

UNIVERSITY OF BUCHAREST

**Semiclassical and Boson
Descriptions of the Wobbling
Motion in Odd-A Nuclei**

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Abstract

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Chapter 1

Introduction

Ground-state nuclear shapes with spherical symmetry or axial symmetry are predominant across the chart of nuclides. Near closed shells, the deformation is indeed sufficient that models based on spherical symmetries can be used to describe nuclear properties (e.g., energies, quadrupole moments, and so on). Besides the spherical and axially-symmetric shapes, the existence of triaxial nuclear deformation was theoretically predicted a long time ago [1]. The rigid triaxiality of nuclei is defined by the asymmetry parameter γ , giving rise to unique quantum phenomena (this parameter will be characterized later on). The quantum mechanical properties of the rigid triaxial shapes drew a lot of attention within the nuclear physics community lately, since the description of nuclear properties for the deformed nuclei represents a great challenge from both an experimental and a theoretical standpoint (e.g., great progress for the experimental evidence of strong nuclear deformation has only been possible after the 2000s). It is worth mentioning that some experiments concerning alpha-alpha particle reactions induced in heavy nuclei in the early 1960s (e.g., [2]) helped to produce decent amount of data related to the rotational in the high-spin region ($\geq 20\hbar$). Within the experimental studies made by Morinaga et al., the alpha reactions which were induced in the nuclei were generated by the formation of a so-called *compound nucleus*. This system may exist at a large spin value due to the absorption of the angular momentum from the incident particle (i.e., spin values up to $\approx 25 \hbar$ can be obtained from a 50 MeV alpha particle energy - relative to the target nucleus [2]).

The physics of *high-spin* states have been studied from the early 1950s, with the major breakthrough on the theoretical side made by Bohr and Mottelson [1].

The elusive properties of nuclear rotation were described in terms of the rotational degrees of freedom associated with other nuclear degrees of freedom (e.g., particle-vibration, quadrupole-quadrupole, parity, and so on).

Chapter 2

Deformed Nuclei

2.1 Nuclear deformation

Most of the nuclei across the nuclide chart are spherical or symmetric in their ground state. Moreover, for the axially symmetric nuclei (i.e, either *oblate* or *prolate*), there is a prolate over oblate dominance. The spherical shell model only describes nuclei near the closed shells. On the other side, for the nuclei that lie far from closed shells, a deformed potential must be employed.

In the case of even-even nuclei, unique band structures resulting from the vibrations and rotations of the nuclear surface (as proposed by Bohr and Mottelson [1] in the *Geometric Collective Model* - GCM) appear in the energy range 0-2 MeV.

Within the GCM, the nucleus is described as a classical charged liquid drop. For the low-lying energy spectrum, usually, the compression of nuclear matter and the nuclear skin thickness are neglected. This results in the final picture of a liquid drop with a constant nuclear density and a sharp surface [3].

2.1.1 Collective coordinates

The nuclear surface can be described via an expansion of the spherical harmonic functions, with some time-dependent parameters as *expansion coefficients*. The

expression of the nuclear shape is shown below [3]:

$$R(\theta, \varphi, t) = R_0 \left(1 + \sum_{\lambda=0}^{\infty} \sum_{-\lambda}^{\lambda} \alpha_{\lambda\mu}(t) Y_{\lambda}^{\mu}(\theta, \varphi) \right) . \quad (2.1)$$

In 2.1, R denotes the nuclear radius as a function of the spherical coordinates θ, φ expressing the direction, and the time t , while R_0 is the radius of the spherical nucleus when all the expansion coefficients vanish. It is worth mentioning that the expansion coefficients $\alpha_{\lambda\mu}$ act as *collective coordinates*, since the time-dependent amplitudes describe the vibrations of the nuclear surface.

2.1.2 Nuclear radius under rotation

To get a grasp at the physical meaning behind the deformation parameters that are used to describe the nuclear surface, it is instructive to see what happens when the system undergoes a rotation transformation.

The function $R(\theta, \varphi)$ describes the original (non-rotated) nuclear shape. Rotating the system will result in the change of the angular coordinates (θ, φ) to (θ', φ') , which will correspond to a new function $R'(\theta', \varphi')$. Moreover, both nuclear surfaces (i.e., the non-rotated and the rotated one) must hold the equality:

$$R'(\theta', \varphi') = R(\theta, \varphi) \quad (2.2)$$

The rotational invariance of R employs that $R'(\theta, \varphi)$ must have the same functional form, but the expansion coefficients $\alpha_{\lambda\mu}$ must be rotated, meaning:

$$\sum_{\lambda\mu} \alpha'_{\lambda\mu} Y'_{\lambda\mu}(\theta, \varphi) = \sum_{\lambda\mu} \alpha_{\lambda\mu} Y_{\lambda\mu}(\theta, \varphi) . \quad (2.3)$$

Note that in Eq. 2.3, the spherical harmonics $Y'_{\lambda\mu}$ are obtained via the usual rotation matrices. Finally, the invariance of Eq. 2.1 is achieved if the set of parameters $\alpha_{\lambda\mu}$ transform similarly to a *spherical tensor with angular momentum* λ [4], that is:

$$\alpha'_{\lambda\mu} = \sum_{\mu'} \mathcal{D}_{\mu\mu'}^{(\lambda)} \alpha_{\lambda\mu'} . \quad (2.4)$$

Besides the spherical tensor character, the collective coordinates also have the following properties (emerging from Eq. 2.1):

- Complex Conjugation.

$$Y_{\lambda\mu}^*(\theta, \varphi) = (-1)^\mu Y_{\lambda-\mu}(\theta, \varphi), \quad (2.5)$$

$$\alpha_{\lambda\mu}^* = (-1)^\mu \alpha_{\lambda-\mu}. \quad (2.6)$$

- Parity - the coordinates $\alpha_{\lambda\mu}$ must undergo the same change of sign under a parity transformation as the spherical harmonics, in order to keep the invariance of the nuclear surface.

$$(r, \theta, \varphi) \xrightarrow{P} (r, \pi - \theta, \pi + \varphi),$$

$$Y_{\lambda\mu}(\theta, \varphi) \xrightarrow{P} Y_{\lambda\mu}(\pi - \theta, \pi + \varphi) = (-1)^\lambda Y_{\lambda\mu}(\theta, \varphi).$$

Therefore, the parity of the expansion coefficients are:

$$\pi(\alpha_{\lambda\mu}) = (-1)^\lambda. \quad (2.7)$$

2.1.3 Multipole deformations

In the expansion of the nuclear surface defined by Eq. 2.1, the different values for λ will determine different effects regarding the physical aspects of the nucleus. As such, the first values of λ will be examined in terms of the physical meaning.

Monopole mode This corresponds to the first value of $\lambda = 0$. This is the simplest mode of *deformation* of a nuclear surface. Within this approximation, the spherical harmonic Y_0^0 is constant, which would imply that any non-vanishing values for α_{00} will correspond to the change in radius of the nucleus. This kind of excitation is also called *breathing mode* of the nucleus [1, 3]. The energy required for this kind of excitation mode is very large, since it implies a compression of the nuclear matter. As a result, this mode is irrelevant in the low-lying excited spectra of atomic nuclei.

Dipole mode Corresponds to $\lambda = 1$. In reality, this type of mode does not manifest itself as a deformation of the nucleus, but rather as a shift of the

nuclear center of mass. In the lowest order $\lambda = 1$, the shift is in fact a translation of the entire nucleus, and it does not represent an actual nuclear excitation.

Quadrupole mode Excited modes that correspond to $\lambda = 2$. These are the most important collective excitations that take place inside the nucleus. The loss of axial symmetry, triaxial deformations, and other shape-specific transitions that happen within the nucleus are mostly described (and very accurately) via the quadrupole effects.

Octupole mode This corresponds to the next increasing value of $\lambda = 3$, representing the main asymmetric excitations of a nucleus with states of negative-parity. The specific shape of a nuclear system governed by octupole deformations is similar to that of a pear.

Hexadecapole deformations Excitations which correspond to $\lambda = 4$. Within the nuclear theory, this is considered the highest angular momentum which can still provide relevant information for the nuclear phenomena that are studied. Currently, there is no clear evidence for pure excitations with hexadecapole nature, however, these excitations seem to have a major role in the admixture to quadrupole excitations for the ground-state shape of heavy nuclei [3].

The multipole deformations for the cases $\lambda = 1, 2, 3$ and $\lambda = 4$ discussed above are pictorially shown in Fig. 2.1. Excitations with higher angular momentum than the mentioned ones have practically no application within the study of atomic nuclei. Moreover, one can also see that there is an intrinsic limitation on the maximal value of λ , which dictates the smallness of the individual bumps of the surface (see Fig. 2.1). These bumps are described by the spherical harmonics Y_λ^μ , and they decrease in size with increasing values of λ , but with the physical limitation given by the size of the nucleon diameter.

2.1.4 Quadrupole Deformation

One of the most important excitation modes (vibrational degrees of freedom) is the quadrupole deformation, corresponding to $\lambda = 2$. In the case of pure quadrupole



FIGURE 2.1: Graphical representation of the first few modes of excitations of the nuclear surface. The figure is taken from Ref. [3].

deformation, the nuclear surface will be given by the following expression:

$$R(\theta, \varphi) = R \left(1 + \sum_{\mu} \alpha_{2\mu} Y_2^{\mu}(\theta, \varphi) \right). \quad (2.8)$$

From this expression, the term α_{00} is of second order in $\alpha_{2\mu}$ and it can be neglected further on. This term also reflects the conservation of volume [3, 4]. The real and independent degrees of freedom from the above expression are: α_{20} , the real and imaginary parts of α_{21} , and the real and imaginary parts of α_{22} , respectively.

More insight in regard to the quadrupole shape of the nucleus can be achieved if one expresses R in terms of Cartesian coordinates. The spherical harmonics will attain a new form, depending on the Cartesian components of the unit vector pointing in a direction defined by (θ, φ) :

$$\xi = \sin \theta \cos \varphi, \quad \eta = \sin \theta \sin \varphi, \quad \zeta = \cos \theta, \quad (2.9)$$

with the condition $\xi^2 + \eta^2 + \zeta^2 = 1$. With the expressions of the spherical harmonics as functions of (ξ, η, ζ) , the nuclear radius will change accordingly (Cartesian expression $R = R(\xi, \eta, \zeta)$). A relationship between the Cartesian components and the spherical ones for the deformation can be also obtained if one writes all coefficients $\alpha_{2\mu}$ as functions of α_{ij} (with $i, j = \xi, \eta, \zeta$). Since the Cartesian deformations can be regarded as closely related to a stretch/contraction of the nucleus in a given direction, a first interpretation of the physical meaning behind the parameters $\alpha_{2\mu}$ can be established:

- α_{20} : describes the stretching of the z axis with respect to the y and x axes.
- α_{2-2} and α_{22} : give the relative length of the x axis compared to the y axis. Moreover, it also gives the oblique deformation in the $x - y$ plane.
- α_{2-1} and α_{21} : describe an oblique deformation, but with respect to the z axis.

With the set of parameters defined above, the shape and orientation of the nucleus can have arbitrary values (the coefficients $\alpha_{2\mu}$ are mixing the shape and orientation), thus making the parametrization somewhat problematic. In order to fix that, the geometry can be changed if one considers the *principal axis system* (the PA reference system is a coordinate system in which the moments of inertia associated with the nucleus are diagonal). When using this reference frame, the number of parameters is still unchanged, however their physical significance becomes clearer. By denoting the new coordinate system with primed letters, nuclear radius will be described as a function $R = R(\xi', \eta', \zeta')$, with the conditions that $\alpha'_{ij} = 0$, $i \neq j$. The condition will further imply that the newly expressed parameters ($\alpha'_{2\mu}$) have the following form:

$$\begin{aligned}\alpha'_{2\pm 1} &= 0 , \\ \alpha'_{2\pm 2} &\equiv a_2 , \\ \alpha'_{20} &\equiv a_0 ,\end{aligned}\tag{2.10}$$

where the conveniently denoted terms a_2 and a_0 are some functions that depend on the Cartesian components $\alpha_{\xi,\xi}$, $\alpha_{\eta,\eta}$, $\alpha_{\zeta,\zeta}$. From this set of equations the physical significance of the five real and independent parameters is clearer:

- a_0 is indicating the stretch of z' axis w.r.t. the x' and y' axes.
- a_2 is indicating the asymmetry between the lengths of x' and y' axes, respectively.
- the three *Euler angles* $\Theta = (\theta_1, \theta_2, \theta_3)$. These angles will determine the orientation of the PA system (x', y', z') with respect to the laboratory-fixed frame (x, y, z) .

One can now clearly see the advantage of working within the PA system: rotation and shape vibration degrees of freedom can be completely separated. A change

in the Euler angles will result in a pure rotation of the nucleus (without changing its shape), while a change in shape will be affected exclusively by the a_0 and a_2 parameters. If $a_2 = 0$, then the nucleus has a shape with axial symmetry around the z axis (equal axis lengths along the x and y directions).

Another way of describing the excitations of quadrupole type is to adopt the parameters introduced by A. Bohr [5]. These two parameters can be viewed as a set of polar coordinates in the space generated by (a_0, a_2) and they are defined as:

$$\begin{aligned} a_0 &= \beta_2 \cos \gamma , \\ a_2 &= \frac{1}{\sqrt{2}} \beta_2 \sin \gamma , \end{aligned} \quad (2.11)$$

where the numeric factor $\frac{1}{2}$ was added such that the following relation holds true:

$$\sum_{\mu} |\alpha_{2\mu}|^2 = \sum_{\mu} |\alpha'_{2\mu}|^2 = a_0^2 + 2a_2^2 = \beta_2^2 . \quad (2.12)$$

It is worth mentioning that the Eq. 2.12 is rotationally invariant, having the same value in the laboratory and the principal axes systems.

Now that the shape of the nucleus (i.e., the nuclear surface radius R) can be described consistently with via the parameters defined in Eq. 2.11, one can calculate the stretching of the nuclear radius along any of the directions is given in terms of (β, γ) as follows:

$$\delta R_k = \sqrt{\frac{5}{4\pi}} \beta \cos\left(\gamma - \frac{2\pi k}{3}\right) . \quad (2.13)$$

2.1.4.1 Axial quadrupole deformations

Using this set of new coordinates, the expression of the nuclear radius for axially quadrupole-deformed nuclei is given as:

$$R(\theta, \varphi) = R_0 (1 + \beta_2 Y_2^0(\theta, \varphi)) . \quad (2.14)$$

In Eq. 2.14, the parameter β_2 is called the *quadrupole deformation parameter*, and its value dictates whether the nucleus is *oblate* - $\beta_2 < 0$ (i.e., a flattened sphere), *prolate* - $\beta_2 > 0$ (i.e., an elongated sphere, like a rugby ball), or *spherical* - $\beta_2 = 0$.



FIGURE 2.2: A graphical representation with the stretching of the nuclear axis δR_k for $k = 1, 2, 3$, corresponding to the increase in axis lengths along the x , y , and the z directions, respectively. The representation used an arbitrary value for the quadrupole deformation $\beta_2 = 0.3$. Figure was reproduced according to the calculations done in [3].

The nuclear shapes that are characterized only by β_2 (i.e., $\gamma = 0$) have shapes that correspond to spheroids. These shapes are axially symmetric, meaning that they only have one deformed axis. For the spherical case $\beta_2 = 0$, all three axes have the same lengths, meaning that the shape of the nucleus is in fact a sphere.

For the axially-symmetric quadrupole deformations, the parameter β_2 can be related to the axes of the spheroid via the formula [3]:

$$\delta R_k = \sqrt{\frac{5}{4\pi}} \beta_2 \cos\left(\gamma - \frac{2\pi k}{3}\right) , \quad (2.15)$$

with $k = 1, 2, 3$ indices that correspond to each of the three principal axes x' , y' , and z' , respectively. The stretching of the nuclear axis in a particular direction (denoted by k in the above formula) varies according to the change in γ , for a fixed value of β_2 .

Taking a look at Fig. 2.2, one can see the variations of the three axes with γ . When $\gamma = 0^\circ$ the nucleus is elongated along the z' axis, but the x' and y' axes are identical (the prolate case) - axial shape. As γ increases, the x' axis grows, while the other two axes decrease in size, making a region with *triaxial shapes* - all three axes are unequal in magnitude. Symmetry is reached again at $\gamma = 60^\circ$, however the x' and z' axes are equal this time but longer than y' axis, making the nucleus look like a flattened shape (the oblate case) - axial shape. This pattern is repeated every $\gamma = 60^\circ$, where axial shapes emerge, with alternating prolate/oblate shapes.



FIGURE 2.3: Beta-gamma plane divided into six regions. The first part, delimited from $\gamma = 0^\circ$ to $\gamma = 60^\circ$ can be considered as the representative one, while the others can be reproduced from this interval.

It is possible to summarize the various nuclear shapes that can occur with the help of a diagram within in the (β, γ) plane. The repeating pattern of the nuclear shapes is graphically represented in Fig. 2.3. One can see that the oblate axially symmetric shapes that occur at $\gamma = 60^\circ, 180^\circ$ and 300° are identical, and only the axes naming scheme differs. The triaxial shapes are also repeated each 60° .

Regarding the characteristics of Fig. 2.3, the triaxial regions have basically identical shapes, only the axes orientations are different. Moreover, the associated Euler angles are also different, leading to the conclusion that identical physical shapes - including the space orientation - can be represented by different sets of deformation parameters (β, γ) and Euler angles.

2.1.4.2 Non-Axial quadrupole deformations

Besides the nuclei characterized by a *spheroidal* shape, where two of the three principal axes have the same length and the quadrupole deformation parameter

β_2 is the key parameter that describes this kind of shapes, there are also *triaxial* nuclei (or non-axial deformed nuclei).

The triaxial shapes are defined by the γ degree of freedom: the parameter which describes the asymmetry between the length of the three axis of the nucleus (e.g., it describes a stretching along an axis that is perpendicular to the symmetry axis). The nuclear radius for the axially-asymmetric quadrupole deformations is given by:

$$R(\theta, \varphi) = R_0 \left(1 + \beta_2 \cos \gamma Y_2^0(\theta, \varphi) + \frac{1}{\sqrt{2}} \sin \gamma (Y_2^2(\theta, \varphi) + Y_2^{-2}(\theta, \varphi)) \right), \quad (2.16)$$

which is different from Eq. 2.14. As it was already mentioned, the values $\gamma = 0^\circ$ and $\gamma = 60^\circ$ correspond to symmetric prolate and oblate shapes, respectively. Between these values, the triaxial region exist, with *maximal triaxiality* reached at $\gamma = 30^\circ$. The deformation parameters (β, γ) are also called the Hill-Wheeler set [6].

In Eq. 2.16, the spherical harmonics are expressed as follows:

$$\begin{aligned} Y_2^0(\theta, \varphi) &= \frac{1}{4} \sqrt{\frac{5}{\pi}} (3 \cos(\theta)^2 - 1) , \\ Y_2^2(\theta, \varphi) &= \frac{1}{4} e^{2i\varphi} \sqrt{\frac{15}{2\pi}} \sin(\theta)^2 , \\ Y_2^{-2}(\theta, \varphi) &= \frac{1}{4} e^{-2i\varphi} \sqrt{\frac{15}{2\pi}} \sin(\theta)^2 , \end{aligned} \quad (2.17)$$

and substituting these terms in $R(\theta, \varphi)$, Eq. 2.16 will become [1, 7]:

$$R(\theta, \varphi) = R_0 \left[1 + \sqrt{\frac{5}{16\pi}} \beta \left(\cos \gamma (3 \cos \theta^2 - 1) + \sqrt{3} \sin \gamma \sin \theta^2 \cos 2\varphi \right) \right]. \quad (2.18)$$

Regarding the nuclear shapes that were described in Fig. 2.3, the redundancies of the (β, γ) variables are:

- for $\beta_2 > 0$ the nucleus is *prolate* for $\gamma = 0^\circ, 120^\circ, 240^\circ$.
- for $\beta_2 > 0$ the nucleus is *oblate* for $\gamma = 60^\circ, 180^\circ, 300^\circ$.

- for $\gamma = 0^\circ, 180^\circ$, the symmetry axis is the z -axis of the intrinsic frame
- for $\gamma = 120^\circ, 300^\circ$, the symmetry axis is the x -axis of the intrinsic frame
- for $\gamma = 60^\circ, 240^\circ$, the symmetry axis is the y -axis of the intrinsic frame

2.1.4.3 Lund Convention

The so-called Lund convention [7] somewhat solves this repetitiveness, by selecting a rotational axis according to the set of rules described below:

- The quadrupole deformation parameter β_2 is always positive: $\beta_2 \geq 0$
- The rotation around the smallest axis (s -axis) implies the constraint on the triaxiality parameter $0^\circ \leq \gamma \leq 60^\circ$.
- The rotation around the longest axis (l -axis) implies the constraint on the triaxiality parameter $-120^\circ \leq \gamma \leq -60^\circ$.
- The rotation around the medium/intermediate axis (i -axis) implies the constraint on the triaxiality parameter $-60^\circ \leq \gamma \leq 0^\circ$.

Fig. 2.4 aims at depicting the mechanism behind the Lund convention. The graphical representations organized in Table 2.1 show the possible nuclear shapes, depending on the number of deformation axes; namely, if there is only one deformation axis, then the nuclear shape is *axial-symmetric* (oblate or prolate) and if there are two deformation axes, then the nucleus is *triaxial* (axially-asymmetric).

2.1.4.4 Alternative description of the quadrupole deformation

Considering the Lund convention and the Eq. 2.15, one can re-write the set of stretching values as follows:

$$\frac{R_x - R_0}{R_0} = \sqrt{\frac{5}{4\pi}} \beta_2 \cos \left(\gamma - \frac{2}{3}\pi \right), \quad (2.19)$$

$$\frac{R_y - R_0}{R_0} = \sqrt{\frac{5}{4\pi}} \beta_2 \cos \left(\gamma - \frac{4}{3}\pi \right), \quad (2.20)$$

$$\frac{R_z - R_0}{R_0} = \sqrt{\frac{5}{4\pi}} \beta_2 \cos \gamma. \quad (2.21)$$

$$(2.22)$$



FIGURE 2.4: Representation of the nuclear shapes in the (β, γ) plane, using the Lund convention [7] previously discussed. The figure was taken from the work of Matta [8].

For the axially symmetric deformation (i.e., $\gamma = 0$), the quadrupole parameter β_2 can be derived as follows:

$$\beta_2 = \frac{4}{3} \sqrt{\frac{\pi}{5}} \frac{\tilde{R}}{R_0} , \quad (2.23)$$

where $\tilde{R} = (R_z - R_x)$ is the difference between the major (R_z) and minor (R_x) axes of the ellipsoid. This equation for β_2 shows how for oblate deformations, $\beta_2 < 0$ (implying that $R_z < R_x$), while for prolate deformations $\beta_2 > 0$ (implying that $R_z > R_x$). Within literature, usual values for β_2 range from 0.2 - 0.3 (known as *normal deformations*) to 0.4 - 0.6 (known as *superdeformations*).

Another possible description of the nuclear deformation that is specific to small deformations, is given in terms of the parameter ϵ_2 , with the connection to β_2 via the formula [9]:

$$\epsilon_2 \approx \frac{\tilde{R}}{R_0} = \frac{3}{4} \sqrt{\frac{5}{\pi}} \beta_2 = 0.946 \beta_2 . \quad (2.24)$$

Shape	n.o. deformed axes	Side view (zx -plane)	Top view (yx -plane)
Prolate	1		
Oblate	1		
Triaxial	2		

TABLE 2.1: Deformed ellipsoidal shapes of the nuclei. A generic ellipsoid is shown at the top of the table. The parameters a , b , and c represent lengths of differing magnitude of the nuclear ellipsoid.

2.1.5 Nuclear Shapes and Softness

Regarding Table 2.1, a discussion about the implications of the nuclear shapes in terms of some specific phenomena is necessary. Indeed, the shell-model (which will be briefly discussed in the next chapter) considers the motion of the individual nucleons, that are *confined* in nucleonic orbitals, where each nucleon will occupy an orbit with a quantized value of angular momentum. The interpretation of the gamma-ray spectra of different nuclei can be properly described through the excitations if individual nucleons between different orbits, but only for nuclei that are near closed shells. Unfortunately, the same cannot be said about nuclei that lie far from a shell closure, where tools like *Collective Model - C.M.* [1] help understand the properties of these nuclei. One can see that any additional nucleon to the closed shells will imply a departure from the spherical view of a nucleus, with deformations along one of the axes of that nucleus. With the help of C.M., the energy spectrum of many nuclei can be understood and described in terms of 1) a rotation around an axis that is perpendicular to the deformation axis, but also in terms of a 2) motion of the nucleus as a whole (i.e., collective behavior) in tandem

with one coming from a single nucleon (i.e., single-particle behavior). As an example, nuclei in the region $N = 82$ were extensively studied, and the properties of a given nuclide are not only determined by the specific orbital occupied by valence nucleons (e.g., proton orbitals such as $s_{1/2}$, $h_{11/2}$ or neutron orbitals such as $f_{7/2}$, $h_{9/2}$), but also the proportion of each shell that is filled with protons and neutrons, respectively. The nuclei in this closed shell $N = 82$ region are considered as perfect examples of evolutions from the single-particle motion, and the evolution to a collective behavior can be emphasized around the *midshell* at $N = 104$. These midshell nuclei have a deformation that is present along only one axis: *axially symmetric*. Every orbital will cause the nucleus to change its shape towards either a prolate or an oblate one. The change in prolate/oblate type of deformation will depend on the value of the quadrupole moment [10], quantity used to evaluate the so-called Nilsson levels [11] (a detailed discussion about the Nilsson orbitals will be made in the following chapter), or Nilsson diagrams: single-particle energies as a function of nuclear deformation. The slope of a Nilsson level is related to the expectation value of the quadrupole moment, via the expression [7]:

$$\frac{de_k}{d\beta} = - \langle j | q | j \rangle \quad (2.25)$$

with e_k representing the energy of the single-particle state $|j\rangle$, β is the deformation, and q is the quadrupole operator. Each nucleon that occupies an orbit with a given slope will contribute to an overall deformation: one nucleon that occupies a downward sloping orbital which for positive β will drive the nucleus to a prolate shape, while the other type of nucleon that occupies an upward sloping orbital will drive the nucleus to an oblate shape. The competition between these two polarizing effects will result in the axial asymmetry.

In triaxial nuclei (*axially-asymmetric*), a number of low-lying nuclear configurations can exist, leading to different shapes. When the nucleus has a dynamic degree of triaxiality (via the γ deformation parameter), it is said to be a *γ -soft nucleus*.

The γ -soft nuclei tend to exist when both the protons and neutrons occupy the top and bottom of their shells, respectively. The opposite also holds true [12]. The conditions for γ -soft nuclear deformations are realized, for example, in $N \approx 90$ nuclei, where the Fermi surfaces are located near the top of the proton shell ($h_{11/2}$) and bottom of the neutron shell ($i_{13/2}$).

It is interesting that a single nucleus does not necessarily holds a single fixed shape. If the potential energy surface (PES) is relatively flat with respect to the triaxiality parameter γ (meaning that there is no constrain with regards to the minimum value of γ), the shape can oscillate within an interval of deformation. Such a feature characterizes the γ -softness of the nucleus itself.

Chapter 3

Nuclear Models

3.1 Introduction

In the following, it is worth to make a discussion about the nuclear models that are used by theoreticians in order to describe phenomena that are specific to rotating nuclei and high-spin regime. Since the focus of this work emerges from a *class* of properties that usually apply to the high-spin region (but this does not necessarily also imply a high-energy region), it makes sense to give an insight in the tools that fit the best the underlying effects.

3.2 Shell model

The fact that an atomic nucleus can have a structure that behaves rather similarly as its *parent* (i.e., the atom) in terms of changing the number of constituents, has been enforced by the experimental observations that were done across time. The sharp and discrete discontinuities of nuclear properties, such as the nucleon separation energy, point to the fact that nucleus can be explained through the existence of *shells*. Some examples of observations which indicate this are:

- When adding a nucleon to a nucleus, there are certain places where the *binding energy* of the next nucleon becomes considerably smaller than the previous one.



FIGURE 3.1: The first excited energy states 2^+ of nuclei with even Z and N graphically represented with respect to the proton number. Each line represents a set of isotopes. Figure taken from Ref. [8].

- Separation energies for both the protons and neutrons suffer drastic changes, having strong deviations from the predictions of the semi-empirical mass formula [13], the discontinuities being represented by major shell closures (complete filling) [14].
- The neutron absorption cross-section has a substantial decrease in value at the neutron magic numbers
- Great abundance of nuclides where Z and N are magic numbers.

The sudden discontinuities occur at specific values of the proton Z and neutron N numbers: these are called *magic numbers*. Currently, these magic numbers correspond to Z or $N = 2, 8, 20, 28, 50, 82, 126$, and they represent the so-called major shells. There are also two *weakly magic numbers*: 40 and 64.

One can examine the values for the first excited states 2^+ that are shown in Figs. 3.1, 3.2. Indeed, these values show some peaks, each peak corresponding to a particular magic number. This results are part of the work of Raman et al [15], where the transition probabilities from the ground state to the first-excited 2^+ state in even-even nuclei were evaluated.



FIGURE 3.2: The first excited energy states 2^+ of nuclei with even Z and N graphically represented with respect to the neutron number. Each line represents a set of isotopes. Figure taken from Ref. [8].

The shell model starts from the basic assumption that the nucleus is a *mean-field potential*, that is a potential for which the motion of a single nucleon is caused by all the other nucleons (the nucleon is moving inside an average potential generated by all the other constituents of the nucleus). Of course, all the nucleons that are under the influence of such a mean field potential occupy the energy levels which correspond to a series of (sub)shells that agree with the Pauli exclusion principle. Having a general expression for the potential that properly reproduces all the magic numbers (and the observed nuclear properties) is the main goal.

Since the model starts from the concept of independent (non-interacting) particle motion within an average potential, finding each energy will be equivalent of solving the Schrödinger equation:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_i(r) + V(r) \psi_i(r) = e_i \psi_i(r) \quad (3.1)$$

where e_i represents the energy (eigenvalue) and ψ_i represents the wave-function (eigenstates), while $V(r)$ is the nuclear potential whose expression must be evaluated.

The choice of $V(r)$ will be dictated by the reproduction of various experimental

data (such as nuclear saturation, scattering, nuclear reactions, and so on). For the motion of an independent particle, an obvious first attempt would be the *simple harmonic oscillator* (SHO), which has the known expression:

$$V(r) = \frac{1}{2}m(\omega_i r)^2 , \quad (3.2)$$

with ω_i as the frequency of the basic harmonic-like motion of the particle in the nucleus. With Eq. 3.2, the motion of the nucleon has a straightforward expression:

$$\frac{\hbar^2}{2m}\nabla^2\psi_i(r) + \frac{1}{2}m(\omega r)^2\psi_i(r) = e_i\psi_i(r) . \quad (3.3)$$

This Schrödinger equation has its energy eigenvalues under to form:

$$e_N = \left(N + \frac{3}{2}\right)\hbar\omega , \quad (3.4)$$

where N is the number of oscillator quanta which describes each major shell (also called the *principal quantum number*). One should keep in mind that such an expression is typical for a three-dimensional and isotropic harmonic oscillator. The principal quantum number N is furthermore defined as:

$$N = 2(n - 1) + l , \quad (3.5)$$

with n and l being the *radial* quantum number and *orbital angular momentum* quantum number, respectively, taking values $n = 1, 2, 3, \dots$ and $l = 0, 1, 2, \dots, n - 1$. In this first approximation, all the levels with the same principal quantum number N are *degenerate*, with a maximal degeneracy given by $2(2l+1)$. However, by using only the SHO term as the expression of $V(r)$, only the first three magic numbers are reproduced, meaning that some additional term(s) might be needed in order to consistently obtain the series of magic numbers.

A next step is to use the fact that the experimentally observed short range of the strong nuclear force: the steepness of the SHO can be corrected with an *attractive* term proportional to l -squared. This acts as a centrifugal term which provides an angular momentum barrier, lifting the degeneracy between the levels with the same principal quantum number N and different values for the orbital angular momentum l . This SHO+ l^2 step is still not enough though. The last step is to add a so-called *spin-orbit* coupling term of the form $\vec{l} \cdot \vec{s}$. This term comes from the

consideration that the nucleon-nucleon interaction has a spin dependence, and the potential depends on the intrinsic spin s (\vec{s}) and the orbital angular momentum l (\vec{l}) of a nucleon. Since $\vec{j} = \vec{l} + \vec{s}$, two possible states emerge from a single value of l (depending on whether \vec{s} is parallel or anti-parallel to \vec{l}). The final expression of the terms SHO+ \vec{l}^2 + $\vec{l} \cdot \vec{s}$ will consist in the *Modified Harmonic Oscillator* (HMO).

$$V(r) = \frac{1}{2}(\omega r)^2 + B \vec{l}^2 + A \vec{l} \cdot \vec{s}. \quad (3.6)$$

For the sake of simplicity, the centrifugal term will be denoted within formulas without the vector symbol. Since the intrinsic spin of a nucleon is $s = 1/2$, for a given value of l , there can be two values for the *total angular momentum* (a.m.) $j = l \pm 1/2$: one for each spin orientation with respect to the direction of the orbital a.m. Moreover, for each value of $l = 0, 1, 2, 3, 4, \dots$, there is a similar notation $l = s, p, d, f, g, \dots$, respectively. Regarding the spectroscopic notation, usually, the value of j is considered as a subscript; nl_j (for example $1p_{1/2}$ and $1p_{3/2}$). What it is worth mentioning is that for high enough shells, there can be splittings between $j + 1/2$ and $j - 1/2$ that are large enough to lower the $j + 1/2$ state from one oscillator shell n to one located below $n - 1$. These types of levels are called *intruder states* and they have opposite parity $\pi = (-1)^l$ with respect to the shell that these levels will occupy.

Going back to the expression of the $\vec{l} \cdot \vec{s}$ term from Eq. 3.6 and denoting it with $V_{ls}(r)$, it is shown by Casten [9] that its contribution to the total potential can be regarded as a surface effect. Due to this, its form can be expressed as a function that depends on the radial coordinate as such [9]:

$$V_{ls}(r) = -a_{ls} \frac{\partial V(r)}{\partial r} \vec{l} \cdot \vec{s}, \quad (3.7)$$

where $V(r)$ is the expression for a central potential and a_{ls} is a strength constant.

Now that an expression for the nuclear potential that is able to reproduce all the magic numbers has been formulated, it is also possible to formulate the total energy of a single-particle within the average potential that is generated by all the other nucleons within the nucleus. Thus, the Hamiltonian of this simple system

(the modified oscillator) can be formulated as such:

$$\begin{aligned} H &= -\frac{\hbar^2}{2m}\nabla^2 + V_{\text{SHO}} + (l^2)_{\text{term}} + (\vec{l} \cdot \vec{s})_{\text{term}} = -\frac{\hbar^2}{2m}\nabla^2 + V_{\text{MHO}}, \\ H &= -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m(\omega r)^2 + Bl^2 + A\vec{l} \cdot \vec{s}. \end{aligned} \quad (3.8)$$

The evolution from each term in the shell-model potential (that is the first approximation as a SHO, then SHO+ l^2 , and finally SHO+ $l^2 + \vec{l} \cdot \vec{s}$ or modified oscillator potential) is illustrated in Fig. 3.3, where it can be seen how each extra term introduces a new degeneracy within the energy states, with the complete reproduction of the magic numbers in the third column. Moreover, the *intruder* levels can be observed, where levels with $j = l + 1/2$ from a particular n are so low, that they lie below an $n - 1$ adjacent level.

Another, more realistic potential that can be used in order to reproduce the specific shell model calculation is the so-called Woods-Saxon potential. Because of the short-range character of the strong nuclear force, it is safe to assume that this potential should behave in the same manner as the density distribution of the nucleons. Since for medium and heavy nuclei, the Fermi-like functions (distributions) are the ones that best fit the experimentally measured data, this potential should have the following form [16]:

$$V_{\text{ws}}(r) = -\frac{V_0}{1 + e^{\frac{r-R_0}{a}}}. \quad (3.9)$$

This mean-field potential contains the terms V_0 that represents the depth of the potential (≈ 50 MeV, in order to reproduce the experimental separation energies for the nucleons), the surface thickness a (also called the diffuseness parameter, giving information about how fast the potential drops to zero) with a value of approximately 0.5 fm, while R_0 is the nuclear radius with $R_0 = r_0 A^{1/3}$ and $r_0 = 1.2$ fm. The nature of this potential is of *central type* and, unfortunately, Eq. 3.9 in its pure form is not enough the reproduce the higher magic numbers. As such, the addition of a spin-orbit term, similarly as in the case of MHO potential, is required [17]:

$$V_{\text{total}} = V_{\text{ws}}^{\text{central}} + V_{ls}(r)\vec{l} \cdot \vec{s}. \quad (3.10)$$



FIGURE 3.3: The energy levels obtained via calculation of the shell model potential using the simple oscillator (SHO), the SHO amended with a centrifugal term l^2 , and finally the modified oscillator (MHO) that contains a spin-orbit term. The ‘correct’ magic numbers are the ones in the right-most column.

Figure is adapted from Refs. [8],[14].

The only good quantum numbers in the case of the WS potential are the total a.m. j and the parity $\pi = (-1)^l$. The expectation value of the spin-orbit term $\vec{l} \cdot \vec{s}$ can be given as:

$$\langle ls \rangle = \hbar^2 \begin{cases} \frac{l}{2} & \text{for } j = l + \frac{1}{2} \\ -\frac{l+1}{2} & \text{for } j = l - \frac{1}{2} \end{cases}. \quad (3.11)$$



FIGURE 3.4: The shape of the Woods-Saxon potential, defined by Eq. 3.9. The parameters are arbitrarily chosen as: $V_0 = 50$ MeV, $R = 5.57$ fm, and $a = 0.5$ fm.

and the spacing between two levels can be furthermore expressed as [17]:

$$\Delta E_{ls} = \frac{2l+1}{2} \hbar^2 \langle V_{ls} \rangle . \quad (3.12)$$

The experimental evidence points to the fact that $V_{ls}(r)$ is negative, meaning that states with $j = l - 1/2$ are shifted higher than $j = l + 1/2$. Some characteristics of the WS potential are the following:

1. It increases with the increase of R , meaning that it has an *attractive nature*
2. It flattens out for large enough A in the center of the nucleus
3. It rapidly goes to zero as R increases (given by the diffuseness parameter), indicating its short-range nature
4. When $R = R_0$ (that is for the nucleons near the surface), a large force towards the center of the nucleus is experienced by the these nucleons.

Fig. 3.4 shows the shape of a typical Woods-Saxon potential. Aiming at a final Hamiltonian which describes the motion of the nucleon within the mean-field



FIGURE 3.5: A schematic representation with the three kind of potentials used to describe the shell model: harmonic oscillator, Woods-Saxon, and for completeness, the square-well.

potential, the formula can be readily obtained:

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V_{ws}^{\text{central}} + (\vec{l} \cdot \vec{s})_{\text{term}}, \quad (3.13)$$

$$H = -\frac{\hbar^2}{2m} \nabla^2 - \frac{V_0}{1 + e^{\frac{r-R_0}{a}}} + A \vec{l} \cdot \vec{s}. \quad (3.14)$$

In addition to the shape of the Woods-Saxon potential, a comparison between it, a SHO, and the square-well-like potential is made in Fig 3.5.

The difference between the pure form of the Woods-Saxon potential and the total potential, where the spin-orbit contribution is amended, can be seen in Fig. 3.6.

So far, the general discussion concerning the nuclear models was for the case where each nucleon is treated as an *independent* particle moving in an average potential (mean-field potential) which represents an *effective* interaction of all the other nucleons with the nucleon under study. However, such an assumption is not accurate enough (especially for the nuclei that lie far away from the closed shells), and this problem should be treated within a *many-body* approach: considering the mutual interaction between the nucleons. These interactions are also called *residual interactions* [9, 18]. With these residual interactions, an accurate depiction of the nucleus might be achieved, and in the following sections, the *Deformed Shell Model*



FIGURE 3.6: The left side represents the energy levels calculated for the Woods-Saxon potential given by Eq. 3.9, and the right side shows the single-particle energies with the spin-orbit correction added, as in Eq. 3.10. Figure adapted from Ref. [10].

will be employed, reaching to the famous Nilsson model/theory of describing the nucleus.

3.3 Deformed Shell Model

In the previous section, the discussion was focused on an approximate description of the (independent) motion of a nucleon within an average potential. That potential is generated by the interaction of that nucleon with all the remaining

nucleons within the compounding nucleus. Indeed, for spherical nuclei, the model described previously works really well and it is a successful tool in reproducing and predicting the properties of nuclear states, especially if the excited states have nucleonic configurations that are dominated by a single nucleon or a very small number of ‘extra’ nucleons.

For nuclei that are even in both the proton number and the neutron number (i.e., even-even nuclei), the nuclear ground-state has a spin and parity that are properly reproduced by the *spherical shell model*: $I^\pi = 0^+$. In a nucleus with complete shells, the *net spin* must be zero while for the nucleus with one nucleon missing from a complete shell closure (a hole), that ground-state spin should equal to the total a.m. j value of the orbital which that particular hole is occupying. Moreover, the parity of the ground-state for a given nucleus is determined by the orbital a.m. value l :

$$\pi = (-)^l \rightarrow \begin{cases} +1 & \text{for even-}l \text{ levels} \\ -1 & \text{for odd-}l \text{ levels} \end{cases}. \quad (3.15)$$

For odd-odd nuclei, one can find the ground-state (g.s.) spin and parity via the coupling of the spin and parity of the last two valence nucleons [14, 18]. The coupling rules that are allowed in the odd-odd nucleus were determined more than 50 years ago by Gallagher et al. [19]:

$$I = j_p + j_n \text{ if } j_p = l_p \pm \frac{1}{2} \text{ and } j_n = l_n \pm \frac{1}{2}, \quad (3.16)$$

$$I = |j_p - j_n| \text{ if } j_p = l_p \pm \frac{1}{2} \text{ and } j_n = l_n \mp \frac{1}{2}. \quad (3.17)$$

3.3.1 Deformed Shell Model - Nilsson Model

The idea that some nuclei are deformed in their ground-state was enforced experimentally a long time ago by measuring quantities such as density distributions, nuclear quadrupole moments [9] and so on. The non-spherical shapes are given by the existence of nucleonic configurations that lie away from the major shell closure. In Chapter 2 the description of the nuclear shapes was treated, using the well-known formula for the parametrization of the nuclear radius in terms of the collective coordinates (see Eq. 2.1), resulting in the known nuclear shapes:

spherical, axially-symmetric (that is prolate or oblate), and *axially-asymmetric* (or triaxial).

Developed by Nilsson in 1955 [20] for treating the *deformed nuclei* proved to be a big pillar within the nuclear community, especially for the study of medium and heavy nuclei. In essence, this tools is a modified shell model which allows for deformations to be taken into account by the use of the *anisotropic harmonic oscillator* (AHO). Similarly as for the basic shell model, the goal is to obtain an expression for the single-particle energies of a nucleon. The basic Hamiltonian corresponding to this kind of system is shown below [18]:

$$H = H_0 + a_1 \vec{l} \cdot \vec{s} + a_2 l^2 , \quad (3.18)$$

where H_0 is a Hamiltonian for the AHO. The general expression for this kind of oscillator is of the form:

$$H_{\text{AHO}} \equiv H_0 = -\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) . \quad (3.19)$$

In the general expression of the single-particle Hamiltonian, the constants a_1 and a_2 are usually determined via adjustments to the experimental results. It can be seen that the centrifugal-like term l^2 , which simulates a flattening of the oscillator potential, and the $\vec{l} \cdot \vec{s}$ term are still present here, as it was the case for the spherical shell model. However, the explicit form of Eq. 3.18 is as follows:

$$\begin{aligned} H_{\text{Nil}} = & -\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) - 2\kappa\hbar\omega_0(\vec{l} \cdot \vec{s}) \\ & - 2\kappa\hbar\omega_0\mu(l^2 - \langle l^2 \rangle_N) . \end{aligned} \quad (3.20)$$

Obviously, the parameters κ and μ act as strength parameters for the spin-orbit coupling term and the centrifugal term, respectively. The last term is a correction, which was originally considered as μl^2 , but it was pointed by Gustafson et al. [21] that the shift in energy is way too large for big values of N (principal quantum number). As a result, taking the current expression for the correction term helps to compensate. The three *oscillator frequencies* are chosen to be inversely proportional to the semi-axis lengths of the deformed ellipsoid (denoted by a_x , a_y , and a_z) such that:

$$\omega_r = \omega_0 \frac{R_0}{a_r} , \quad r = x, y, z . \quad (3.21)$$

For the spherical case, the oscillator frequency $\hbar\omega_0$ is set to $41A^{-1/3}$ MeV (calculation for this value arise from the shell model with SHO [18]). For the axially-symmetric case, one can choose the z -axis as symmetry axis, implying that thw oscillator frequencies along the x and y axes are equivalent (that is $\omega_x = \omega_y \equiv \omega_{\perp}$).

Following the calculations done in [18], one can express the two relevant oscillator frequencies in terms of a deformation parameter ϵ_2 (whose dependence on the quadrupole deformation parameter β_2 has been shown in Eq. 2.24) as such:

$$\omega_{\perp}^2 = \omega_0^2 \left(1 + \frac{2}{3}\epsilon_2\right) , \quad (3.22)$$

$$\omega_z^2 = \omega_0^2 \left(1 - \frac{4}{3}\epsilon_2\right) . \quad (3.23)$$

Moreover, a dependence on the deformation parameter itself is employed for the frequency ω_0 that appears in the expressions for ω_{\perp} and ω_z , respectively:

$$\omega_0 = \left(1 - \frac{4}{3}\epsilon_2^2 - \frac{16}{27}\epsilon_2^3\right)^{-1/6} , \quad (3.24)$$

where $\bar{\omega}_0$ can be considered a constant written as $\bar{\omega}_0 = (\omega_x\omega_y\omega_z)^{1/3} = \text{const}$ (coming from the harmonic oscillator at zero deformation and also considering the conservation of the nuclear volume).

The energy eigenvalues ϵ_q for the nucleonic state ψ_q belonging to a deformed nucleus can be determined within the Nilsson model by solving the Schrödinger equation associated to each nucleon in particular:

$$H_{\text{Nil}}\psi_q = \epsilon_q\psi_q , \quad (3.25)$$

where the index q denotes a set with all the relevant quantum numbers. This set is also called the *asymptotic quantum numbers*, and they are used to specify a *Nilsson orbital*. The well-known notation is as follows (still considering the z -axis as the symmetry axis):

$$\Omega^{\pi} [Nn_z\Lambda] . \quad (3.26)$$

- Λ is the projection of the particle's orbital a.m. along the symmetry axis (component of l along z)



FIGURE 3.7: A schematic drawing that shows the geometrical interpretation of the Nilsson asymptotic quantum numbers (see text). This figure is inspired from Ref. [22]

- N the principal quantum number of the major shell. It also determines the parity as $\pi = (-1)^N$, making the notation from Eq. 3.26 somewhat redundant in terms of explicitly specifying it
- n_z is the number of oscillator quanta along the symmetry axis. More precisely, it gives the number of nodes for the wave-function of that particle along the direction of the z -axis
- Ω is the projection of the particle's total a.m. along the symmetry axis (i.e., \mathbf{j}). Moreover, the projection of the intrinsic spin of a nucleon onto the symmetry axis can have the values $\Sigma = \pm \frac{1}{2}$, so that $\Omega = \Lambda + \Sigma = \pm \frac{1}{2}$.

Fig. 3.7 shows the geometrical meaning of the asymptotic quantum numbers for the Nilsson model. Indeed, for a single nucleon orbiting a deformed core, the vector \mathbf{R} represents the angular momentum of a *rotating nucleus* (having a collective character, since it emphasizes the motion of the nucleus as a whole), the vector \mathbf{I} represents the total a.m. of the entire nucleus, \mathbf{j} is the total a.m. of the single-particle (that is $\mathbf{j} = \mathbf{j} + \mathbf{s}$). However, two more quantum numbers should be mentioned: the projection of the total a.m. \mathbf{I} onto the symmetry axis, denoted by K , and the projection of the same vector onto the laboratory axis, referred to as M .

Regarding the quantum numbers sketched in Fig. 3.7, there is an important aspect which needs to be specified about the two projections K and Ω , respectively, since it would make the understanding of the orbital motion of nucleons more concise. Indeed, it is clear that compared to the spherical case, where different orientations are irrelevant to the energy spectrum of nucleons, here in the deformed case, different directions in space lead to different energies. The orientation is in fact specified by the *magnetic sub-state* of the nucleon, i.e., the projection of the total angular momentum on the symmetry axis. This projections is denoted by Ω for the single-particle, however, because the rotational angular momentum \mathbf{R} in the axially deformed is perpendicular to the symmetry axis for low-lying states, then it will have no contribution to K , meaning that one can use Ω and K interchangeably.

3.3.2 Single-particle states in deformed nuclei

It is instructive to go into detail about the quantum numbers defined in Eq. 3.26 since the orbits which characterize the nucleons with such numbers help to point out the nature of nuclear deformations that take place.

The quantum numbers N , n_z and Λ are good quantum numbers only when the nuclear deformation is large, meaning that ϵ (or equivalently β) tends to infinity: also the reason why they are called asymptotic quantum numbers. However, the numbers Ω and π remain good quantum numbers even for low and moderate deformations for the nucleus. It should be noted that if N is even, then $(\Lambda + n_z)$ is also even. Similarly, if N is odd, then the sum of the other two quantum numbers must also be odd [9].

Since the eigenvalues of the Hamiltonian H_{Nil} ultimately depend on the deformation parameter ϵ , each nucleon will have an orbit (energy) that is deformation dependent. At no deformation (i.e., the spherical case), all the energy levels for a single-particle state will have a $2j + 1$ degeneracy. This translates to the fact that all $2j + 1$ possible orientations of \vec{j} are equivalent, when referring to any arbitrary axis of choice. On the other side, when the potential is deformed, this will no longer hold: the energy levels in the deformed potential will depend on the spatial orientation of the orbit itself: the energy depends on the component of \vec{j} along the symmetry axis of the core.



FIGURE 3.8: A simple sketch showing the single-particle orbits for the $j = 7/2$ nucleonic state, along the symmetry axis for a *prolate* deformation. The actual projections are $\Omega_1 = \frac{1}{2}$, $\Omega_2 = \frac{3}{2}$, $\Omega_3 = \frac{5}{2}$, and $\Omega_4 = \frac{7}{2}$. The figure was inspired from Ref. [14].

As an example, a nucleon from the $f_{7/2}$ shell will be considered. This nucleon can have eight possible components for \vec{j} , this is the range $\Omega = [-\frac{7}{2}, \frac{7}{2}]$. Because of the reflection symmetry for nuclei for either of the two possible directions of the symmetry axis, the positive components of Ω will have the same energy as the negative ones: leading to a degeneracy of the levels. Now, the single-particle $f_{7/2}$ state will split up into four new states when deformation emerges: $\Omega = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$ and all have negative parity. In Fig. 3.8 an illustration with the different orbits of the odd particle is given, for both the prolate deformed nuclei as well as for oblate ones. Similarly, the orbits of the same state are pictorially represented in Fig. 3.9.

From Figs. 3.8 - 3.9, it can be seen that the first orbit (denoted by orbit 1) lies closest to the core in the prolate case, while in the oblate case this is true for orbit 4. This plays the role in the interaction strength, meaning that for the prolate case, the orbit 1 will interact the strongest with the *core*, while in the oblate case, it is the orbit 4 which has the strongest interaction with the bulk core. Moreover, the strength of interaction indicates the magnitude of the energies for each projection: the stronger the interaction between the orbit and the core, the more tightly bound these states are and lie lower in energy. For prolate deformations, the orbits with smallest Ω ‘prefer’ to lie lower in energy (interacting strongly with the core). For



FIGURE 3.9: A simple sketch showing the single-particle orbits for the $j = 7/2$ nucleonic state, along the symmetry axis for a *oblate* deformation. The actual projections are $\Omega_1 = \frac{1}{2}$, $\Omega_2 = \frac{3}{2}$, $\Omega_3 = \frac{5}{2}$, and $\Omega_4 = \frac{7}{2}$. The figure was inspired from Ref. [14].

oblate deformations, the situation is opposite: orbits with the maximal Ω have the strongest core interactions and therefore lie lowest in energy.

Another way of looking at the coupling of the single-particle with the bulk core can be given in terms of overlaps of their corresponding wave-functions (eigenstates). Indeed, a nucleon lying in the lowest Ω orbit will have a *maximum* wave-function overlap with a prolate core. On the other hand, nucleons lying in the highest Ω orbits will have maximum overlap of the wave-function with an oblate core. The overlap gives the overall binding energy between the two systems (i.e., core and particle) as explained in the previous paragraph. Discussion about the wave-function overlap and the nuclear density distribution [23, 24] will be made in the following chapters.

The induced degeneracy due to deformation for a particle state l_j is shown in Fig. 3.10, for the same example of the nucleon with the orbit $f_{7/2}$.

Obviously, the sketch shown in Fig. 3.10 is just an instructive example, and it does not represent an accurate description of the single-particle energies for deformed nuclei. In fact, if the potential is deformed, the quantum numbers l and j are not



FIGURE 3.10: The effect of deformation for the particle state $f_{7/2}$. It can be seen that indeed, as it was mentioned within the text, Ω_1 component lies lowest in energy for the oblate deformation, and Ω_4 component lies the lowest in energy for an oblate deformation.

valid anymore (that is, the angular momentum is no longer a constant of motion for non-spherical potentials). A proper description of the single-particle orbits are represented by the so-called *Nilsson diagrams*, where the energy for each state is represented as a function of the deformation parameter. Remember that the energies are in fact the eigenvalues of the Schrödinger equation associated to the initial Nilsson deformed Hamiltonian (see Eq. 3.25).

The spectrum of one-particle orbits plays an invaluable role within the nuclear structure and the study of deformed nuclei: the picture of one-particle motion in deformed potential works for deformed nuclei much better than the case of single-particle motion in spherical potentials for spherically shaped nuclei. Multiple quantitative analyses have been performed on experimental data of well-deformed (especially odd- A) nuclei, from light (^{25}Mg , ^{25}Al) to heavy (^{169}Tm , ^{175}Yb , ^{177}Yb) [25]. Examples with this kind of diagrams are shown in Figs. 3.11 - 3.12.

It can be seen that each state within a Nilsson diagram is represented as a solid line or a dashed line, depending on its parity (remember that the parity quantum number is given by $(-1)^N$ or, equivalently, by $(-1)^l$). The labelling from the Figs. 3.11 - 3.12 is consistent with the one defined in the previous subsection.



FIGURE 3.11: A Nilsson diagram for protons or neutrons, with Z or $N \leq 50$. Picture reproduced from Ref. [11].



FIGURE 3.12: A Nilsson diagram for neutrons, with $82 \leq N \leq 126$. Picture reproduced from Ref. [11].

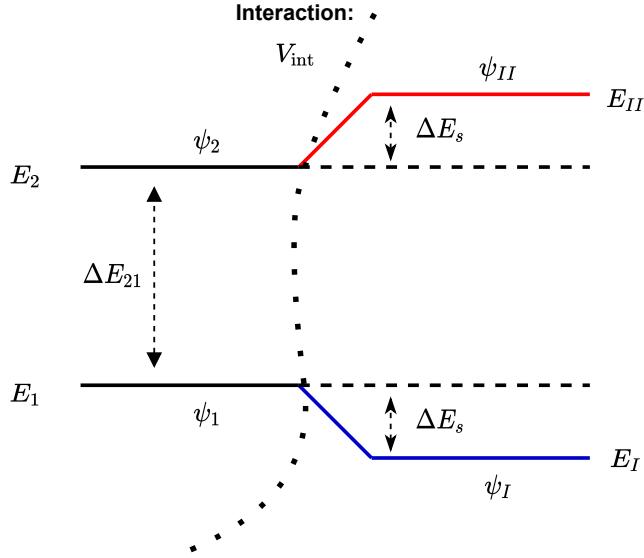


FIGURE 3.13: Defining the mixing between two different states, with two corresponding energies and wave-functions. Interaction is illustrated via the curved line and V_{int} term.

Another important aspect which can be seen in the Nilsson diagrams (for some orbits) is the ‘crossing’ between states with different quantum numbers. In order to fully understand this concept, it is instructive to go into detail about *two-state mixing*.

Two-state mixing

In the work of Casten [9], an analytical approach is given for treating the mixing of two different states (energy levels). It starts from the basic idea of two initial levels, each with its corresponding energy E_1 and E_2 , and their associated wave-functions (denoted here with ψ_1 and ψ_2). Any interaction between them results in the mixing matrix element $\langle \psi_1 | V_{\text{int}} | \psi_2 \rangle$, where V_{int} is the arbitrary interaction between the states. This is sketched in Fig. 3.13.

This problem can be solved by finding the final energies and wave-functions, this being done via the diagonalization procedure of a 2×2 matrix, where the main diagonal contains the two energies and off-diagonal terms represent the interaction itself. The final states will be denoted here with (E_I, ψ_I) for the energies and (ψ_I, ψ_{II}) for the wave-functions. As a general rule, the mixing depends on the initial separation $\Delta E_{21} = (E_2 - E_1)$ and the matrix element $\langle \psi_1 | V_{\text{int}} | \psi_2 \rangle$. Given a large spacing, the effect of a given matrix element will be quenched. Moreover, even for

a small matrix element, it can introduce a large mixing if the energy separation between the states is small (that is, the unperturbed states are lie close in energy).

A reduction from these two parameters can be performed, obtaining a single universal mixing expression that is valid for any arbitrary interaction and any initial spacing. As a first step, one should define the ratio between the spacing of the unperturbed states (ΔE_{21}) and the strength of the matrix element:

$$R = \frac{\Delta E_{21}}{V_{\text{int}}} . \quad (3.27)$$

With this quantity, the newly perturbed energies E_I and E_{II} are readily obtained [9]:

$$E_I = \frac{1}{2}(E_1 + E_2) + \frac{\Delta E_{21}}{2} \sqrt{1 + \frac{4V_{\text{int}}^2}{\Delta E_{21}^2}} , \quad (3.28)$$

$$E_{II} = \frac{1}{2}(E_1 + E_2) - \frac{\Delta E_{21}}{2} \sqrt{1 + \frac{4V_{\text{int}}^2}{\Delta E_{21}^2}} . \quad (3.29)$$

Even more useful would be to find the amount by which each energy is shifted after the interaction. This is denoted in Fig. 3.13 by ΔE_S and its expression depends on ΔE_{12} as such:

$$|\Delta E_S| = |E_{II} - E_2| = |E_I - E_1| = \frac{\Delta E_{21}}{2} \left[\sqrt{1 + \frac{4}{R^2}} - 1 \right] . \quad (3.30)$$

The two perturbed wave functions are as follow:

$$\begin{aligned} \psi_I &= \alpha\psi_1 + \beta\psi_2 , \\ \psi_{II} &= -\beta\psi_1 + \alpha\psi_2 , \end{aligned} \quad (3.31)$$

where the two amplitudes α and β must verify the condition $\alpha^2 + \beta^2 = 1$ and:

$$\beta = \frac{1}{\left\{ 1 + \left[\frac{R}{2} + \sqrt{\frac{R^2}{4} + 1} \right]^2 \right\}^{1/2}} \quad (3.32)$$

It is noteworthy to point out that the amplitude β is in fact a function that only depends on R (i.e., the ratio between the unperturbed energy splitting and the



FIGURE 3.14: **Left:** The dependence of R (see text) on the mixing amplitude β . **Right:** The dependence of R (see text) on the energy shift of the perturbed states (ΔE_S).

interaction strength). Similarly, by dividing the shift in energy ΔE_S to the initial splitting ΔE_{21} , one will obtain an expression that is independent of the initial level spacing:

$$\frac{|\Delta E_S|}{\Delta E_{21}} = \frac{|E_{II} - E_2|}{\Delta E_{21}} = \frac{|E_I - E_1|}{\Delta E_{21}} = \frac{1}{2} \left[\sqrt{1 + \frac{4}{R^2}} - 1 \right] \quad (3.33)$$

The importance of these formulae will be now emphasized through a numerical example. First of all, the evolution of the ratio of the unperturbed shift and the interaction can be graphically represented as a function of the small mixing amplitude β by the use of Eq. 3.32. The graphical representation is shown in Fig. 3.14. Following this analysis, also in Fig. 3.14 the shape of R as a function of the energy shift of the perturbed states can be visualized.

For an arbitrary case where two initial states are separated by, say $\Delta_{21} = 0.07$ MeV, and they become *perturbed* via the interaction with a strength $V_{\text{int}} = 0.03$ MeV, this gives a value of $R = 3.5$ and, moreover, the mixing amplitude is $\beta = 0.256$. The two states will both be shifted by only $\Delta E_S = 5.31$ keV (accounting for about 7.6% of the initial separation). Indeed, for this particular example, the perturbation results in an energy shift that is rather small compared to the initial state spacing.

Besides the numerical example discussed above, there are also two extremely important limiting situations when two states interact via a perturbation. The first one is the so-called *strong mixing limit*, when the two initial states are degenerate



FIGURE 3.15: The *strong mixing* limit for two energy levels that are interacting via a perturbation. The initial two levels are degenerate, such that their splitting is null.

(i.e., there is practically no spacing between them and $\Delta_{21} = 0$). In this situation, the analytical expressions from Eq. 3.30 fail to provide a quantitative analysis, but from Eq. 3.29 a small adjustment of the expression will give rise to the following:

$$E_{I,II} = \frac{1}{2} [(E_1 + E_2) \pm 2V_{\text{int}}] = E_0 \pm V_{\text{int}}, \quad (3.34)$$

where the initial (common) energy of the two degenerate states is denoted by E_0 . The above equation indicates the important fact that the energy shift which the two states suffer via the perturbation is only given by the *mixing matrix element*. This means that the final separation energy for a two-state isolated system can never be closer than twice the interaction strength ($2V$). In the degeneracy case, the values for β and α are readily obtained: ($\beta = \alpha = \frac{1}{\sqrt{2}} = 0.707$), such that the states are completely mixed. Consequently, the mixed wave-functions of two (initially) degenerate states do not depend on the strength V_{int} between them. The limiting case of *strong mixing* of two degenerate levels is sketched in Fig. 3.15.

The second limiting case is called *weak mixing limit*, corresponding to a very large value of R (meaning that the initial separation of the states is very large compared to the magnitude of the interaction itself). The shift in energy of the perturbed states in this case is given by:

$$\frac{|\Delta E_S|}{\Delta E_{21}} = \frac{1}{R^2}. \quad (3.35)$$

A graphical representation for the weak mixing is shown in Fig. 3.16.

As a final step in the analysis of the two-state mixing, it is worth mentioning a corner-case which will help to get a better grasp of the Nilsson orbitals. Consider two states (say ψ_1 and ψ_2) whose energies are parametrized in terms of some argument c_{nuc} which is relevant for the nuclear structure of that system (e.g., c_{nuc} could be a quadrupole deformation and the two initial states are in fact Nilsson

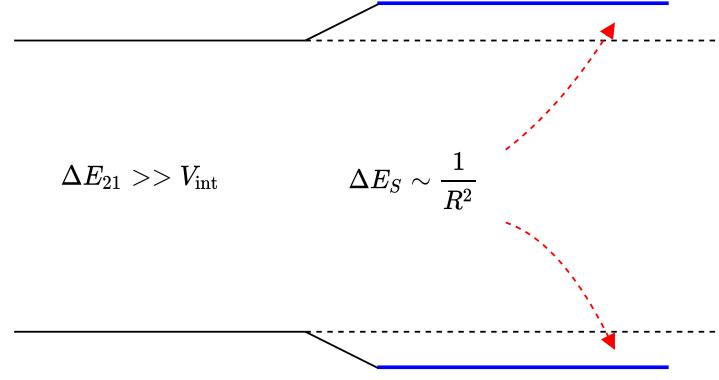


FIGURE 3.16: The *weak mixing* limit for two energy levels that are interacting via a perturbation. The interaction strength is much smaller than the initial spacing between states, resulting in a very small energy splitting ΔE_S .

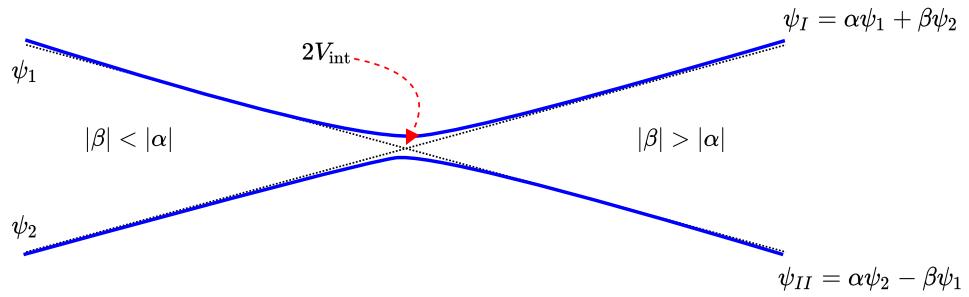


FIGURE 3.17: A sketch showing the concept of *non-crossing* between two states. Arrow represents the closest point at which the two states can interact with each other (i.e., the inflection point).

orbits). The remarkable ‘feature’ of this hypothesis is that if there indeed exists mixing between the two states, they can never cross each other. The two mixed states will always repel and they can never be closer than twice the mixing matrix element V_{int} after mixing occurs. In Fig. 3.17, the behavior of non-crossing for the mixed states is sketched. The point at which the two states are the closest to each other represents the case when the wave-functions contain similar admixtures of each of the initial states (unperturbed). The *inflection point* can be seen in Fig. 3.17, where the behavior of the final states ψ_I and ψ_{II} can be seen.

Nilsson orbitals

With the concept of two-state mixing clearly depicted, it is instructive to go further into the Nilsson orbitals and their significance. Recalling Fig. 3.10, the splitting of a j orbital into $j + 1/2$ magnetic sub-states can be viewed as a set of orbitals (energies) where the nucleon orbits around the bulk nucleus with an orbit that

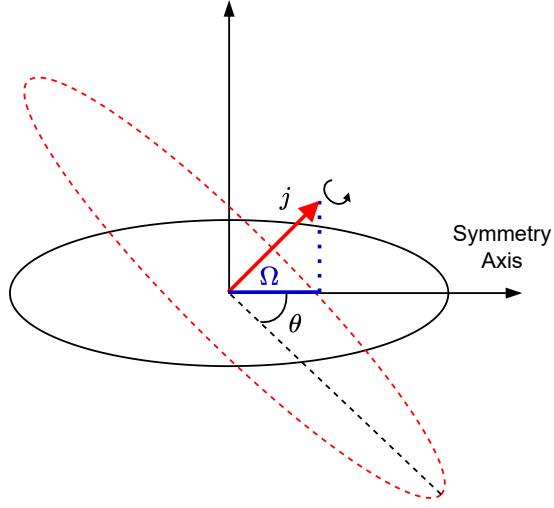


FIGURE 3.18: The orbit of a single particle orbiting the deformed nucleus, defined by the projection of the particle's a.m. Ω (on the symmetry axis) and the tilting angle θ . Figure inspired from Ref. [9]

has a certain *tilt* angle θ (see the orbits depicted in Figs. 3.8 and 3.8). The tilting angle is conceptually showed in Fig. 3.18, where a magnetic sub-state with given Ω is shown. For that particular orbit, the angle is given by the expression [9, 14]:

$$\begin{aligned} \sin \theta &= \frac{\Omega}{j}, \\ \theta &= \arcsin\left(\frac{\Omega}{j}\right). \end{aligned} \quad (3.36)$$

The change of θ is rather slow for low Ω projections, while rapid changes take place at high Ω values. As a numerical example, the change in θ is studied for the orbits $j = \{9/2, 11/2, 13/2\}$, with their corresponding projections. The evolution with Ω for different orbits can be seen in Fig. 3.19.

The simplistic shapes within the splitting of an orbital j into multiple sub-states (see Fig. 3.10) emerge from the considerations regarding the change in tilting angle θ and the observation that the difference in energy is rather slight (high) depending on low (high) Ω values.

Based on this discussion, it is clear that a full Nilsson diagrams is constructed with the configuration mixing of different j values, configuration which is superimposed on state-splitting via the Ω projections. With this idea, one can state that *no two*

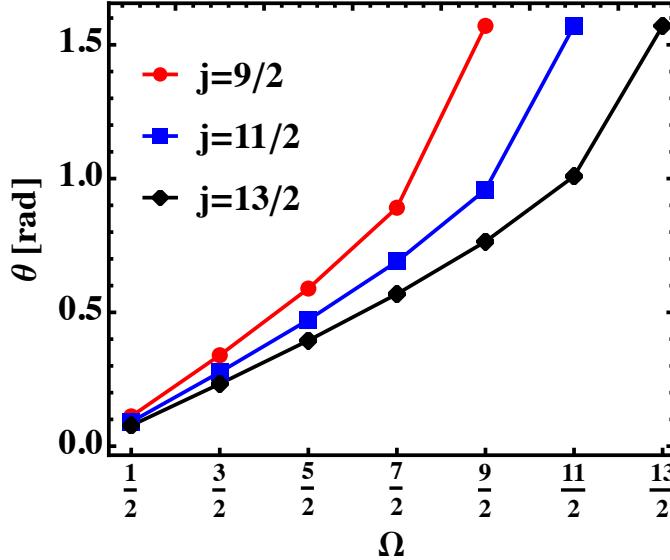


FIGURE 3.19: The change in θ with increasing values of Ω , for given orbitals j .

lines in the Nilsson diagram with similar Ω values can cross each other. As two such orbits come close to each other, they must repel as shown in Fig. 3.17. Explaining the behavior of the lines that appear in the Nilsson diagrams 3.11 - 3.12 is straightforward: each line represents a Nilsson state, starting out in a straight line and then sloping downward or upward, depending on the angle of the orbit relative to the bulk nucleus. The *curving* of an orbit starts when it approaches another level with the same quantum number Ω and parity π . Thus, the structure of any Nilsson diagram relies on three main features [9]:

- the Ω splitting
- repulsion between two levels
- single-particle shell model energies

Taking a closer look at the second Nilsson diagram previously shown (see Fig. 3.12), there are two orbits within the 82-126 neutron shell that can be analyzed in terms of *mixing*: $f_{7/2}$ and $h_{9/2}$. Obviously, the lack of deformation implies a degeneracy of these orbits, but when deformation occurs, splitting kicks in. The angle of the orbital orientation θ depends on the ratio $\frac{\Omega}{j}$ (recall formula $\theta = \arcsin \frac{\Omega}{j} \approx \frac{\Omega}{j}$ for low Ω). Small tilting angles will occur due to i) small values of Ω or ii) high j . As a result, the energies for the orbits $\Omega = 1/2, 3/2, 5/2$ belonging to the $h_{9/2}$ shell are decreasing in energy faster with deformation than those from $f_{7/2}$ orbit. Consequently, the different rates of decrease of the Nilsson

energies will overcome any small spherical energy separation $f_{7/2} - h_{9/2}$, making the orbits with low Ω to approach each other: mixing becoming more pronounced. But as discussed in the section devoted to *two-state mixing*, two orbits defined by the same quantum numbers cannot cross each other, so they will repel, leading to the *inflection point*. The points can be seen, for example, when looking at the $\Omega = 5/2$ and $\Omega = 7/2$ orbits, corresponding to $f_{7/2}$ and $h_{9/2}$, respectively.

Lastly, an alternative form of the Nilsson Hamiltonian should be expressed, taking into consideration the already studied nuclear radius (see Eq. 2.1 which describes the shape of the nuclear surface) and the fact that until now, only the *quadrupole* effects have been relevant to the discussion about deformed potentials in nuclei. Indeed, for quadrupole deformations, the nuclear radius can be simplified to:

$$R(\theta, \varphi) = R_0 (1 + \beta Y_2^0(\theta, \varphi)) . \quad (3.37)$$

The single-particle Hamiltonian can be written in the general form, starting from the expression Eq. 3.20:

$$\begin{aligned} H_{\text{Nil}} = & -\frac{\hbar^2}{2m} + \frac{1}{2}m(\omega_0 r)^2 - \frac{4}{3}\sqrt{\frac{\pi}{5}}m(\omega_0 r)^2\epsilon Y_2^0(\theta, \varphi) - 2\kappa\hbar\omega_0(\vec{l} \cdot \vec{s}) \\ & - 2\kappa\hbar\omega_0\mu(l^2 - \langle l^2 \rangle_N) . \end{aligned} \quad (3.38)$$

The expression for the oscillator frequencies were already given (defined as functions of the deformation parameter ϵ), and they keep the same form (see Eqs. 3.23 - 3.24). It is worth mentioning that both forms of H_{Nil} are equivalent, and allow to describe the structure of the deformed nuclei in the limits of large deformations (via Eq. 3.20) and small deformations (via Eq. 3.38). Within literature, the two parameters κ and μ have usually values around 0.06 for the former and (0 \sim 0.7) for the latter. As previously shown, the relationship between the ϵ and β deformation parameters is given by $\epsilon = 3/4\sqrt{5/\pi}\beta$.

When the deformations are small, j is a good quantum number, and the Eq. 3.38 represents a Hamiltonian for the AHO (which it was discussed) plus a *perturbation* that is proportional to $\epsilon r^2 Y_2^0$. One can consider the eigenstates of the Hamiltonian as some states labelled by the quantum numbers Nlj and m typical to the spherical case. Casten shows that if the angular part Y_2^0 is treated as a perturbation, it is

possible to obtain a shift in energies relative to $\epsilon = 0$ [9]:

$$\Delta E_{Nljm} = -\frac{4}{3}\sqrt{\frac{\pi}{5}}m\omega_0^0\epsilon \langle Nljm| r^2 Y_2^0 | Nljm \rangle . \quad (3.39)$$

Furthermore, one can perform a separation of the radial and the angular parts while using the known relation for a harmonic oscillator potential:

$$\frac{1}{2}m\omega_0^2 \langle Nljm| r^2 | Nljm \rangle = \frac{1}{2}\hbar\omega_0 \left(N + \frac{3}{2} \right) , \quad (3.40)$$

and, together with the evaluation of the matrix elements for spherical harmonics, the final expression for the energy shift at small deformations is:

$$\Delta E_{Nljm} = -\frac{2}{3}\hbar\omega_0 \left(N + \frac{2}{3} \right) \epsilon \frac{[3K^2 - j(j+1)] [\frac{3}{4} - j(j+1)]}{(2j-1)j(j+1)(2j+1)} , \quad (3.41)$$

with the projection of the total a.m. on the z axis replacing the projection m . Based on Eq. 3.41, the following properties for a Nilsson diagram (within the small deformation regime) emerge:

- There is a K^2 dependence for the energy shifts
- The quadrupole deformation parameter (albeit ϵ or β) shows a clear linear dependence for ΔE_{Nljm}
- Another linear dependence for the shifts is induced by the principal (oscillator) quantum number N .
- When the deformation parameter is positive, there are more downward sloping orbits than upward ones. (Example discussed below)

For a value of j greater than $1/2$, the terms $[3K^2 - j(j+1)]$ and $3/4 - j(j+1)$ are negative, resulting in the following types of orbits: [14]:

$$\text{downward sloping: } K < \sqrt{\frac{j(j+1)}{3}} = \frac{j}{1.8} \approx 0.65j , \quad (3.42)$$

$$\text{upward sloping: } K > 0.65j . \quad (3.43)$$

It was already shown that the angular orientation (i.e., the tilting angle θ) of an orbit is given by $\theta = \arcsin(K/j)$. Checking to see for what value of θ the

ratio $K/j = 0.65$ corresponds to, this will lead to $\theta = 40^\circ$. Consequently, the physical implication is that any larger *tilt* of an orbit within a prolate quadrupole deformation is energetically unfavorable.

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