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SYMMETRIES IN NUCLEI, MOLECULES AND ATOMIC CLUSTERS

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ABSTRACT

Staggering effects reveal several structural similarities between the rotational spectra of nuclei and diatomic molecules. The $\Delta I = 2$ staggering effect, first observed in superdeformed nuclear bands, has also been detected in certain electronically excited rotational bands of diatomic molecules, where it has been attributed to interband interactions (bandcrossings). In addition, a $\Delta I = 1$ staggering effect seems to appear in certain rotational bands of diatomic molecules. Interpretations of this effect in terms of algebraic models including octupole or clustering degrees of freedom, as well as by comparison to the $\Delta I = 1$ staggering patterns appearing in light actinides, have been attempted. Finally, the description of magic numbers of metallic clusters in terms of the 3-dimensional q-deformed harmonic oscillator, related to the modified harmonic oscillator of Nilsson, reveals certain similarities between the structure of nuclei and atomic clusters.

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Staggering effects reveal several structural similarities between the rotational spectra of nuclei and diatomic molecules. The $\Delta I = 2$ staggering effect, first observed in superdeformed nuclear bands, has also been detected in certain electronically excited rotational bands of diatomic molecules, where it has been attributed to interband interactions (bandcrossings). In addition, a $\Delta I = 1$ staggering effect seems to appear in certain rotational bands of diatomic molecules. Interpretations of this effect in terms of algebraic models including octupole or clustering degrees of freedom, as well as by comparison to the $\Delta I = 1$ staggering patterns appearing in light actinides, have been attempted. Finally, the description of magic numbers of metallic clusters in terms of the 3-dimensional q-deformed harmonic oscillator, related to the modified harmonic oscillator of Nilsson, reveals certain similarities between the structure of nuclei and atomic clusters.

1. Introduction

Several *staggering* effects are known in nuclear spectroscopy:

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, 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) 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) 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, ...

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 in superdeformed nuclear bands. 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 and, in addition, the effect is not clearly larger than the relevant experimental errors.

On the other hand, rotational spectra of diatomic molecules are known to show great similarities to nuclear rotational spectra, having in addition the advantage that observed rotational bands in several diatomic molecules are much longer than the usual rotational nuclear bands. We have been therefore motivated to make a search for staggering effects in rotational bands of diatomic molecules. The questions to which we have hoped to provide answers are:

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

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

Furthermore, we have made a systematic study of the $\Delta I = 1$ staggering observed in the light actinides, since the systematics of the staggering patterns observed there can be useful for the interpretation of the $\Delta I = 1$ staggering patterns observed in diatomic molecules.

In Sections 2 and 3 of the present work the $\Delta I = 2$ and $\Delta I = 1$ staggering in rotational bands of diatomic molecules will be considered respectively, while in Section 4 the $\Delta I = 1$ staggering in the light actinides will be studied.

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

2.1. $\Delta I = 2$ staggering in superdeformed nuclear bands

In nuclear physics 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

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

is used, where $E(I)$ denotes the energy of the level with angular momentum I. The deviation of the γ-ray transition energies from the rigid rotator behavior can be

measured by the quantity

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

Using the rigid rotator expression

$$E(I) = AI(I+1), \quad (3)$$

one can easily see that in this case $\Delta E_{2,\gamma}(I)$ vanishes. In addition the perturbed rigid rotator expression

$$E(I) = AI(I+1) + B(I(I+1))^2, \quad (4)$$

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

$$\omega = \frac{dE(I)}{dI}, \quad (5)$$

which for discrete states takes the approximate form

$$\omega = \frac{E(I+2) - E(I)}{\sqrt{(I+2)(I+3)} - \sqrt{I(I+1)}}. \quad (6)$$

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

$$\omega = \frac{E(I+2) - E(I)}{2} = \frac{E_{2,\gamma}(I)}{2}. \quad (7)$$

Examples of superdeformed nuclear bands exhibiting staggering are shown in Figs 1–2 of Ref. [1]. We say that $\Delta I = 2$ staggering is observed if the quantity $\Delta E_2(I)$ exhibits alternating signs with increasing ω (i.e. with increasing I, according to Eq. (7)). The following observations can be 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. 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, with the exception of a few points.

2.2. Analysis of experimental data

In the case of molecules 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

$$E^R(I) - E^P(I) = E_{v_{upper}}(I+1) - E_{v_{upper}}(I-1) = DE_{2,v_{upper}}(I), \quad (8)$$

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

where in general

$$DE_{2,v}(I) = E_v(I+1) - E_v(I-1). \quad (10)$$

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

$$\Delta E_{2,v}(I) = \frac{1}{16}(6DE_{2,v}(I) - 4DE_{2,v}(I-2) - 4DE_{2,v}(I+2) + DE_{2,v}(I-4) + DE_{2,v}(I+4)). \quad (11)$$

Results for several rotational bands in different electronic and vibrational states of various diatomic molecules are shown in Figs 3–9 of Ref. [1]. Ref. [1] in addition contains detailed references regarding the contents of this section. 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. Several observations can be made:

1) In all cases shown, the "upper" bands (which happen to be electronically excited) exhibit $\Delta I = 2$ staggering which is 2 to 3 orders of magnitude larger than the experimental error, while the corresponding "lower" bands (which, in the cases studied, correspond to the electronic ground state of each molecule), show some effect smaller than the experimental error.

2) There is no uniform dependence of the $\Delta I = 2$ staggering on the angular momentum I. In some cases of long bands, though, it appears that the pattern is a sequence of points exhibiting small staggering, interrupted by groups of 6 points each time showing large staggering. For example, in the odd levels of the $v = 1$ $C^1\Sigma^+$ band of YD the first group of points showing appreciable $\Delta I = 2$ staggering appears at $I = 13$–23 and the second group appears at $I = 27$–37, while in the even levels of the same band the first group appears at $I = 12$–22 and the second group at $I = 26$–36. Also in the odd levels of the $v = 0$ $A^6\Sigma^+$ band of CrD the first group appears at $I = 15$–25 and the second at $I = 27$–37, while in the even levels of the same band the first group appears at $I = 14$–24 and the second group at $I = 26$–36.

3) In all cases shown, the results obtained for the odd levels of a band are in good agreement with the results obtained for the even levels of the same band. For example, the regions showing appreciable staggering are approximately the same in both cases. In addition, the positions of the local staggering maxima in each pair of figures are closely related. In the odd levels of the YD band mentioned in 2), for example, maximum staggering appears at $I = 19$ and $I = 31$, while in the even levels of the same band the maxima appear at $I = 18$ and $I = 32$.

4) In several cases the $\Delta I = 2$ staggering of a band can be calculated from two different sets of data. For example, the $\Delta I = 2$ staggering of the $v = 1$ $C^1\Sigma^+$ band of YD can be calculated from the data on the 1–1 $C^1\Sigma^+$–$X^1\Sigma^+$ transitions, but it can also be calculated from the data on the 1–2 $C^1\Sigma^+$–$X^1\Sigma^+$ transitions. The results concerning points showing staggering larger than the experimental error come out completely consistently from the two calculations, while the results concerning points exhibiting staggering of the order of the experimental error come out randomly. The best example of disagreement between staggering pictures of the same band calculated from two different sets of data is offered by the $v = 2$ $X^1\Sigma^+$ band of YD, which shows staggering of the order of the experimental error.

5) When considering levels of the same band, in some cases the odd levels exhibit larger staggering than the even levels, while in other cases the opposite is true. In the $v = 1$ $C^1\Sigma^+$ band of YD, for example, the odd levels show staggering larger than that of the even levels, while in the $v = 2$ $C^1\Sigma^+$ band of YD the odd levels exhibit staggering smaller than that of the even levels.

2.3. Discussion

The observations made above can be explained by the assumption that the staggering observed is due to the presence of one or more bandcrossings. The following points support this assumption:

1) It is known 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. 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. (10)), 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. (11). This fact explains why points showing appreciable staggering appear 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. As we have already seen, 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. 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 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 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 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. Similarly, in the case of the YD molecule the observed spectra are influenced by Y and Ne atomic lines, while in the case of the CrH molecule there are Ne and Cr atomic lines influencing the molecular spectra.

5) The fact that consistency between results for the same band calculated from two different sets of data is observed 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 experimantal error, or even smaller, appear to be random, points towards the absence of any real effect in these regions.

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

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. The effect seen in the Ce isotopes is very similar to the mid-band disappearance of staggering seen, for example, in the $v = 1$ $C^1\Sigma^+$ band of YD.

In conclusion, there are several examples of $\Delta I = 2$ staggering in electronically excited bands of diatomic molecules. 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, 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. These facts emphasize 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.

3. $\Delta I = 1$ staggering in rotational bands of diatomic molecules

3.1. Formalism

In this section 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.

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

4) In several cases the $\Delta I = 2$ staggering of a band can be calculated from two different sets of data. For example, the $\Delta I = 2$ staggering of the $v = 1$ $C^1\Sigma^+$ band of YD can be calculated from the data on the 1–1 $C^1\Sigma^+$–$X^1\Sigma^+$ transitions, but it can also be calculated from the data on the 1–2 $C^1\Sigma^+$–$X^1\Sigma^+$ transitions. The results concerning points showing staggering larger than the experimental error come out completely consistently from the two calculations, while the results concerning points exhibiting staggering of the order of the experimental error come out randomly. The best example of disagreement between staggering pictures of the same band calculated from two different sets of data is offered by the $v = 2$ $X^1\Sigma^+$ band of YD, which shows staggering of the order of the experimental error.

5) When considering levels of the same band, in some cases the odd levels exhibit larger staggering than the even levels, while in other cases the opposite is true. In the $v = 1$ $C^1\Sigma^+$ band of YD, for example, the odd levels show staggering larger than that of the even levels, while in the $v = 2$ $C^1\Sigma^+$ band of YD the odd levels exhibit staggering smaller than that of the even levels.

2.3. Discussion

The observations made above can be explained by the assumption that the staggering observed is due to the presence of one or more bandcrossings. The following points support this assumption:

1) It is known 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. 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. (10)), 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. (11). This fact explains why points showing appreciable staggering appear 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. As we have already seen, 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. 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 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 can be attributed

quantity

$$\Delta E_{1,\gamma}(I) = \frac{1}{16}(6E_{1,\gamma}(I) - 4E_{1,\gamma}(I-1) - 4E_{1,\gamma}(I+1) + E_{1,\gamma}(I-2) + E_{1,\gamma}(I+2)), \quad (12)$$

where

$$E_{1,\gamma}(I) = E(I+1) - E(I). \quad (13)$$

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

In the case of molecules the experimentally determined quantities regard the R branch and the P branch, as we have already seen in Eqs (8)-(9). In order to be able to use an expression similar to that of Eq. (12) for the study of $\Delta I = 1$ staggering in molecular bands we need transition energies similar to those of Eq. (13), i.e. transition energies between levels differing by one unit of angular momentum. However, Eqs (8) and (9) 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 (8) or (9) all of its levels with even I

$$E_{v_{upper}}(2) = E^R(1) - E^P(1), \quad (14)$$

$$E_{v_{upper}}(4) = E_{v_{upper}}(2) + E^R(3) - E^P(3), \ldots \quad (15)$$

$$E_{v_{lower}}(2) = E^R(0) - E^P(2), \quad (16)$$

$$E_{v_{lower}}(4) = E_{v_{lower}}(2) + E^R(2) - E^P(4), \ldots \quad (17)$$

In order to be able to determine the levels with odd I from Eqs (8) and (9) in an analogous way, one needs $E(1)$. Then

$$E_{v_{upper}}(3) = E_{v_{upper}}(1) + E^R(2) - E^P(2), \quad (18)$$

$$E_{v_{upper}}(5) = E_{v_{upper}}(3) + E^R(4) - E^P(4), \ldots \quad (19)$$

$$E_{v_{lower}}(3) = E_{v_{lower}}(1) + E^R(1) - E^P(3), \quad (20)$$

$$E_{v_{lower}}(5) = E_{v_{lower}}(3) + E^R(3) - E^P(5), \ldots \quad (21)$$

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

$$E(I) = T_v + B_v I(I+1) - D_v[I(I+1)]^2 + H_v[I(I+1)]^3 + L_v[I(I+1)]^4, \quad (22)$$

which is usually given in the experimental papers. Preliminary results indicate, 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 (8) and (9), 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, 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. One can 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 (16), (17), ... In the next step, however, which is

$$E_{v_{lower}}(20) = E_{v_{lower}}(18) + E^R(18) - E^P(20), \tag{23}$$

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. (23) 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. (12),

$$\Delta E_{1,v}(I) = \frac{1}{16}(6DE_{1,v}(I) - 4DE_{1,v}(I-1) - 4DE_{1,v}(I+1) + DE_{1,v}(I-2) + DE_{1,v}(I+2)), \tag{24}$$

where

$$DE_{1,v} = E_v(I) - E_v(I-1). \tag{25}$$

3.2. Analysis of experimental data

In Ref. [2] we have made a preliminary application of the formalism described above to the 0–0 bands of the $A^6\Sigma^+$–$X^6\Sigma^+$ system of CrD. Ref. [2] in addition contains detailed references regarding the contents of this section. We have focused our attention on the ground $X^6\Sigma^+$ state, which is known to be free from $\Delta I = 2$ staggering effects, while the $A^6\Sigma^+$ state is known to exhibit $\Delta I = 2$ staggering effects, which are fingerprints of interband interactions (bandcrossings). The following observations have been made:

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 several cases, in which no interpolation of missing experimental data is needed, almost constant $\Delta I = 1$ staggering (of different magnitude in each case) is seen. $E(1)$ has been calculated using the Dunham expansion (Eq. (22)). The experimental errors are very small (of the order of 0.001 cm^{-1} for the R and P branches), making 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 and the form of

Eq. (22) 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 one can see that the error of B_v will be of the order of 0.002 cm^{-1}. Therefore the error of $E(1)$ will be of the order of 0.004 cm^{-1}, which is much smaller than the $\Delta I = 1$ staggering seen in these cases.

4) In cases in which a missing experimental value has been determined in the way indicated by Eq. (23), the "jump" observed in the staggering at the point corresponding to the interpolation shows the sensitivity of the staggering to small errors in the transition energies. For example, in the case that R(18) is missing, as we see from Eq. (23) the "jump" is due to the fact that $E(20)$ is determined from the relevant Dunham expansion. It is easily seen that an error of the order of 0.002 cm^{-1} in B_v (as estimated in 3)) can cause an error of the order of 0.84 cm^{-1} in $E(20)$, for which the first term in the Dunham expansion is $420B_v$. Indeed, "jumps" of the order of 1 cm^{-1} are seen.

3.3. Algebraic models

As we have seen in the previous subsection, there is some preliminary evidence for $\Delta I = 1$ staggering of constant magnitude in the $v = 0$ bands of the ground $X^6\Sigma^+$ 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. 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^-, ... 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.

3.3.1. The spf-Interacting Boson Model

In the spf-IBM, which possesses an u(11) symmetry, s, p, and f bosons (i.e. bosons with angular momentum 0, 1, and 3, respectively) are used. Octupole bands are described in the su(3) limit, which corresponds to the chain

$$\mathrm{u}(11) \supset \mathrm{u}(10) \supset \mathrm{su}(3) \supset \mathrm{o}(3) \supset \mathrm{o}(2). \tag{26}$$

The relevant basis is

$$|N, N_b, \omega_b, (\lambda_b, \mu_b), K_b, I, M>, \tag{27}$$

where N is the total number of bosons labelling the irreducible representations (irreps) of u(11), N_b is the total number of negative parity bosons (p and f) labelling the irreps of u(10), ω_b is the "missing" quantum number in the decomposition u(10)$\supset$su(3), (λ_b, μ_b) are the Elliott quantum numbers 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

$$E(N_b, \lambda_b, \mu_b, I) = \alpha + \beta N_b + \gamma N_b^2 + \kappa C(\lambda_b, \mu_b) + \kappa' I(I+1), \tag{28}$$

where

$$C(\lambda,\mu) = \lambda^2 + \mu^2 + \lambda\mu + 3\lambda + 3\mu. \tag{29}$$

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. (6) one obtains

$$\Delta E(I) = \begin{cases} -(\beta + \gamma(2N-1) + 18\kappa N), & \text{for } I = \text{even}, \\ +(\beta + \gamma(2N-1) + 18\kappa N), & \text{for } I = \text{odd}. \end{cases} \tag{30}$$

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. (24) one has

$$\Delta E(I) = \begin{cases} +(\beta + \gamma(2N-1) + 18\kappa N), & \text{for } I = \text{even}, \\ -(\beta + \gamma(2N-1) + 18\kappa N), & \text{for } I = \text{odd}. \end{cases} \tag{31}$$

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 also be used in molecular physics as an extension of the molecular vibron model, 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.

3.3.2. The spdf-Interacting Boson Model

In the spdf-Interacting Boson Model, which possesses a u(16) symmetry, s, p, d, and f bosons (i.e. bosons with angular momentum 0, 1, 2, and 3, respectively) are taken into account. Octupole bands are described in the su(3) limit, which corresponds to the chain

$$\mathrm{u(16)} \supset \mathrm{u_a(6)} \otimes \mathrm{u_b(10)} \supset \mathrm{su_a(3)} \otimes \mathrm{su_b(3)} \supset \mathrm{su(3)} \supset \mathrm{o(3)} \supset \mathrm{o(2)}. \tag{32}$$

The relevant basis is

$$|N, N_a, N_b, \omega_b, (\lambda_a, \mu_a), (\lambda_b, \mu_b), (\lambda, \mu), K, I, M>, \tag{33}$$

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 $su_a(3)$ and $su_b(3)$. The energy eigenvalues are given by

$$E(N_b, \lambda_a, \mu_a, \lambda_b, \mu_b, \lambda, \mu, I) =$$

$$\alpha + \beta N_b + \gamma N_b^2 + \kappa_a C(\lambda_a, \mu_a) + \kappa_b C(\lambda_b, \mu_b) + \kappa C(\lambda, \mu) + \kappa' I(I+1), \qquad (34)$$

with $C(\lambda, \mu)$ defined as in Eq. (29).

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. (24) one has

$$\Delta E(I) = \begin{cases} +(\beta + \gamma - 2k_a(4N+1) + 18k_b + 4k(N+1)) & \text{for } I = \text{even}, \\ -(\beta + \gamma - 2k_a(4N+1) + 18k_b + 4k(N+1)) & \text{for } I = \text{odd}. \end{cases} \qquad (35)$$

Therefore $\Delta I = 1$ staggering of constant amplitude is predicted, since N is a constant for a given nucleus, representing the number of valence nucleon pairs counted from the nearest closed shells.

In comparison with the molecular vibron model, 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 inequality of the masses of the two atoms composing a diatomic molecule 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 in the context of molecules the f boson suffices, i.e. one can remain within the framework of the u(11) model.

3.3.3. The Vector Boson Model

In the Vector Boson Model (VBM), 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 $(\lambda, \mu) = (1, 0)$, i.e. they are two distinct bosons of angular momentum 1. Octupole bands are described in the su(3) limit of the VBM, which corresponds to the chain

$$\mathrm{u}(6) \supset \mathrm{su}(3) \otimes \mathrm{u}(2) \supset \mathrm{so}(3) \otimes \mathrm{u}(1). \qquad (36)$$

The relevant basis is

$$|N, (\lambda, \mu), (N, T), K, I, T_0 >, \qquad (37)$$

where N is the total number of bosons labelling the irreps of u(6), (λ, μ) are the Elliott quantum numbers 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)$\supset$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, their irreps (λ, μ) and (N, T) being related by

$$N = \lambda + 2\mu, \qquad T = \lambda/2. \tag{38}$$

The energy eigenvalues are given by

$$E(N, \lambda, \mu, K, I, T_0 = T) = aN + a_6 N(N+5) + a_3 C(\lambda, \mu) + b_3 I(I+1) + a_1 \frac{\lambda^2}{4}, \tag{39}$$

with $C(\lambda, \mu)$ defined as in Eq. (29).

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. (24) one obtains

$$\Delta E(I) = \begin{cases} +(6a_3 + a_1), & \text{for } I = \text{even}, \\ -(6a_3 + a_1), & \text{for } I = \text{odd}. \end{cases} \tag{40}$$

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.

3.3.4. The Nuclear Vibron Model

An alternative interpretation of the low lying negative parity states appearing in the light actinides has been given following the assumption that alpha clustering is important in this region. An algebraic model appropriate for the description of clustering effects in nuclei is the Nuclear Vibron Model, which uses s and d bosons for the description of nuclear collectivity, plus s' and p bosons for taking into account the distance separating the center of the cluster from the center of the remaining nucleus. The chain corresponding to the su(3) limit of this model is

$$\mathrm{u(6)} \otimes \mathrm{u(4)} \supset \mathrm{su_a(3)} \otimes \mathrm{u_b(3)} \supset \mathrm{su_a(3)} \otimes \mathrm{su_b(3)} \supset \mathrm{su(3)} \supset \mathrm{o(3)} \supset \mathrm{o(2)}, \tag{41}$$

where the subscript a labels the subalgebras of u(6), while the subscript b labels the subalgebras of u(4). The relevant basis is

$$|N, M, (\lambda_a, \mu_a), n_p, (\lambda, \mu), \chi, I, M>, \tag{42}$$

where N is the number of the s and d bosons related to the u(6) algebra, M is the number of the s' and p bosons related to the u(4) algebra, (λ_a, μ_a) are the Elliott quantum numbers related to $\mathrm{su}_a(3)$, n_p is the number of p bosons, (λ, μ) are the Elliott

quantum numbers related to su(3), χ is the Vergados "missing" quantum number in the decomposition su(3)$\supset$o(3), while I and M represent the angular momentum and its z-component respectively, as usual. The energy eigenvalues are given by

$$E(n_p, \lambda_a, \mu_a, \lambda, \mu, I) = \epsilon_p n_p + \alpha_p n_p(n_p+3) + \kappa_d C(\lambda_a, \mu_a) + \kappa C(\lambda, \mu) + \kappa' I(I+1), \quad (43)$$

with $C(\lambda, \mu)$ defined as in Eq. (29).

The ground state band is characterized by $(\lambda_a, \mu_a) = (2N, 0)$, $n_p = 0$, $(\lambda, \mu) = (2N, 0)$ (i.e. it contains N bosons of positive parity and no p-boson of negative parity), while the negative parity band is characterized by $(\lambda_a, \mu_a) = (2N, 0)$, $n_p = 1$, $(\lambda, \mu) = (2N+1, 0)$ (i.e. it contains N bosons of positive parity plus one p-boson of negative parity). Then from Eq. (24) one has

$$\Delta E(I) = \begin{cases} +(\epsilon_p + 4\alpha_p + 4\kappa(N+1)), & \text{for } I = \text{even}, \\ -(\epsilon_p + 4\alpha_p + 4\kappa(N+1)), & \text{for } I = \text{odd}. \end{cases} \quad (44)$$

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

It is not obvious how this model could be applied in the case of diatomic molecules. However, we have opted to describe it here along with the other algebraic models, since it will be needed in the next section.

We conclude that the various algebraic models, describing low lying negative parity bands in terms of octupole deformation or in terms of alpha clustering, predict odd–even staggering ($\Delta I = 1$ staggering) of constant amplitude. In all cases the staggering results from the fact that the negative parity states belong to an irrep different from the one in which the positive parity states composing the ground state band sit.

3.4. Discussion

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. 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 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 [3]. The physical origins of such variations are an interesting problem. Some insight into this can be gained from the study of $\Delta I = 1$ staggering patterns in octupole bands of light actinides, which will be the subject of the next section.

4. $\Delta I = 1$ staggering in octupole bands of light actinides

4.1. Introduction

Rotational nuclear spectra have been long attributed to quadrupole deformations, corresponding to nuclear shapes produced by the revolution of an ellipsis around its maximum or minimum axis and rotating around an axis perpendicular to their axis of symmetry. In addition, it has been suggested that octupole deformation occurs in certain regions, most notably in the light actinides and in the $A \approx 150$ mass region, corresponding to pear-like nuclear shapes. In even nuclei exhibiting octupole deformation the ground state band, which contains energy levels with $I^\pi = 0^+, 2^+, 4^+, 6^+, \ldots$, is accompanied by a negative parity band containing energy levels with $I^\pi = 1^-, 3^-, 5^-, 7^-, \ldots$. After the first few values of angular momentum I the two bands become interwoven, forming a single octupole band with levels characterized by $I^\pi = 0^+, 1^-, 2^+, 3^-, 4^+, 5^-, \ldots$. (It should be noted, however, that in the light actinides alternative interpretations of these bands in terms of alpha clustering have been proposed.)

It has been observed that in octupole bands the levels with odd I and negative parity ($I^\pi = 1^-, 3^-, 5^-, \ldots$) are displaced relatively to the levels with even I and positive parity ($I^\pi = 0^+, 2^+, 4^+, \ldots$), i.e. *odd–even staggering* or $\Delta I = 1$ *staggering* occurs.

The dependence of the amplitude of the staggering effect on the angular momentum I presents much interest. The situation up to now had as follows:

1) As we have seen in subsection 3.3, algebraic models of nuclear structure appropriate for the description of octupole bands, like the spf-Interacting Boson Model (spf-IBM) with u(11) symmetry, the spdf-IBM with u(16) symmetry, and the Vector Boson Model (VBM) with u(6) symmetry, predict $\Delta I = 1$ 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. In other words, $\Delta I = 1$ staggering takes alternatively positive and negative values of equal absolute value as I increases.

2) As we have also seen in subsection 3.3, 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, also predict $\Delta I = 1$ staggering of constant ampli-

tude.

3) Older experimental work 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.

4) As we have seen in subsection 3.2, recent work on experimental data for diatomic molecules shows that in some rotational bands $\Delta I = 1$ staggering of constant amplitude seems to appear, while in other bands a variety of shapes, reminiscent of beats, are exhibited.

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

1) Which patterns of behaviour of the amplitude of the $\Delta I = 1$ staggering appear? Are these patterns related to the ones seen in diatomic molecules?

2) Can these patterns be interpreted in terms of the existing models, or in terms of any other theoretical description?

4.2. Formalism

Traditionally the odd–even staggering ($\Delta I = 1$ staggering) in octupole bands, as well as in gamma bands, has been estimated quantitatively through use of the expression

$$\delta E(I) = E(I) - \frac{(I+1)E(I-1) + IE(I+1)}{2I+1}, \tag{45}$$

where $E(I)$ denotes the energy of the level with angular momentum I. This expression vanishes for

$$E(I) = E_0 + AI(I+1), \tag{46}$$

but not for

$$E(I) = E_0 + AI(I+1) + B(I(I+1))^2. \tag{47}$$

Therefore it is suitable for measuring deviations from the pure rotational behaviour.

On the other hand, one can use Eq. (12), as already described in subsection 3.1. This is what we are going to use in this section.

4.3. Analysis of 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 and which show no backbending (i.e. bandcrossing) behaviour. Using the R_4 ratio,

$$R_4 = \frac{E(4)}{E(2)}, \tag{48}$$

a well known characteristic of collective behaviour, we see that 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 $2.4 \geq R_4 \geq 2$). A special case is ^{218}Ra, for which it has been argued 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, can be found in in Fig. 1, Fig. 2, and Fig. 3 of Ref. [4], respectively. Ref. [4] in addition contains detailed references regarding the contents of this section. In all cases the experimental errors are of the size of the symbol used for the experimental point and therefore negligible. 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 other patterns, 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 $I = 10-18$).

These observations bear considerable similarities to $\Delta I = 1$ staggering patterns found in rotational bands of diatomic molecules. In particular:

1) Staggering patterns of almost constant amplitude have been found in some rotational bands of the CrD and AgH molecules.

2) Staggering patterns resembling the "beat" structure have been seen in several bands of the AgH molecule.

The following comments are also in place:

1) In all cases bands not influenced by bandcrossing effects have been considered, in order to make sure that the observed effects are "pure" single-band effects. The only exception is ^{220}Th, which shows signs of bandcrossings at 10^+ and 13^-, which, however, do not influence the relevant staggering pattern. A special case is ^{218}Ra, which shows a rather irregular dependence of $E(I)$ on I. As we have already mentioned, it has been argued that this nucleus is an example of a new type of tran-

sitional nuclei in which the octupole deformation dominates over all other types of deformation.

2) 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.

3) The present findings are partially consistent with older work. 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.

4.4. Interpretation of the experimental observations

As we have seen in the previous subsection, various $\Delta I = 1$ staggering patterns occur in the octupole bands of the light actinides. On the other hand, in subsection 3.3 we have seen that the various algebraic models describing low lying negative parity bands in terms of octupole deformation or in terms of alpha clustering, predict odd–even staggering ($\Delta I = 1$ staggering) of constant amplitude.

It should be noticed, as already remarked in subsection 4.3, that the experimental data indicate that the value of I at which the first vanishing of the staggering amplitude occurs increases as a function of R_4, i.e. as the rotational limit is approached. The higher the value of I at which the first vanishing occurs, the more smooth the decrease of the staggering as a function of I is. We see, therefore, that as the rotational limit is approached, the experimental data approach more and more the constant staggering prediction provided by the various algebraic models. The best example is provided by ^{228}Th, the most rotational among the nuclei studied here.

Although the algebraic models mentioned above are sufficient for providing an explanation for $\Delta I = 1$ staggering in the cases in which this appears as having almost constant amplitude, it is clear that some additional thinking is required for the many cases in which the experimental results show a "beat" pattern, as in subsection 4.3 has been exhibited.

A simple explanation for the appearance of "beat" patterns can be given by the following assumptions:

1) It is clear that in each nucleus the even levels form the ground state band, which starts at zero energy, while the odd levels form a separate negative parity band, which starts at some higher energy. Let us call E_0 the bandhead energy of the negative parity band.

2) It is reasonable to try to describe the ground state band by an expression like

$$E_+(I) = AI(I+1) - B(I(I+1))^2 + C(I(I+1))^3 + \cdots \qquad (49)$$

where the subscript + reminds us of the positive parity of these levels. Such expansions in terms of powers of $I(I+1)$ have been long used for the description of nuclear collective bands. They also occur if one considers Taylor expansions of the energy expressions provided by the Variable Moment of Inertia Model (VMI) model and the $su_q(2)$ model. Notice that fits to experimental data 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. Eq. (49) has been long used in molecular spectroscopy as well, under the name of Dunham expansion.

3) In a similar way, it is reasonable to try to describe the negative parity levels by an expression like

$$E_-(I) = E_0 + A'I(I+1) - B'(I(I+1))^2 + C'(I(I+1))^3 + \cdots \tag{50}$$

where the subscript $-$ reminds us of the negative parity of these levels, while E_0 is the above mentioned bandhead energy. In analogy to the previous case one expects to have $A' > 0$, $B' > 0$, $C' > 0$, ...

4) In the above expansions it is reasonable to assume that $A > A'$, $B > B'$, $C > C'$, ... The reason is the following: Eq. (49) corresponds to the ground state band, which is expected to possess quadrupole deformation, while Eq. (50) corresponds to the negative parity states, for which in addition octupole deformation should show up. One should expect that the states with larger deformation (the negative parity states) should correspond to larger values of the moment of inertia Θ, and therefore to smaller values of the coefficient of the $I(I+1)$ term, which is essentially $1/(2\Theta)$. As a result one should have $A > A'$, and, by analogy, one can assume $B > B'$, $C > C'$, ... This is admitedly a quite weak argument, which is however driving to interesting results, as we shall soon see.

Using Eqs (49) and (50) in Eqs (12) and (13) we find the following results

$$\begin{aligned}\Delta E(I) = E_0 &- (A-A')(I^2+2I+2) + (B-B')\left(I^4+4I^3+13I^2+18I+\frac{23}{2}\right) \\ &-(C-C')\left(I^6+6I^5+33I^4+92I^3+\frac{357}{2}I^2+\frac{333}{2}I+68\right) \\ &+45C'(I+1)+\cdots, \quad \text{for} \quad I = \text{even},\end{aligned} \tag{51}$$

$$\begin{aligned}\Delta E(I) = -E_0 &+ (A-A')(I^2+2I+2) - (B-B')\left(I^4+4I^3+13I^2+18I+\frac{23}{2}\right) \\ &+(C-C')\left(I^6+6I^5+33I^4+92I^3+\frac{357}{2}I^2+\frac{333}{2}I+68\right) \\ &-45C'(I+1)+\cdots, \quad \text{for} \quad I = \text{odd}.\end{aligned} \tag{52}$$

On these results the following comments can be made:

1) The expression for odd I is the opposite of the expression with even I. This means that in the relevant staggering plot the staggering points for even I and the

staggering points for odd I shall form two lines which are reflection symmetric with respect to the horizontal axis.

2) For even I the behaviour of the staggering amplitude is as follows: At low I it starts from a positive value, because of the presence of E_0. As I increases, the second term, which is essentialy proportional to I^2, becomes important. (E_0 is expected to be much larger than $(A-A')$.) This term is negative (since $A > A'$), thus it decreases the amplitude down to negative values. At higher values of I the third term, which is essentially proportional to I^4, becomes important. (Remember that usually B is 3 orders of magnitude smaller than A.) This term is positive (since $B > B'$), thus it increases the amplitude up to positive values. At even higher values of I the fourth term, which is essentially proportional to I^6, becomes important. (Remember that usually C is 3 orders of magnitude smaller than B.) This term is negative (since $C > C'$), thus it decreases the amplitude again down to negative values, and so on.

3) For odd I the behaviour of the staggering amplitude is exactly the opposite of the one described in 2) for even I. The amplitude starts from a negative value and then becomes consequently positive (because of the second term), negative (because of the third term), again positive (because of the fourth term), and so on.

4) When drawing the staggering figure one jumps from an even I to an odd I, then back to an even I, then back to an odd I, and so on. It is clear therefore that a "beat" pattern appears.

The following additional comments are also in place:

1) In the case of a single band (i.e. in the case of $A = A'$, $B = B'$, $C = C'$, etc), the first contribution to the staggering measure $\Delta E(I)$ is the last term in Eqs (51), (52), which comes from the $C(I(I+1))^3$ term in the energy expansion (see Eqs (49), (50)). This is understandable: Since Eq. (12) is a discrete approximation of the fifth derivative of the function $E(I)$, as it has already been remarked, the terms up to $B(I(I+1))^2$ are "killed" by the derivative, while the $C(I(I+1))^3$ term gives a contribution linear in I.

2) The last term in Eqs (51), (52) does not influence significantly the behaviour of the staggering pattern, since C is usually 6 orders of magnitude smaller than A and 3 orders of magnitude smaller than B.

3) One could argue that the above reasoning is valid only for the case of rotational or near-rotational bands, for which the expansions of Eqs (49), (50) are known to be adequate (although one should be reminded at this point that the VMI model describes quite well not only rotational, but also transitional and even vibrational nuclei). One can attempt to mend this problem by adding to the expansions of Eqs (49) and (50) a linear term, in the spirit of the Ejiri formula, the Variable Anharmonic Vibrator Model (VAVM), and the u(5) and o(6) limits of the Interacting Boson Model

$$E_+(I) = A_1 I + AI(I+1) - B(I(I+1))^2 + C(I(I+1))^3 + \cdots, \qquad (53)$$

$$E_-(I) = E_0 + A'_1 I + A'I(I+1) - B'(I(I+1))^2 + C'(I(I+1))^3 + \cdots. \qquad (54)$$

Then Eqs (51) and (52) get modified as follows

$$\Delta E(I) = E_0 - (A_1 - A_1')\left(I + \frac{1}{2}\right) - (A - A')(I^2 + 2I + 2)$$

$$+ (B - B')\left(I^4 + 4I^3 + 13I^2 + 18I + \frac{23}{2}\right) - \cdots, \quad \text{for} \quad I = \text{even}, \qquad (55)$$

$$\Delta E(I) = -E_0 + (A_1 - A_1')\left(I + \frac{1}{2}\right) + (A - A')(I^2 + 2I + 2)$$

$$- (B - B')\left(I^4 + 4I^3 + 13I^2 + 18I + \frac{23}{2}\right) + \cdots, \quad \text{for} \quad I = \text{odd}. \qquad (56)$$

We see that the extra term, which is proportional to $(A_1 - A_1')$, plays the same role as the term proportional to $(A - A')$ in shaping up the behaviour of the staggering amplitude. Therefore the conclusions reached above for rotational nuclei apply equally well to vibrational and transitional nuclei as well.

4) This type of explanation of the staggering patterns seems to be outside the realm of the form of the algebraic models presented above. Even if one decides to include higher order terms of the type $(I(I+1))^2$, $(I(I+1))^3$, etc, in these models, by including in the Hamiltonian higher powers of the relevant Casimir operator, these terms will appear with the same coefficients for both the ground state band and the negative parity band, even though these two bands belong to different irreps. The only possible contributions to the staggering will then come from terms like the last term in Eqs (51) and (52), which comes from the term $(I(I+1))^3$, and similar terms coming from higher powers of $I(I+1)$. However, the term $(I(I+1))^3$ in the framework of the algebraic models already corresponds to 6-body interactions, which are usually avoided in nuclear structure studies.

We conclude therefore that the "beat" pattern 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.

4.5. Discussion

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.

It has also been demonstrated that various algebraic models, including octupole degrees of freedom or based on the assumption that alpha clustering is important in this region, predict $\Delta I = 1$ staggering of amplitude constant as a function of the angular molentum I. Although this description becomes reasonable in the rotational

limit, it cannot explain the "beat" patterns appearing in both the rotational and the vibrational regions.

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 (expansions in powers of $I(I+1)$) with slightly different sets of coefficients, the difference in the coefficients being attributed to the octupole deformation which is present in the negative parity band.

The "beat" patterns found here in the octupole bands of the light actinides bear striking similarities to the "beat" patterns seen in the rotational bands of some diatomic molecules, like AgH. It is expected that an explanation of the "beat" behaviour in terms of two Dunham expansions with slightly different sets of coefficients should be equally applicable in this case.

It is also of interest to check if "beat" patterns appear in other kinds of bands as well. Preliminary results indicate that such patterns appear in some gamma bands (^{164}Er, ^{170}Yb), as well as in a variety of negative parity bands. Further work in this direction is needed.

5. Quantum algebraic symmetries in atomic clusters

In the previous sections we have studied staggering phenomena in nuclear and molecular spectra, revealing certain structural similarities between these physical systems. Structural similarities exist also between nuclei and atomic clusters. Both of these systems exhibit magic numbers, different in each case. An interpretation of the magic numbers of several kinds of metallic clusters can be given in terms of the 3-dimensional q-deformed harmonic oscillator, which can in addition reproduce the results of the modified harmonic oscillator, first used in nuclear structure by Nilsson. The main difference is that the spin–orbit interaction, which plays a crucial role in the formation of magic numbers in nuclei, is absent in the case of atomic clusters. Discussions of the description of the magic numbers of metallic clusters in terms of the 3-dimensional q-deformed harmonic oscillator can be found in Refs [5], [6], while reviews of applications of quantum algebraic techniques in nuclei and molecules can be found in Refs [7], [8], and [9].

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