Collective and single-particle motion of nuclei with reflection asymmetry

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Abstract. The collective model of nuclear coherent quadrupole-octupole oscillations and rotations gives a specific test for the influence of Coriolis interaction between the even-even core and the unpaired nucleon on the split parity-doublet spectra in odd-mass nuclei. It provides model estimations for the angular momentum projection K on the intrinsic symmetry axis and the related intrinsic nuclear structure. Based on this result we propose a study of the connection between collective shape characteristics and the intrinsic reflection-asymmetric shell structure of the nucleus. The analysis of the Coriolis interaction with deformed reflection-asymmetric shell-model calculations shows consistency with the results of the model of coherent quadrupole-octupole motion.

1 Introduction

The observed split parity-doublet spectra of odd-mass nuclei provide rich information about the interaction between collective and single-particle motion in the nuclear system. In particular, the behaviour of the energy difference between two opposite parity counterparts in dependence on the angular momentum carries specific information on the Coriolis coupling between the odd particle and the even-even core [1]. On the other hand, in some cases, the angular momentum of the ground state and/or its projection K are not unambiguously determined, which requires a careful analysis of the related dynamic characteristics of odd-A nuclei. The observation of E1 transitions between opposite parity counterparts provides additional interesting information about the contribution of reflection asymmetric (octupole) deformation modes on the complicated single-particle and rotation-vibration motion of the system. These phenomena represent a challenging subject of study within both the collective and microscopic model approaches in nuclear structure.

Starting by recently implemented analysis [1] in the framework of the collective model of coherent quadrupole-octupole motion [2], in the present work we propose the involvement of a deformed shell model formalism, as a necessary tool to study in detail the interaction between single-particle and collective degrees of freedom in nuclei. The aim of the work is to examine the consistency between the collective and shell model approaches in the estimation of the Coriolis interaction in odd-A nuclei. In this aspect we examine the possibility to incorporate the deformed shell model analysis into the framework of the collective quadrupole-octupole formalism.

2 Coherent quadrupole–octupole motion with Coriolis interaction

We consider that the even–even core of an odd nucleus is allowed to oscillate with respect to the quadrupole β_2 and octupole β_3 axial deformation variables mixed through a centrifugal (rotation-vibration) interaction. The unpaired nucleon contributes to the collective motion of the total system through the Coriolis interaction. The collective Hamiltonian of the odd nucleus can then be taken in the form [1]

$$H_{qo} = -\frac{\hbar^2}{2B_2}\frac{\partial^2}{\partial\beta_2^2} - \frac{\hbar^2}{2B_3}\frac{\partial^2}{\partial\beta_3^2} + \frac{1}{2}C_2{\beta_2}^2 + \frac{1}{2}C_3{\beta_3}^2 + \frac{X(I,K,\pi a)}{d_2\beta_2^2 + d_3\beta_3^2}\ , \quad (1)$$

where B_2 and B_3 are the effective quadrupole and octupole mass parameters and C_2 and C_3 are the stiffness parameters for the respective oscillation modes. The last part of (1) represents the centrifugal term in which the Coriolis interaction is taken into account

$$X(I,K,\pi a) = \frac{1}{2}\left[d_0 + I(I+1) - K^2 + \pi a\delta_{K,\frac{1}{2}}(-1)^{I+1/2}\left(I+\frac{1}{2}\right)\right]. \quad (2)$$

The decoupling parameter a is defined between the unpaired particle states $a = \langle\mathcal{F}_K|\hat{j}_+|\mathcal{F}_{-K}\rangle$ (with $K = 1/2$). However, in the collective model framework it is taken as a fitting parameter. The sign of its contribution in the potential energy depends on the total intrinsic parity $\pi = \pm$ of the system (see below). The parameter d_0 characterizes the shape of the potential in the ground state.

The Schrödinger equation for the Hamiltonian (1) is solved in polar variables $\beta_2 = \sqrt{d/d_2}\,\eta\cos\phi$ and $\beta_3 = \sqrt{d/d_3}\,\eta\sin\phi$, with $d = (d_2 + d_3)/2$. By assuming a coherent interplay between the quadrupole and octupole modes, the following correlations between the stiffness, inertia and mass parameters are imposed $d_2/(dC_2) = d_3/dC_3 = 1/C$, $d_2/dB_2 = d_3/dB_3 = 1/B$. As a result the energy spectrum is obtained in the following analytic form

$$E_{n,k}(I,K,\pi a) = \hbar\omega\left[2n + 1 + \sqrt{k^2 + bX(I,K,\pi a)}\right], \quad (3)$$

where $\omega = \sqrt{C/B}$, $n = 0,1,2,...$ and $b = 2B/(\hbar^2 d)$. The quantum number $k = 1,2,3,...$ comes from the separation of the variables ϕ and η. The quadrupole-octupole eigenfunction $\Phi^{\pm} = \psi(\eta)\varphi^{\pm}(\phi)$ includes the Laguerre polynomials for the variable η in the part $\psi(\eta)$ [2] and the function $\varphi^{\pm}(\phi) = \sqrt{2/\pi}\sin\left(k\phi + [1-(-1)^k]\pi/4\right)$ for the variable ϕ, with $k = k_+ = 1$ for φ^+ and $k = k_- = 2$ for φ^-. The quantum number k provides an energy difference between states with the same angular momentum and opposite parity. The total wave function has the form

$$\begin{aligned}\Psi^{\pi}_{nIMK}(\eta,\phi) &= \psi^I_n(\eta)\varphi^{\pm}(\phi)\sqrt{\frac{2I+1}{16\pi^2}} \\ &\times\left(D^I_{M\,K}(\theta)\mathcal{F}_K \pm (-1)^{I+K}D^I_{M\,-K}(\theta)\mathcal{F}_{-K}\right), \quad (4)\end{aligned}$$

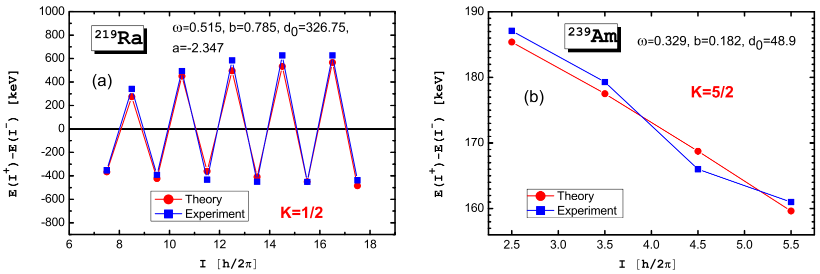

Figure 1. Experimental and theoretical parity-doublet splitting in ^{219}Ra and ^{239}Am.

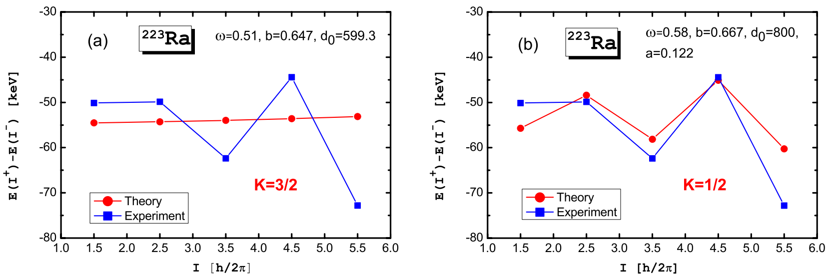

Figure 2. Experimental and theoretical parity doublet-splitting in ^{223}Ra with (a) $K = 3/2$ and (b) $K = 1/2$. Data from [3].

where the total intrinsic parity $\pi = \pi_\varphi \cdot \pi_\chi$ is determined by the parity π_φ of the even-core oscillation function $\varphi^\pm(\phi)$ and the parity of the single-particle function $\mathcal{F}_K$.

Eq. (3) has been applied to describe the split parity-doublet structure of the spectra in a wide range of odd-mass nuclei [1]. Reasonable model descriptions have been obtained also for the available B(E1) and B(E2) transition probabilities in these spectra. In addition the model analysis shows that the parity-doublet splitting, given by the quantity $\Delta E(I^\pm) = E(I^+) - E(I^-)$ exhibits a staggering behaviour as a function of the angular momentum when the spectrum is perturbed by the Coriolis interaction. This is illustrated in Fig. 1(a) for the spectrum of ^{219}Ra with $K = 1/2$. In Fig. 1(b) it is shown that for the nucleus ^{239}Am with $K \neq 1/2$ (reduced Coriolis interaction) a smooth behavior of the parity splitting is observed.

The doublet-splitting analysis allows a detailed estimation of the possible values of the angular momentum projection K on which the parity-doublet structure is built. This is illustrated in Fig. 2 for the nucleus ^{223}Ra. It is seen in Fig. 2(a) that the experimentally assumed value $K = 3/2$ does not support the staggering behaviour of the parity splitting observed in the experimental data. Fig. 2(b) shows that if the value $K = 1/2$ is assumed, the staggering behaviour of $\Delta E(I^\pm)$ is reproduced. In such a way the staggering effect indicates a strong contribution of an intrinsic $K = 1/2$ configuration which is related to the Coriolis coupling interaction. The considered example suggests a possibility to get information about the single-particle orbitals which contribute to the K-configurations associated with the particular collective spectrum of the nucleus.

The above result naturally indicates the need of a deeper microscopic analysis of the single-particle motion in odd-mass nuclei with quadrupole-octupole degrees of freedom and its relation to the collective motion of the system. As a step in this direction we propose the involvement of the quadrupole-octupole deformed shell model formalism which is considered to be capable of describing the single-particle motion in the field of the reflection asymmetric deformed even-even core of the nucleus. The first important task, that will be addressed in the next section, is to estimate the contribution of the Coriolis interaction on the basis of the shell model calculations and to compare the result with the estimations suggested by the above collective model approach.

3 Coriolis interaction by the quadrupole-octupole deformed shell model

To examine the Coriolis interaction from the intrinsic point of view, we refer to the shell model analysis. As far as the considered nuclei are characterized by shape deformations with a presence of reflection asymmetry, we use the formalism of the quadrupole-octupole deformed shell model for which a numerical code is available [4].

The Hamiltonian of the model is

$$H_{\text{ws}} = T + V_{\text{ws}} + V_{\text{s.o.}} + \frac{1}{2}(1+\tau_3)V_{\text{Coul}}, \tag{5}$$

where

$$V_{\text{ws}}(r,\theta,\phi) = -V_0\left[1+\exp\left(\frac{r-R(\theta,\phi)}{a(\theta,\phi)}\right)\right]^{-1}$$

is the Woods-Saxon potential with quadrupole, octupole and higher-multipolarity deformations up to β_6

$$R(\theta,\varphi) = c(\hat{\beta})R_0\left(1+\sum_{\lambda=2}^{6}\beta_\lambda Y_{\lambda 0}(\theta,\varphi)\right), \quad \hat{\beta}\equiv(\beta_2,\beta_3,\beta_4,\beta_5,\beta_6).$$

$V_{\text{s.o.}}$ and V_{Coul} are the spin-orbit and Coulomb terms whose analytic form is given in [4]. The quantity $c(\hat{\beta})$ is the scaling (volume) factor, also given in [4].

The Hamiltonian (5) is diagonalized in the deformed harmonic-oscillator basis $|n_\rho n_z \Lambda\Sigma\rangle$ in cylindrical coordinates $\eta = [(M\omega_\perp)/\hbar]\,\rho^2$, $(\rho^2 = x^2+y^2)$, $\xi = \sqrt{(M\omega_z)/\hbar}\,z$

$$|n_\rho n_z \Lambda\Sigma\rangle = \psi^{\Lambda}_{n_\rho}(\rho)\psi_{n_z}(z)\psi_\Lambda(\varphi)\chi(\Sigma)$$

where [5]

$$
\begin{aligned}
\psi_{\Lambda}(\varphi) &= \frac{1}{\sqrt{2\pi}} e^{i\Lambda\varphi} \\
\psi_{n_z}(z) &= \frac{1}{(\sqrt{\pi}2^{n_z}n_z!)^{1/2}} \left(\frac{M\omega_z}{\hbar}\right)^{\frac{1}{4}} e^{-\frac{\xi^2}{2}} H_{n_z}(\xi) \\
\psi_{n_\rho}^{\Lambda}(\rho) &= \frac{\sqrt{n_\rho!}}{\sqrt{(n_\rho+|\Lambda|)!}} \left(\frac{2M\omega_\perp}{\hbar}\right)^{\frac{1}{2}} e^{-\frac{\eta}{2}} \eta^{\frac{|\Lambda|}{2}} L_{n_\rho}^{|\Lambda|}(\eta)
\end{aligned} \tag{6}
$$

and $\chi(\Sigma)$ is the spin part with $\Sigma = \pm 1/2$.

By using the above formalism one is capable to determine the single-particle orbital in the deformed Woods-Saxon potential occupied by the odd particle in the odd-A nuclear system. Since in the deformed system the intrinsic angular momentum j is not a good quantum number, this orbital is characterized by the quantum number $\Omega = \Lambda + \Sigma$, which can be interpreted as the third projection of j. Due to the axial symmetry Ω appears equal to the third projection K of the total angular momentum I. Thus the solution of the deformed shell model problem could provide an intrinsic estimation for the quantum number K.

Hence the following question naturally arises. Is it possible to apply consistently both the collective model of sec. 2 and the deformed shell model so as to determine unambiguously the intrinsic structure with the quantum number K on which the split parity doublets in odd-A nuclei are built? If so, one can further try to solve simultaneously the eigenvalue problem for the collective Hamiltonian (1) and the single-particle Hamiltonian (5) providing a useful tool to study the interaction between collective and intrinsic degrees of freedom in nuclei.

The following two items represent important steps in the addressing of the above question. First, the shell model Hamiltonian requires constant values for the quadrupole and octupole deformation variables β_2 and β_3 as input values. On the other hand the model of coherent quadrupole-octupole motion does not impose static deformations. Therefore, one has either to include the shell model solution into the collective model problem as a function of both deformation variables, or to try to determine their mean values in the collective model and to apply them as an input for the shell model calculation. Since this task is not straightforwardly solvable, in the present work we use the experimentally estimated values of β_2 and β_3 as the shell model input.

Second, once the quantum number K is determined in the shell model one has to be able to determine the Coriolis decoupling strength. The principal way to do this is to diagonalize the Coriolis interaction together with the single-particle Hamiltonian. However, this is also not an easily solvable problem because one needs to calculate the Coriolis operator matrix elements in cylindrical coordinates. Another more direct approach is to start by the following expression for the decoupling parameter a (see for example [6])

$$
a = \sum_{Nj} c_{Nj}^2 \left(j + \frac{1}{2}\right) (-1)^{j-\frac{1}{2}}. \tag{7}
$$

It corresponds to a diagonalization of the deformed shell model Hamiltonian in the basis of the spherical harmonic oscillator $|Nlj\Omega\rangle$. Here c_{Nj} are the decomposition coefficients of the single-particle wave function in the harmonic oscillator basis

$$\mathcal{F} = \sum_{Nj} c_{Nj} |Nlj\Omega\rangle. \tag{8}$$

The expression (7) is valid for $\Omega = K = 1/2$. To make it useful in the case of anisotropic oscillator basis (6) one needs to switch to the coefficients in the respective decomposition of the single-particle wave function

$$\mathcal{F} = \sum_{Nn_z} c_{Nn_z} |Nn_z\Lambda\Sigma\rangle. \tag{9}$$

By inserting the completeness condition for the harmonic oscillator functions

$$\sum_{Nj} |Nlj\Omega\rangle\langle Nlj\Omega| = 1 \tag{10}$$

in (9) one has

$$\begin{aligned}\mathcal{F} &= \sum_{Nn_z}\sum_{Nj} \langle Nlj\Omega|Nn_z\Lambda\Sigma\rangle c_{Nn_z} |Nlj\Omega\rangle \\ &= \sum_{Nn_z}\sum_{Nj} C^{Nlj\Omega}_{Nn_z\Lambda\Sigma} c_{Nn_z} |Nlj\Omega\rangle, \end{aligned} \tag{11}$$

where $C^{Nlj\Omega}_{Nn_z\Lambda\Sigma}$ are the overlap integrals connecting the spherical and anisotropic harmonic oscillator basis functions. By comparing Eqs. (11) and (8) one finds the relation

$$c_{Nj} = \sum_{Nn_z} C^{Nlj\Omega}_{Nn_z\Lambda\Sigma} c_{Nn_z}. \tag{12}$$

Since the coefficients c_{Nn_z} are determined in the deformed harmonic oscillator formalism presented above, the coefficients c_{Nj} can be obtained through Eq. (12) after calculating the overlap integrals. The Coriolis decoupling parameter can be subsequently calculated by inserting the result of (12) into Eq. (7). One should remark that the above consideration would be useful for not very large deformations for which a reasonable number of terms will be enough to determine the coefficients c_{Nj} in (12). The application of the method of overlap integrals to calculate the Coriolis decoupling interaction is the subject of forthcoming work.

In the present work we apply an approximative but more straightforward approach to estimate the strength of the Coriolis interaction by using the solution of the deformed shell model problem in the stretched basis (6). It is based on the possibility to establish a correspondence between the spherical and anisotropic harmonic oscillator levels contributing to the forming of the physical wave function in a given

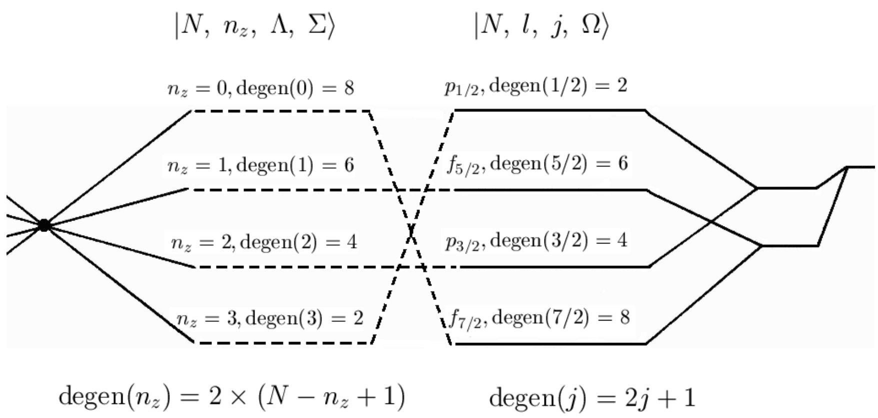

Figure 3. Schematic correspondence between levels-degeneracies of the deformed harmonic oscillator and spherical harmonic oscillator with spin-orbit interaction for $N = 3$.

major shell N. So, we notice that the states of the anisotropic harmonic oscillator with given N have the same-fold splitting as the levels of the spherical harmonic oscillator with spin orbit interaction and the same N. Furthermore, the respective subsets of states are characterized with the same numbers for the level-degeneracy. To clarify this statement we remark that the degeneracy of the states in the anisotropic harmonic oscillator is given by

$$\mathrm{degen}(n_z) = 2(N - n_z + 1), \tag{13}$$

while that for the states of the spherical harmonic oscillator with spin-orbit interaction is

$$\mathrm{degen}(j) = 2j + 1. \tag{14}$$

For example consider $N = 3$. The anisotropic oscillator subset contains 4 states characterized by

$$n_z = 0, \mathrm{degen} = 8 \quad n_z = 1, \mathrm{degen} = 6 \quad n_z = 2, \mathrm{degen} = 4 \quad n_z = 3, \mathrm{degen} = 2.$$

For the spherical oscillator set one has

$$p_{1/2}, \mathrm{degen} = 2 \quad p_{3/2}, \mathrm{degen} = 4 \quad f_{5/2}, \mathrm{degen} = 6 \quad f_{7/2}, \mathrm{degen} = 8.$$

The above example is illustrated schematically in Fig. 3. It is seen that the same set of partition numbers $(2, 4, 6, 8)$ characterizes both oscillator schemes. We suppose that if a given anisotropic oscillator level accommodates a given number of particles, then the same number of particles should be accommodated in the corresponding level of the spherical oscillator. Thus we assume the following relation

$$2j + 1 = 2(N - n_z + 1). \tag{15}$$

This relation provides a correspondence between the spherical oscillator j-orbitals and the anisotropic oscillator states n_z which contribute to the construction of the physical wave functions in the spherical and stretched bases, respectively. One should however have in mind that such a correspondence does not mean a mapping of both bases onto each other. It is only a relation between two quantum numbers of different bases providing the same level-degeneracy structure of the spectrum. Having this remark in mind one can introduce in the deformed shell model problem an analogue of the quantum number j as a function of the stretched-basis quantum number n_z

$$j \rightarrow j(N, n_z) = N - n_z + \frac{1}{2}. \tag{16}$$

Using the above correspondence one can relate the spherical oscillator decomposition coefficients c_{Nj} of the single-particle wave function to the "stretched" coefficients c_{Nn_z}. Assuming a weak mixing of the different major shells, N, we consider $c^2_{Nn_z} \approx c^2_N c^2_{n_z}$, where c^2_N and $c^2_{n_z}$ are the decomposition coefficients of the wave function in the quantum numbers N and n_z, respectively. The coefficients c^2_N and $c^2_{n_z}$ are obtained on the output of the deformed shell model code [4]. Then using Eq. (7) one can introduce the following expression for the Coriolis decoupling factor in the stretched basis

$$a_{\text{dsm}} = \sum_{N=0}^{N\text{max}} \sum_{n_z=0}^{N} c^2_N c^2_{n_z} \left(j(N, n_z) + \frac{1}{2} \right) (-1)^{j(N,n_z)-\frac{1}{2}} \ . \tag{17}$$

We applied Eq. (17) with the use of the deformed shell model calculations to estimate the quantity a_{dsm} in the nuclei ^{223}Ra and ^{239}Pu. For each nucleus we made the calculations for several alternative sets of deformation parameters β_2 and β_3. In ^{239}Pu the considered deformation parameters are taken from available experimental estimations. In ^{223}Ra only β_2 was known from an experimental estimation [7] while for β_3 we took several "testing" values. Calculations for the Coriolis decoupling factor (17) were performed only for the cases when the angular momentum projection Ω_{dsm} of the odd particle is obtained equal to $1/2$.

The results of calculations are shown in Table 1. The respective values of the decoupling parameter from the coherent quadrupole-octupole model of sec. 2, denoted by a_{qoc}, are also given for comparison. The boxed numbers correspond to the cases of a closer consistence between the results of the deformed shell model and coherent quadrupole–octupole model calculations. We see that most of the examined pairs (β_2, β_3) in ^{239}Pu predict $\Omega_{\text{dsm}} = 1/2$ and thus allow the calculation of a_{dsm}. The obtained a_{dsm}- values vary in physically reasonable limits from -1.3 to -0.4. The closest values of both model factors $a_{\text{dsm}} = -0.43$ and $a_{\text{qoc}} = -0.3$ at $\beta_2 = 0.227$ and $\beta_3 = 0.091$ indicate the physical relevance of this deformation region for the nucleus ^{239}Pu. In ^{223}Ra the calculations outline a deformation region including $\beta_2 = 0.192$ and $\beta_3 = 0.01$ where both model calculations are consistent.

The obtained results are preliminary and just provide a test for the way in which both microscopic and collective models can be applied to a consistent study of the

Table 1. Coriolis decoupling factor $a_{\rm dsm}$, Eq. (17), from deformed shell model calculations for ^{223}Ra and ^{239}Pu at different sets of deformation parameters. The values $a_{\rm qoc}$ of the decoupling factor from the coherent quadrupole-octupole model are given in the last column for comparison. $\Omega_{\rm dsm}$ is the third angular momentum projection of the odd particle obtained by the deformed shell model.

Nucl.	β_2 Ref.	β_3 Ref.	$\Omega_{\rm dsm}$	$a_{\rm dsm}$	$a_{\rm qoc}$
^{239}Pu	0.286 [7]	0.091 [8]	1/2	-1.30	-0.3
	0.370 [9]	0.091 [8]	7/2	–	-0.3
	$\boxed{0.227}$ [3]	$\boxed{0.091}$ [8]	1/2	$\boxed{-0.43}$	$\boxed{-0.3}$
	0.312 [9]	0.091 [8]	5/2	–	-0.3
	0.213 [9]	0.091 [8]	1/2	-0.56	-0.3
	0.293 [9]	0.091 [8]	1/2	-1.92	-0.3
	0.204 [9]	0.091 [8]	1/2	-0.6	-0.3
^{223}Ra	0.192 [7]	0.150 [test1]	3/2	–	0.122
	0.192 [7]	0.100 [test2]	5/2	–	0.122
	0.192 [7]	0.050 [test3]	5/2	–	0.122
	$\boxed{0.192}$ [7]	$\boxed{0.010}$ [test4]	1/2	$\boxed{0.264}$	$\boxed{0.122}$

interaction between single-particle and collective motions in odd-mass nuclei. Certainly, a number of further calculations has to be done including other nuclei and regions in order to make a definite conclusion about such a possibility. This is a subject of forthcoming work.

4 Summary

In summary, starting by the analysis of Coriolis interaction effects in odd-mass nuclei within the framework of the collective model of coherent quadrupole-octupole motion, we outlined several ways in which the formalism of the deformed shell model can be involved in the study. The most general way appears to be based on the direct diagonalization of the Coriolis interaction in stretched coordinates. As a more straightforward way we pointed out the application of overlap integrals between deformed and spherical oscillator functions allowing one to use the known analytic expression for the Coriolis term in the spherical basis. We suggested an even more direct way to use this expression by assuming a correspondence between the spherical and deformed oscillator states obeying equal degeneracies. The test of this approach on the nuclei ^{223}Ra and ^{239}Pu provides reasonable estimations for the Coriolis decoupling parameter and moreover shows a consistency with the analysis in the collective model. The obtained results indicate the possibility of further consistent studies of the interaction between single-particle and collective degrees of freedom in nuclei.

Acknowledgements

This work is supported by DFG and by the Bulgarian Scientific Fund under contract F-1502/05.

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