function of the angular momentum I [21, 22]. Although this description becomes reasonable in the rotational limit, it cannot explain the "beat" patterns appearing in both the rotational and the vibrational regions. The detailed study of limits other than the su(3) ones for these models remains an interesting open problem.

A simple explanatation of the "beat" behaviour has been given by describing the even I levels of the ground state band and the odd I levels of the negative parity band by two Dunham expansions [42] (expansions in powers of $I(I+1)$) with slightly different sets of coefficients, the difference in the coefficients being attributed to Coriolis couplings of the negative parity band to other negative parity bands. However, the microscopic origins of the "beat" behavior need further elucidation.

In the present work we have in addition addressed the question of the possible existence of $\Delta I = 1$ staggering (i.e. of a relative displacement of the odd levels with respect to the even levels) in rotational bands of diatomic molecules, which are free from $\Delta I = 2$ staggering (i.e. free from interband interactions/bandcrossings). The main conclusions drawn are:

1) The YD bands studied indicate that there is no $\Delta I = 1$ staggering, which could be due to the mass asymmetry of this molecule.

2) The CrD bands studied indicate that there is $\Delta N = 1$ staggering, which is, however, due to the spin–rotation and spin–spin interactions present in the relevant states.

3) Based on the above results, we see that $\Delta I = 1$ staggering is a sensitive probe of

deviations from the pure rotational behaviour. Since the method of its calculation from the experimental data leads, however, to error accumulation, one should always calculate the $\Delta I = 1$ staggering measure for the same band from two different sets of data and check the consistency of the results, absence of consistency meaning absence of any real effect.

It is desirable to corroborate the above conclusions by studying rotational bands of several additional molecules.

References

[1] A. Bohr and B. R. Mottelson, *Nuclear Structure Vol. II: Nuclear Deformations* (World Scientific, Singapore, 1998).

[2] D. Bonatsos, Phys. Lett. B **200**, 1 (1988).

[3] P. Schüler *et al.*, Phys. Lett. B **174**, 241 (1986).

[4] W. R. Phillips, I. Ahmad, H. Emling, R. Holzmann, R. V. F. Janssens, T.-L. Khoo and M. W. Drigert, Phys. Rev. Lett. **57**, 3257 (1986).

[5] I. Ahmad and P. A. Butler, Annu. Rev. Nucl. Part. Sci. **43**, 71 (1993).

[6] P. A. Butler and W. Nazarewicz, Rev. Mod. Phys. **68**, 349 (1996).

[7] C. S. Wu and Z. N. Zhou, Phys. Rev. C **56**, 1814 (1997).

[8] S. Flibotte *et al.*, Phys. Rev. Lett. **71**, 4299 (1993).

[9] S. Flibotte *et al.*, Nucl. Phys. A **584**, 373 (1995).

[10] B. Cederwall *et al.*, Phys. Rev. Lett. **72**, 3150 (1994).

[11] P. J. Twin *et al.*, Phys. Rev. Lett. **57**, 811 (1986).

[12] P. J. Nolan and P. J. Twin, Ann. Rev. Nucl. Part. Sci. **38**, 533 (1988).

[13] R. V. F. Janssens and T. L. Khoo, Ann. Rev. Nucl. Part. Sci. **41**, 321 (1991).

[14] D. Bonatsos, C. Daskaloyannis, S. B. Drenska, N. Karoussos, J. Maruani, N. Minkov, P. P. Raychev, and R. P. Roussev, Phys. Rev. A **60**, 253 (1999).

[15] G. A. Leander, R. K. Sheline, P. Möller, P. Olanders, I. Ragnarsson and A. J. Sierk, Nucl. Phys. A **388**, 452 (1982).

[16] H. J. Daley and F. Iachello, Ann. Phys. (N.Y.) **167**, 73 (1986).

[17] B. Buck, A. C. Merchant and S. M. Perez, Phys. Rev. C **57**, R2095 (1988).

[18] J. Engel and F. Iachello, Phys. Rev. Lett. **54**, 1126 (1985).

[19] J. Engel and F. Iachello, Nucl. Phys. A **472**, 61 (1987).

[20] A. Georgieva, P. Raychev and R. Roussev, J. Phys. G **8**. 1377 (1982); **9**, 521 (1983); Bulg. J. Phys. **12**, 147 (1985).

[21] D. Bonatsos, C. Daskaloyannis, S. B. Drenska, N. Karoussos, J. Maruani, N. Minkov, P. P. Raychev, and R. P. Roussev, in *HNPS: Advances in Nuclear Physics (Proceedings of the 10th Hellenic Symposium on Nuclear Physics)*, ed. P. Demetriou and N. Vodinas (Giahoudi-Giapouli, Thessaloniki, 2000) p. 231.

[22] D. Bonatsos, C. Daskaloyannis, S. B. Drenska, N. Karoussos, N. Minkov, P. P. Raychev, and R. P. Roussev, Phys. Rev. C **62**, 024301 (2000).

[23] J. F. C. Cocks *et al.*, Phys. Rev. Lett. **78**, 2920 (1997).

[24] N. Schulz *et al.*, Phys. Rev. Lett. **63**, 2645 (1989).

[25] A. Artna-Cohen, Nucl. Data Sheets **80**, 157 (1997).

[26] Y. A. Akovali, Nucl. Data Sheets **77**, 271 (1996).

[27] A. Artna-Cohen, Nucl. Data Sheets **80**, 227 (1997).

[28] Y. A. Akovali, Nucl. Data Sheets **77**, 433 (1996).

[29] A. Artna-Cohen, Nucl. Data Sheets **80**, 723 (1997).

[30] G. Herzberg, *Molecular Spectra and Molecular Structure, Vol. I: Spectra of Diatomic Molecules* (Van Nostrand, Toronto, 1950).

[31] R. S. Ram and P. F. Bernath, J. Mol. Spectrosc. **171**, 169 (1995).

[32] R. S. Ram and P. F. Bernath, J. Mol. Spectrosc. **172**, 91 (1995).

[33] R. S. Ram, C. N. Jarman, and P. F. Bernath, J. Mol. Spectrosc. **161**, 445 (1993).

[34] R. S. Ram, P. F. Bernath, and S. P. Davis, J. Mol. Spectrosc. **175**, 1 (1996).

[35] D. Bonatsos, C. Daskaloyannis, S. B. Drenska, G. A. Lalazissis, N. Minkov, P. P. Raychev, and R. P. Roussev, Phys. Rev. A **54**, R2533 (1996).

[36] W. Nazarewicz and P. Olanders, Nucl. Phys. A **441**, 420 (1985).

[37] M. J. A. de Voigt, J. Dudek and Z. Szymanski, Rev. Mod. Phys. **55**, 949 (1983).

[38] F. X. Xu, C. S. Wu and J. Y. Zeng, Phys. Rev. C **40**, 2337 (1989).

[39] D. Bonatsos, E. N. Argyres, S. B. Drenska, P. P. Raychev, R. P. Roussev and Yu. F. Smirnov, Phys. Lett. B **251**, 477 (1990).

[40] M. A. J. Mariscotti, G. Scharff-Goldhaber and B. Buck, Phys. Rev. **178**, 1864 (1969).

[41] P. P. Raychev, R. P. Roussev and Yu. F. Smirnov, J. Phys. G **16**, L137 (1990).

[42] J. L. Dunham, Phys. Rev. **41**, 721 (1932).

[43] K. Neergård and P. Vogel, Nucl. Phys. A **145**, 33 (1970); **149**, 217 (1970).

[44] P. Vogel, Phys. Lett. B **60**, 431 (1976).

[45] S. G. Rohoziński and W. Greiner, Phys. Lett. B **128**, 1 (1983).

[46] G. M. Barrow, *Introduction to Molecular Spectroscopy* (McGraw-Hill, London, 1962).

[47] D. Bonatsos, N. Karoussos, C. Daskaloyannis, S. B. Drenska, N. Minkov, P. P. Raychev, R. P. Roussev, and J. Maruani, in *4th European Workshop on Quantum Systems in Chemistry and Physics (Marly-le-Roi, 1999)*, ed. J. Maruani, R. McWeeny, C. Minot, Y. G. Smeyers and S. Wilson (Kluwer, Dordrecht, 2000).

[48] H. J. Krappe and U. Wille, Nucl. Phys. A **124**, 641 (1969).

[49] J. M. Brown and D. J. Milton, Molec. Phys. **31**, 409 (1976).

[50] R. M. Gordon and A. J. Merer, Can. J. Phys. **58**, 642 (1980).