Parity mixing in the single particle states of quadrupole-octupole deformed nuclei

N Minkov$^1$, S Drenskা$^1$, M Strecker$^2$ and W Scheid$^2$

$^1$ Institute of Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Tzarigrad Road 72, BG–1784 Sofia, Bulgaria
$^2$ Institut für Theoretische Physik der Justus-Liebig-Universität, Heinrich-Buff-Ring 16, D–35392 Giessen, Germany
E-mail: nminkov@inrne.bas.bg

Abstract. The effect of parity mixing in the single particle (s.p.) states of odd-mass nuclei with quadrupole-octupole deformations is examined through a reflection-asymmetric deformed shell model. A strong coupling scheme between the parity mixed s.p. state and a coherent quadrupole-octupole vibration mode in the core is considered. The Coriolis decoupling factor is obtained in a projected form corresponding to the good total parity of the system. The average s.p. parity and the decoupling factor are evaluated in several nuclei as functions of the quadrupole and octupole deformation parameters $\beta_2$ and $\beta_3$. It is found that the average s.p. parity obtains various dominant (+ or −) values in the ($\beta_2$, $\beta_3$)-plane, while the s.p. wave function is strongly fragmented into components with different parities. It is shown that by comparing the behaviour of the decoupling factor in the ($\beta_2$, $\beta_3$)-plane to values obtained in a collective quadrupole-octupole model one can determine physically reasonable regions for the deformation parameters.

1. Introduction
In odd-mass atomic nuclei with quadrupole-octupole shapes the coupling of the collective rotations and vibrations to the single-particle (s.p.) motion of the unpaired nucleon provides a split parity-doublet structure of the spectrum [1, 2]. It is known that the octupole deformation of the core can induce respective deformation in the s.p. potential [3]. In this situation, known as a strong coupling, the state of the odd nucleon appears without good parity. On its turn the parity-mixed s.p. state couples to the core state in a way that the total state of the nucleus remains with a good parity. The relevant wave function of the total state can be constructed if a particular model assumption for the behaviour of the core with respect to the reflection asymmetric (octupole) degree of freedom is made.

In the present work a coupling of the particle to a core performing coherent quadrupole-octupole vibrations and rotations [4] is considered. It will be seen that such a coupling scheme provides a reasonable physical framework to examine the effect of the parity mixing in the s.p. state on the total behaviour of the system as well as on the interaction between the collective and s.p. motions of the nucleus. The magnitude of the parity mixing is characterized by the expectation value of the parity operator in the s.p. state. For the s.p. states with $z$-projection of the angular momentum $K = 1/2$ the effect of the Coriolis interaction between the odd particle
and the rotating core has to be considered. Below it will be seen that the way in which this
should be done essentially depends on the parity mixing.

The purpose of the present work is to examine the behaviour of the parity mixing and its
effect on the Coriolis interaction in some odd-mass nuclei in dependence on the quadrupole
and octupole deformations. The numerical evaluation of the Coriolis decoupling factor and the
average parity is realized within a deformed shell model with reflection asymmetry in the basis
of the axially deformed harmonic oscillator (ADHO) [5].

In sec. 2 the general Hamiltonian of the quadrupole-octupole vibrating and rotating core
plus particle is considered. In sec. 3 the particle-core coupling scheme is considered. In sec. 4
the decoupling factor is determined. Numerical results and discussions are given in sec. 5.

2. Hamiltonian of quadrupole–octupole vibrating and rotating core plus particle
The Hamiltonian of an odd-mass nucleus with quadrupole–octupole degrees of freedom can be
written in the form

\[ H = H_{\text{qoc}} + H_{\text{sp}} + H_{\text{coriol}}, \]  

(1)

where \( H_{\text{qoc}} \) corresponds to the collective quadrupole-octupole vibrations and rotation of the
system, \( H_{\text{sp}} \) describes the motion of the odd particle (neutron or proton) in the field of the
even-even core, while \( H_{\text{coriol}} \) represents the Coriolis interaction between the core and the particle.
The quadrupole and octupole vibration modes in \( H_{\text{qoc}} \) can be mixed through a centrifugal term
if a dependence of the moment of inertia on the respective deformation variables \( \beta_2 \) and \( \beta_3 \)
is assumed. The Coriolis part \( H_{\text{coriol}} \) can be superposed to the centrifugal term yielding the
Hamiltonian [4]

\[ H' = H_{\text{qoc}} + H_{\text{coriol}} = -\frac{\hbar^2}{2B_2} \frac{\partial^2}{\partial \beta_2^2} - \frac{\hbar^2}{2B_3} \frac{\partial^2}{\partial \beta_3^2} + \frac{1}{2} C_2 \beta_2^2 + \frac{1}{2} C_3 \beta_3^2 \]

\[ + \frac{\hat{j}^2 - \hat{I}_z^2 - \hat{I}_+ \hat{j}_- - \hat{I}_- \hat{j}_+}{2(d_2 \beta_2^2 + d_3 \beta_3^2)}, \]  

(2)

where \( B_2 \) and \( B_3 \) are effective quadrupole and octupole mass parameters and \( C_2 \) and \( C_3 \) are
stiffness parameters for the respective oscillation modes. Here \( \hat{I}_\pm = \hat{I}_x \pm i \hat{I}_y \) are the total angular
momentum operators, while \( \hat{j}_\pm = \hat{j}_x \pm i \hat{j}_y \) are the spherical components of the total intrinsic
particle angular momentum \( \hat{j} \). In [4] the s.p. Hamiltonian \( H_{\text{sp}} \) was not considered explicitly
and the contribution of the Coriolis part in (2) was treated phenomenologically by taking the
decoupling factor as a free adjustable parameter. The Schrödinger equation for the Hamiltonian
(2) was solved by assuming certain relations between the quadrupole and octupole stiffness and
mass parameters which provide a coherent interplay between the both degrees of freedom. The
obtained energy spectrum has a split parity-doublet structure with the wave function of the
quadrupole-octupole oscillating core \( \Phi_{\text{vib}} \equiv \Phi_{\text{core}} \) determining core vibrating states with given
parity \( \pi_c = (\pm) \) [4].

In the present work the single particle Hamiltonian \( H_{\text{sp}} \) is considered explicitly which allows
one first, to construct an appropriate total wave function carrying detailed information for the
motion of the odd nucleon in the reflection asymmetric s.p. potential, and second, to implement
respectively a fully microscopic treatment of the Coriolis interaction by directly calculating the
decoupling factor. For this purpose \( H_{\text{sp}} \) is taken in a form including a Woods-Saxon potential
with axial quadrupole and octupole deformations [5]

\[ H_{\text{sp}} = T + V_{\text{ws}} + V_{\text{s.o.}} + V_c, \]  

(3)
where $V_\text{ws}(r, \beta) = V_0 \left[1 + \exp\left(\frac{\text{dist}_\Sigma(r, \beta)}{a}\right)\right]^{-1}$ is the Woods-Saxon potential with $\beta = (\beta_2, \beta_3, \beta_4, \beta_5, \beta_6)$ and dist$_\Sigma(r, \beta)$ being the distance between the point $r$ and the nuclear surface represented by $R(\theta, \beta) = c(\beta)R_0 \left[1 + \sum_{\lambda=2,3,...} \beta_\lambda Y_{\lambda 0}(\cos \theta)\right]$. ($c(\beta)$ is a volume conserving factor). $V_{\text{o.o.}}$ and $V_c$ are the spin-orbit and Coulomb terms whose analytic form is given in [5]. Hamiltonian (3) can be diagonalized in the ADHO basis $|Nn\Lambda\Omega\rangle$. Due to the axial symmetry, $\Omega$ is equal to the third projection $K$ of the total angular momentum $I$. The wave function for the odd particle is obtained as an expansion in the ADHO basis functions

$$\mathcal{F}_\Omega = \sum_{Nn\Lambda} C_{Nn\Lambda}^{\Omega} |Nn\Lambda\Omega\rangle. \quad (4)$$

The Hamiltonian (3) can be applied in the two cases of reflection-symmetric ($\beta_3 = 0$) and reflection-asymmetric ($\beta_3 \neq 0$) deformations of the s.p. potential. The respective s.p. wave functions, $\mathcal{F}_\Omega$, correspond to states with a good parity $\pi_{\text{sp}} = (+)$ or $(-)$ ($\beta_3 = 0$) and to mixed-parity states without determined parity ($\beta_3 \neq 0$). Since the parity of the basis states $|Nn\Lambda\Omega\rangle$ is given by $(-1)^N$, in the first case the expansion (4) contains only terms with $N = \text{even}$ ($\pi_{\text{sp}} = +$), or $N = \text{odd}$ ($\pi_{\text{sp}} = -$). In the second case both terms with even and odd $N$ are present in (4).

Thus in the case of a mixed s.p. state the expansion (4) contains components with both parities $\pi_{\text{sp}} = (-1)^N = +1$ and $-1$. Then the wave function $\mathcal{F}_\Omega$ can be written as

$$\mathcal{F}_\Omega = \sum_{\pi_{\text{sp}}=\pm 1} \mathcal{F}_{\Omega}^{(\pi_{\text{sp}})} = \mathcal{F}_{\Omega}^{(+)} + \mathcal{F}_{\Omega}^{(-)}, \quad (5)$$

where $\mathcal{F}_{\Omega}^{(+)}$ contains only the positive parity components, while $\mathcal{F}_{\Omega}^{(-)}$ contains the negative ones with

$$\hat{\pi}_{\text{sp}} \mathcal{F}_\Omega^{(\pm)} = \pm \mathcal{F}_\Omega^{(\pm)}. \quad (6)$$

Then the action of the s.p. parity operator $\hat{\pi}_{\text{sp}}$ on the function $\mathcal{F}_\Omega$ gives

$$\hat{\pi}_{\text{sp}} \mathcal{F}_\Omega = \mathcal{F}_\Omega^{(+)} - \mathcal{F}_\Omega^{(-)}. \quad (7)$$

The parity mixing in a given s.p. state is characterized by the expectation (average) value of the parity operator in this state

$$\langle \hat{\pi}_{\text{sp}} \rangle = \langle \mathcal{F}_\Omega | \hat{\pi}_{\text{sp}} | \mathcal{F}_\Omega \rangle = \sum_{Nn\Lambda} (-1)^N |C_{Nn\Lambda}^{\Omega}|^2.$$

### 3. Total particle-core wave function

The total wave function for the Hamiltonian (1) with the ansatz (2) and (3) can be given in a symmetrized form providing a good total parity $\pi$ and $\mathcal{R}_1$ invariance of the system

$$\Psi_{IMK}^\pi = \frac{1}{2} N (1 + \mathcal{R}_1) D_{MK}^I(\theta)(1 + \pi \hat{P}) \Phi_{\text{core}}^{\pi_{\text{sp}}} \mathcal{F}_K. \quad (8)$$

Here, $D^I_{MK}(\theta)$ is the rotation function and $N$ is a normalization factor. The operator $\hat{P} = \hat{\pi}_c \hat{\pi}_{\text{sp}}$ is a composition of the core and s.p. parity operators $\hat{\pi}_c$ and $\hat{\pi}_{\text{sp}}$, respectively. The operator $\mathcal{R}_1$ represents a rotation by an angle $\pi$ about an axis perpendicular to the intrinsic z-axis and acts on the rotation, core and s.p. parts of the wave function, respectively, as follows

$$\mathcal{R}_1 D_{MK}^I = (-1)^I D_{MK}^I, \quad \mathcal{R}_1 \Phi_{\text{core}}^{\pi_{\text{sp}}} = \hat{\pi}_c \Phi_{\text{core}}^{\pi_{\text{sp}}} = \pi_c \Phi_{\text{core}}^{\pi_{\text{sp}}}, \quad \mathcal{R}_1 \mathcal{F}_K = \mathcal{F}_{-K}. \quad (9)$$
where characterized by the function \( \phi \) negative (right side) ground-state parity. The respective expressions for the decoupling factor Eqs. (15) and (16) in [4]. The full core wave function has the form \( \Phi \) presented by ground state (states shifted down), and \( \psi \) quadrupole-octupole deformation where \( \eta \) is the “radial” part obtained in terms of Laguerre polynomials for the effective quadrupole-octupole deformation \( \eta \) [see Eq. (14) in [4]].

The s.p. wave function \( F_K \) represents a mixture of two parts \( F_K^{\pm} \) with opposite parities. Under the above condition the operator \( 1 + \pi \hat{P} \) projects out the component \( F_K^{(+)} \) or \( F_K^{(-)} \) from \( F_K \) providing a good total parity of the states in the split parity-doublet spectrum. Thus, if the lowest (ground) state (gs) of the doublet has a positive total parity, \( \pi_{gs} = (+) \), the projected component is \( F_K^{(+)} \), while for a negative-parity of the ground state, \( \pi_{gs} = (-) \), the projected component is \( F_K^{(-)} \). These two situations are shown schematically in Fig. 1. In the limiting case of \( \beta_3 = 0 \), the good parity of the s.p. state \( \pi_{sp} = (+) \), or \( (-) \) is restored. Then only the component \( F_K^{(+)} \) or \( F_K^{(-)} \) remains non-zero and the scheme reduces to a s.p. wave function \( F_K^{sp} \equiv F_K^{(+)} \), or \( F_K^{(-)} \) with a good parity.

4. Decoupling factor for a parity-mixed s.p. state

When the system possesses reflection asymmetry the standard definition [1] for the Coriolis decoupling factor, \( a = \langle F_{1/2} | \hat{j}_+ | F_{-1/2} \rangle \), needs to be modified in dependence on the considered core+particle coupling scheme. The modified decoupling factor \( a_{pc} \) (‘pc’ means particle-core) is determined through the matrix element

\[
-\langle \Psi_{IM_{1/2}}^{\pi} | \hat{j}_- | \Psi_{IM_{1/2}}^{\pi} \rangle = N^2 (-1)^{I+1/2} (I + 1/2) \cdot a_{pc}.
\]

Thus for the total wave function (8) with the transformation properties (9) and (7) the factor \( a_{pc} \) is obtained in the form

\[
a_{pc} = \frac{1}{2} \pi_c \left( \langle F_{1/2} | \hat{j}_+ | F_{-1/2} \rangle + \pi_{pc} \langle \hat{\pi}_{sp} F_{1/2} | \hat{j}_+ | F_{-1/2} \rangle \right) = \frac{1}{2} \pi_c \left( (1 + \pi_{pc}) a^{(+)} + (1 - \pi_{pc}) a^{(-)} \right),
\]

where

\[
a^{(+)} = \langle F_{1/2}^{(+)} | \hat{j}_+ | F_{1/2}^{(+)} \rangle, \quad a^{(-)} = \langle F_{1/2}^{(-)} | \hat{j}_+ | F_{1/2}^{(-)} \rangle,
\]

Figure 1. Particle-core states coupling for split parity-doublets with positive (left part) and negative (right side) ground-state parity. The respective expressions for the decoupling factor \( a_{pc} = \pm \pi a^{(\pm)} \) are also given.

The core parity \( \pi_c \) is fixed so as \( \pi_c = (+) \) for the split doublet counterparts containing the ground state (states shifted down), and \( \pi_c = (-) \) for the states shifted up. According to the model of coherent quadrupole–octupole motion [4] the lower \( \pi_c = (+) \) oscillating-core state is characterized by the function \( \phi = \sqrt{2/\pi} \cos (\phi) \), while the next upper \( \pi_c = (-) \) state is presented by \( \phi = \sqrt{2/\pi} \sin (2\phi) \), where \( \phi \) is the quadrupole–octupole angular variable [see Eqs. (15) and (16) in [4]]. The full core wave function has the form \( \Phi_{core}(\eta, \phi) = \psi(\eta) \phi^{\pi}(\phi) \), where \( \psi(\eta) \) is the “radial” part obtained in terms of Laguerre polynomials for the effective quadrupole-octupole deformation \( \eta \) [see Eq. (14) in [4]].
Table 1. Particular forms of the decoupling factor $a_{pc}$ in dependence on the ground-state parity $\pi_{gs}$ and the parity $\pi$ of a given state.

| $\pi$  | $\pi_{gs}$  | $a_{pc}$ |
|-------|-------------|----------|
| (+)   | (+)         | $a^{(+)}$|
| (+)   | (-)         | $a^{(-)}$|
| (-)   | (+)         | $-a^{(+)}$|
| (-)   | (-)         | $a^{(-)}$|

with $\langle F_{1/2}^{(+)} | \hat{j}_{+} | F_{-1/2}^{(-)} \rangle = \langle F_{1/2}^{(-)} | \hat{j}_{+} | F_{-1/2}^{(+)} \rangle = 0$. The factors $a^{(+)}$ and $a^{(-)}$ represent projected matrix elements of the operator $\hat{j}_{+}$ in the subspaces of positive and negative parity components of the s.p. wave function, respectively. By using the expansion (4) they are obtained in the form

$$a^{\pm} = \sum_{Nn_{z} \Lambda} \sum_{N' n'_{z} \Lambda'} C^{4*}_{Nn_{z} \Lambda} C^{\frac{3}{2}}_{N' n'_{z} \Lambda} \times \langle N' n'_{z} \Lambda' \frac{1}{2} | \hat{j}_{+} | Nn_{z} - \Lambda - \frac{1}{2} \rangle,$$

where the matrix element of $\hat{j}_{+}$ between ADHO basis states (with $N$ even or odd) can be calculated through an available analytic expression [6] (see also Table 1 in Ref. [7]).

It can be straightforward seen, that according to Eq. (11), the decoupling factor $a_{pc}$ is reduced to $\pi a^{(\pm)} = \pm a^{(\pm)}$ when the downwards shifted sequence (containing the ground state) has positive total parity $\pi_{gs} = (+)$, and to $-\pi a^{(\pm)} = \mp a^{(\pm)}$ when this sequence has negative total parity $\pi_{gs} = (-)$. This is illustrated in Table 1 (see also Fig. 1). (Note that $\pi_{gs}$ is the total parity in the ground state, while $\pi_{c}$ is the core parity considered to be always $(+)$ in the ground state.) From Table 1 it is seen that for a given state $I^{\pi}$ in the parity-doublet one can shortly write

$$a_{pc} = \pi \pi_{gs} a^{(\pi_{gs})} = \pm \pi a^{(\pm)}.$$

(14)

Now one can easily obtain a correspondence between the values of the decoupling factor $a_{qoc}$ fitted in the model of coherent quadrupole–octupole motion [4] and the values of the projected decoupling factors $a^{(\pm)}$ in the present scheme. One has

$$a_{coll} = \pi a_{qoc} \leftrightarrow \pi \pi_{gs} a^{(\pi_{gs})} = \pm \pi a^{(\pm)} = a_{pc},$$

which gives

$$a_{qoc} \leftrightarrow \pi_{gs} a^{(\pi_{gs})} = \pm a^{(\pm)}.$$

(15)

In the limiting case $\beta_{3} = 0$ of a good s.p. parity the quantity $a_{pc}$ reduces to the standard Coriolis decoupling factor.

5. Numerical results and discussion

The numerical behaviour of the average s.p. model parity $\langle \hat{\pi}_{sp} \rangle$ and of the parity-projected decoupling factor $a_{pc}$ was examined as a function of the quadrupole and octupole deformations in several odd-mass nuclei. Numerical calculations were performed on a net in the two-dimensional space of the parameters $\beta_{2}$ and $\beta_{3}$.

In Fig. 2 the behaviour of the average s.p. model parity in the nuclei $^{237}$U, and $^{249}$Cm is shown (upper plots) as a function of the octupole deformation $\beta_{3}$ at $\beta_{2}$ corresponding to the...
experimentally estimated quadrupole deformations of the respective even-even core nuclei and (lower plots) as a two-dimensional function (contour plot) in the plane \((\beta_2, \beta_3)\). From the upper plots it is seen that \(\langle \tilde{\pi}_{sp} \rangle\) smoothly changes with the increasing of \(\beta_3\). In \(^{237}\text{U}\) the average parity starting by \(-1\) at \(\beta_3 = 0\) goes through the zero value at \(\beta_3 \approx 0.15\) and further increases to \(\langle \tilde{\pi}_{sp} \rangle \approx 0.3 - 0.4\). This is an interesting observation showing that a presence of a dominant parity is possible at large \(\beta_3\) deformations. In \(^{249}\text{Cm}\) \(\langle \tilde{\pi}_{sp} \rangle\) smoothly approaches the zero value for \(\beta_3 \approx 0.2\) indicating the presence of a deformation region with strong parity mixing. Actually, the two-dimensional contour plots show that in the most regions in the \((\beta_2, \beta_3)-\) plane the s.p. state is characterized with some dominant parity instead of becoming totally mixed \((\langle \tilde{\pi}_{sp} \rangle \sim 0)\). Another important result is that in the considered nuclei the s.p. wave functions appear strongly fragmented into various Nilsson orbitals with different parities. This is indicated in Fig. 2 (upper plots) where the contributions (in %) of the largest \([N, n_z, \Lambda]\) components of the wave function are given for certain \(\beta_3\) deformations.

The behaviour of the quantity \(a^{(+)}\) (which determines the decoupling factor \(a_{pc}\) in the cases of a ground state with \(K = 1/2^+\)) as a function of \(\beta_2\) and \(\beta_3\) in the nucleus \(^{239}\text{Pu}\) is illustrated in Fig. 3. The left plot shows a two-dimensional surface containing the values of \(a^{(+)}\) in the \((\beta_2, \beta_3)-\) regions with \(K = 1/2\). The right plot contains a contour which corresponds to the intersection of the two-dimensional surface with the plane determined by the decoupling parameter value \(a_{coll} = -0.34\) fitted in the collective model [4]. This contour outlines deformation regions for...
Figure 3. The decoupling factor $a_{pc} = a^{(+)}$ in $^{239}$Pu as a function of $\beta_2$ and $\beta_3$. The flat area at $a^{(+)} = 0$ in the left plot and the white area in the contour plot (right) correspond to $K \neq 1/2$, which the microscopically calculated decoupling factor $a_{pc}$ provides a reasonable description of the split parity-doublet structure, perturbed by the Coriolis interaction, of the experimental spectrum in $^{239}$Pu. Two experimental guesses for the quadrupole deformation, $\beta_2 = 0.227$ (from an experimental data base for $^{239}$Pu) and 0.286 (from the core nucleus $^{238}$Pu) and one for the octupole deformation, $\beta_3 = 0.091$ (also from $^{238}$Pu), are given in the right plot of Fig. 3. It is seen that the couple of $^{238}$Pu core-deformations ($\beta_2 = 0.286$, $\beta_3 = 0.091$) lies exactly on the contour, while the value $\beta_2 = 0.227$ suggests a slightly larger octupole deformation $\beta_3 = 0.117$ for the odd-mass nucleus $^{239}$Pu. This result shows that by comparing the behaviour of the microscopically obtained decoupling factor $a_{pc}$ in the $(\beta_2, \beta_3)$-plane to a value obtained in the collective model one can determine physically reasonable regions of quadrupole and octupole deformations in the considered nucleus. However, more detailed analysis of the possible deformation values and the corresponding dominant s.p. parity $\langle \hat{\pi}_{sp} \rangle$ should be done in order to draw a definite conclusion.

Finally, the obtained results indicate the possibility for a consistent collective and microscopic model description of the split parity-doublet spectra in odd-mass nuclei. This is the subject of further work.

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