Outline

1. Infinitely deep potential well in three dimensions

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1. Spherical infinitely deep potential well in three dimensions

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1. Spherical infinitely deep potential well in three dimensions

2. Axial infinitely deep potential well in three dimensions

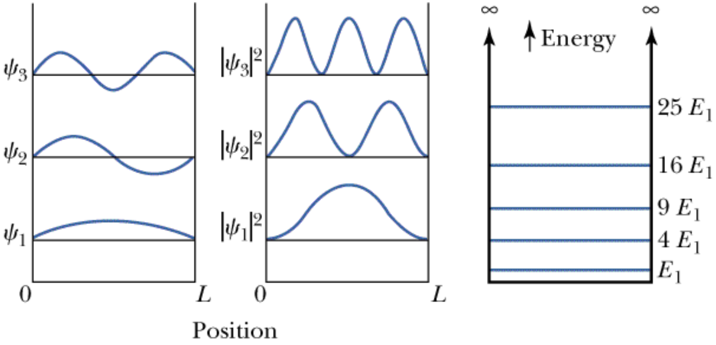
Outline

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

$$k = \frac{1}{\hbar}\sqrt{2mE} = \frac{n\pi}{L} \quad \text{or}$$
$$E = n^2\frac{\pi^2\hbar^2}{2mL^2} = n^2E_1 \qquad E_1 = \frac{h^2}{8mL^2}$$

- 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

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

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

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

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

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

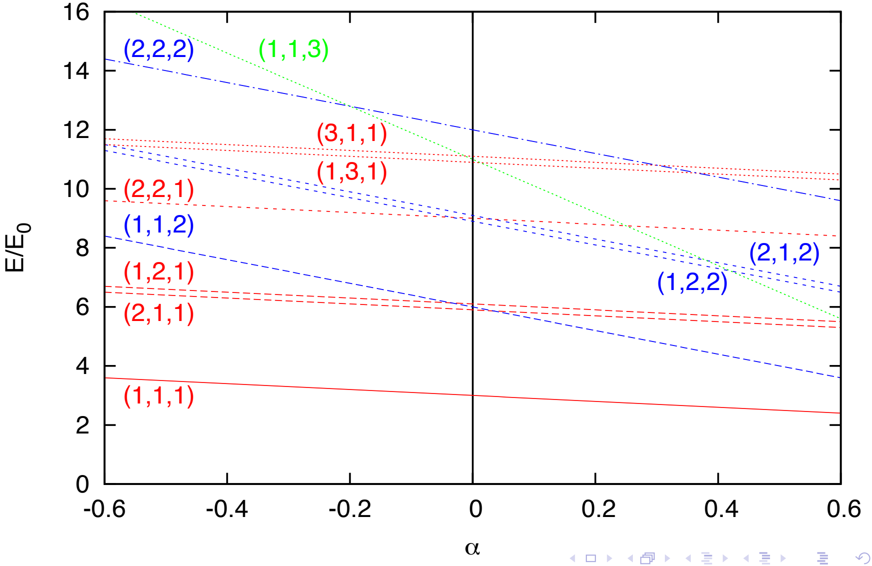
Axial infinitely deep potential well in three dimensions

- 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?

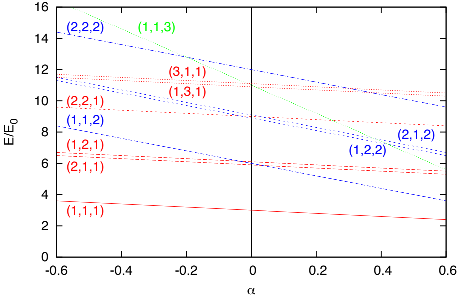
- If deformation reduces energy of a system why atoms do not deform? Indeed, all atoms are found to be spherical, but the deformed shell model features we investigated are generic. Should they be applicable to atoms as well?
- The answer is in the central role and tiny size of a nucleus.
- Since the 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

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

- Since

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

the volume conservation implies

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

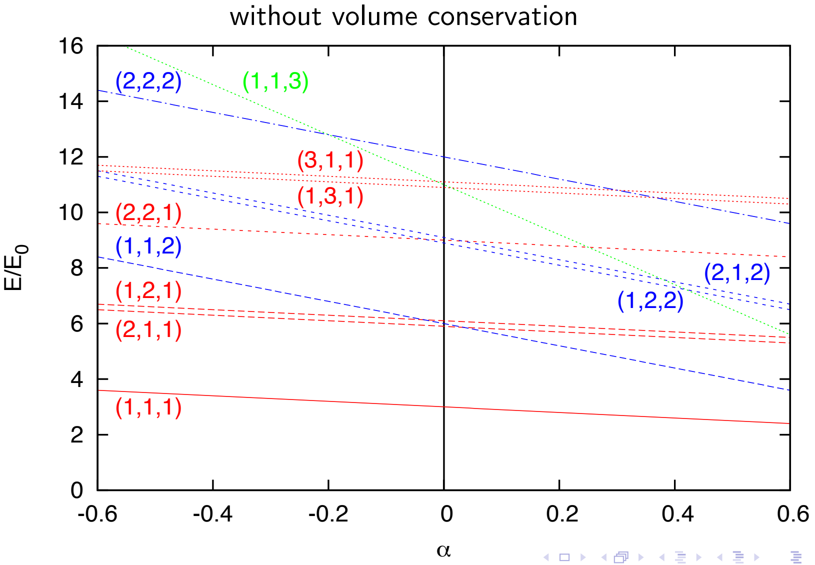
Volume conservation

- The energies including volume conservation conditions are

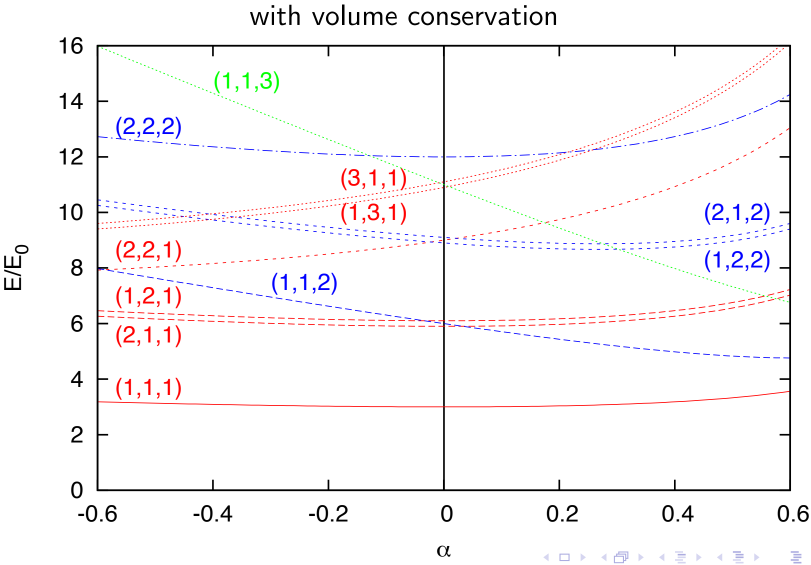
$$\begin{aligned} E_{n_x,n_y,n_z} &= \frac{\pi^2\hbar^2}{2m}\frac{n_x^2}{L_x^2} + \frac{\pi^2\hbar^2}{2m}\frac{n_y^2}{L_y^2} + \frac{\pi^2\hbar^2}{2m}\frac{n_z^2}{L_z^2} = \\ &= \frac{\pi^2\hbar^2}{2mL}\left(n_x^2\left(\frac{L}{L_\perp}\right)^2 + n_y^2\left(\frac{L}{L_\perp}\right)^2 + n_z^2\left(\frac{L}{L_\parallel}\right)^2\right)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

- 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

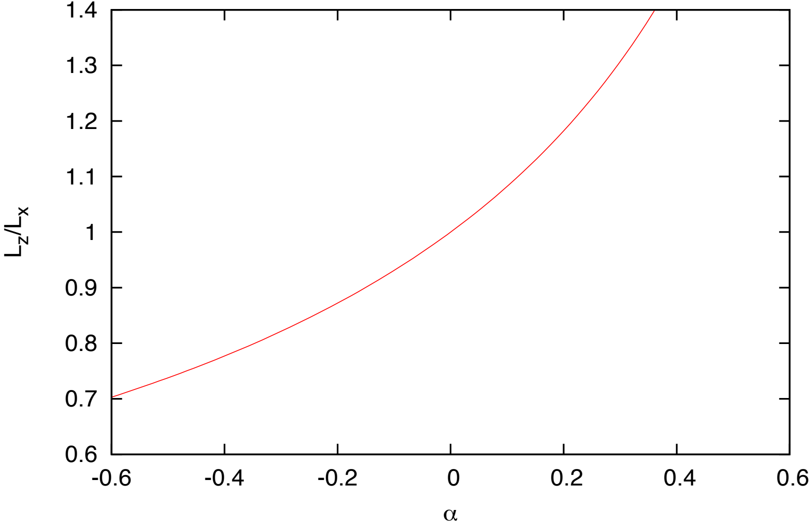


Axes ratio

- 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

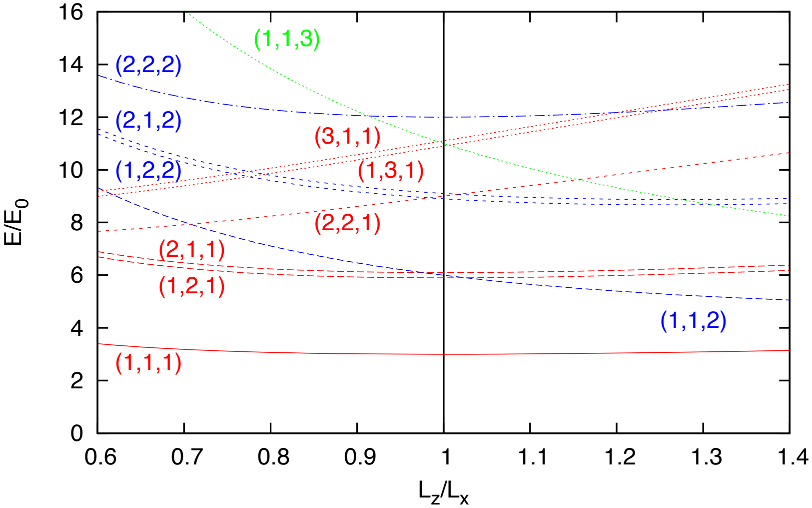
$$\begin{aligned}
\frac{L}{L_{\parallel}} &= \sqrt{1-\alpha} \\
\frac{L_{\perp}}{L} &= \sqrt[4]{1-\alpha} \\
\frac{L_{\perp}}{L_{\parallel}} &= \sqrt{1-\alpha}\sqrt[4]{1-\alpha} = \sqrt[4]{(1-\alpha)^3} \\
\frac{L_{\parallel}}{L_{\perp}} &= \frac{1}{\sqrt[4]{(1-\alpha)^3}} \qquad (18)
\end{aligned}$$

Axes ratio as a function of α



Axial infinitely deep potential well in three dimensions

with volume conservation as a function of axis ratio

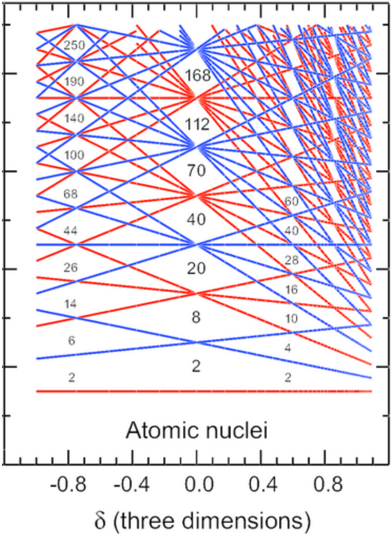


The Nilsson model

- 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.

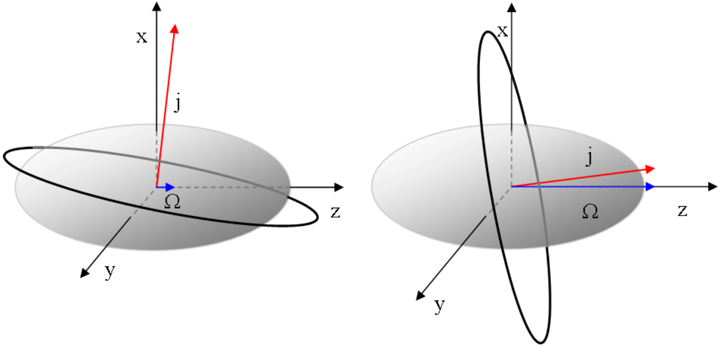


The total angular momentum in Nilsson model

- 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.

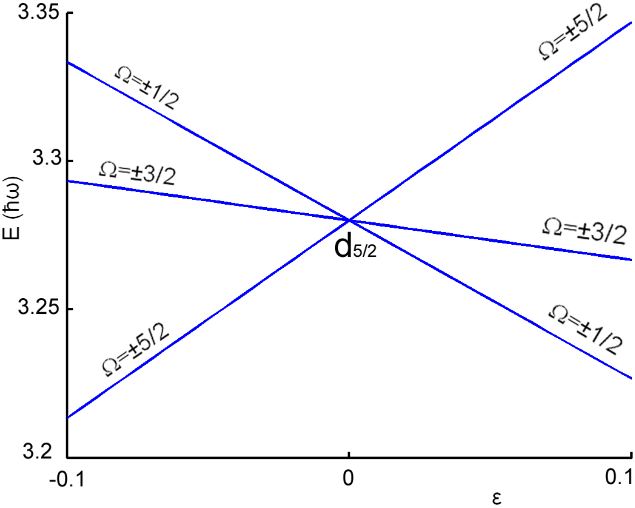
The Ω quantum number

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

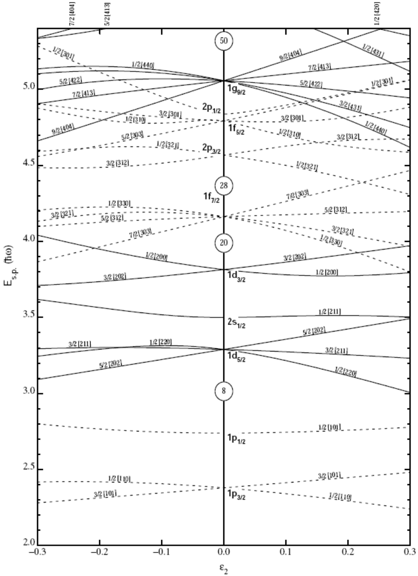


- Since the potential is attractive large overlap results in energy gains (lowering of state energy) small overlap results in increased energy.

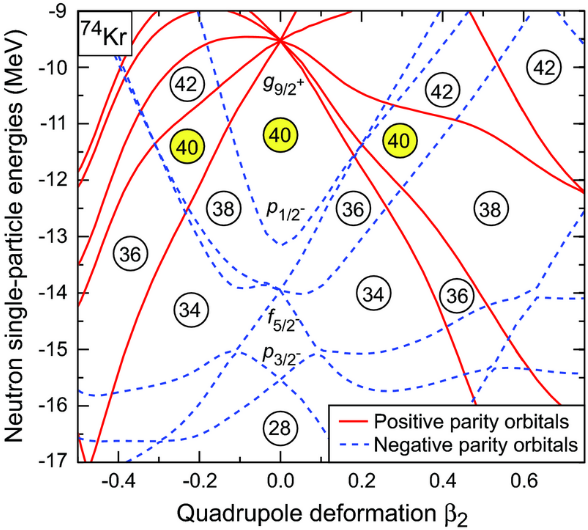
Nilsson model energy splitting



The Nilsson diagram



The Nilsson diagram



Outline

1. Single particle vs. collective behaviour

Outline

1. Single particle vs. collective behaviour
2. Deformation of a sphere

Outline

1. Single particle vs. collective behaviour
2. Deformation of a sphere
3. Surface vibrations

Outline

1. Single particle vs. collective behaviour
2. Deformation of a sphere
3. Surface vibrations
4. Static deformation

Outline

1. Single particle vs. collective behaviour
2. Deformation of a sphere
3. Surface vibrations
4. Static deformation
5. Euler angles

Outline

1. Single particle vs. collective behaviour
2. Deformation of a sphere
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4. Static deformation
5. Euler angles
6. Intrinsic reference frame

Outline

1. Single particle vs. collective behaviour
2. Deformation of a sphere
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7. Nuclear rotor

Outline

1. Single particle vs. collective behaviour
2. Deformation of a sphere
3. Surface vibrations
4. Static deformation
5. Euler angles
6. Intrinsic reference frame
7. Nuclear rotor
8. Quadrupole deformation parameters

Nuclear single-particle behaviour

- Spherical and deformed shell models view nucleus as a collection of fermions occupying single-particle states in a potential well.
- These models can successfully predict properties of nuclear states with configuration dominated by a single nucleon, or, to some extend, by relatively small number of nucleons.
- We discussed example application of these models in predicting spins, parities, magnetic, and quadrupole moments of states with a single nucleon, or a pair of nucleons outside an even-even core.
- Nuclear properties which are determined by a single nucleon are often referred to as the single-particle properties.
- In numerous cases nuclear behaviour can be described in therms of the single particle properties, however, in equally numerous examples the single particle description is far from being adequate.

Nuclear collective behaviour

- Experimental data suggest that in many nuclei ground states or low-energy excitations involve a coordinated, large-amplitude motion of many nucleons.
- Nuclear properties which are determined by such a coordinated, large-amplitude motion of many nucleons are often referred to as collective properties.
- Surprisingly, collective properties are often quite simple to describe in terms of deformation of nuclear surface.
- Examples are provided by nuclear vibrations around spherical shape or nuclear rotation of a deformed shape.
- Note, however, that explaining nuclear collective phenomena in terms of the single-particle motion can be very complicated, if at all possible.

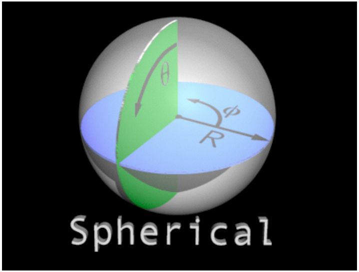
Comments on collective and single-particle behaviour

- Nuclear surface or nuclear potential are good examples of a collective behaviour in itself.
- Indeed, we discussed the nuclear potential as resulting from averaged two-body interactions of all nucleons in nuclei.
- Nuclear surface, in turn, results from a superposition of density distribution of all nucleons in a nucleus.
- Both are in principle very complicated if addressed in terms of the superposition of single-particle properties but have simple and intuitive interpretation in terms of the collective properties.
- Nuclei provide numerous examples of emergence of simple patterns in complex systems which is an active part of research in nuclear science.

Spherical shell

- Let us first consider a spherical shell.
- The shell is defined by a constant radius.
- A spherical shell is easily defined in the spherical coordinate system by

$$R(\theta, \phi) = R_0 = \text{const.} \tag{1}$$



Deformed shell

- Let us now deformed the shell by changing the radius slightly with respect to R_0.
- This, in principle, can be a complicated task since now the radius becomes a function of the polar and azimuthal angles θ and ϕ.
- Any deformation of the spherical shell can be represented as a series of spherical harmonics which are functions of the polar and azimuthal angles θ and ϕ.
- The spherical harmonics are the same functions which represent the orbital motion in the shell model. Recall that they have a rank l and m $Y_{l,m}(\theta, \phi)$ and spherical harmonics of different rank are different functions of the polar and azimuthal angle.
- In the shell model the rank l and m defined the orbital angular momentum and the magnetic quantum number. Here, the rank defines different deformation of the shell.

Deformed shell

- The deformed shell as a function of the polar and azimuthal angles is defined by

$$\begin{aligned} R(\theta,\phi) &= R_0\,[1+ \\ &\alpha_{1,-1}Y_{1,-1}(\theta,\phi)+\alpha_{1,0}Y_{1,0}(\theta,\phi)+\alpha_{1,1}Y_{1,1}(\theta,\phi)+ \\ &\alpha_{2,-2}Y_{2,-2}(\theta,\phi)+\alpha_{2,-1}Y_{2,-1}(\theta,\phi)+ \\ &\alpha_{2,0}Y_{2,0}(\theta,\phi)+\alpha_{2,1}Y_{2,1}(\theta,\phi)+\alpha_{2,2}Y_{2,2}(\theta,\phi)+\ldots] \\ &= R_0\left[1+\sum_{l=1}^{\infty}\sum_{m=-l}^{l}\alpha_{l,m}Y_{l,m}(\theta,\phi)\right] \qquad (2) \end{aligned}$$

- In this expansion coefficient $\alpha_{l,m}$ is the amplitude of the deformation defined by the spherical harmonics of the rank l, m. For applet showing deformations of a particular rank this link

Nuclear deformation

- The expansion of the deformed shape into spherical harmonics is used in many field of science and can be done for gravity, electromagnetic fields, liquid drop, as well as for deformed nuclear shapes.
- In the nuclear case the important factor is the incompresibility of the nuclear matter which implies volume conservation.
- Moreover the nuclear deformation should not change the position of the centre of mass of a nucleus.
- As we argued in an example given in lecture 3 for small deformations the rank $l = 1$ (dipole) deformation shifts the centre of mass without changing the shape.
- Thus, the amplitudes which define independent deformations are these for rank $l = 2$ (quadrupole) and higher.
- The coefficients for the dipole deformation are adjusted to ensure the constant volume and position of the centre of mass.

Time dependent amplitudes

- Let us consider the case of small deformations with time dependent amplitudes $\alpha_{l,m}(t)$.
- The conservation of nuclear volume imposes conditions on these amplitudes. There is a restoring force preventing these amplitudes to grow large and driving the shape of a nucleus towards sphericity.
- This is completely analogues to the surface vibration of the droplet of a liquid around the spherical shape.
- In the nuclear case the restoring force can be estimated based on the liquid drop model by calculating change in the energy associated with surface deformation at a constant volume.
- In the lowest order approximation time-dependent amplitudes describe harmonic oscillations of the nuclear surface around the spherical shape.

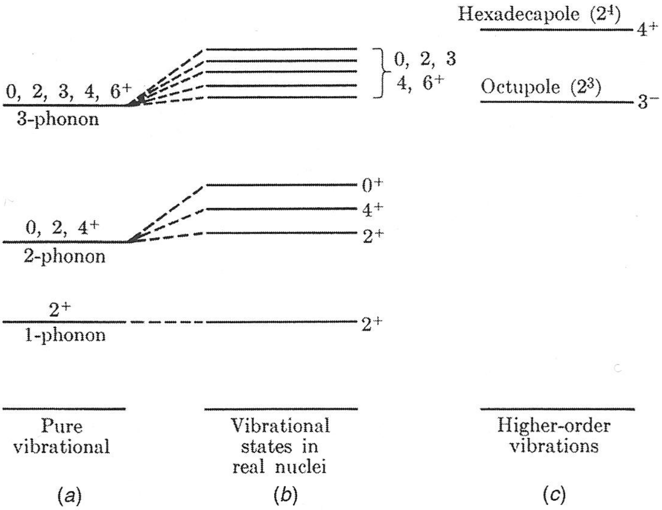
Harmonic vibrations of various ranks

- This applet shows harmonic surface vibrations of various ranks, starting with
    1. $l = 0$ (monopole breathing mode) violating volume conservation
    2. $l = 1$ (dipole) shifting centre of mass
    3. $l = 2$ (quadrupole)
    4. $l = 3$ (octupole)
    5. $l = 4$ (hexadecupole)
- Vibrational mode of surface at a given rank is called a phonon of a given rank (for example quadrupole phonon or octupole phonon).
- Phonon of a given rank carries angular momentum l and parity $(-1)^l$ defined by its rank.
- Low energy excitations in vibrational nuclei are define by the number of excited phonons and coupling of their angular momenta.

The phonon model

- The phonon model explains low-energy collective excitations of nuclei as resulting from surface vibrations.In this model there is an energy associated with an excitation of a phonon.
- The ground state at zero energy is the zero-phonon state.
- The first excited state is the one-phonon state. The excitation energy of this state is equal to the excitation energy of the phonon. The spin and parity of that state is the rank and parity of the phonon.
- For example for a quadrupole vibrator the first excited state has spin 2 and parity $(-1)^2 = +1$. For a quadrupole vibrator the first excited state has spin 3 and parity $(-1)^3 = -1$.
- The next group of excited states are the two-phonon states. Excitation energy is twice of the first excited state. Spins/parity of these states are defined by the coupling of two phonon angular momenta, in general from 0^+ to $2l^+$.

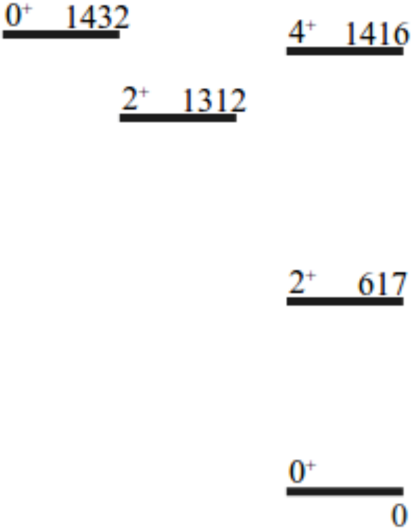
The phonon model



The phonon model

- In general, the energy of the phonon grow with its rank. Therefore the energy of a quadrupole phonon is smaller than the energy of a octupole phonon, etc.
- In the simplest version the phonon model predicts that the energy for a multi-phonon state is the number of phonons times the energy of a single phonon.
- This is true for non-interacting phonons. If phonons interact, multiphonon states of different spin are shifted in various degree by the interactions.
- These shifts are evidence of non-harmonicity in the phonon model.
- Data on vibrational nuclei indicate large degree of anharmonicity.

Anharmonicity in ^{112}Cd



The phonon model

- The phonon model predicts existence of electromagnetic transitions between the ground state and excited states.
- On the absorption of a photon by a vibrational nucleus the photon energy is converted into the phonon energy (phonon excitation). The energy of the photon has to be equal to the energy of the phonon plus recoil energy of the nucleus.
- A phonon state can also de-excite with an emission of a photon. The number of phonons in the deexcitation decreases by one, the energy of the photon is the energy of the phonon less the recoil energy of the nucleus.
- Note that electromagnetic transitions can change the number of phonons by one only. Transitions changing the number of phonons by more or less then one are forbidden.

Static deformation

- Let us come back to the expansion of the radius in terms of spherical harmonics

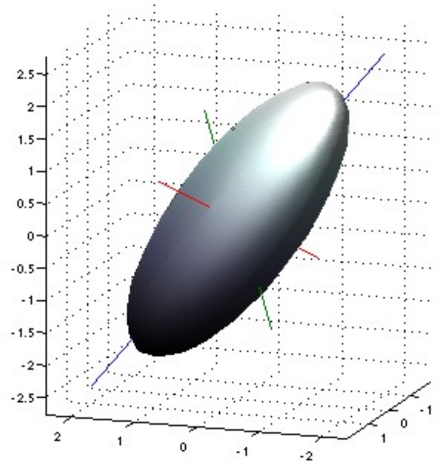
$$R = R_0 \left[1 + \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \alpha_{l,m} Y_{l,m}(\theta, \phi) \right] \tag{3}$$

- If we fix the axis of the coordinate frame and if the amplitudes α are constant in time we have a case of static deformation.
- Static deformations of a globe with fixed axes were shown by the applet we discussed earlier.
- We also discussed in Lecture 3 that an object with static deformation defines a coordinate system in space.
- In particular we have discussed the system with ellipsoidal (quadrupole) deformation.

Euler angles

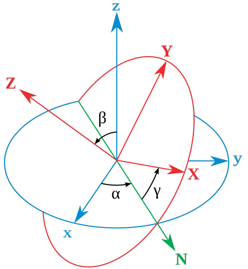
- For a deformed object we can distinguish two reference frames
  1. Ours, which we will referred to as the lab reference frame.
  2. Objects, which we will referred to as the intrinsic or the body-fixed reference frame.
- For example, for a triaxial potential well the intrinsic reference frame is defined by the three axes of the well. The same is true for triaxial ellipsoidal deformation.
- It is important to recognize that for nuclei the intrinsic reference frame can have any orientation with respect to the lab reference frame as we can hardly control orientation of nuclei (although it is possible in some cases).

Intrinsic (body-fixed) and lab-fixed referenced frames



The Euler angles

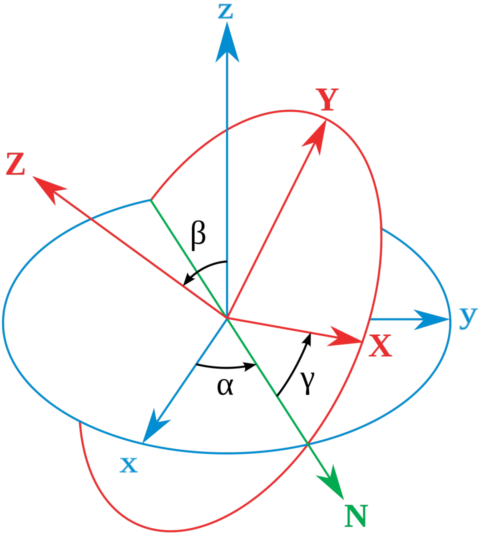
- It is important to recognize that for nuclei the intrinsic reference frame can have any orientation with respect to the lab reference frame as we can hardly control orientation of nuclei (although it is possible in some cases).
- One way to specify the mutual orientation of two reference frames of the common origin is to use the Euler angles.



The Euler angles

- Here are the steps to define Euler angles between the (x, y, z) axes of the lab frame (red) and the (x', y', z') axes of the intrinsic frame (blue).
  1. Define the line of nodes (green) as $\vec{N} = \vec{z} \times \vec{z'}$, this line is perpendicular to the plane defined by the z and the z' axes of both coordinate frames.
  2. Angle α is between the x' axis and the line of nodes.
  3. Angle β is the angle between the z' and z axis.
  4. Angle γ is the angle between the line of nodes and the x axis.
- Rotation by angle α about the z' axis, β about the x' axis and γ about the z' axis (which at the time of this rotation overlaps with the z axis) brings the intrinsic frame onto the lab frame.

The Euler angles



Quadrupole rotor vs. nuclear vibrator

- For simplicity, let us concentrate on the first independent deformation which is of rank 2 (quadrupole).
- Remember that the dipole is not independent as it moves the centre of mass and changes volume.
- In the nuclear rotor model the Euler angles become time dependent coordinates while the deformation parameters in the intrinsic system are static. See this applet.
- This should be contrasted with the vibrator model in which the deformation parameters are time-dependent but the intrinsic frame and Euler angles can not be defined. See this applet.

Quadrupole deformation parameters

- Let us try to estimate how many parameters are needed to describe static quadrupole deformation.
- Let us start with the number of amplitudes: there are five coefficients for the deformation of rank 2: $\alpha_{2,-2}$, $\alpha_{2,-1}$, $\alpha_{2,0}$, $\alpha_{2,1}$, $\alpha_{2,2}$
- These coefficients are in principle complex, implying 10 coefficients.
- But the surface is real. This fact imposes a conditions for the amplitudes reducing the number of independent coefficients to five.
- Furthermore, there is a relation between these five amplitudes and three Euler angles defining the orientation of the intrinsic coordinate frame.
- For quadrupole only two amplitudes are truly independent. Thus two parameters fully define quadrupole deformation in the intrinsic reference frame.

Bohr-Wheeler parametrization

- The two parameters of static quadrupole deformation in the intrinsic system are often chosen as the Bohr-Wheeler parameters β and γ.
- The deformed surface in terms of these parameters is defined as

$$\begin{aligned} R(\theta,\phi) &= R_0(1+\beta\cos\gamma\, Y_{2,0}(\theta,\phi)+ \\ &\quad \frac{1}{\sqrt{2}}\beta\sin\gamma(Y_{2,2}(\theta,\phi)+Y_{2,-2}(\theta,\phi))) \end{aligned} \tag{4}$$

- The axes lengths of the ellipsoid in the intrinsic reference frame are

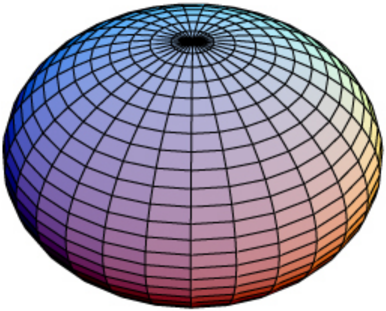
$$\begin{aligned} R_{x'} &= R_0(1+\sqrt{\frac{5}{4\pi}}\beta\cos(\gamma-120^\circ)) \\ R_{y'} &= R_0(1+\sqrt{\frac{5}{4\pi}}\beta\cos(\gamma+120^\circ)) \\ R_{z'} &= R_0(1+\sqrt{\frac{5}{4\pi}}\beta\cos(\gamma)) \end{aligned} \tag{5}$$

Axial quadrupole deformation

- In the Bohr-Wheeler parametrization the parameter β defines the elongation along the z' axis in the intrinsic reference frame.
- The parameter γ defines the length difference between the x' and the y' axes of the quadrupole-deformed shape in the intrinsic frame.
- Thus the parameter γ defines the triaxiality of the shape.
- Let us consider the special case of $\gamma = 0^\circ$). For $\gamma = 0^\circ$ $R_{x'} = R_{y'}$ and the shape is axially symmetric with the z' axis being the axis of symmetry.
- For the axial case of $\gamma = 0^\circ$ positive values of β correspond to the prolate deformation while negative values of β correspond to the oblate deformation.

Axial quadrupole deformation

Quadrupole deformation (Left) oblate, $\beta < 0$ (Right) prolate, $\beta > 0$



Axial rotor

- So far everything looks dandy. Something must be wrong!
- Some of you may, and all of you should feel uncomfortable by now due to the fact that there is no clear way to define the intrinsic system for an axial rotor.
- The z' axis is fine, this is the symmetry axis of the deformation.
- But what about the x' and y' axes? For an axially symmetric deformation there is no clear way to define the direction of the x' and the y' axes.
- As a matter of fact there is an infinite number of ways to do it, anyone of them equivalent to any other.
- This has a profound consequences for the rotor.

Quantum quadrupole axial rotor

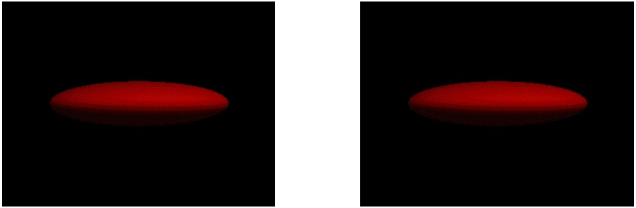
- The first consequence for an axial rotor in quantum mechanical description is the observation that rotation around the symmetry axis does not result in a new state.
- Truly, the rotation around the symmetry axis changes the phase factor of the wave function only.
- Since the energy of a state does not depend on the phase factor (depends on the wave function squared) all the states which are related by rotation around the symmetry axis have the same energy.
- This means that there are no quantum mechanical excitations related to rotation about the symmetry axis.
- The excitation must then involve rotation about the axis perpendicular to the symmetry axis.

Quantum quadrupole axial rotor

- The property of the quantum axial rotor defined in the previous slide is sometimes expressed by stating that "quantum mechanics" forbids rotation around a symmetry axis.
- This is clearly wrong, the rotation is allowed it generates the phase factor but does not generate excitations.
- In fact, rotations shown in this applet, this applet, and this applet in quantum mechanics correspond to the same single state and the same energy, independent of rotational frequency.
- In contrast, the rotation show in this applet corresponds to different energy states if the rotational frequency is different.

Quantum quadrupole axial rotor

- From now we rotate perpendicular to the symmetry axis.
- The next property of the quantum quadrupole axial rotor to be recognized is a symmetry with respect to the rotation by 180° about the axis perpendicular to the symmetry axis.
- In quantum mechanics there is no distinction between a quantum quadrupole axial rotor and a quantum quadrupole axial rotor rotated by 180° around the symmetry axis.



$$E_I = \frac{\hbar^2}{2J} I(I+1) \tag{6}$$

Quantum quadrupole axial rotor

- Rotational excitations energies of a quantum quadrupole axial rotor are
- I is the angular momentum (spin) of the state, J is the moment of inertia.
- As a consequence of the 180° symmetry with respect to rotation about the axis perpendicular to the symmetry axis only even values of I are allowed for excited levels.
- Consequently the energy levels are

Spin I	0	2	4	6	8
Energy E	0	$6\frac{\hbar^2}{2J}$	$20\frac{\hbar^2}{2J}$	$42\frac{\hbar^2}{2J}$	$72\frac{\hbar^2}{2J}$

Analogy with di-atomic molecules

- Rotational spectra for nuclear quantum quadrupole axial rotor are analogues to the rotational spectra of di-atomic molecules with both atoms being of the same kind, like for example H_2.
- In the di-atomic molecules with both atoms of the same kind there is the same restriction for rotation only about the axis perpendicular to the symmetry axis, and the symmetry of rotation by 180° around the axis perpendicular to the symmetry axis.
- Consequently, the di-atomic molecules of this type have the excitation spectra as defined on the previous slide with even-spin states only.

Analogy with di-atomic molecules

- Rotational excitation spectra are different for di-atomic molecules with two atoms of a different kind, like for example HCl.
- The energies are still given by

$$E_I = \frac{\hbar^2}{2J} I(I+1) \tag{7}$$

- For HCl, however, there is no symmetry between the rotation by 180° about the axis perpendicular to the symmetry axis, since this rotation exchanges H with Cl
- Consequently, odd-spin state are allowed and present in excitation spectrum of HCl.
- Nuclear analog of HCl is a rotor with axial octupole deformation.