Deformed (Nilsson) shell model

Introduction to Nuclear Science

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Outline

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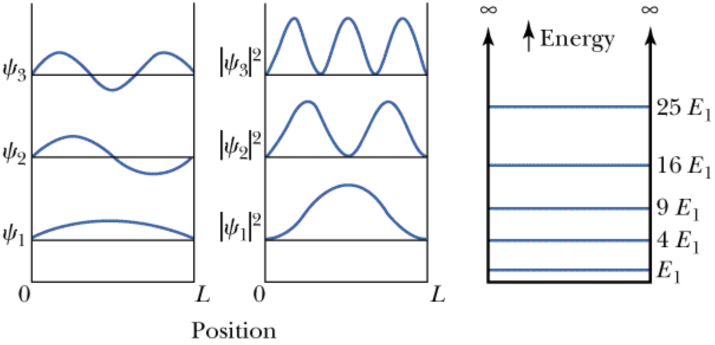
Towards the deformed shell model

- We learnt in the previous lecture that residual pairing interactions in nuclei couple nucleons of the same kind occupying the same orbitals into pairs of zero spin and positive parity.
- We also said that residual proton-neutron interaction leads to configuration mixing and drives a nucleus towards deformation.
- The data supports this hypothesis, we considered the systematics of the energy of the first excited state in nuclei near Z=50 as an evidence, another one comes from a complete failure of the spherical shell model in predicting spins of nuclei far from the magic numbers.
- Therefore, let us analyze impact of the deformation on a nuclear system and develop tools to deal with non-spherical shapes and shells.
- We will start with a non-spherical infinitely deep potential well which captures all important feature of a deformed shell model.

Infinitely deep potential well in one dimension

If the well is infinitely deep the Schrödinger equation requires that the wave function vanishes on the boundaries.



Infinitely deep potential well in one dimension

- For the well on the graph

$$\psi(0) = 0 \quad \psi(L) = 0 \quad \Longrightarrow \quad \psi(x) = A\sin(\frac{n\pi}{L}x)$$

- But at the same time

$$\psi(x) = A\sin(kx) \qquad \hbar k = \sqrt{2mE}$$

- This leads to

$$k = \frac{1}{\hbar}\sqrt{2mE} = \frac{n\pi}{L} \quad \text{or}$$

$$E = n^2\frac{\pi^2\hbar^2}{2mL^2} = n^2 E_1 \qquad E_1 = \frac{h^2}{8mL^2}$$

- Note that the wave function for the ground state is symmetric with respect to the middle of the well (has positive parity), for the next state the wave function is asymmetric (has negative parity) etc.

Infinitely deep potential well in three dimensions

- In a Cartesian space the coordinates x, y and z are independent of each other.
- Therefore we can think about a three-dimensional infinitely deep potential well as about three independent wells constraining particle motion along each of the independent coordinate.
- A consequence of that fact is separation of variables in the Schrödinger equation, the three-dimensional equation can be split into three one-dimensional equations.
- The wave function is a product of three one-dimensional wave function, each being a solution for the one-dimensional equation for each of the coordinates.
- The energy is the sum of three energies corresponding to the solution for the one-dimensional equation for each of the coordinates.

Separation of variables

- For the potential

$$V(x, y, z) = V(x) + V(y) + V(z) \tag{1}$$

- For the wave function

$$\Psi(x, y, z) = \Psi(x)\Psi(y)\Psi(z) \tag{2}$$

- For the equation

$$\begin{aligned}
E\Psi(x, y, x) &= \left\{-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x, y, z)\right\}\Psi(x, y, z) \\
&= \Psi(y)\Psi(z)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\Psi(x) + \\
&\quad \Psi(x)\Psi(z)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dy^2} + V(y)\right)\Psi(y) + \\
&\quad \Psi(x)\Psi(y)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z)\right)\Psi(z)
\end{aligned}$$

Infinitely deep potential well in three dimensions

- Let us denote the dimensions of the well along the x, y and z coordinates as L_x, L_y and L_z.
- The wave functions are

$$\begin{aligned}\Psi_{n_x,n_y,n_z}(x,y,z) &= \Psi_{n_x}(x)\Psi_{n_y}(y)\Psi_{n_z}(z) = \\ &= \sin(n_x\pi\frac{x}{L_x})\sin(n_y\pi\frac{y}{L_y})\sin(n_z\pi\frac{z}{L_z}) \end{aligned} \tag{4}$$

- Note that $n_x > 0$, $n_y > 0$ and $n_z > 0$ otherwise $\Psi_{n_x,n_y,n_z} = 0$.
- The energies are

$$\begin{aligned}E_{n_x,n_y,n_z} &= \frac{\pi^2\hbar^2}{2m}\frac{n_x^2}{L_x^2} + \frac{\pi^2\hbar^2}{2m}\frac{n_y^2}{L_y^2} + \frac{\pi^2\hbar^2}{2m}\frac{n_z^2}{L_z^2} = \\ &= \frac{\pi^2\hbar^2}{2m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)\end{aligned} \tag{5}$$

Spherical infinitely deep potential well in three dimensions

- Note that for $L_x = L_y = L_z = L$ the well has spherical symmetry.
- The energies are

$$E_{n_x,n_y,n_z} = \frac{\pi^2\hbar^2}{2mL}\left(n_x^2 + n_y^2 + n_z^2\right) = E_0\left(n_x^2 + n_y^2 + n_z^2\right) \qquad (6)$$

  with $E_0 = \frac{\pi^2\hbar^2}{2mL}$

- Let us denote a state with a set of quantum numbers n_x, n_y and n_z as (n_x, n_y, n_z).
- For the ground state $n_x = n_y = n_z = 1$ the label is $(1,1,1)$ and energy is $E_{(1,1,1)} = 3E_0$.
- Next there are three excited state of the same energy with quantum numbers $(1,1,2)$, $(1,2,1)$ and $(2,1,1)$. The energies are $E_{(1,1,2)} = E_{(1,2,1)} = E_{(2,1,1)} = 6E_0$

Degenerate states

- Let us have a closer look at the three states at energy $E = 6E_0$.
- The quantum numbers $(1, 1, 2)$, $(1, 2, 1)$ and $(2, 1, 1)$ indicate that they have a different quantum numbers, thus, they have different wave functions.
- Different wave functions indicate different states. But for $L_x = L_y = L_z = L$ the energy $E = E_0(n_x^2 + n_y^2 + n_z^2)$ is the same for all three states. States of different wave function but the same energy are called degenerate states.
- The level of degeneracy is the number of states at a given energy. For states at the energy $E = 6E_0$ the level of degeneracy is three.
- Note that the next level is also degenerate with the level of degeneracy of three, quantum numbers $(2, 2, 1)$, $(2, 1, 2)$ and $(1, 2, 2)$ and energy $E = 9E_0$.

Spherical infinitely deep potential well in three dimensions

- Here are the parameters of low-energy states in spherical infinitely deep potential well in three dimensions

Energy	Degeneracy	Quantum numbers
$3E_0$	1	$(1,1,1)$
$6E_0$	3	$(1,1,2)$, $(1,2,1)$, $(2,1,1)$
$9E_0$	3	$(2,2,1)$, $(2,1,2)$, $(1,2,2)$
$11E_0$	3	$(1,1,3)$, $(1,3,1)$, $(3,1,1)$
$12E_0$	1	$(2,2,2)$

- In this model the energies are the energies of the major shells, the degeneracy defines the number of particles or occupancy of the shell.
- The most important consequence of the deformation is a change in energy and the level of degeneracy of shells.
- The deformation destroys spherical shell gaps and open new gaps and different magic numbers.

Deformed shapes

- The simplest deviation from spherical symmetry is for one dimension of the well to be different of the other two, with the other two being equal.
- This corresponds to axially symmetric potential well with the non-equal dimension being along the symmetry axis, and the other two dimension being perpendicular to the symmetry axis.
- Traditionally, the symmetry axis is taken as the z axis of the coordinate frame $L_z \neq L_x = L_y$.
- We can distinguish two cases of axial deformation, prolate $L_z > L_x = L_y$ and oblate $L_z < L_x = L_y$.
- These are the cases we are going to analyze. There is also the triaxial case $L_z \neq L_y \neq L_x$ which is absolutely legitimate, but we have no time to analyze it.

Axial infinitely deep potential well in three dimensions

- Let us define $L_x = L_y = L$.
- For convenience it is also good to define a single parameter α which measures how different is the L_z from L. Let us do it in this way

$$\left(\frac{L}{L_z}\right)^2 = 1 - \alpha \tag{7}$$

- Here is why. The energy for the axially deformed well is

$$\begin{aligned} E_{n_x,n_y,n_z} &= \frac{\pi^2\hbar^2}{2m}\frac{n_x^2}{L_x^2} + \frac{\pi^2\hbar^2}{2m}\frac{n_y^2}{L_y^2} + \frac{\pi^2\hbar^2}{2m}\frac{n_z^2}{L_z^2} = \\ &= \frac{\pi^2\hbar^2}{2mL}\left(n_x^2 + n_y^2 + n_z^2\left(\frac{L}{L_z}\right)^2\right) = \\ &= E_0(n_x^2 + n_y^2 + n_z^2(1-\alpha)) = E_0(n_x^2 + n_y^2 + n_z^2 - n_z^2\alpha) \end{aligned} \tag{8}$$

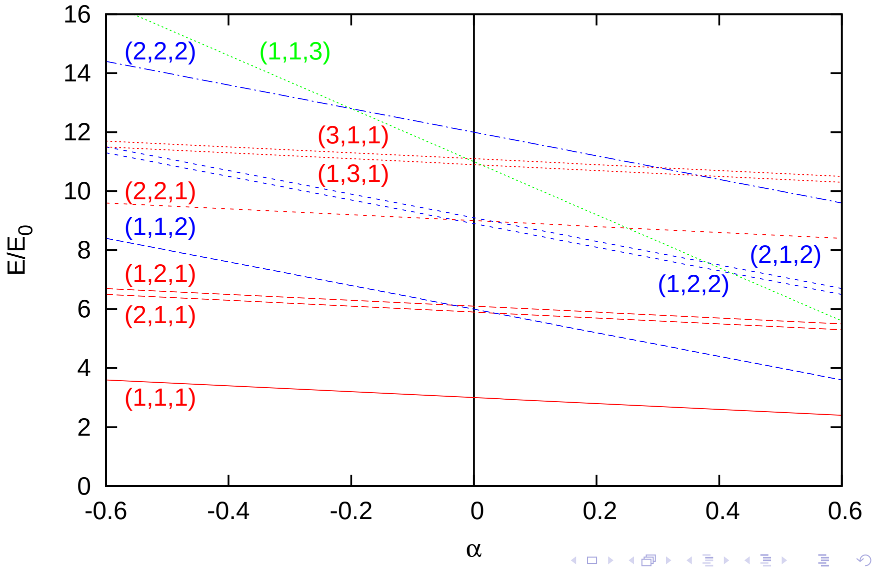
Axial infinitely deep potential well in three dimensions

- Note that the energy for the deformed well is a sum of the energy E_S for the spherically symmetric well plus the deformation energy E_D which depends on the parameter α

$$
\begin{aligned}
E_{n_x,n_y,n_z} &= E_0(n_x^2 + n_y^2 + n_z^2 - n_z^2\alpha) = E_S + E_D \\
E_S &= E_0(n_x^2 + n_y^2 + n_z^2) \\
E_D &= = -\alpha n_z^2 E_0
\end{aligned}
\tag{9}
$$

- For α=0 the energy sequence of the spherically symmetric well is recovered
- For $\alpha \neq 0$ the degeneracy of levels is changed.
- Consider the $(1, 1, 2)$, $(1, 2, 1)$, $(2, 1, 1)$ states degenerate at $6E_0$ for spherical symmetry. The deformation term will impact the $(1, 1, 2)$ differently than the $(2, 1, 1)$ and $(1, 2, 1)$ states as the n_z quantum number is different for the $(1, 1, 2)$ than for $(2, 1, 1)$ and $(1, 2, 1)$

Axial infinitely deep potential well in three dimensions



Why does the energy change?

- Recall that the energy is directly proportional to the frequency of the wave function or inversely proportional to the wave length.
- The wave function has nodes at the boundaries of the well, thus the wave length is define by the size of the well.
- If the well gets larger the wave length of the wave function increases, the frequency decreases and energy is reduced.
- In a contrary, if the well size decreases the wave length decreases, the frequency increases and the energy increases.
- Recall that

$$L_z = L\frac{1}{\sqrt{1-\alpha}} \approx L(1+\frac{1}{2}\alpha) \tag{10}$$

thus for positive α the well becomes prolate, the L_z increases and energy decreases, while for the negative α L_z decreases and energy increases.

Why atoms do not deform?

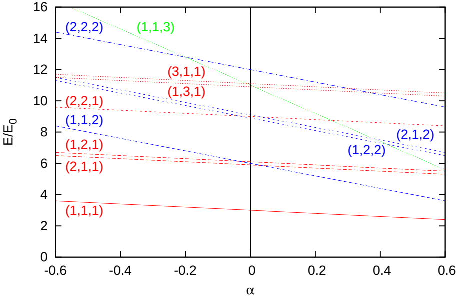
- If deformation reduces energy of a system why atoms do not deform? Indeed, all atoms are found to be spherical, but the deformed shell model features we investigated are generic. Should they be applicable to atoms as well?
- The answer is in the central role and tiny size of a nucleus.
- Since the force bounding atom comes from the nucleus and this force dominates any other forces, if this force has spherical symmetry the whole atom does.
- Object of any shape when looked from afar looks point-like. A point has the same symmetry as a sphere.
- This is the case for nucleus in atoms. Even if deformed it is separated by electrons by a large distance, so the impact of the nuclear deformation on the shape of an atom is minimal. However, there is an impact on the structure of the atomic levels (hyperfine structure).

Why atoms do not deform?

- The size of the atom is $\sim$0.1 [nm] the size of a nucleus $\sim$1 [fm]=10^{-4} [nm]. Thus electrons are separated from a nucleus by a distance which is $\sim$10000 times larger than the nucleus.
- Nuclear deformation is not larger than the size of a nucleus.
- On average for an electron to see a nucleus deformed it is similar for a human being to see a deformation of a soccer ball (1 foot in diameter) from a plane being 10000 feet above the ground.
- Good luck.

What is wrong with what we have done so far?

- We obtained a very nice and hopefully reasonably easy to understand figure showing the change of magic numbers as a function of deformation parameter α.



- But is this figure right?
- The answer is negative. We have forgotten a very important point: the volume conservation.

Volume conservation

- In previous lectures we discussed incompressibility of nuclear matter.
- This implies that nuclear deformation has to conserve volume.
- The deformation we considered so far made one of the dimensions of the well longer or shorter while keeping the other two together.
- This deformation does not conserve the volume.
- To conserve the volume when axially deforming the well we need to make the dimensions perpendicular to the symmetry axis shorter when the dimension along the axis gets longer, or the other way around.
- This implies that all three axes need to change the length while deformation occurs.
- Change of the axes length has a direct impact on state energies.

Volume conservation

- The volume of the well is

$$V_{x,y,z} = L_x * L_y * L_z \tag{11}$$

- Let us take as a reference the volume of the undeformed sphere

$$V = L^3 \tag{12}$$

  this is the volume to be conserved.

- Let us define the length of the dimensions parallel and perpendicular to the deformation axis

$$\begin{aligned} L_{\parallel} &= L_z \\ L_{\perp} &= L_x = L_z \end{aligned} \tag{13}$$

Volume conservation

- The volume conservation calls for

$$V_{x,y,z} = L_x * L_y * L_z = L_{\perp}^2 * L_{\parallel} = L^3 = V \tag{14}$$

- Since

$$\left(\frac{L}{L_{\parallel}}\right)^2 = \left(\frac{L}{L_z}\right)^2 = 1-\alpha \quad \text{or} \quad \frac{L}{L_{\parallel}} = \sqrt{1-\alpha} \tag{15}$$

the volume conservation implies

$$\frac{L_{\perp}}{L} = \sqrt{\frac{L}{L_{\parallel}}} = \sqrt[4]{1-\alpha} \tag{16}$$

Volume conservation

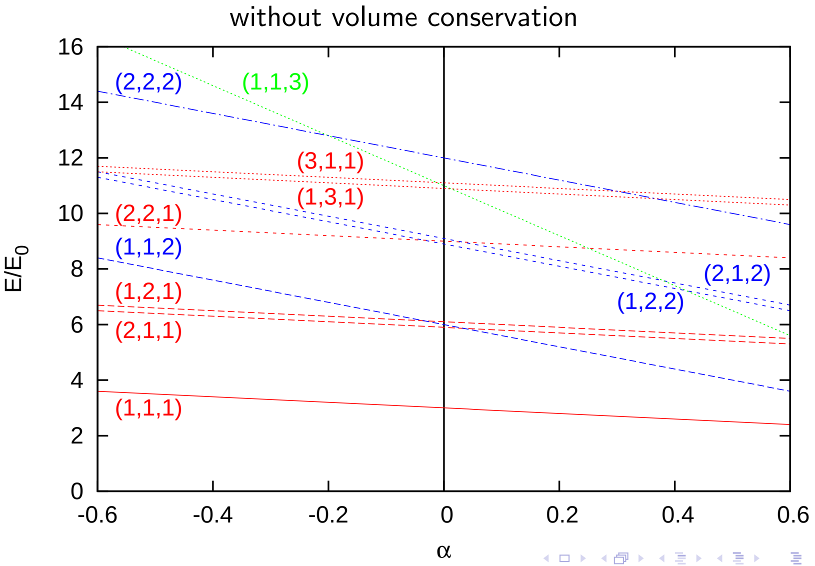
- The energies including volume conservation conditions are

$$
\begin{aligned}
E_{n_x,n_y,n_z} &= \frac{\pi^2\hbar^2}{2m}\frac{n_x^2}{L_x^2} + \frac{\pi^2\hbar^2}{2m}\frac{n_y^2}{L_y^2} + \frac{\pi^2\hbar^2}{2m}\frac{n_z^2}{L_z^2} = \\
&= \frac{\pi^2\hbar^2}{2mL}\left(n_x^2\left(\frac{L}{L_\perp}\right)^2 + n_y^2\left(\frac{L}{L_\perp}\right)^2 + n_z^2\left(\frac{L}{L_\parallel}\right)^2\right) = \\
&= E_0\left((n_x^2+n_y^2)\frac{1}{\sqrt{1-\alpha}} + n_z^2(1-\alpha)\right) \qquad (17)
\end{aligned}
$$

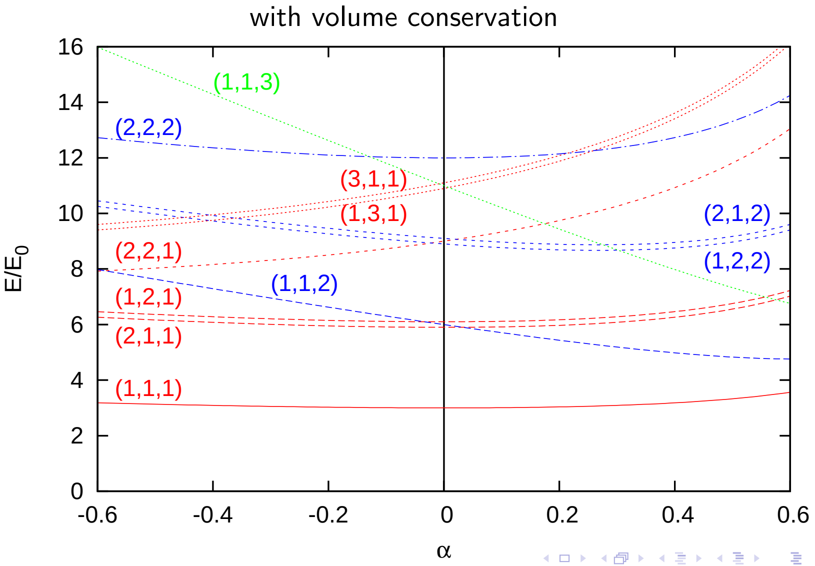
- Volume conservation changes the diagram, in particular, the energies as a function of deformation are not linear any more.

- Things get complicated, but for a reason.

Axial infinitely deep potential well in three dimensions



Axial infinitely deep potential well in three dimensions

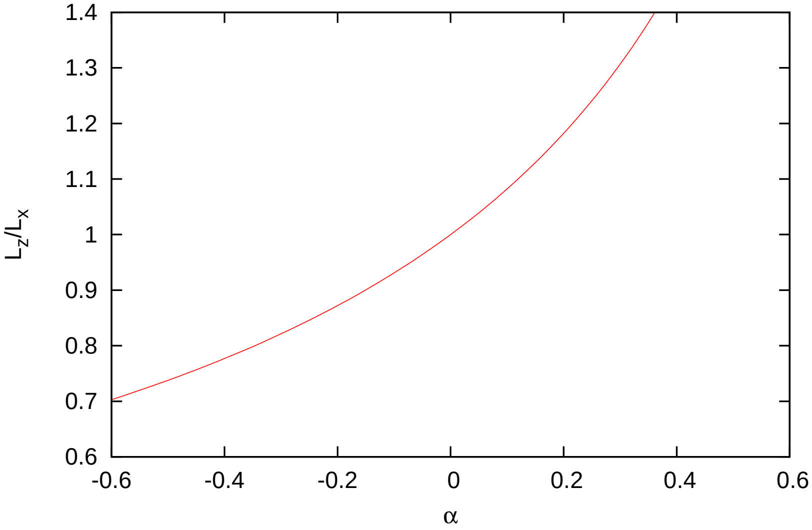


Axes ratio

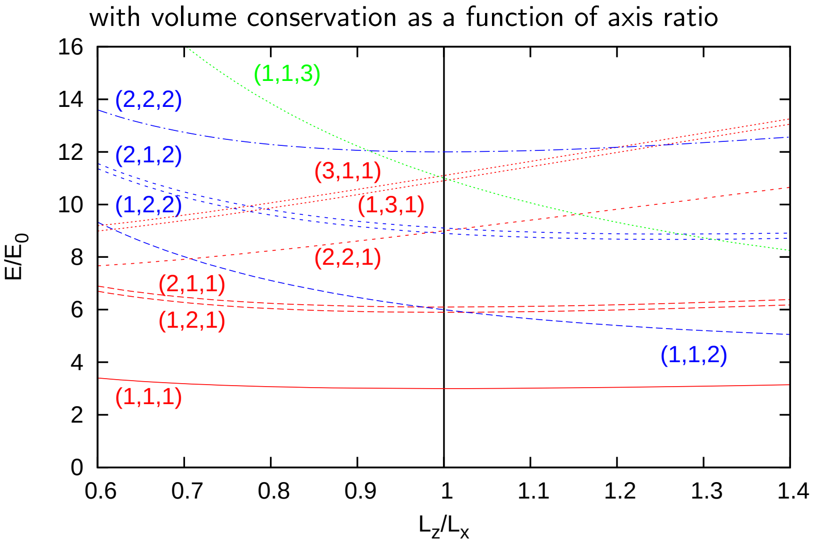
- The deformation parameter α which we used may not be the most intuitive to think about (although it was useful).
- Something more intuitive is the axes ratio.
- Let us express the axes ratio as a function of α

$$\begin{aligned}
\frac{L}{L_{\parallel}} &= \sqrt{1-\alpha} \\
\frac{L_{\perp}}{L} &= \sqrt[4]{1-\alpha} \\
\frac{L_{\perp}}{L_{\parallel}} &= \sqrt{1-\alpha}\sqrt[4]{1-\alpha} = \sqrt[4]{(1-\alpha)^3} \\
\frac{L_{\parallel}}{L_{\perp}} &= \frac{1}{\sqrt[4]{(1-\alpha)^3}}
\end{aligned} \tag{18}$$

Axes ratio as a function of α



Axial infinitely deep potential well in three dimensions

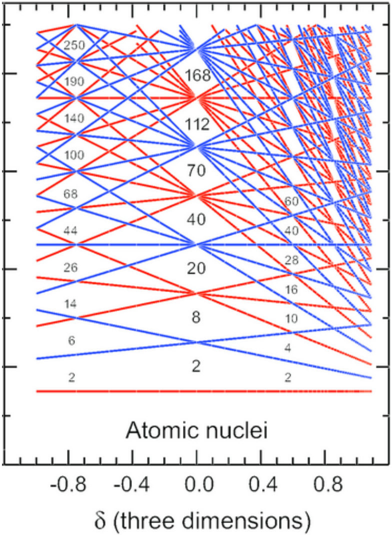


The Nilsson model

- What we have done for the three dimensional potential well has been done with a great success for nuclear harmonic oscillator potential in 3 dimensions including the flat bottom correction and spin-orbit terms to model deformed nuclear potential
- The deformed shell model he developed is often referred to as the Nilsson model.
- As for the three dimensional potential well the Nilsson model predicts that shells and shell gaps are modified by the deformation.
- The main achievement of the Nilsson model is correct explanation of ground state spins and parities of a large number of nuclei, as well its ability to be expanded into a model for rotation of deformed odd-mass nuclei (later this week).

Three dimensional deformed harmonic oscillator

Note: without volume conservation, flat bottom or spin-orbit splitting.

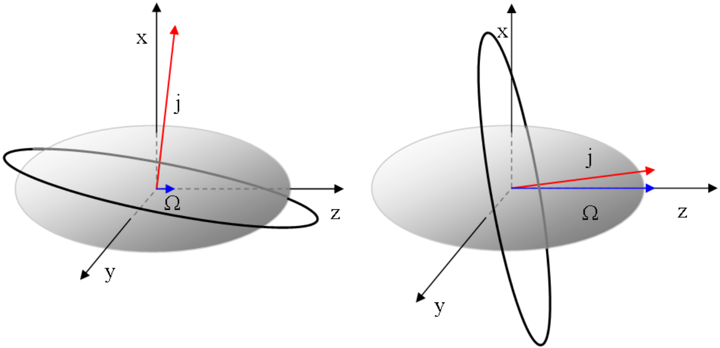


The total angular momentum in Nilsson model

- One of the consequence of deformation is configuration mixing. For example the $d_{5/2}$ and the $d_{3/2}$ states which are separate for the spherical shell model mix in the Nilsson model.
- As a consequence of mixing the total angular momentum does not have a well defined value in a deformed shell model, for example for a mixture of $d_{5/2}$ and the $d_{3/2}$ states the total angular momentum is a mixture of $j = \frac{5}{2}$ and $j = \frac{3}{2}$
- However, in the axially-symmetric Nilsson model deformation the projection of the total angular momentum on the symmetry axis (analogues to the magnetic m-quantum number) has a well defined half-integer value.
- This quantum number in the Nilsson model is referred to as Ω.

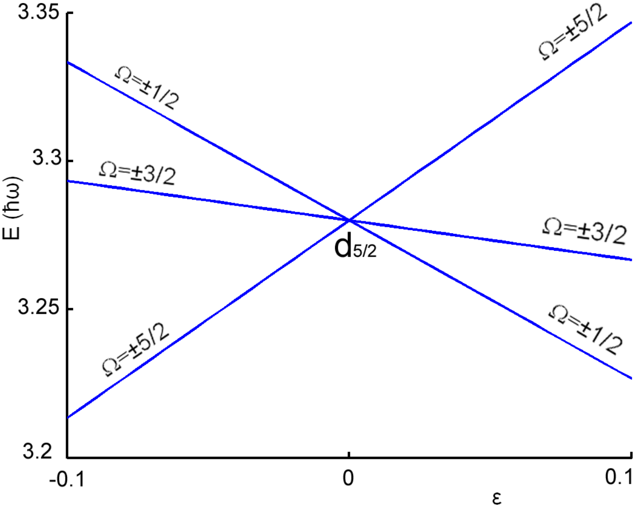
The Ω quantum number

- The Ω quantum number defines the overlap of the orbital with the deformed core.

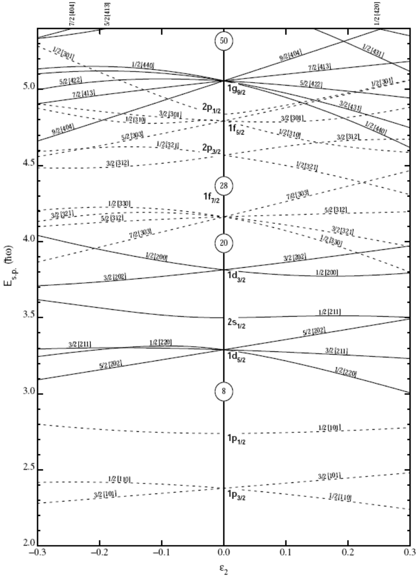


- Since the potential is attractive large overlap results in energy gains (lowering of state energy) small overlap results in increased energy.

Nilsson model energy splitting



The Nilsson diagram



The Nilsson diagram