

Evolution of Collectivity in the Forming of Octupole Structure in Nuclear Rotational Bands

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Abstract.

We study the evolution of octupole collectivity in the structure of nuclear rotational bands in the framework of a Quadrupole-Octupole Rotation Model (QORM). The model formalism is capable of reproducing the different angular momentum regions in alternating parity bands together with the respective beat staggering patterns. The obtained result clearly indicates the presence of a critical angular momentum region where the separate sequences of negative and positive parity levels merge into a single octupole rotational band. The implemented model analysis outlines the mechanism of forming octupole band structure and the respective evolution of nuclear complex shape properties. Also, we have studied the effect of K-mixing and its influence on the model predictions for reduced transition probabilities in octupole bands.

1 Introduction

Recently a model formalism applicable to rotation motion of nuclei with octupole deformations has been proposed [1]. It provides a useful theoretical tool in the study of rotation motion in nuclear systems with complex quadrupole–octupole shapes. This Quadrupole–Octupole Rotation Model (QORM) is based on the point symmetry group theory which allows a principal way to construct a rotational Hamiltonian for octupole deformations superposed on the top of a quadrupole shape. It suggests specific properties of collective motion characterized by “wobbling”-type modes. On this basis QORM provides detailed

explanation and successful description [2, 3] of the fine staggering effects [5] observed in nuclear octupole bands.

In the present work we extend the model formalism by including the lowest states of the spectrum in which the octupole shape properties are not well pronounced. This development allows one to reproduce the angular momentum region where the separate sequences of negative and positive parity levels merge into a single octupole rotational band. Our purpose is to obtain a consistent QORM description of all angular momentum regions in the spectrum as well as to study the evolution of collectivity in the forming of octupole structure in nuclear rotational bands. Also, we study the effect of K-mixing in the octupole band structure and its influence on the respective model predictions for reduced transition probabilities. As it will be seen below the QORM concept provides a wide range of specific spectroscopic properties of nuclear quadrupole-octupole deformed systems.

2 The Quadrupole–Octupole Rotation Model

2.1 QORM Hamiltonian

The basic ingredient of QORM is the collective octupole Hamiltonian

$$\hat{H}_{oct} = \hat{H}_{A_2} + \sum_{r=1}^2 \sum_{i=1}^3 \hat{H}_{F_r(i)} \quad (1)$$

constructed by the irreducible representations A_2 , $F_1(i)$ and $F_2(i)$ ($i = 1, 2, 3$), of the octahedron (O) point-symmetry group, where

$$\begin{aligned} \hat{H}_{A_2} &= a_2 \frac{1}{4} [(\hat{I}_x \hat{I}_y + \hat{I}_y \hat{I}_x) \hat{I}_z + \hat{I}_z (\hat{I}_x \hat{I}_y + \hat{I}_y \hat{I}_x)], \quad (2) \\ \hat{H}_{F_1(1)} &= \frac{1}{2} f_{11} \hat{I}_z (5 \hat{I}_z^2 - 3 \hat{I}^2), \\ \hat{H}_{F_1(2)} &= \frac{1}{2} f_{12} (5 \hat{I}_x^3 - 3 \hat{I}_x \hat{I}^2), \\ \hat{H}_{F_1(3)} &= \frac{1}{2} f_{13} (5 \hat{I}_y^3 - 3 \hat{I}_y \hat{I}^2), \quad (3) \\ \hat{H}_{F_2(1)} &= f_{21} \frac{1}{2} [\hat{I}_z (\hat{I}_x^2 - \hat{I}_y^2) + (\hat{I}_x^2 - \hat{I}_y^2) \hat{I}_z], \\ \hat{H}_{F_2(2)} &= f_{22} (\hat{I}_x \hat{I}^2 - \hat{I}_x^3 - \hat{I}_x \hat{I}_z^2 - \hat{I}_z^2 \hat{I}_x), \\ \hat{H}_{F_2(3)} &= f_{23} (\hat{I}_y \hat{I}_z^2 + \hat{I}_z^2 \hat{I}_y + \hat{I}_y^3 - \hat{I}_y \hat{I}^2). \end{aligned}$$

The different terms in the above Hamiltonian (cubic combinations of angular momentum operators in body fixed frame) generate rotation degrees of freedom

for the system in correspondence to various octupole shapes with a magnitude determined by the model parameters a_2 and f_{r_i} ($r = 1, 2; i = 1, 2, 3$).

We consider that the octupole degrees of freedom are superposed on the top of the leading quadrupole deformation of the system. So we take the quadrupole rotation Hamiltonian with the presence of a non-axial deformation term

$$\hat{H}_{quad} = A\hat{I}^2 + A'\hat{I}_z^2 + C(I_x^2 - I_y^2). \quad (4)$$

It provides the general energy scale for rotation motion of the nucleus. In addition we assume the presence of a high order quadrupole–octupole interaction, restricting ourselves to its diagonal term in the total angular momentum space

$$\hat{H}_{qoc} = f_{qoc} \frac{1}{I^2} (15\hat{I}_z^5 - 14\hat{I}_z^3\hat{I}^2 + 3\hat{I}_z\hat{I}^4). \quad (5)$$

The non-axial term $C(I_x^2 - I_y^2)$ in (4) is involved for completeness and is given in addition to the originally considered quadrupole Hamiltonian Eq. (19) in Ref. [1]. It assumes that even for nuclei with axial quadrupole deformation in the ground state the excitation of octupole degrees of freedom (both axial and non axial) at higher angular momenta might cause the appearance of non-axial quadrupole degrees of freedom as well.

Eqs. (2)–(5) represent the rotation part of the model Hamiltonian which has rather clear geometrical meaning in terms of the point symmetry and shape characteristics of the system. The appearance of angular momentum operators in the octupole Hamiltonian (1) in powers higher than two has been motivated on the basis of the octahedron point symmetry and discussed in terms of the properties of the angular momentum and octupole operators [1]. It is important to remark that the Hamiltonian (2)–(5) represents a particular case of a more general class of rotational Hamiltonians given in the form [4]

$$H = h + \sum_{\alpha} h_{\alpha} I_{\alpha} + \sum_{\alpha, \beta} h_{\alpha, \beta} I_{\alpha} I_{\beta} + \sum_{\alpha, \beta, \gamma} h_{\alpha, \beta, \gamma} I_{\alpha} I_{\beta} I_{\gamma} + \dots, \quad (6)$$

which is an infinite power series in I_{α} ($\alpha = x, y, z$). The coefficients in (6) depend on the intrinsic structure of the system and could be determined by means of various microscopic approaches (see [4] and references therein). From a geometrical point of view these coefficients can be restricted by using an appropriate point symmetry group, when assumptions for the shape properties of the system are made. Actually, such is the case of the present QORM rotational Hamiltonian. The above general point symmetry approach allows a detailed study of many-folded symmetry axes and suggests quite interesting angular momentum properties related to critical point phenomena and different kinds of bifurcation effects in the rotating quantum mechanical systems at all.

2.2 Low-Energy Extension of QORM

So far we presented a collective Hamiltonian constructed under the assumption of clearly determined shape characteristics of the nucleus. However, the physics is more complicated and the experimental data for nuclei with octupole deformations show more dynamic evolution in collectivity with related shape effects observed in rotational spectra. Here, the important point is that the octupole deformation seems to appear and gradually stabilize to a quadrupole–octupole shape configuration at some high enough angular momentum region of the spectrum. For an example (which is also the case of our interest) in the alternating parity bands of light rare earth nuclei this is the region of angular momenta $I \sim 7 - 8$ [6]. Below this region the negative parity states are shifted up with respect to the positive parity states and both together do not form a single rotational band. The reason is that the system undergoes a tunnelling between two reflection asymmetric (octupole) shape orientations (up and down) separated by a slightly pronounced potential barrier. As a result a strong parity splitting effect is observed. This situation can be described approximately as a vibration of the system with respect to some octupole deformation in a symmetric double-well potential. (In the simplest case one may consider the axial octupole deformation $Y_{3,0}$ with the parameter $\beta_{3,0}$). For the higher angular momenta $I > 7 - 8$ the potential barrier becomes higher and the tunnelling effect sharply decreases. There the vibration mode is reduced and the octupole shape properties of the system are stabilized. Then the rotation mode becomes favorable and a well formed single octupole band can be observed. This process is explained reasonably in terms of the Dinuclear System Model [7].

The above considered higher angular momentum region ($I > 7 - 8$) is the original area of application for the QORM rotational Hamiltonian (2)–(5). In order to consider the lowest part of the spectrum $I < 7 - 8$ we need to take into account the strong parity effect due to the octupole vibration mode. The involvement of the respective vibration Hamiltonian part in the model (including solution of the Schrödinger equation in octupole deformation parameter) is the subject of a forthcoming work.

In the present work we involve a phenomenological term capable to reproduce the abnormal ordering of the odd and even levels by generating a strong but fast vanishing (near $I = 7 - 8$) parity splitting effect. Therefore, we take an energy expression of the form

$$\hat{H}_{low} = E_0 \left(1 - \frac{(-1)^I}{1 + bI^3} \right). \quad (7)$$

This term effectively reproduces the effect of the vibration mode. More generally it could be interpreted as a low level energy term carrying the bandhead properties of the spectrum. We remark that in the present development of QORM formalism Eq. (7) replaces Eqs. (22) and (23) in [1]. The parameter b in the

denominator of (7) determines the rapidity of decrease of the parity splitting with the increase of the angular momentum. In the framework of QORM it is restricted (as it will be shown below) so the effect of \hat{H}_{low} vanishes near the region where the octupole band is formed.

The so involved low energy term (7) suggests the presence of a *critical angular momentum region* for the forming of octupole band structure which could be interpreted as a region of a transition from the quadrupole to a complex quadrupole–octupole shape structure of the system. Thus QORM matches two separate dynamical manifestations of collectivity represented both by the term (7) and the rotational terms (2)–(5).

Below it will be demonstrated that the application of this formalism to particular spectra rather precisely outlines the respective angular momentum regions where such a transition might take place. Moreover, we shall see that in these regions the model provides perfect matching not only for the energy level structure but also for the angular momentum characteristics of the system and the related staggering effects which are known as extremely sensitive properties of the collective dynamics.

3 Nuclear Octupole Bands in QORM. Odd-Even Staggering Effect.

3.1 Model Spectrum and Numerical Results

Eqs. (2)–(5) together with Eq. (7) represent the total Hamiltonian of the collective Quadrupole–Octupole Rotation Model (QORM) [1]. The yrast rotational spectrum of the system is obtained by minimizing the energy in the diagonal Hamiltonian terms with respect to the third projection, K , of the collective angular momentum I in the states $|I, K\rangle$, and subsequently diagonalizing the total Hamiltonian.

The so determined energy spectrum is built on different intrinsic K -configurations which provide a $\Delta I = 1$ staggering behavior of rotational energy. The changing quantum number K implies the presence of a wobbling type collective motion resulting from the complicated shape characteristics of the system.

Generally the structure of the QORM spectrum depends on the quadrupole and octupole shape parameters A, A', C and f_{1i}, f_{2i} ($i = 1, 2, 3$), respectively, on the high order interaction parameter f_{qoc} and the low energy parameters E_0 and b . However, for a given nucleus only few of them can be considered as free model parameters, while the others vary in very narrow limits. So, A and A' are kept reasonably close to the known quadrupole shapes, E_0 and b are determined to reproduce the region of the forming octupole band, and furthermore three parameters of the off-diagonal octupole matrix elements can be excluded since in the intrinsic frame of reference three octupole degrees of freedom are related to the orientation angles.

We have applied the above QORM formalism to the alternating parity bands

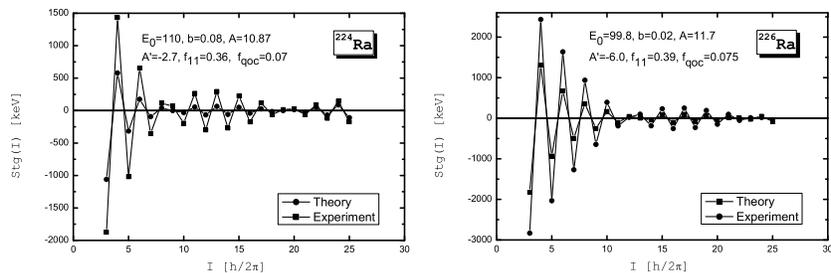


Figure 1. $\Delta I = 1$ staggering patterns for the octupole bands in $^{224,226}\text{Ra}$, experiment (data from [6]) and theory (the parameter values are given in keV).

in the light actinide nuclei $^{224,226}\text{Ra}$ and $^{224,226}\text{Th}$ covering all angular momentum regions of the spectrum (including the lowest inverse ordered odd-even levels). As a result we reproduced successfully the complete $\Delta I = 1$ staggering patterns observed in these bands. This is demonstrated in Figure 1 (for $^{224,226}\text{Ra}$) and Figure 2 ($^{224,226}\text{Th}$) where the fourth (discrete) derivative of the energy difference $\Delta E(I) = E(I+1) - E(I)$,

$$Stg(I) = 6\Delta E(I) - 4\Delta E(I-1) - 4\Delta E(I+1) + \Delta E(I+2) + \Delta E(I-2) \quad (8)$$

is plotted as a function of the angular momentum.

The parameters of the model fits are displayed in the figures. We remark that only the diagonal terms of the model Hamiltonian have been included in the fits. As it will be discussed later the involvement of the off-diagonal terms should be led by the treatment of the reduced transition probabilities which are very sensitive to the structure of the Hamiltonian eigenstates. Anyway, our current consideration assumes small contributions of these terms with the respective parameter values being less than an order smaller compared to the diagonal parameters. The latter condition keeps the third angular momentum projection K as an asymptotically good quantum number.

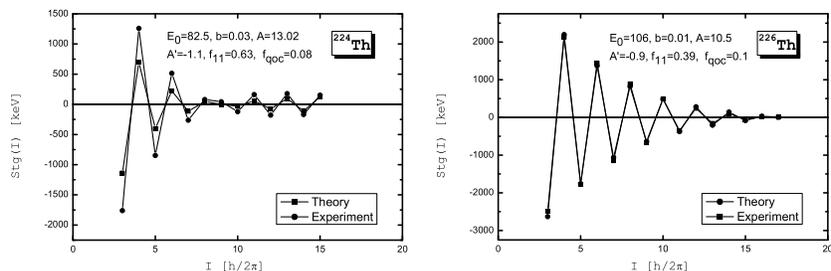


Figure 2. $\Delta I = 1$ staggering patterns for the octupole bands in $^{224,226}\text{Th}$, experiment (data from [8, 9]) and theory (the parameter values are given in keV).

Despite of this “diagonal” restriction we see that the model reproduces all typical characteristics of the octupole band structure including the subsequently appearing beat staggering regions in the spectrum. In all cases the agreement between theory and experiment is remarkable. A sample comparison between theoretical and experimental results for energy levels and the quantity $Stg(I)$ is given in Table 1 for ^{226}Ra .

Table 1. Energy levels (in keV) and the respective values of the quantity $Stg(I)$ (in keV), Eq. (8), at given angular momentum I for the octupole band in ^{226}Ra (QORM description and experiment). The values of the quantum number K which minimize the diagonal part of QORM Hamiltonian are also given.

I	K	E_{th}	E_{exp}	$Stg(I)_{th}$	$Stg(I)_{exp}$
1	1	215.1	253.7		
2	2	60.2	67.7		
3	3	262.9	321.5	-1823.8	-2831.5
4	4	218.4	211.7	1309.2	2436.5
5	4	377.2	447.0	-928.3	-2032.4
6	5	421.4	416.7	673.0	1638.5
7	5	573.6	627.2	-494.0	-1270.2
8	6	668.7	669.6	358.1	937.3
9	7	827.1	858.2	-252.6	-644.1
10	7	960.4	960.3	169.4	393.4
11	8	1129.7	1133.5	-102.1	-186.8
12	8	1292.6	1281.6	46.2	23.2
13	9	1473.2	1448.0	2.0	99.7
14	9	1659.2	1628.9	-45.5	-184.2
15	10	1848.9	1796.5	80.6	233.8
16	10	2053.0	1998.7	-98.2	-254.1
17	11	2249.1	2174.9	97.2	250.6
18	12	2462.0	2389.8	-84.9	-228.0
19	12	2666.0	2579.3	66.6	191.3
20	13	2882.0	2801.1	-45.6	-145.9
21	13	3092.3	3006.7	23.3	97.3
22	14	3307.3	3232.7	0.0	-51.7
23	14	3520.4	3454.9	-24.4	12.5
24	15	3730.6	3685.6	49.9	19.7
25	15	3943.0	3921.9	-76.3	-42.7
26	16	4144.3	4158.2		
27	16	4352.6	4405.9		
28	17	4541.1	4650.7		

3.2 Critical Region in the Forming of the Octupole Band

An important feature of our model description is the correct reproduction of the major “beat” points in the respective staggering patterns. First of all the theoretical patterns clearly indicate the angular momentum region where the separate sequences of negative and positive parity levels merge into a single octupole rotational band. The model description clearly identifies it as a critical region in which the octupole band is formed. This is provided by the respective fast reduction of the low energy term [Eq. (7)] which separates the alternative parity states. In Figure 3 we demonstrate the above merging process for the spectrum of ^{226}Ra . The observed change in collectivity appears consistently with the appearance of the first beat in the corresponding energy staggering pattern. For example in the case of $^{224-226}\text{Ra}$ (see Figure 1) this happens in the region near $I \sim 10$, while in ^{226}Th (Figure 2) the critical region is shifted to $I \sim 15$.

It is important to remark that the presence of the octupole forming region is typical for the considered light actinide nuclei and identifies them as the best examples of octupole deformed nuclear systems. The wider systematics of actinide and rare earth nuclei shows that this type of collective properties is gradually reduced towards the respective middshell regions [10]. In the latter cases only the lowest part of the staggering pattern is observed, where the amplitude slightly decreases with angular momentum but does not reach any beat (octupole forming) region.

Further, our model formalism successfully describes the second and third staggering regions in the experimental staggering patterns of $^{224,226}\text{Ra}$ by reproducing correctly the respective changes in the phase of oscillations. This result gives a relevant model interpretation of the fine structure of the so formed (at the high angular momenta) rotational bands in terms of the high order quadrupole-octupole interaction.

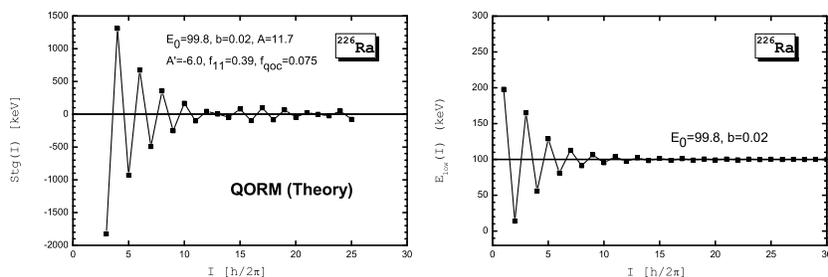


Figure 3. Theoretical $\Delta I = 1$ staggering patterns for ^{226}Ra and the respective behavior of the low energy term Eq. (7) (the parameter values are given in keV).

4 K-Mixing Effects and Reduced Transition Probabilities in QORM

The QORM formalism suggests some general features of the electromagnetic (EM) transitions in a rotating quadrupole–octupole system.

In the simpler case of a diagonal model interaction the general expression for the reduced transition probabilities can be written as [11]

$$B(E\lambda; I_1 \rightarrow I_2) = \langle I_1 K_1 \lambda \mu | I_2 K_2 \rangle^2 \langle K_2 | T_\mu^\lambda | K_1 \rangle^2, \quad (9)$$

where T_μ^λ is the transition operator with multipolarity λ and $\mu = K_2 - K_1$. The quantum numbers K_1 and K_2 correspond to the energy minima in the respective states. The first term in Eq. (9) is the kinematic (Clebsch-Gordan) factor with $I_1 = I + 1$ and $I_2 = I$ being the angular momenta of two neighboring states of the band. The second term in Eq. (9), which depends on the intrinsic states of the system also depends on K but is considered to be slightly changed along the band [11]. So in our present analysis we take it constant.

The changing quantum number K provides a staggering behavior of the Clebsch-Gordan coefficient in Eq. (9) as a function of the angular momentum. As a result a staggering effect in the electromagnetic transition probabilities of octupole bands is predicted. This is demonstrated in Figures 4-6 for the “diagonal” spectrum of ^{226}Th (see the parts labelled as “diagonal Hamiltonian”) where the respective model behavior of the E1, E2 and E3 reduced probabilities is shown.

Indications for staggering effects in the EM transitions of octupole bands are available in Ref. [13], [14] and [15]. However it seems that the predictions of Eq. (9) overestimate their magnitude. Therefore, we suggest that a more realistic consideration is required in which the K -mixing interactions are taken into account. As it is known from the analysis of the model energy spectrum the effect of jumps in K is strongly reduced by the non-diagonal (K -mixing)

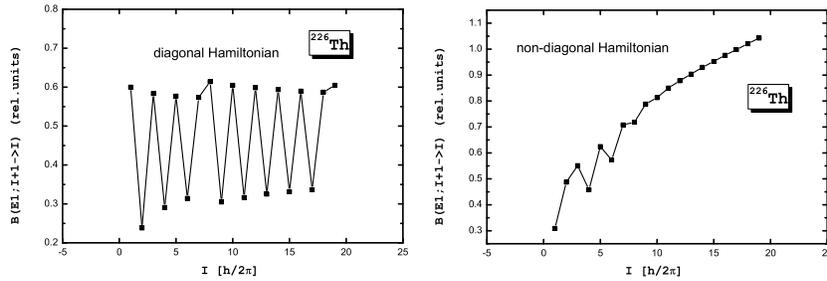


Figure 4. Theoretical predictions for $B(E1)$ transition probabilities in ^{226}Th as functions of the angular momentum. The values of non-diagonal Hamiltonian parameters are $f_{12} = 0.057$ and $f_{22} = 0.035$.

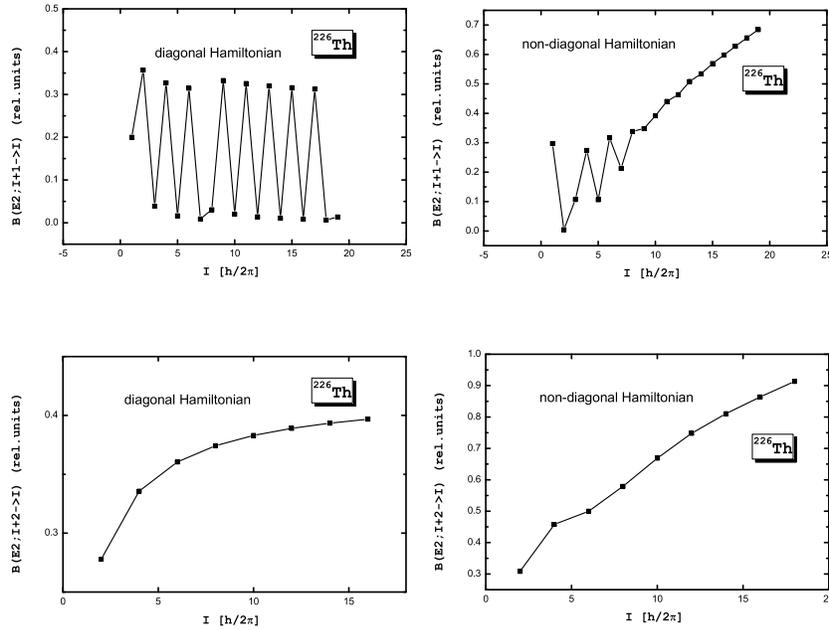


Figure 5. Theoretical predictions for $B(E2)$ transition probabilities in ^{226}Th as functions of the angular momentum. The values of non-diagonal Hamiltonian parameters are $f_{12} = 0.057$ and $f_{22} = 0.035$.

Hamiltonian terms. They provide a decrease in the energy staggering amplitude for the higher angular momentum region (see Figure 4 of [1]). In the same way the mixing interaction will reduce the staggering effect generated by the kinematic factor in Eq. (9). On the other hand taking this interaction into account in the EM transition rates one would be able to determine quite precisely the relative role of the diagonal and off-diagonal Hamiltonian terms which is not unambiguously fixed in the energy levels. So we have developed the model formalism to calculate electromagnetic transitions between K -mixed collective states.

The general assumption of the K -mixing analysis is that any collective state with given angular momentum is characterized with some “main” value of K , let us denote it by \tilde{K}_0 , while the amplitudes of the other K ’s admixtures decrease with the deviation away from the main value (for example see [16]). In terms of QORM, \tilde{K}_0 naturally corresponds to the projection which provides the minimum in the energy for the diagonal part of the Hamiltonian. This state can

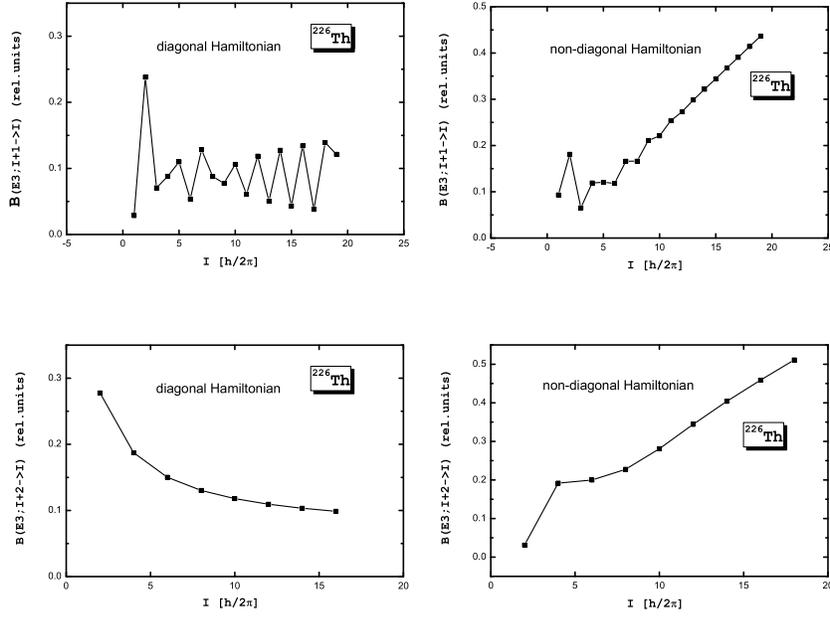


Figure 6. Theoretical predictions for $B(E3)$ transition probabilities in ^{226}Th as functions of the angular momentum. The values of non-diagonal Hamiltonian parameters are $f_{12} = 0.057$ and $f_{22} = 0.035$.

be expanded in the pure K basis as

$$|I\tilde{K}_0\rangle = \sum_{K=-I}^I a_{K}^{\tilde{K}_0} |IK\rangle. \quad (10)$$

The coefficients $a_{K}^{\tilde{K}_0}$ are obtained after diagonalizing the QORM Hamiltonian in the pure K basis $|IK\rangle$ and have the meaning of mixing amplitudes. The set $\{a_{K}^{\tilde{K}_0}\}_{K=-I, \dots, I}$ carries the full information about the QORM interactions and therefore provides complete specification of the model states including the EM transition strength which relates two states with given “main” K - values.

Now we can write the general expression for an electric transition between K - mixed states of the type (10) as follows:

$$B(E\lambda; I_1\tilde{K}_1 \rightarrow I_2\tilde{K}_2) = \frac{1}{2I_1 + 1} \sum_{\mu} \left| \langle I_2\tilde{K}_2 | T_{\mu}^{\lambda} | I_1\tilde{K}_1 \rangle \right|^2, \quad (11)$$

with

$$\begin{aligned}
\langle I_2 \tilde{K}_2 | T_\mu^\lambda | I_1 \tilde{K}_1 \rangle &= \sum_{K' K''} a_{K'}^{\tilde{K}_1} a_{K''}^{\tilde{K}_2}{}^* \langle I_2 K'' | T_\mu^\lambda | I_1 K' \rangle = \\
&= \sum_{K' K''} a_{K'}^{\tilde{K}_1} a_{K''}^{\tilde{K}_2}{}^* (-1)^{I_2 - K''} [(2I_2 + 1)(2I_1 + 1)]^{1/2} \begin{pmatrix} I_2 & \lambda & I_1 \\ -K'' & \mu & K' \end{pmatrix} Q_{intr}^\lambda
\end{aligned} \tag{12}$$

where Q_{intr}^λ has the meaning of an intrinsic multipole momentum corresponding to the second term in Eq. (9), so for a given λ we take it constant. (See [11] and [12])

Eq. (12) provides reduced probabilities for transitions between the K -mixed states of the octupole bands in QORM. However, it can be applied to any K -mixing model scheme for which the mixing amplitudes of the states ($a_K^{\tilde{K}_0}$) can be obtained at least numerically. Note that the presence of these amplitudes on the right hand side of (12) does not allow to use the advantage of the Wigner-Eckart theorem, so one needs to carry out the entire summation over K' and K'' . In the special case of a diagonal non-mixing interaction one can easily see that Eq. (12) reduces to the form of Eq. (9).

We have applied Eq. (12) to the model states of ^{226}Th after including the non-diagonal terms in the model interaction. The respective “ K -mixed” model predictions for the E1, E2 and E3 reduced probabilities are presented in Figures 4-6 compared with the respective “non-mixed” results. The difference between the diagonal and non-diagonal Hamiltonian cases is remarkable. We clearly see that the involvement of the K -mixing terms reduces the staggering effects in the higher angular momenta. This is quite well pronounced in the case of the E1 transitions (Figure 4). It is interesting to note that similar behavior is observed for the experimental E1 transition matrix elements in ^{226}Ra (see Table 2 in [14]). So, the result in Figures 4-6 indicates the crucial role of the non-diagonal QORM interaction in the determining the electromagnetic properties of a rotating quadrupole–octupole deformed system. In this respect the inclusion of transition properties in the model fits appears to be very important with the need of further new experimental data.

5 Concluding Remarks

In conclusion, we demonstrated that QORM successfully reproduces the entire structure of alternating parity bands in light actinide nuclei including the angular momentum regions below and above the critical region of forming the octupole band. The implemented model analysis clearly outlines the evolution of collectivity between different modes of nuclear motion, vibration and rotation, based on the quadrupole and octupole degrees of freedom and their interaction. In such a way the considered QORM formalism suggests a wide range of specific spectroscopic properties of nuclear quadrupole–octupole deformed systems such

as the fine staggering effects in energy levels and electromagnetic transitions as well as the effects of K -mixing. They can be a subject of further studies both from the theoretical and experimental point of view.

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