Chapter 6

Nuclear Structure

The experimental information outlined in the previous two chapters on
- i- energy level positions
- ii- static moments
- iii- transition rates
- iv- reaction cross section

provides us with the information for the nuclear structure studies.

Partly because of the complexity of quantum-mechanical many-body systems ⟶ Model construction is a necessary step toward a proper theory for understanding nuclei.

We examine two classes of nuclear structure models
- i- Microscopic
- ii- Macroscopic

Microscopic model:

In this model we use many-body Hamiltonian based on individual nucleons interacting with each other through a two-body pot.

After solving $H\Psi_n = E_n\Psi_n$, the eigenfuncs. Ψ_n may be used to calculate observables and the results compared with exponents.

Macroscopic model:

Many observed properties of a nucleus involve the motion of many nucleons collectively.

H is expressed in terms of a bulk or macroscopic coords. of the system such as mass, radius, and volume.

6-1 Variational Model:

We have seen that the nucleus may be looked as a drop of fluid.

Here we extend the analogy to nuclear excitation due to vibrational motion

Assumption: At equilibrium the shape of the nucleus is spherical

i.e. → Pot. energy = Min., when the shape is spherical

→ No rotational deg. of freedom

→ Vibrational motion stands out more clearly.

In practice, for many nuclei the most stable shpe is deformed one.

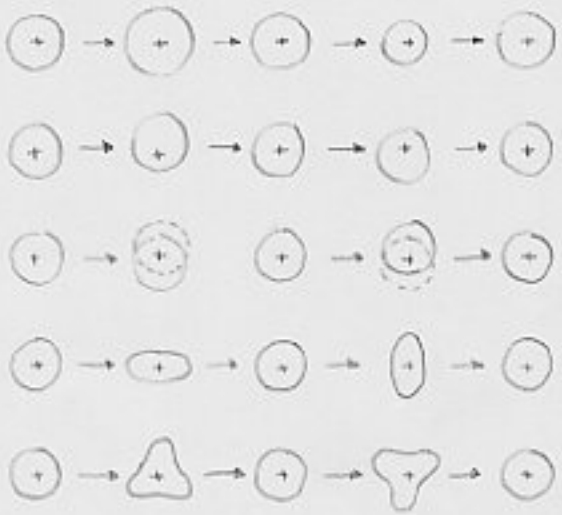
a) Monopole

b) Isoscalar Dipole

c) Isovector

d) Quadrupole

e) Octupole



Breathing mode:

When a nucleus aquires an excess energy, for example, from Coulomb excitation due to a charged particle nearby,

⟶ it can be set into vibration around its equilibrium.

We can envisage several different types of vibaration for a nucleus, (Fig.).

Case a) Monopole,

Respiration type motion, ⟶ density vibration

For even-even spherical nucleus, the ground state $J_i^\pi = 0^+$

To preserve the nuclear shape, breathing mode excitation

generates $J_f^\pi = 0^+$

Ex. Doubly magic nuclei ^{16}O, ^{40}Ca, ^{90}Zr and ^{208}Pb, a low-lying excited state $J_f^\pi = 0^+$ is found (among the others).
→ may be identified as a breathing mode state.

On the other hand;
Since nuclear matter is rather stiff against compression

→ main part of the breathing mode strength is expected to be much higher in energy.

The peak location ~ $80\, A^{-1/3}$ MeV

Shape Vibaration;

In this type of vibaration (more commonly observed type)

density = const.

Since the amount of the energy imparted to the drop is usually too small to change its density, the motion simply involves a change in the shape.

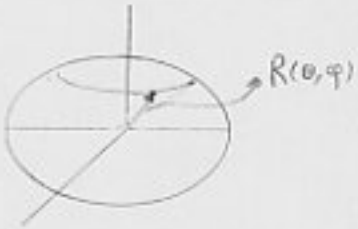
For a drop of fluid;

$$R(\theta,\varphi) = R_0 \left\{ 1 + \sum_{\lambda\mu} \alpha_{\lambda\mu}(t)\, Y_{\lambda\mu}(\theta,\varphi) \right\} \qquad \text{surface func.}$$

where density = const.

$\alpha_{\lambda\mu}(t)$: Shape parameters (determines departure from spherical shape)

R_0 : The radius of equivalent sphere



$$R(\theta,\varphi) = R^*(\theta,\varphi) \longrightarrow \alpha_{\lambda\mu}(t) = (-)^{\mu} \alpha^*_{\lambda,-\mu}$$

If <u>rotational</u> symmetry ($R(\theta,\varphi) = R(\varphi)$), $\alpha_{\lambda\mu}$ <u>are not</u> indep. of each other.

If nuclear matter is <u>incompressible</u>;

$$\text{Volume conservation} \longrightarrow \frac{4}{3}\pi R_0^3 = \int_0^{\pi}\int_0^{2\pi}\int_0^{R(\theta,\varphi)} r^2 \sin\theta \, dr\, d\theta\, d\varphi$$

$$\longrightarrow \quad \alpha_{00} = -\left(\frac{1}{4\pi}\right) \sum_{\lambda\mu} |\alpha_{\lambda\mu}|^2$$

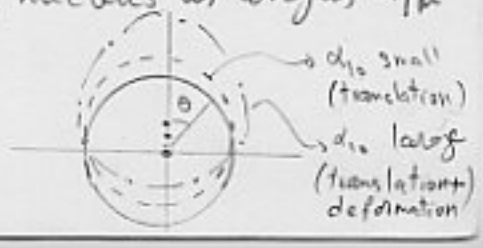
For small deformation $\alpha_{\lambda\mu}$ are small $\longrightarrow |\alpha_{\lambda\mu}|^2$ too small

$\longrightarrow \alpha_{00}$ second order small quantity

Remark: $\lambda = 1$ terms are usually excluded from the sum, because they correspond to a <u>trivial</u> translation of of the total nucleus as long as $\alpha_{1\mu}$ are small (in the isoscalar case).

Ex.: If $\alpha_{11} = \alpha_{1,-1} = 0$ (isoscalar case)

$$R(\theta,\varphi) = R_0 (1 + \alpha_{10} Y_{10}) = R_0 \left(1 + \alpha_{10}\sqrt{\tfrac{3\pi}{4}}\cos\theta\right)$$



Case b) $\lambda = 1$ $T = 0$ (isoscalar dipole mode)

oscillation about a fixed point in lab frame.

In this excitation the internal structure of the nucleus does not change (all the nucleons move together).

This mode of excitation is of no interest.

Case c) $\lambda = 1$ $T = 1$ (isovector case)

Corresponds to dipole oscillations of neutrons and protons in opposite dir.

→ This is the cause of giant dipole resonances.

Case d) $\lambda = 2$

→ Quadrupole oscillation of the nucleus

$Q > 0$ deformation → prolate shape ⬭

$Q < 0$ " → oblate shape ○

→ There is a quadrupole vibration

Case e) $\lambda = 3$

$\rightarrow$ Octupole vibration

Since $\alpha_{\lambda\mu}$ represent the deformation of the nucleus from its equlibrium;

$$\rightarrow \quad T = \frac{1}{2} \sum_{\lambda\mu} D_\lambda |\dot{\alpha}_{\lambda\mu}|^2 \qquad (1) \qquad \dot{\alpha}_{\lambda\mu} = \frac{d\alpha_{\lambda\mu}}{dt}$$

$$V = \frac{1}{2} \sum_{\lambda\mu} C_\lambda |\alpha_{\lambda\mu}|^2 \qquad (2)$$

Where instead of the coords. of the nucleons we have used shape parameters (appropriate Cannonical variables).

D_λ: has a role equivalent to <u>mass</u>

with the assumptions $\begin{cases} 1- \text{incompressible liquid} \\ 2- \text{classical irrotational flow} \end{cases}$

$$\rightarrow \quad D_\lambda = \frac{\rho}{\lambda} R_0^5 \qquad \rho: \text{density of nuclear matter}$$

Min. Pot. energy is chosen to be at $\alpha_{\lambda\mu} = 0$
((2) follows from this choice).

$\rightarrow$ No linear dependence of V on $\alpha_{\lambda\mu}$

$\rightarrow$ The leading order: quadratic

For small oscillations $\rightarrow$ higher order terms in V may be ignored.

$$C_\lambda = \frac{1}{4\pi}(\lambda-1)(\lambda+2)\,\alpha_2 A^{2/3} - \frac{5}{2\pi}\frac{\lambda-1}{2\lambda+1}\,\alpha_3 \frac{Z(Z-1)}{A^{1/3}}$$

↑ surface term ↑ Coulomb term

Note: $4\pi\sigma \sim r_0^2 = \alpha_2$ $\quad R_0 = r_0 A^{1/3}$

↑ surface tension

$$H_\lambda = \frac{1}{2}\sum_\mu \left\{ C_\lambda |\alpha_{\lambda\mu}|^2 + D_\lambda |\dot{\alpha}_{\lambda\mu}|^2 \right\} \quad (1)$$

$$H = \frac{1}{2}\sum_{\lambda\mu} \left\{ C_\lambda |\alpha_{\lambda\mu}|^2 + D_\lambda |\dot{\alpha}_{\lambda\mu}|^2 \right\} \quad (2)$$

(if different modes of excitation are decoupled from each other.)

↑ Generalized coords. ↑ Generalized velocities

$$\Pi_{\lambda\mu} \equiv \frac{\partial H}{\partial \dot{\alpha}_{\lambda\mu}} = D_\lambda \dot{\alpha}^*_{\lambda\mu}$$

Generalized Momenta

Canonically conjugate to $\alpha_{\lambda\mu}$

We postulate; (Tr. to quantum Hamiltonian)

$$[\Pi_{\lambda\mu}, \alpha_{\lambda'\mu'}] = \frac{\hbar}{i}\delta_{\lambda\lambda'}\delta_{\mu\mu'}$$

(operators)

$$[\alpha_{\lambda\mu}, \alpha_{\lambda'\mu'}] = [\Pi_{\lambda\mu}, \Pi_{\lambda'\mu'}] = 0 \quad (3)$$

$$H = \frac{1}{2}\sum_{\lambda\mu}\left\{ C_\lambda |\alpha_{\lambda\mu}|^2 + \frac{1}{D_\lambda}|\Pi_{\lambda\mu}|^2 \right\} \quad (4)$$

If different mode of excitation (different λ) are decoupled from each other and any other degrees of freedom $\longrightarrow$ H_λ, C_λ, D_λ are consts. of motion

Differentiating (1) w.r.t time $\longrightarrow$ $D_\lambda \frac{d^2\alpha_{\lambda\mu}}{dt^2} + C_\lambda \alpha_{\lambda\mu} = 0$

Comparing with $\frac{d^2x}{dt^2} + \omega^2 x = 0$

$\rightarrow$ For small oscillations, the amplitude $\alpha_{\lambda\mu}$ undergoes harmonic oscillation with frequency:

$$\omega_\lambda = \sqrt{\frac{C_\lambda}{D_\lambda}} \qquad \text{(indep. of } \mu\text{)}$$

$$E = \sum_{\lambda\mu} \left(n_{\lambda\mu} + \frac{1}{2}\right) \hbar \omega_\lambda \qquad n_{\lambda\mu}: \text{positive integers}$$

Since $-\lambda \leq \mu < \lambda$ $\rightarrow$ the degeneracy of an excited state with a fixed λ is $(2\lambda+1)$-fold.

The elementary exciations of the surface vibrations of a nucleus can be regarded quasi-particles — phonons.

A vibrational quantum of energy is called phonon since it is a form of mechanical energy.

Each phonon is a boson carrying $\lambda\hbar$ units of angular momentum and having a parity $\Pi = (-)^{\lambda}$.

It is convenient to use the occupation number representation;

We introduce new operators $b_{\lambda\mu}$;

$$\alpha_{\lambda\mu} = \left(\frac{\hbar}{2D_\lambda \omega_\lambda}\right)^{1/2} \left[b_{\lambda\mu} + (-)^{\mu} b^{\dagger}_{\lambda,-\mu} \right]$$

$$\Pi_{\lambda\mu} = \left(\frac{\hbar D_\lambda \omega_\lambda}{2}\right)^{1/2} \left[b^{\dagger}_{\lambda\mu} - (-)^{\mu} b_{\lambda,-\mu} \right]$$

Equ. (3) (P117) $\longrightarrow$ $\left[b_{\lambda\mu}, b^{\dagger}_{\lambda'\mu'} \right] = \delta_{\lambda\lambda'} \delta_{\mu\mu'}$

$$\left[b_{\lambda\mu}, b_{\lambda'\mu'} \right] = \left[b^{\dagger}_{\lambda\mu}, b^{\dagger}_{\lambda'\mu'} \right] = 0$$

$$\rightarrow H = \sum_{\lambda\mu} \left(b^{\dagger}_{\lambda\mu} b_{\lambda\mu} + \frac{1}{2} \right) \hbar\omega_\lambda$$

$$b_{\lambda\mu} |n_{\lambda\mu}\rangle = \sqrt{n_{\lambda\mu}}\, |n_{\lambda\mu}-1\rangle \qquad b^{\dagger}_{\lambda\mu} |n_{\lambda\mu}\rangle = \sqrt{n_{\lambda\mu}+1}\, |n_{\lambda\mu}+1\rangle$$

$$|n_{\lambda\mu}\rangle = \frac{1}{\sqrt{n_{\lambda\mu}!}} \left(b^{\dagger}_{\lambda\mu} \right)^{n_{\lambda\mu}} |0\rangle$$

$$N_{\lambda\mu} \equiv b^{\dagger}_{\lambda\mu} b_{\lambda\mu} \qquad N_{\lambda\mu} |n_{\lambda\mu}\rangle = n_{\lambda\mu} |n_{\lambda\mu}\rangle$$

$$H = \sum_{\lambda\mu} \left(N_{\lambda\mu} + \frac{1}{2} \right) \hbar\omega_\lambda$$

$$\rightarrow E = \sum_{\lambda\mu} \left(n_{\lambda\mu} + \frac{1}{2} \right) \hbar\omega_\lambda \qquad E_{n_{\lambda\mu}} = \left(n_{\lambda\mu} + \frac{1}{2} \right) \hbar\omega_\lambda$$

$$L_z = \hbar \sum_{\lambda\mu} \mu N_{\lambda\mu} \qquad \langle n_{\lambda\mu} | L_z | n_{\lambda\mu} \rangle = \hbar \mu n_{\lambda\mu}$$

Two-phonon wave funcs. $b^+_{\lambda\mu} b^+_{\lambda'\mu'} |0\rangle$ describe states with well-defined

$$\begin{cases} E = \hbar(\omega_\lambda + \omega_{\lambda'}) & \text{energy} \\ \Pi = (-)^{\lambda+\lambda'} & \text{parity} \\ M = \mu + \mu' & z\text{-component of total angular mom.} \end{cases}$$

In this case Λ does not have <u>well-defined</u> value.

The wave func. of a state with <u>well-defined</u> angular momentum Λ lying within the limits $|\lambda - \lambda'| \leq \Lambda \leq \lambda + \lambda'$ can be constructed as:

$$|\Lambda M\rangle = \sum_{\mu\mu'} (\lambda\mu, \lambda'\mu' / \Lambda M)\, b^+_{\lambda\mu} b^+_{\lambda'\mu'} |0\rangle$$

If $\lambda = \lambda'$ from the symmetry of $\begin{cases} \text{i- } |\Lambda M\rangle \text{ under } (1 \rightleftarrows 2) \\ \text{ii- } (\lambda\mu, \lambda\mu' / \Lambda M) = (-)^{2\lambda - \Lambda} (\lambda\mu', \lambda\mu / \Lambda M) \end{cases}$

$\longrightarrow \Lambda = 0, 2, \ldots 2\lambda$ (only)

For two-phonon system with $\lambda = \lambda' = 2 \rightarrow \Lambda = 0, 2, 4$

" three " " " $\lambda = \lambda' = \lambda'' = 2 \rightarrow \Lambda = 0, 2, 4, 6$

With increasing the number of phonons <u>of the same type</u>

$\longrightarrow$ the states can classified using <u>group theoretical methods</u>.

Quadrupole and Octupole Vibrations:

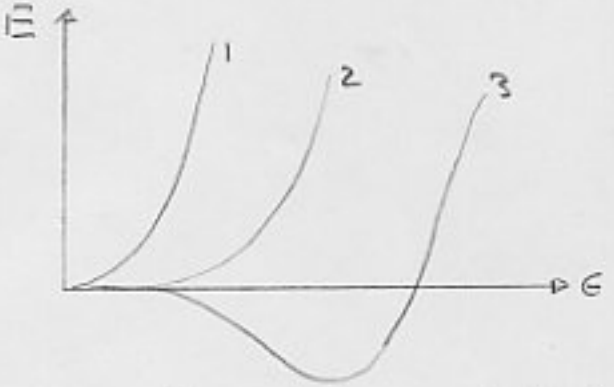
For an even-even nucleus the ground state: $J^{\pi} = 0^{+}$

→ may be regarded as Zero-phonon state

The excited state has $J^{\pi} = \lambda^{(-1)^{\lambda}}$

If $J=0$ → A spherically density dist. corresponds → to the equilibrium state with lowest energy

However; although a spherically dist. corresponds → to a condition of equilibrium it is not always → the case that the equilibrium is stable.



Dependence of the ground state energy on the nuclear deformation parameter.

ϵ: Deformation parameter

(for example eccentricity)

E: Ground state energy

(case I) In a stable equilibrium for spherical shape $\frac{\partial E}{\partial \epsilon} = 0 \rightarrow \epsilon_{Min} = 0$ (Min. of E at $\epsilon = 0$)

This happens in doubly magic nuclei (1) and nearby nuclei (2)

Case II) As the number of nucleons in the unfilled outer shell increases ⟶ the polarizing effect of these nucleons leads to violation of the spherical symmetry (3)

⟶ $\frac{\partial E}{\partial \epsilon} = 0 \quad \epsilon \neq 0_{min}$

In the case of spherical nuclei, the collective excitation corresponds to ⟶ vibrations of the surface of the nucleus about the equilibrium shape.

$\omega_\lambda = \sqrt{\frac{C_\lambda}{D_\lambda}}$ (P116,117) ⟶ The energy $\hbar\omega_\lambda$ of the surface vibrations increases monotonically with increasing λ.

Collective excited states are defined by the quantum numbers:

n : Number of phonons

Λ : Angular momentum (total)

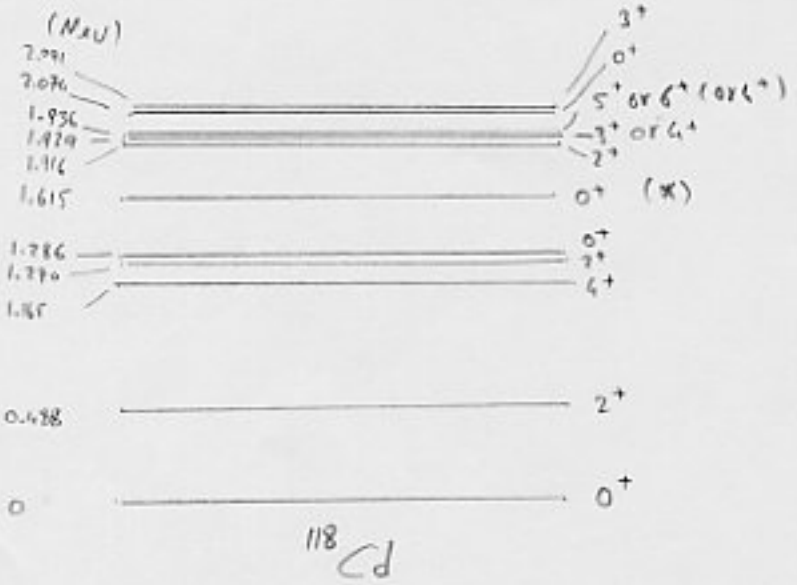
$\Lambda = 1$ case may be ignored ($\alpha_{1\mu} = 0$ assumption) because the nucleus transforms as a whole (isoscalar case)

Low-energy spectra of spherical nuclei,
($\lambda = 2$ quadrupole vibrations):

i) $\lambda = 2$ $n = 1$ $J^{\pi} = \Lambda^{(-)^{\lambda}} = 2^{+}$

ii) $\lambda = 2$ $n = 2$ $J^{\pi} = 0^{+}, 2^{+}, 4^{+}$ (degenerate)

iii) $\lambda = 2$ $n = 3$ $J^{\pi} = 0^{+}, 2^{+}, 3^{+}, 4^{+}, 6^{+}$ ≈



$3\hbar\omega_2$ ——— $0^{+}, 2^{+}, 3^{+}, 4^{+}, 6^{+}$

$2\hbar\omega_2$ ——— $0^{+}, 2^{+}, 4^{+}$

$\hbar\omega_2$ ——— 2^{+}

——— 0^{+}

Quadrupole vibration of ^{118}Cd up to 3-phonon excitations.

(*) May not be a member of the vibrational spectrum.

The first excited states ($\hbar\omega_2$) predicted by the vibrational model have been observed in most even-even nuclei

Splitting between the energies (triplet states for n=2 ... etc..) can not be explained in this simple vibrational model, because there is no J-dependence in the energy.

In this model quantitative calculations of the spectra for even-even nuclei have not been successfull

$$\omega_\lambda = \sqrt{\frac{C_\lambda}{D_\lambda}} \xrightarrow{\text{neglecting coulomb ter.}} \hbar\omega_2 = \frac{a}{A^{1/2}}$$

→ the energy of the first excited state should be a monotonic func. of A.

However, empirical data show that the energy of the first excited state of even-even nuclei depends strongly on the structure of the nuclei (large values for the magic nuclei)

This indicates → the limited applicability of this model.

Acc. to the model the ratio of the second to the first excited state must be 2.

$$\frac{E_2}{E_1} = \frac{2\hbar\omega}{\hbar\omega} = 2$$

large deviations $\frac{E_2}{E_1} \to 3$ $\xrightarrow{\text{implies}}$ large quadrupole moments

$\xrightarrow{\text{connected}}$ non-spherical equilibrium shape (Ground state)

$\xrightarrow{\text{Therefore}}$ the low-energy levels of these nuclei are associated with the rotation of the nuclei rather than with the surface vibrations.

Examples of one-phonon ($n=1$) octupole ($\lambda=3$) excitations are found in the form of a low-lying 3^- state in all closed shell nuclei ^{16}O, ^{40}Ca, ^{90}Zr, ^{208}Pb.

Remark: $E = 41\, A^{-1/3}$ Mev typical energy of exciting a nucleon up one major shell. (we shall see later. Single Particle picture)

$\longrightarrow$ $E = 16$ Mev in ^{16}O, $E = 7$ mev in ^{208}Pb

One-phonon octupole excitation ($J^\pi = 3^-$) observed in closed shell nuclei ^{16}O and ^{208}Pb are much lower in energy than these values $\xrightarrow{\text{indicating}}$ many nucleons are acting in an coherent or collective manner to lower the energy required to excite the state.

Electromagnetic transitions:

The vibrational model also predicts electromagnetic tr. rates between states consisting of different numbers of excitation phonons.

In tr. of $n \longrightarrow n-1$ phonon state,

one quantum of energy $\hbar\omega$ is emitted.

$O_{\lambda\mu}(E\lambda) \sim b_{\lambda\mu}$ $\quad$ $b_{\lambda\mu}$: annihilation op for a phonon with multipolarity $(\lambda\mu)$.

Because of collective nature (coherent nature) $\longrightarrow$

Nucl. excitations induced predominantly by quadrupole vibrations have large $W(E2)$ from the one-phonon state to the ground state, compared with Weisskopf single-particle estimates.

Similar case happens for E3-trs. in states excited by octupole vibrations.

$\langle n'|b|n\rangle = \sqrt{n}\,\delta_{n',n-1} \longrightarrow B(E\lambda, n\to n-1) \sim n$

$\longrightarrow B(E\lambda, 2\to 1) > B(E\lambda, 1\to 0)$ (in the same nucleus)

$\langle n'|b\ldots b|n\rangle \ll \langle n'|b|n\rangle$

↑ higher order

(emission of more than one phonon)

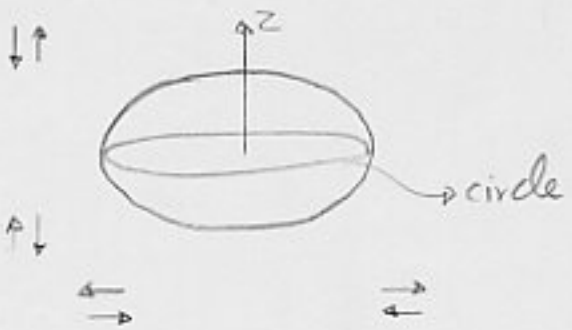
These points are observed to be correct in vibrational nuclei

In our discussion we have assumed that the vibration is an axially symmetric.

Axially symmetric vibration: Vibration along x- and y- dirs. are always equal to each other, only their ratio to that along z-axis is changing as a func. of t.

$R_x(t) = R_y(t)$

$\frac{R_x(t)}{R_z(t)} = f(t)$



This type of vibration is generally known as β-vibration.

More generally;

γ-vibrations: The nucleus deforms into an ellipsoidal shape in the equatorial dir.

i.e., Section of nucleus in x-y plane at any instant of t is an ellipse rather than a circle.

In addition to purely harmonic vibrational motion, anharmonic terms may be present.

Furthermore, vibrations may also be coupled to other modes of excitation in realistic situations.

If the amplitude of vibration is large, the above treatment will no longer apply.

If the vibration is energic enough ⟶

deformation leading to fission

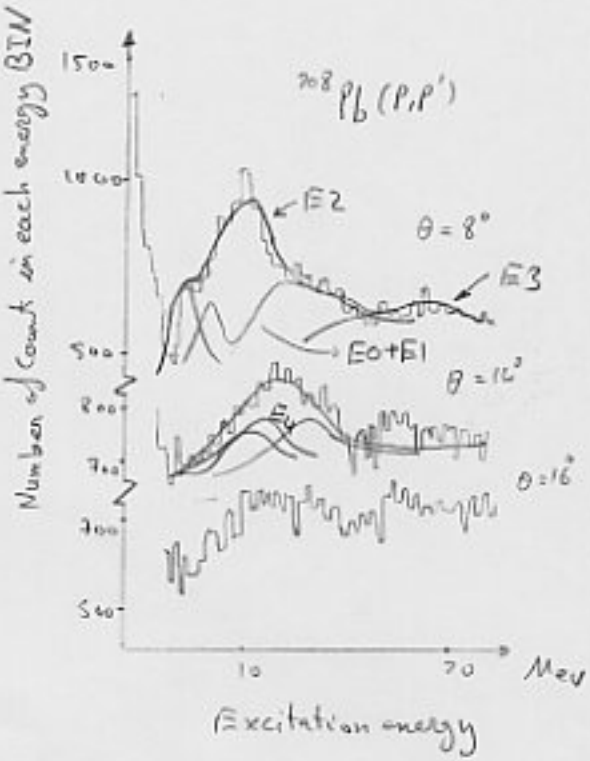
In this case there must be:

1- Superposition of many different vibrational modes
2- The vibrational modes must strongly be coupled to each other.

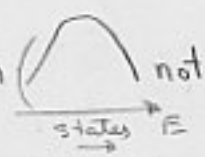
6-2 Giant Resonances:

Both { 1- strength / 2- width } of these resonances are much larger than typical resonances built upon single-particle (non-collective) resonances.

They occur at energies at tens of Mev above the grand state.



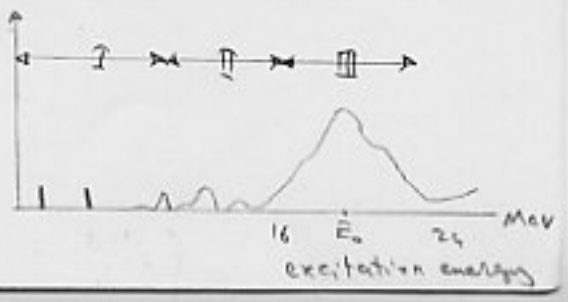
Diff. cross-section of $^{208}Pb(P,P')$ with 200Mev protons at different scattering angles

In the energy region where giant resonances appear, the density of states is sufficiently high and the number of open decay channels sufficiently large that → states in a given energy region ( not) can not be very different from each other in character.

As a result → We expect only smooth variations of reaction cross sections when the nucleus is excited.

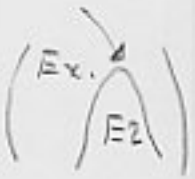
Remark: Resonances in I and II regions can be explained by shell structure, while that one in III region have collective basis.

$E_0 \sim A^{-1/3}$ for heavy and medium nuclei



For most giant resonances;

The excitation strengths are found to be indep. of the prob, used to excite the nucleus (γ-ray, electron, proton, α-particle, ^{16}O ion).

Furthermore both $\begin{cases} 1\text{-width} \\ 2\text{-location of the peak of the strength dist.} \end{cases}$ 

in different nuclei vary smoothly as a func. of A (without any significant dependence on the detailed structure of the nucleus involved).

↓

Ex.

$E_1 \simeq 78\, A^{-1/3}$ isovector giant resonances (location of peak) (well described)

The cause of giant resonances is the collective excitation of nucleons.

$\Delta E \simeq 41\, A^{-1/3}$ energy gap between two major shells

1P-1h
Two major shell excitation
$\Pi = +$ excitation

1P-1h
One major shell excitation
$\Pi = -$ excitation (in general)

Parity of states produced by 1h-1P excitations

up one (odd) major shell = −

up two (even) " " = +

" 0 − major shell = + (rearrangement of the particles in the same shell (0hω-excitation))

nhω-excitations with n>2 are less probable because of larger amount of energy involved.

Giant dipole resonance:

They are excitations of the $J^{\pi} = 1^-$ strength by promoting nucleons up one major shell.

In light nuclei observed peaks of strength occur around 25 MeV in the excitation energy (E1)

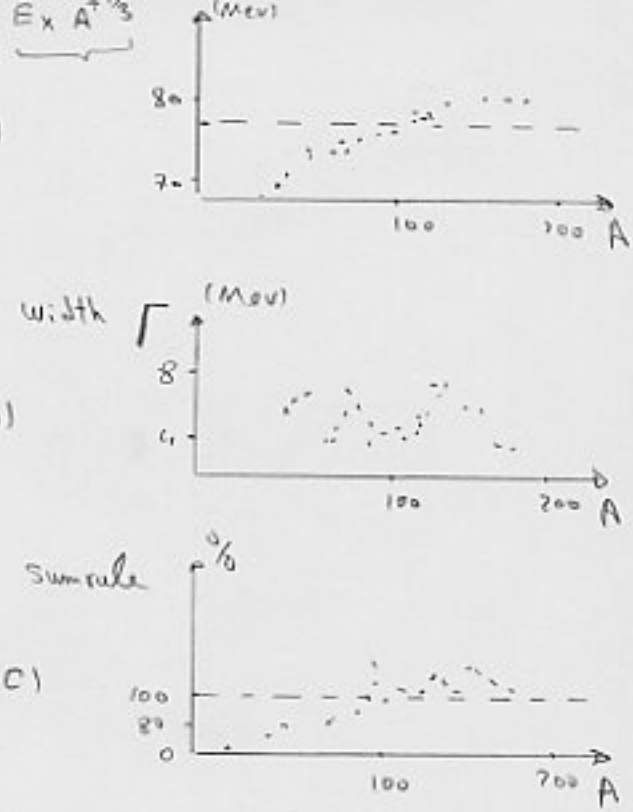
In heavy nuclei the values are lower (the energy levels are close together)

In ^{208}Pb : it is just below 14 MeV (E1) (P129)

a) Variation of peak location

b) " " width

c) " " isovector giant dipole resonance as a func. of nucleon number



Isovector dipole resonance

$E_1 \approx 78 A^{-1/3}$ is fairly consistant with empirical data (Fig. a).

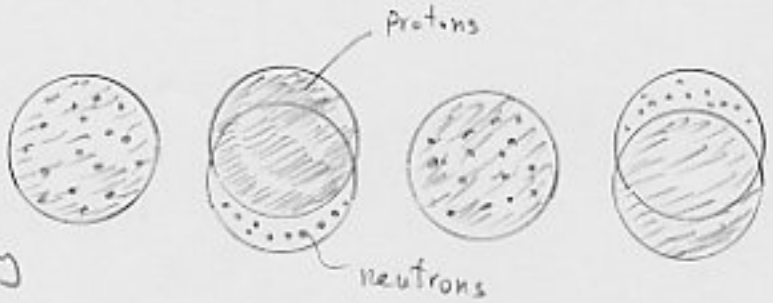
The peak position is higher than that expected of a simple one-two excitation process of $41 A^{-1/3}$ Mev.

The difference is caused by the residual interaction between the nucleons which → pushes the isovector excitation to a higher energy.

The width of resonance $\approx$ 6 Mev without noticeable dependence to A (Fig. b)

An explanation of giant dipole resonance based on the collective motion of nucleons is provided by the Goldhaber-Teller model.

In this model the neutrons and protons vibrate collectively but in opposite phase with respect to each other.



Isovector dipole

→ The center of mass of the entire nucleus is stationary

In contranst, in isoscalar case the entire nucleus is oscillating around some equilibrium position in the lab. frame.

→ These oscillations don't correspond to the excited states and they are of no interest.

Sum rule quantities:

Another useful way to study giant resonances is to find out % total possible tr. strength (represented by the observed (cross-section)

$$S = \int_0^\infty \sigma(E)\, dE \qquad \text{for a certain multipolarity } \Lambda$$

$\uparrow$ all final states

$S \equiv S(\text{initial states})$

For isovector dipole trs.;

$$S(J^\pi = 1^-) = \int_0^\infty \sigma(E)\, dE = \frac{2\pi^2 \hbar^2 \alpha}{M_p} \frac{NZ}{A} \simeq 60 \frac{NZ}{A} \text{ Mev-fm}^2$$

(Thomas-Reiche-Kuhn (TRK) sumrule)

Ref.: de-Shalit and Feshbach, Theoretical Nucl. Phys., Wiley, New York, 1974. PP. 709-713.

Assumption in derivation:
1- No velocity dependent term in nucleon-nucleon int.
2- Antisymmetrization among all nucleons is ignored

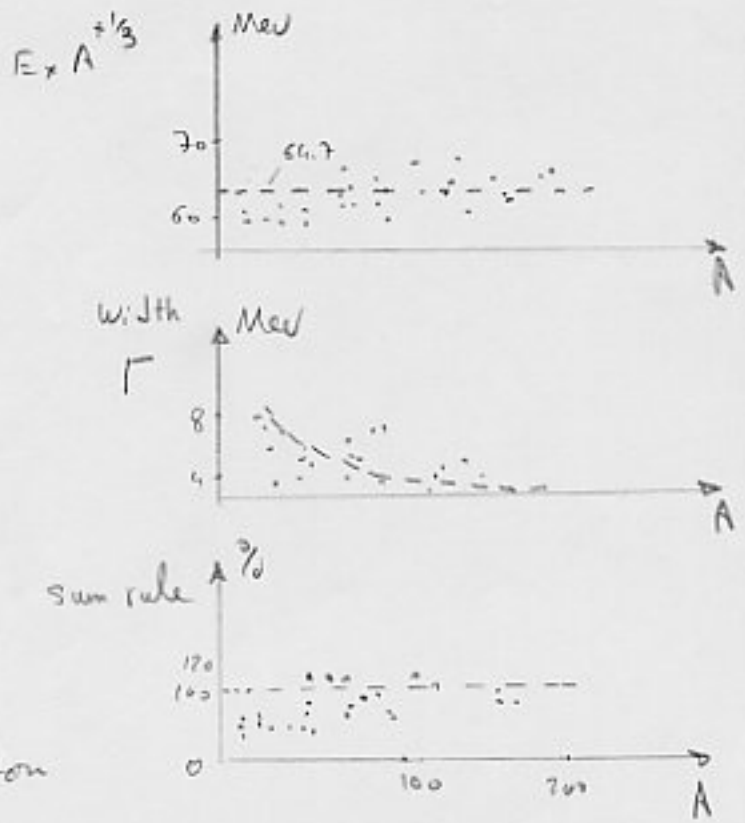
The correction for antisymmetrization effects is a multiplicative factor $(1+\eta)$ $\quad \eta \simeq 0.5$

Fig (c) (P132) represents a comparison of the total strength obtained experimentally and those given by the TRK sum rule (with $\eta = 0$) for the isovector dipole trs.

As long as $\eta \approx 0.5$ (accepted value) we see that the measured giant dipole cross sections exhaust large fractions of the total possible strengths.

Besides isovector dipole excitation, other giant resonances have also been observed in recent years.

Both giant quadrupole (E2) and giant octopole (E3) resonances have been observed.



a) Vibration of peak location

b) " " width

c) " " total strength

of isoscalar giant quadrupole resonances as a func. of nuclear number A.

6-5 Magic Number and Single-Particle Energy

We have treated nucl. binding energy as a smooth func. of A, N, Z.

$$E_B(Z,N) = \alpha_1 A - \alpha_2 A^{2/3} - \alpha_3 \frac{Z(Z-1)}{A^{1/3}} - \alpha_4 \frac{(N-Z)^2}{A} + \Delta$$

Superimposed on this global picture, there are local variations that are useful in understanding nucl. Phys.

For example:

Nuclei with $\begin{cases} Z = 2, 8, 20, 40, 82 \\ \text{or} \\ N = 2, 8, 20, 50, 82, 126 \end{cases}$ (magic numbers)

are known to be special:

1- Energies of the first few excited states are higher than those in nearby nuclei.

2- Single neutron and single proton removal energies, S_n and S_p are much larger than those in the neighboring even-even nuclei

$$S_n(Z,N) = E_B(Z,N) - E_B(Z,N-1)$$

$$S_p(Z,N) = E_B(Z,N) - E_B(Z-1,N)$$

3- The intrinsic shape of the ground states is spherical (as can be seen from observations such as el-mag. trs.)

Doubly magic nuclei:

$^4He \begin{cases} Z=2 \\ N=2 \end{cases}$, $^{16}O \begin{cases} Z=8 \\ N=8 \end{cases}$ $^{40}Ca \begin{cases} Z=20 \\ N=20 \end{cases}$ $^{90}Zr \begin{cases} Z=40 \\ N=50 \end{cases}$ $^{208}Pb \begin{cases} Z=82 \\ N=126 \end{cases}$

The existance of magic numbers may be explained by → Independent-Particle Model

In this model:

1- There is no int. between the nucleons
2- The effect of all other nucleons is replaced by → a mean-field

$$H = \sum_i \epsilon(i)\, n_i \qquad \text{(single particle terms)}$$

$\epsilon(i)$: The energy of each single particle state

n_i : Number op. (it measures the occupancy (0 or 1) of a single particle state i)

The magic numbers are the consequence of that the nuclear single-particle spectrum is not a smooth one, there are relatively large gaps between groups of single particle states

Harmonic Oscillator Single-particle Spectrum:

A simple model:

$$h(r_i) = -\frac{\hbar^2}{2\mu_i}\nabla_i^2 + V(r_i)$$ one-body Hamiltonian

$V(r_i)$ represents the average effect of all the other nucleon-nucleon int. on nucleon i

There is still residual two-body int. that gives → information about the detailed nucl. properties

We will not be concerned with it here.

$$V(r_i) = \frac{1}{2}\mu_i \omega_0^2 r_i^2$$ assumption (3-dim. isotropic osc.)

$$\begin{cases} V(r) = -V_0 - \frac{1}{2}\mu\omega_0^2 r^2 & \text{inside} \\ V(r) = 0 & \text{outside} \end{cases}$$ for light nuclei

$$\xi\frac{d^2\psi}{d\xi^2} + \frac{3}{2}\frac{d\psi}{d\xi} + \frac{1}{2}\left[\epsilon - \frac{1}{2}\xi - \frac{\ell(\ell+1)}{2\xi}\right]\psi = 0 \qquad (1)$$

where $\xi = \frac{\mu\omega_0^2 r^2}{\hbar}$ $\qquad \epsilon = \frac{E+V_0}{\hbar\omega_0}$

For large ξ $\longrightarrow$ $\frac{d^2\psi}{d\xi^2} - \frac{1}{4}\psi \approx 0 \qquad (2)$

$\longrightarrow \psi \sim e^{-\xi/2}$ $(\xi \to \infty)$

For small values of ξ;

$$\frac{d^2\psi}{d\xi^2} + \frac{3}{2\xi}\frac{d\psi}{d\xi} - \frac{l(l+1)}{4\xi^2}\psi \simeq 0 \qquad (3)$$

$\longrightarrow \psi \sim \xi^s$ (We seek)

$\longrightarrow s(s-1) + \frac{3}{2}s - \frac{l(l+1)}{4} = 0$

We choose positive root $s = \frac{l}{2}$ (since ψ must be finite at $\xi = 0$)

$\longrightarrow \psi \sim e^{-\xi/2}\, \xi^{l/2}\, W(\xi) \qquad (4)$

$W(\xi)$: A polynomial finite at $\xi = 0$

(4) in (1) $\longrightarrow \xi W'' + (l + \frac{3}{2} - \xi) W' + \frac{1}{2}(\epsilon - l - \frac{3}{2}) W = 0$

Sol. $\longrightarrow$ A confluent hypergeometric func.

$$W(\xi) = F(-\tfrac{1}{2}\epsilon + \tfrac{1}{2}l + \tfrac{3}{4},\ l + \tfrac{3}{2};\ \xi)$$

Where

$$F(\alpha, \gamma; \xi) = 1 + \frac{\alpha}{\gamma}\frac{\xi}{1!} + \frac{\alpha(\alpha+1)}{\gamma(\gamma+1)}\frac{\xi^2}{2!} + \frac{\alpha(\alpha+1)(\alpha+2)}{\gamma(\gamma+1)(\gamma+2)}\frac{\xi^3}{3!} + \cdots$$

which is terminated if α is negative integer or zero.

The sol. will be a polynomial only in the case when;

$$-\frac{1}{2}\epsilon + \frac{1}{2}\ell + \frac{3}{4} = -(n-1) \qquad n = 1, 2, 3, \cdots$$

$$\rightarrow \quad \epsilon = 2\underbrace{(n-1)+\ell}_{N} + \frac{3}{2} \equiv N + \frac{3}{2}$$

$$E_N = -V_0 + (N + \tfrac{3}{2})\hbar\omega \qquad N = 0, 1, 2, \cdots$$ Principal quantum number

$$\psi_{n\ell}(r) = C_{n\ell}\, e^{-\frac{\alpha^2 r^2}{2}}\, r^{\ell}\, F(1-n, \ell+\tfrac{3}{2}, \alpha^2 r^2)$$

where $$C_{n\ell} = \frac{1}{\Gamma(\ell+\frac{3}{2})}\sqrt{\frac{2\Gamma(\ell+n+\frac{1}{2})}{\Gamma(n)}}\;\alpha^{\ell+\frac{3}{2}} \qquad \alpha = \left(\frac{\mu\omega_0}{\hbar}\right)^{1/2}$$

$\ell \leq N$, ℓ and N have the same parity

$\ell = N, N-2, \cdots 1$ or 0

$(n\ell)$ identifies the state

1S; 1P; 2S; 1d; 2P; 1f; 3S; 2d; 1g ...

The number of states in a harmonic osc. shell permitted by the Pauli principle for protons or neutrons is given by;

$$D_N = 2 \sum_{\substack{\text{allowed } \ell \\ (\text{odd or even})}}^{N} (2\ell+1) = 2 \sum_{k=1}^{N+1} k = (N+1)(N+2)$$

$$D_{max} = \sum_{N=0}^{N_{max}} D_N = \frac{1}{3}(N_{max}+1)(N_{max}+2)(N_{max}+3)$$

$$\lim_{N_{max} \gg 1} D_{max} = \frac{1}{3}(N_{max}+2)^3$$

where we have used the identity $\sum_{k=1}^{n} k^2 = \frac{1}{6} n(n+1)(2n+1)$

How is ω_0 related to the size of the nucleus (R) and hence to A?

$$\omega_0 \stackrel{?}{=} f(A)$$

N	(nℓ)	D_N	D_{max}
0	1S	2	2
1	1P	6	8
2	2S, 1d	12	20
3	2P, 1f	20	40
4	3S, 2d, 1g	30	70
5	3P, 2f, 1h	42	112
6	4S, 3d, 2g, 1i	56	168

For a nucleon in a harmonic osc. well (in 3-dim.)

$$\langle T \rangle_{mean} = \langle V \rangle = \frac{1}{2} \text{ total energy}$$

↓ measured from the bottom of the well

$$\langle V \rangle = \left\langle \tfrac{1}{2} \mu \omega_0^2 r^2 \right\rangle_N \qquad \text{for one nucleon}$$

$$\left\langle \tfrac{1}{2} \mu \omega_0^2 r^2 \right\rangle_N = \tfrac{1}{2} \left(N + \tfrac{3}{2}\right) \hbar \omega_0$$

$$\rightarrow \langle r^2 \rangle_N = \frac{\hbar}{\mu \omega_0} \left(N + \tfrac{3}{2}\right) \qquad (1)$$

The mean-square radius of a nucleus made of A nucleons is given by the average over all occupied harmonic osc. states for both neutrons and protons;

$$\langle R^2 \rangle = \frac{2}{A} \sum_{N=0}^{N_{max}} D_N \langle r^2 \rangle_N = \frac{2}{A} \sum_{N=0}^{N_{max}} (N+1)(N+2)\left(N+\tfrac{3}{2}\right) \frac{\hbar}{\mu \omega_0} \qquad (2)$$

where we have assumed the number of protons and neutrons are equal.

Using the identity $\sum_{k=1}^{n} k^3 = \left[\frac{n(n+1)}{2}\right]^2$ and those for $\sum k$ and $\sum k^2$ given earlier;

$$\sum_{N=0}^{N_{max}} (N+1)(N+2)\left(N+\tfrac{3}{2}\right) = \frac{1}{4}\left(N_{max}+1\right)\left(N_{max}+2\right)^2\left(N_{max}+3\right)$$

$$\xrightarrow[N_{max} >> 1]{} \frac{1}{4}\left(N_{max}+2\right)^4$$

$$\rightarrow \langle R^2 \rangle = \frac{2}{A} \frac{\hbar}{\mu \omega_0} \frac{1}{4}\left(N_{max}+2\right)^4 \qquad (3)$$

$$\rightarrow \hbar \omega_0 = \frac{1}{A} \frac{\hbar^2}{\mu \langle R^2 \rangle} \frac{1}{2}\left(N_{max}+2\right)^4 \qquad (4)$$

on the other hand:

$$A = 2 \sum_{N=0}^{N_{max}} D_N = \frac{2}{3}(N_{max}+2)^3$$

↓ nadp

$$\rightarrow (N_{max}+2) = \left(\frac{3}{2}A\right)^{1/3}$$

$$\xrightarrow{(4)} \hbar\omega_0 = \frac{1}{A}\frac{\hbar^2}{\mu\langle R^2\rangle}\frac{1}{2}\left(\frac{3}{2}A\right)^{4/3} \qquad (5)$$

For const. density sphere:

$$\rho(r) = \begin{cases} \rho_0 & r \le R \\ 0 & r > R \end{cases}$$

$$V = 4\pi\int_0^\infty \rho(r)\, r^2\, dr = \frac{4\pi}{3}R^3\rho_0$$

$$\langle r^2\rangle = 4\pi\left(\frac{3}{4\pi}\frac{1}{R^3\rho_0}\right)\int_0^\infty \rho(r)\, r^4\, dr = \frac{3}{5}R^2 = \frac{3}{5}(r_0 A^{1/3})^2$$

$\downarrow$ $\psi^*\psi\, r^2 r^2 dr$

$$(5) \rightarrow \hbar\omega_0 = \frac{\hbar^2}{\mu\frac{3}{5}(r_0A^{1/3})^2}\frac{3}{4}\left(\frac{3}{2}A\right)^{1/3} = \frac{5}{4}\left(\frac{3}{2}\right)^{1/3}\frac{\hbar^2}{\mu r_0^2}A^{-1/3}$$

$$\rightarrow \hbar\omega_0 \simeq 41\, A^{-1/3}\ \text{MeV} \qquad (r_0 = 1.2\,\text{f}-)$$

The energy gap between the shells
(energy necessary for excitation)

Spin-Orbit Energy:

In the electron rest frame, the proton is moving

⟶ there is a current present ⟶ electron sees a mag. field B ($\bar{B} = \nabla \times \frac{\bar{E}}{c} = \frac{1}{c}\frac{\bar{P}}{\mu} \times \bar{E} = \frac{1}{c}\frac{\bar{P}}{\mu} \times \left(-\frac{1}{e}\nabla V\right)$) ;

↓ Pot. energy

$$H' = -\bar{M}\cdot\bar{B} = -\frac{\hbar e}{\mu c}\bar{S}\cdot\bar{B}$$

$$= -\frac{\hbar}{\mu^2 c^2}(P \times \nabla V)\cdot S$$

where $\nabla V = \frac{\bar{r}}{r}\frac{\partial V}{\partial r}$, $\bar{r}\times\bar{P} = \hbar\bar{L}$

$$H' = \left(\frac{\hbar}{\mu c}\right)^2 \frac{1}{r}\frac{\partial V}{\partial r} L\cdot S$$

In the nucleus we introduce an additional factor $-\lambda$ characterizing the magnitude of spin-orbit coupling;

$$H' = -\lambda\left(\frac{\hbar}{\mu c}\right)^2 \frac{1}{r}\frac{\partial V}{\partial r} L\cdot S$$

$\begin{cases} -\lambda & \text{for neutrons} \\ \lambda' & = \text{Protons} \end{cases}$

$$2\, L\cdot S = j(j+1) - l(l+1) - s(s+1)$$

$$H = -\frac{a}{r}\frac{\partial V}{\partial r} \qquad a = \frac{\lambda}{2}\left(\frac{\hbar}{\mu c}\right)^2 \times \begin{cases} l & j = l + \frac{1}{2} \\ -(l+1) & j = l - \frac{1}{2} \end{cases}$$

The schrodinger equ.;

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r) - \frac{a}{r}\frac{\partial V}{\partial r} - E \right] \psi = 0$$

$$\psi_{n\ell jm} = \varphi_{n\ell}(r)\, \mathcal{Y}_{\ell s j m}$$

$$\mathcal{Y}_{\ell s j m} = \sum_{m_\ell + m_s = m} (\ell m_\ell, s m_s / j m)\, Y_\ell^{m_\ell}(\theta, \varphi)\, \chi_s^{m_s}$$

$$\frac{d^2\varphi_{n\ell}}{dr^2} + \frac{2}{r}\frac{d\varphi_{n\ell}}{dr} + \frac{2\mu}{\hbar^2}\left[E_{n\ell j} - V(r) + \frac{a_{\ell j}}{r}\frac{dV(r)}{dr} - \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2} \right]\varphi_{n\ell} = 0$$

↓ self consistent

In the presence of spin-orbit int. the degeneracy of energy levels with respect to j is lifted.

In the case of harmonic osc.;

$$V(r) = -V_0 + \frac{1}{2}\mu\omega_0^2 r^2$$

$$-\frac{a}{r}\frac{\partial V}{\partial r} = -a\mu\omega_0^2$$

$$E_{N\ell j} = -V_0 + (N + \tfrac{3}{2})\hbar\omega_0 - a_{\ell j}\mu\omega_0^2$$

$$E_{Nlj} = -V_0 + \left(N + \frac{3}{2}\right)\hbar\omega_0 - \frac{\lambda}{2}\left(\frac{\hbar}{\mu c}\right)^2 \mu\omega_0^2 \times \begin{cases} l & j_> = l + \frac{1}{2} \\ -(l+1) & j_< = l - \frac{1}{2} \end{cases}$$

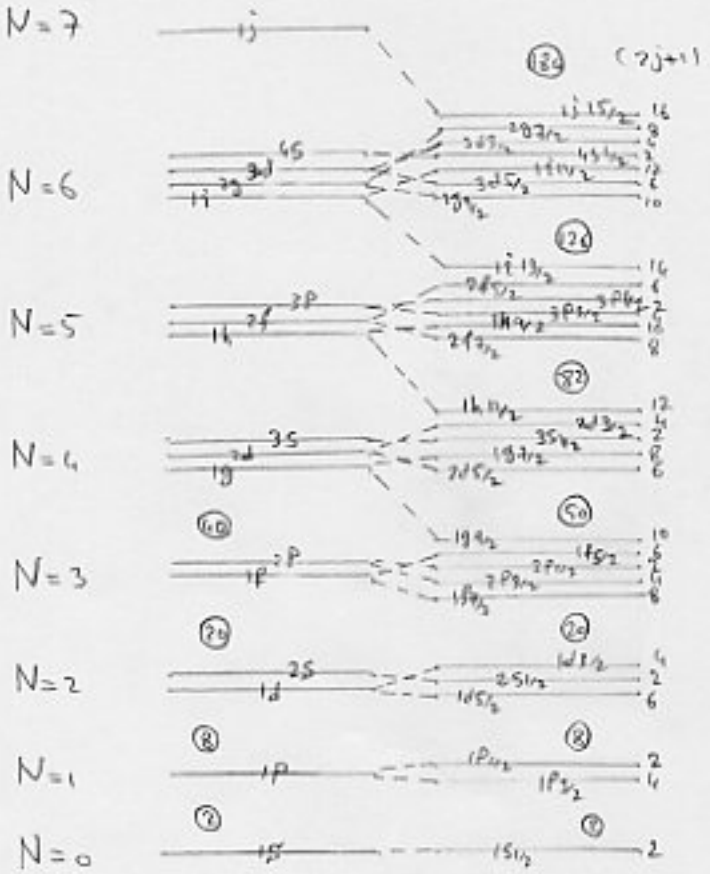
↑ higher in energy

In $j_>$ case for large values of l the last term is comparable with $\hbar\omega_0$;

⟶ The $j_>$ states of the largest l in a shell with N osc. quanta may be moved closer ⟶ to the group of states belonging to the $(N-1)$ shell below.

Note: An L^2-dep. term in H lowers the centroid energy of states with large l values;

⟶ $j_<$ states are prevented from moving up to join the states in the next major shell higher up.



Single-particle energy level positions for the spherical shell model.

Due to spin-orbit int. for neutrons ($-\lambda$) we have magic number 50 instead of 40.

Why there is <u>no</u> doubly magic nucleus with $Z=50$?

Because of Coulomb repulsion, nuclei beyond ^{40}Ca <u>must</u> have an <u>excess</u> of <u>neutrons</u>

For example ^{90}Zr : $(N-Z) = (50-40) = 10$

^{208}Pb : $(N-Z) = (126-82) = 44$

The next higher magic number after 50 is 82.

? : $(N-Z) = (82-50) = 32$ has too large neutron excess

⟶ A doubly-magic nucleus with $Z=50$ can not be formed.

Superheavy Nuclei:

The heaviest closed shell (doubly) nucleus is known to be ^{208}Pb.

Calculations indicate ⟶ $Z=114$ the next stable proton number (magic)

⟶ There may be a possibility that a superheavy element with $A=298$ $(N=184, Z=114)$ can be made in the lab.

Alternatively we may use the known magic number $Z=126$ and form $A=310$ (another candidate)

These exotic elements, however, have not been observed up to now.

Spectroscopic notation:

Each single particle orbit is specified by N, l, j (N: number of H. osc. quanta)

S, P, d, f, g, h, i, j... ⟶ $l = 0, 1, 2, 3, 4, 5, 6, 7 \ldots$

$n l_j$ (n: number of nodes)

There are two conventions to number n, depending whether the node at the origin is counted.

Ex: $\begin{cases} 0\,S_{1/2} \text{ (the node at origin excluded)} \\ 1\,S_{1/2} \end{cases}$

6-6 Many-Body Basis States

Indep variables $\begin{cases} x \\ \alpha \\ \tau \end{cases}$ and other deg. of freedom.

$$\Psi_\alpha \equiv \Psi_\alpha(r_1, \alpha_1, \tau_1; r_2, \alpha_2, \tau_2, \ldots r_A, \alpha_A, \tau_A)$$

But we will use $\bar{r}_i$ and assume that it represents <u>all</u> the other deg. of freedom.

$$H \Psi_\alpha(\bar{r}_1, \bar{r}_2 \ldots \bar{r}_A) = E_\alpha \Psi_\alpha(\bar{r}_1, \bar{r}_2, \ldots \bar{r}_A) \qquad (1)$$

Other properties of the system are obtained from the <u>matrix-elements</u> of the eigenvectors $\Psi_\alpha(\bar{r}_1, \bar{r}_2, \ldots \bar{r}_A)$ for the corresponding <u>operators</u>.

Matrix method to solve the eigenvalue problem:

It is more convenient to solve (1) using a matrix method.

We need,

$$\{\Phi_k(\bar{r}_1, \bar{r}_2, \ldots \bar{r}_A)\} \quad k = 1, 2, \ldots D$$

A complete set of <u>basis</u> states for A-particle system.

D: number of linearly indep. states in the Hilbert space

We assume they are orthogonal and normalized.

$$\Psi_\alpha(\bar{r}_1, \bar{r}_2 \cdots \bar{r}_A) = \sum_{k=1}^{D} C_k^\alpha \Phi_k(\bar{r}_1, \bar{r}_2 \cdots \bar{r}_A) \qquad (2)$$

C_k^α : expansion coeffs. for <u>α-th</u> eigenfunc.

Note: The sol. of (1) is indep. of the basis states chosen.

C_k^α determination:

$$(1) \longrightarrow \langle \Phi_j(\bar{r}_1, \bar{r}_2, \cdots \bar{r}_A) | H | \Psi_\alpha(\bar{r}_1, \bar{r}_2, \cdots \bar{r}_A) \rangle =$$

$$= E_\alpha \langle \Phi_j(\bar{r}_1, \bar{r}_2 \cdots \bar{r}_A) | \Psi_\alpha(\bar{r}_1, \bar{r}_2, \cdots \bar{r}_A) \rangle \qquad (3)$$

$$(2) \text{ in } (3) \longrightarrow \sum_{k=1}^{D} H_{jk} C_k^\alpha = E_\alpha C_j^\alpha \qquad (4)$$

where $H_{jk} \equiv \langle \Phi_j(\bar{r}_1, \bar{r}_2 \cdots \bar{r}_A) | H | \Phi_k(\bar{r}_1, \bar{r}_2 \cdots \bar{r}_A) \rangle$

Eqn. (4) in a matrix form;

$$\begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1D} \\ H_{21} & H_{22} & \cdots & H_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ H_{D1} & H_{D2} & \cdots & H_{DD} \end{pmatrix} \begin{pmatrix} C_1^\alpha \\ C_2^\alpha \\ \vdots \\ C_D^\alpha \end{pmatrix} = E_\alpha \begin{pmatrix} C_1^\alpha \\ C_2^\alpha \\ \vdots \\ C_D^\alpha \end{pmatrix} \qquad (5)$$

The eigenvalues E_α are the roots of the secular eqn.;

$$\det \begin{vmatrix} (H_{11}-E_\alpha) & H_{12} & \cdots & H_{1D} \\ H_{21} & (H_{22}-E_\alpha) & \cdots & H_{2D} \\ \vdots & \vdots & & \\ H_{D1} & H_{D2} & \cdots & (H_{DD}-E_\alpha) \end{vmatrix} = 0 \qquad (6)$$

Once an eigenvalue E_α is found $\longrightarrow C_i^\alpha$, $i=1,2\cdots D$ may be obtained by solving (5)

$\longrightarrow$ This gives the eigenvector corresponding to E_α.

The complete set of eigenvectors for $\alpha=1,2,\cdots D$ may be viewed as a matrix $\{C_i^\alpha\}$

$$R = \begin{pmatrix} C_{11} & C_{12} \cdots C_{1D} \\ C_{21} & C_{22} \cdots C_{2D} \\ \vdots & \\ C_{D1} & C_{D2} \cdots C_{DD} \end{pmatrix}$$

that transforms the Hamiltonian from the basis representation into a diagonal form

$$RH = H' \qquad H' = \begin{pmatrix} H'_{11} & 0 & 0 & \cdots & 0 \\ 0 & H'_{22} & \cdots & & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & & H'_{DD} \end{pmatrix}$$

Single-Partical Basis States:

The many-body basis wave funcs. are usually constructed out of products of single-particle wave funcs $\varphi_i(\bar{r}_j)$.

$$\Phi_k(\bar{r}_1, \bar{r}_2, \cdots \bar{r}_A) = \frac{1}{\sqrt{A!}} \det \begin{vmatrix} \varphi_1(\bar{r}_1) & \varphi_1(\bar{r}_2) \cdots \varphi_1(\bar{r}_A) \\ \varphi_2(\bar{r}_1) & \varphi_2(\bar{r}_2) \cdots \varphi_2(\bar{r}_A) \\ \vdots & \\ \varphi_A(\bar{r}_1) & \varphi_A(\bar{r}_2) \cdots \varphi_A(\bar{r}_A) \end{vmatrix}$$

$$\varphi_i(\bar{r}_j) \equiv \varphi_{K_i}(\bar{r}_j)$$

K_i: quantum numbers

If different set of A single-particle states $\{\varphi_i(\bar{r}_j)\}$ is taken $\longrightarrow$ a different many-body basis state $\{\Phi_k(\bar{r}_1, \bar{r}_2 \cdots \bar{r}_A)\}$ can be constructed.

In principle, the single-particle spectrum is an infinite one ($D \longrightarrow \infty$) extending in energy without an upper bound.

$\longrightarrow$ One must to find a reasonable and realistic approx. schemes such that only a small portion of Hilbert space is adequate to give a reasonable description of the nucl. states we wish to study.

There are many possible ways to specify the single-particle wave funcs. $\varphi_i(\bar{r}_j)$.

In general it is more convenient to take them as eigenfuncs. of a single-particle $h(\bar{r}_i)$

$$h(\bar{r}_i)\varphi_k(\bar{r}_i) = \epsilon_k \varphi_k(\bar{r}_i)$$

where $h(\bar{r}_i) = -\frac{\hbar^2}{2\mu_i}\nabla_i^2 + V(\bar{r}_i)$

In terms of such a single-particle $h(\bar{r}_i)$

$$H = \sum_{i=1}^{A} h(\bar{r}_i) + \sum_{i \neq j = 1}^{A} V(\bar{r}_i, \bar{r}_j)$$

$V(\bar{r}_i, \bar{r}_j)$: residual two-body int.

$$H_{jk} = \delta_{jk} \sum_{n=1}^{A} \epsilon_n + V_{jk} \qquad \text{(matrix elements)}$$

where $V_{jk} \equiv \langle \Phi_j(\bar{r}_1, \bar{r}_2, \ldots \bar{r}_A) | \sum_{p \neq q = 1}^{A} V(\bar{r}_p, \bar{r}_q) | \Phi_k(\bar{r}_1, \bar{r}_2 \ldots \bar{r}_A) \rangle$

Ex.: $\Phi_k(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \varphi_\alpha(r_1) & \varphi_\alpha(r_2) \\ \varphi_\beta(r_1) & \varphi_\beta(r_2) \end{vmatrix} = \frac{1}{\sqrt{2}} \left(\varphi_\alpha(r_1)\varphi_\beta(r_2) - \varphi_\alpha(r_2)\varphi_\beta(r_1) \right)$

$$H = h(r_1) + h(r_2) + V(r_1, r_2)$$

$$\langle \varphi_k(\bar{r}_1, \bar{r}_2) | \left(h(r_1) + h(r_2) \right) | \varphi_k(\bar{r}_1, \bar{r}_2) \rangle =$$

$$\frac{1}{2} \langle \varphi_\alpha(1)\varphi_\beta(2) - \varphi_\alpha(2)\varphi_\beta(1) | h(r_1) + h(r_2) | \varphi_\alpha(1)\varphi_\beta(2) - \varphi_\alpha(2)\varphi_\beta(1) \rangle$$

$$= \frac{1}{2} \left[2(\epsilon_\alpha + \epsilon_\beta) \right] = \epsilon_\alpha + \epsilon_\beta$$

Independant-particle model.

In the basis we have adopted, off diagonal elements come from $V(\vec{r}_p, r_q)$. (two-body part of H).

If residual int. is weak $\longrightarrow$ V_{jk} small

$\longrightarrow$ off-diagonal terms may be ignored.

$\longrightarrow$ $E = \sum_{n=1}^{A} \epsilon_n$

$\longrightarrow$ Many-body eigenvalue prob. is reduced to a much simpler one-body eigenvalue prob.

This is the idea behind the independant particle model.

In reality there is a correlation between nucleons.

In such cases $\longrightarrow$ Linear combinations of products of single particle states are required to describe them

{ i- The independant-particle model no longer applies
ii- The effect of the residual int. must be incorporated into the calculation of many-body wave fncs.

On the other hand it is often the case that a wave func. is dominated by a few many-body basis states. (in particular this is true for the low lying states).

We expect → The many-body eigenvalue prob. may be approximated by diagonalizing H in a small well-chosen subspace of the complete Hilbert space.

6-7 Hartree-Fock Single-Particle Hamiltonian:

$$H = \sum_{i=1}^{A} h'(\bar{r}_i) + \sum_{i \neq j=1}^{A} V'(\bar{r}_i, \bar{r}_j)$$ Complete Nucl. Hamiltonian

↓ nucleon-nucleon int.

$$h'(\bar{r}_i) = -\frac{\hbar^2}{2\mu_i} \nabla_i$$

A large part of nucleon-nucleon int can be represented by an average field which → we may include it as a part of $h'(\bar{r}_i)$.

$$\longrightarrow \quad h'(\bar{r}_i) \longrightarrow h(\bar{r}_i) = -\frac{\hbar^2}{2\mu_i} \nabla_i + V(\bar{r}_i)$$

$$V'(\bar{r}_i, \bar{r}_j) \longrightarrow V(\bar{r}_i, \bar{r}_j) \qquad |V(\bar{r}_i, \bar{r}_j)| \ll |V'(r_i, r_j)|$$

↓ residual nucleon-nucleon int. — Weaker

Variation of the trial wave func.:

In the absence of a two-body residual int., the ground state is given by the configuration with the lowest A single-particle states occupied.

$$|\Phi_0\rangle = |\varphi_1, \varphi_2, \cdots \varphi_A\rangle$$ (Antisymmetrized and Normalized given by slater det.)

If $|\Phi_0\rangle$ is the ground state; (with or without $V(r_i, r_j)$);

$$\longrightarrow \delta \langle \Phi_0 | H | \Phi_0 \rangle = 0 \quad \text{variational cond.} \quad (1)$$

$$\longrightarrow |\Phi_0\rangle \text{ gives } \langle H \rangle_{min}$$

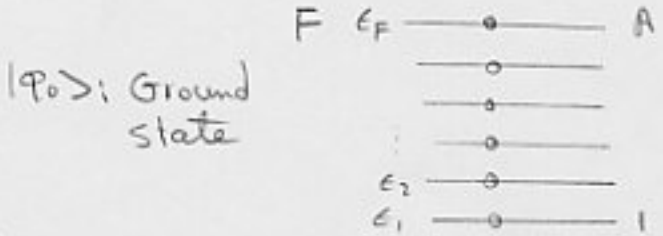
The aim of Hartree-Fock calculation is to find a set of single-particle states that fulfills this cond.

Since variations on $\langle \Phi_0|$ are not indep. of the variations on $|\Phi_0\rangle$,

$$(1) \longrightarrow \langle \delta\Phi | H | \Phi_0 \rangle = 0 \quad (2)$$

$$|\Phi_0\rangle = |1, 2, \cdots A\rangle$$ occupancy representation

i.e. α_2-state (for example ϵ_2)



$|\Phi_0\rangle$: Ground state

A linear combination of such many-body basis states

$$|\Phi\rangle = \sum_{i=0} c_i |\Phi_i\rangle$$

$|\Phi_1\rangle$ (1P-1h) excitation

means that some of the single particle states are partially occupied (fractional value between 0 and 1).

$$|\Phi_0\rangle \xrightarrow{\text{Variation}} |\Phi_0\rangle + |\delta\Phi\rangle = |\Phi_0\rangle + \sum_{kt} \eta_{kt} |\Phi_{kt}\rangle$$

$$|\Phi_{kt}\rangle = |1, 2, \ldots (t-1), (t+1) \ldots, A, K\rangle$$

We ignore 2P-2h excitations.

$|\eta_{kt}| \ll 1$ to ensure the variations are carried out in small steps.

$$(7) \rightarrow \sum_{kt} \eta_{kt} \langle \Phi_{kt} | H | \Phi_0 \rangle = 0$$

Since different variations are indep. of each other;

$$\langle \Phi_{kt} | H | \Phi_0 \rangle = 0$$

$$\rightarrow \langle \Phi_{kt} | \sum_{i=1}^{A} h(r_i) + \sum_{i<j=1}^{A} V(r_i, r_j) | \Phi_0 \rangle = 0$$

For one-body part of H, the only possible nonvanishing matrix elements are those with left and right hand sides differing by no more than the single particle state of a nucleon

For two-body part the occupied single particle state on the left and right differing by no more than two can give non-zero matrix elements.

$$\rightarrow \langle k|h|t\rangle + \sum_{\substack{r \\ \text{all occupied states}}} \langle kr|V(r_1,r_2)|tr\rangle = 0$$

$$|t\rangle = \varphi_t(r) \qquad |k\rangle = \varphi_k(r)$$

$$|kr\rangle = \frac{1}{\sqrt{2}} \begin{vmatrix} \varphi_k(r_1) & \varphi_k(r_2) \\ \varphi_r(r_1) & \varphi_r(r_2) \end{vmatrix} = \frac{1}{\sqrt{2}} \left\{ \varphi_k(r_1)\varphi_r(r_2) - \varphi_r(r_1)\varphi_k(r_2) \right\}$$

$$|tr\rangle = \frac{1}{\sqrt{2}} \begin{vmatrix} \varphi_t(r_1) & \varphi_t(r_2) \\ \varphi_r(r_1) & \varphi_r(r_2) \end{vmatrix} = \frac{1}{\sqrt{2}} \left\{ \varphi_t(r_1)\varphi_r(r_2) - \varphi_r(r_1)\varphi_t(r_2) \right\}$$

$$\langle kr|V(r_1,r_2)|tr\rangle =$$

$$= \frac{1}{2} \langle \varphi_k(r_1)\varphi_r(r_2) - \varphi_r(r_1)\varphi_k(r_2) | V(r_1,r_2) | \varphi_t(r_1)\varphi_r(r_2) - \varphi_r(r_1)\varphi_t(r_2) \rangle$$

$$= \langle \varphi_k(r_1)\varphi_r(r_2)|V(r_1,r_2)|\varphi_t(r_1)\varphi_r(r_2)\rangle$$
$$- \langle \varphi_k(r_1)\varphi_r(r_2)|V(r_1,r_2)|\varphi_r(r_1)\varphi_t(r_2)\rangle$$

where we have used the symmetry relation:

$$\langle \varphi_k(r_1)\varphi_r(r_2)|V(r_1,r_2)|\varphi_t(r_1)\varphi_r(r_2)\rangle = \langle \varphi_r(r_1)\varphi_k(r_2)|V(r_1,r_2)|\varphi_r(r_1)\varphi_t(r_2)\rangle$$

Hartree-Fock Hamiltonian:

It is more instructive to write the relation:

$$\langle k|h|t\rangle + \sum_r \langle kr|V(r_1,r_2)|tr\rangle = 0 \qquad (1)$$

in an operator form.

Remark: Note that we have two sets of single particle states:

$|\alpha\rangle, |\beta\rangle, |\delta\rangle, |\gamma\rangle$ original states (trial)

in old basis

$|r\rangle, |s\rangle, |t\rangle, |k\rangle$ Hartree-Fock single particle states

in new basis

Matrix representation:

$$X = \sum_{a'a''} |a''\rangle\langle a''|X|a'\rangle\langle a'|$$

$$X = \begin{pmatrix} \langle a_1|x|a_1\rangle & \langle a_1|x|a_2\rangle \cdots \\ \langle a_2|x|a_1\rangle & \langle a_2|x|a_2\rangle \cdots \\ \vdots & \end{pmatrix}$$ one-body op.

$$V(r_1, r_2) = \sum_{\alpha\beta\gamma\delta} |\alpha\beta\rangle V_{\alpha\beta\gamma\delta} \langle\gamma\delta|$$

Where $V_{\alpha\beta\gamma\delta} \equiv \langle\alpha\beta|\, V(r_1, r_2)\, |\gamma\delta\rangle$

$|\alpha\beta\rangle$ ad $|\alpha\delta\rangle$ are normalized and antisymmetrized

We define the Hartree-Fock single particle Hamiltonian op. as below;

$$H_{HF} = \underbrace{h}_{(H_0)} + \sum_r \sum_{\alpha\beta\gamma\delta} \langle r|\alpha\beta\rangle V_{\alpha\beta\gamma\delta} \langle\gamma\delta|r\rangle \qquad (2)$$

Indeed equ. (1) is the matrix element of this op. between single particle bra $|k\rangle$ and single particle ket $|t\rangle$.

$\langle\gamma|\alpha\beta\rangle \sim \langle r|\alpha\rangle |\beta\rangle$ except for antisymmetrization in $|\alpha\beta\rangle$

The second term in (2) may be interpreted as the average one-body pot. (mean field), experienced by a nucleon, as a result of two-body ints. with all the other nucleons.

Equ. (1) can also be expressed as an eigenvalue equ. using the op. (2);

$$h|t\rangle + \sum_{r} \sum_{\alpha\beta\gamma\delta} \langle r|\alpha\beta\rangle V_{\alpha\beta\gamma\delta} \langle\gamma\delta|rt\rangle = \epsilon_t |t\rangle \qquad (3)$$

ϵ_t: Hartree-Fock single-particle energy.

The sol. of (3) provides with us a transformation from the set of basis states $|\alpha\rangle, |\beta\rangle, \ldots$ (trial wave-fucs.) to the eigenstates of Hartree-Fock single-particle Hamiltonian $|k\rangle, |t\rangle$.

Starting with an arbitrary set of single-particle wave fucs. (such as Harmonic Osc. wave fucs.) as the trial fucs., we evaluate the quantities $\langle r|\alpha\beta\rangle$ and $\langle\gamma\delta|rt\rangle$ or the equivalent quantity $\langle kr|V|tr\rangle$ in equ. (1) and find $|t\rangle$. Again using this new $|t\rangle$ we repeat the procedure iteratively until the self-consistency is achieved.

Ex.

The energy eigenvalue prob. for an atom with Z-electron:

$$\left[\sum_{i=1}^{Z} -\frac{\hbar^2}{2m}\nabla_i^2 - \frac{Ze^2}{r_i} + \sum_{i>j} \frac{e^2}{|r_i - r_j|} \right] \psi(r_1, r_2 \cdots r_Z) = E\,\psi(r_1, \cdots r_Z) \qquad (1)$$

Assume $\psi(r_1, r_2 \cdots r_Z) = \varphi_1(r_1)\,\varphi_2(r_2) \cdots \varphi_Z(r_Z)$ (2)

(Each of fncs. is normalized to unity).

$$\langle H \rangle = \sum_{i=1}^{Z} \int d^3 r_i\, \varphi_i^*(r_i) \left(-\frac{\hbar^2}{2m}\nabla_i^2 - \frac{Ze^2}{r_i} \right) \varphi_i(r_i)$$
$$+ e^2 \sum_{i>j} \sum_{j} \iint d^3 r_i\, d^3 r_j\, \frac{|\varphi_i(r_i)|^2\, |\varphi_j(r_j)|^2}{|r_i - r_j|} \qquad (3)$$

$$\varphi_i(r_i) \longrightarrow \varphi_i(r_i) + \lambda f_i(r_i) \qquad (4)$$

(this variation should change $\langle H \rangle$ by a term of order λ^2)

$$\int d^3 r_i\, |\varphi_i(r_i) + \lambda f_i(r_i)|^2 = 1$$

$$\longrightarrow \int d^3 r_i \left[\varphi_i^*(r_i) f_i(r_i) + \varphi_i(r_i) f_i^*(r_i) \right] = 0 \qquad (5)$$

(to first order λ)

(4) in (3) $\xrightarrow{\text{the terms linear in } \lambda}$

$$A = \sum_i \int d^3 r_i \left[\varphi_i^*(r_i) \left(-\frac{\hbar^2}{2m}\nabla_i^2 \right) \lambda f_i(r_i) + \lambda f_i^*(r_i) \left(-\frac{\hbar^2}{2m}\nabla_i^2 \right) \varphi_i(r_i) \right]$$
$$= \lambda \sum_i \int d^3 r_i \left\{ f_i(r_i) \left[-\frac{\hbar^2}{2m}\nabla_i^2 \varphi_i^*(r_i) \right] + f_i^*(r_i) \left[-\frac{\hbar^2}{2m}\nabla_i^2 \varphi_i(r_i) \right] \right\}$$

where we have integrated by parts two times, and used the fact that $f_i(r_i) \longrightarrow 0$ as $r_i \to \infty$

$$B = -\lambda \sum_i \int d^3 r_i \left[f_i^*(r_i) \frac{Ze^2}{r_i} \varphi_i(r_i) + \varphi_i^*(r_i) \frac{Ze^2}{r_i} f_i(r_i) \right]$$

$$C = \lambda e^2 \sum_{i>j} \sum_j \int d^3 r_i \int d^3 r_j \frac{1}{|r_i - r_j|} \left\{ \left[f_i^*(r_i) \varphi_i(r_i) + f_i(r_i) \varphi_i^*(r_i) \right] |\varphi_j(r_j)|^2 \right.$$
$$\left. + \left[f_j^*(r_j) \varphi_j(r_j) + f_j(r_j) \varphi_j^*(r_j) \right] |\varphi_i(r_i)|^2 \right\}$$

We can not just set $A+B+C=0$, because we have the constraint (5).

We use Lagrange multipliers:

$$A + B + C + \epsilon (\text{constraint}) = 0$$

$$\rightarrow \sum_i \int d^3 r_i \left\{ f_i^*(r_i) \left[-\frac{\hbar^2}{2m} \nabla_i^2 \varphi_i(r_i) \right] - f_i^*(r_i) \frac{Ze^2}{r_i} \varphi_i(r_i) \right\}$$
$$+ e^2 \sum_{i \neq j} \sum_j \iint d^3 r_i \, d^3 r_j \, f_i^*(r_i) \frac{|\varphi_j(r_j)|^2}{|r_i - r_j|} \varphi_i(r_i)$$
$$- \epsilon_i \int d^3 r_i \, f_i^*(r_i) \varphi_i(r_i) + (\text{complex conjugate term}) = 0$$

Note: $\sum_{i>j} \to \frac{1}{2} \sum_{i \neq j}$ and C is symmetric in $i \leftrightarrow j$

We may treat $f_i(r_i)$ and $f_i^*(r_i)$ independently.
Furthermore, other than being square integrable, they are completely arbitrary,

$\longrightarrow$ the coeffs. of $f_i(r_i)$ and $f_i^*(r_i)$ must separately vanish at each $\bar{r}_i$.

$$\longrightarrow \left[-\frac{\hbar^2}{2m}\nabla_i^2 - \frac{Ze^2}{r_i} + e^2 \sum_{i\neq j} \int d^3 r_i \frac{|\varphi_j(r_j)|^2}{|r_i - r_j|} \right] \varphi_i(r_i) = \epsilon_i \varphi_i(r_i)$$

and the complex conjugate relation.

These are a set of Z simultaneous nonlinear integrodifferential eqns. for the Z-funcs. $\varphi_i(r_i)$.

$$V_i(r_i) = -\frac{Ze^2}{r_i} + e^2 \sum_{i\neq j} \int d^3 r_i \frac{|\varphi_j(r_j)|^2}{|r_i - r_j|}$$

$\rho_j(r_j) = -e\,|\varphi_j(r_j)|^2$ charge densities of all other electrons.

A greater simplification occurs when $V_i(\bar{r})$ is replaced by its angular average.

$$V_i(r) = \int \frac{d\Omega}{4\pi} V_i(\bar{r})$$

$\longrightarrow$ self consitent pot. becomes central.

6-8 Spherical Shell Model

In this model;

1) The nuclear states are described in terms of nucleon deg. of freedom
2) 1p-1h, 2p-2h, - - types of correlation are important
3) We use independent-particle model with a Hartree-Fock single particle basis.
4) By transforming the single particle states to a Hartree-Fock a large part of the nucleon-nucleon interaction (strong) may be included in the average one-body field for a nucleon. ⟶ The residual int. remaining may be weak enough that the nucl. many body eigenvalue prob. may be carried out in a small subset of the complete Hilbert space (otherwise the dim. will be large).

In other words;

If a Hartree-Fock type of single-particle basis is used ⟶ the residual int may be sufficiently weak that most of the many-body basis states are not involved in any significant way in low-lying states of interest to us.

5) Since it is desirable from a practical point of view to reduce the size of the active space as much as possible ⟶ it may become necessary to leave a large number of basis states which individually contribute only a small amount to the nucl. state of interest. To account for the small contributions of these states, the residual int. should be renormalized so that the effect of the truncated space may be taken care of in an average way.

6) Before shell model calculation, there are 3-steps to be carried out:

i - the choice of a single particle basis
ii - the selection of an active space
iii - the derivation of an effective int.
(these three are related to each other and all of them hinge on the single particle basis chosen)

We will be concern with:
1 - Mainly with calculation in the spherical basis.
2 - Single particle basis which includes deformation of the nucl. shape.

Selection of the Shell Model Space:

i- Selection of the space (restriction to a few number)
ii- " " " = effective int.

There are two different ways to carry out the angular momentum coupling:

i- LS coupling scheme

$$L = \sum_{i=1}^{A} l_i \qquad S = \sum_{i=1}^{A} s_i \qquad J = L + S$$

ii- jj coupling scheme

$$j_i = l_i + s_i \qquad J = \sum_{i=1}^{A} j_i$$

Since H is invariant under a rot. of the coord. sys.,

$[H, J] = 0 \longrightarrow$ J: a good quantum number

Also $[H, T] = 0$ (if we ignore the symmetry breaking effects of the el.mag. ints.

$\longrightarrow \langle \alpha, T, J' | H | \alpha, T, J \rangle = 0$ for $J' \neq J$ and/or $T' \neq T$

If the many body basis states are grouped together acc. to their (J, T)-values $\longrightarrow$ H-matrix in the complete shell model space will appear in a block-diagonal space.

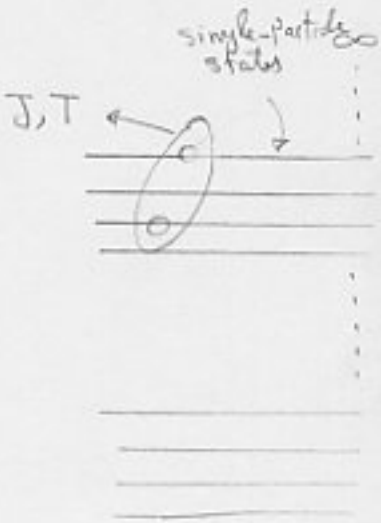
i.e.: Only square blocks of matrix elements along the diagonal corresponding to a given set of (J,T)-values are different from zero.

⟶ The calculation can therefore be carried out separately within the subspace of a specific (J,T) of the full shell model space.

⟶ Angular momentum coupling greatly reduces the size of the active space (for the calculation).

On the other hand:

Unless the number of active single-particle states is finite, the number of A-nucleon states for a given J and T is still infinite.



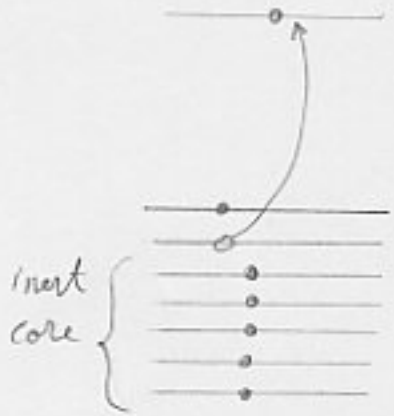
⟶ To construct a finite shell model space, the active single-particle states must be restricted to a small number.

We can do this in two different directions:

1- Since we are interested in a few nuclear states near the ground state region,

⟶ We need only to excite particles occupying single particle states just below the Fermi energy level (these are active or valence nucleons).

2- If nucleons in some of the low-lying single particle states are never excited, they form an inert core and the single-particle states they occupy may be left out of the active space



$$H = H_{core} + H_{core-valence} + H_{valence}$$

H_{core}: may be absorbed into the def. of the zero point of the energy scale for the A-nucleon system (and may be ignored except in the binding energy calculation).

$$H_{core} = \sum \left(h_{core}(r_i) + V_{core}(r_i, r_j) \right)$$

$$H_{core-valence} = \sum V(r_i, r_j)$$

$$H_{valence} = \sum \left(h_{valence}(r_i) + V_{valence}(r_i, r_j) \right)$$

Effective Hamiltonian:

1- We are in a Hartree-Fock single-particle basis -

2- $H = \sum \left(h(r_i) + V(r_i, r_j) \right)$

$$h(r_i) = -\frac{\hbar^2}{2\mu}\nabla_i^2 + V(r_i) + V'(r_i)$$

$V(r_i)$ → mean field; $V'(r_i)$ → other single particle effects (like spin-orbit int.)

$V(r_i, r_j)$: residual int.

Here we wish to make a further transformation:

$$H \longrightarrow H_{eff}$$

such that when the active shell model space is restricted to a manageable size ⟶ the effect of states ignored in the calculation may be accounted for in average way.

The procedure for tr.:

Let d: the dim. of a finite shell model space (active space)
(we are interested to make calculation in this dim.)

$\bar{P}$: the op. that projects out any vector on d-space

$\bar{Q}$: " " " " " the rest of the Hilbert space

H: True Hamiltonian

$H\Psi_i = E_i \Psi_i$ eigenvalue prob. in the complete Hilbert space

Ψ_i: eigenvector $\Psi_i = \sum c_{ij} \phi_i$,

An <u>ideal</u> H_{eff} satisfies the following cond.:

$$H_{eff} P\Psi_i = E_i P\Psi_i$$

⟶ H_{eff} is one which produces the <u>same</u> eigenvalues (in d-space) as those obtained by solving the prob. in the <u>complete</u> space using true H.

In general, it is impossible to satisfy this cond. for all d-eigenvalues in the <u>truncated</u> shell model space.

This is, however, not a problem, since we are interested only in a <u>small</u> number of low-lying states that are <u>much</u> less than d.

$$H_{eff} = H_0 + V_{eff}$$

$$H_0 = \sum_i h(r_i) = \sum_i \epsilon_i n_i$$

ϵ_i : energy n_i : number op. of single particle state i.

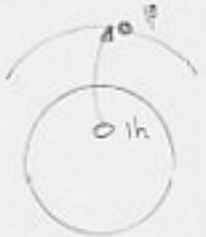
ϵ_i: includes contributions from the core nucleons.

In practice;

It is common to replace ϵ_i by the observed energy level positions of single particle states in the region.

The measured values of ϵ_i may be found in nuclei with one nucleon away from closed shells, where some of the low-lying states are predominantly formed by the coupling of one nucleon or one hole to the ground states of the closed shell nuclei.

Such states are exactly the ones described by Hartree-Fock eigenvectors.



For nuclei away from closed shells, correlations other than 1P-1h play a role ⟶ the Hartree-Fock states are no longer good approx. of the eigenstates of the complete H.

This results in situations where the strength of each single particle state is shared by several nucl. states, (fractional strength).

We assume that V_{eff} remain two-body in nature (three-body and higher orders are negligable).

A formal sol. of V_{eff}:

$$P + Q = I$$

$$P^2 = P \quad \text{and} \quad Q^2 = Q$$

$$H\Psi = E\Psi \quad \text{in complete space} \quad (1) \qquad \text{(we omitted the indices)}$$

$$H = H_0 + V \qquad (2)$$

(1) ⟶ $PH\Psi = PE\Psi$

$$PH(P+Q)\Psi = EP\Psi$$

$$PHP\Psi + PHQ\Psi = EP\Psi \qquad (3)$$

also

(1) $\longrightarrow$ $Q H \Psi = Q E \Psi$

$\longrightarrow$ $Q H P \Psi + Q H Q \Psi = E Q \Psi$ (4)

(3) (4) are two-coupled eqns. for $P\Psi$ and $Q\Psi$,

(4) $\longrightarrow$ $E Q \Psi - Q H Q \Psi = Q H P \Psi$

$\longrightarrow$ $(E - QH) Q \Psi = Q H P \Psi$

$\longrightarrow$ $Q \Psi = \frac{1}{E - QH} Q H P \Psi$ (5)

(5) in (3) $P H P \Psi + P H \frac{1}{E - QH} Q H P \Psi = E P \Psi$

$\longrightarrow$ $P \left\{ H + H \frac{1}{E - QH} Q H \right\} P \Psi = E P \Psi$ (6)

We recall $H = H_0 + V$

H_0: one-body, V: two-body

$\longrightarrow$ $P \left\{ H_0 + V + (H_0 + V) \frac{1}{E - QH} Q (H_0 + V) \right\} P \Psi = E P \Psi$ (7)

i- If all the single particle states are chosen to be eigenfuncs. of $h(r)$

ii- And our truncation of the many body Hilbert space is carried out by restricting the number of active single-particle states

$\longrightarrow$ $P H_0 = H_0 P$ (8)

Since P and Q are mutually exclusive

$$PQ = QP = 0 \qquad (9)$$

$$(7) \rightarrow P\{ \cdots\cdots Q(H_0+V)\}P\psi = EP\psi$$

$Q(H_0+V) = 0$ due to (8,9)

The H_0 term at the mid. of (7)

$$\rightarrow \quad P\left\{H_0 \frac{1}{E-QH} QV\right\} P\psi$$

Since everything to the right of H_0 acts on states in the space projected out by Q

$$PH_0(E-QH)^{-1}QVP\psi \sim PH_0Q(E-QH)^{-1}QVP\psi$$

(equivalent; $PH_0Q = 0$ due to (8,9))

$$(7) \rightarrow P\left\{H_0+V+V\frac{1}{E-QH}QV\right\}P\psi = EP\psi$$

Comparing with $\begin{cases} H_{eff} = H_0 + V_{eff} \\ H_{eff}(P\psi) = E(P\psi) \end{cases}$

$$\rightarrow V_{eff} = V + V\frac{1}{E-QH}QV \qquad \text{formal sol.}$$

Note: $PH_{eff}(P\psi) = E(P\psi)$

But $E(P\psi) = P(EP\psi)$

$$\rightarrow P(H_{eff}(P\psi)) = P(E(P\psi))$$

$$QH = QH_0 + QV = (1-P)H_0 + QV = H_0 - PH_0 + QV = H_0 - H_0P + QV$$

H_0P acts on Q-space $\longrightarrow$ no contribution

$$V\frac{1}{E-QH}QV = VQ\frac{1}{E-H_0-QV}QV$$

$\frac{1}{E-QH}QV$ in Q space; $\frac{1}{E-H_0-QV}$ will not change anything

These are equivalent.

In a Hartree-Fock single particle basis, it is likely;

$$|\langle|V|\rangle| < |\langle|H_0|\rangle|$$

$$\longrightarrow \quad < |\langle|(E-H_0)|\rangle| \quad \text{(perhaps!)}$$

? residual int.

If it is possible $\longrightarrow$ $\frac{1}{E-H_0}QV < 1$

$$(1\pm x)^{-n} = 1 \mp \frac{nx}{1!} + \frac{n(n+1)}{2!}x^2 + \cdots$$

$$(E-H_0-QV)^{-1} = \frac{1}{E-H_0}\left(1 - \frac{1}{E-H_0}QV\right)^{-1}$$

$$= \frac{1}{E-H_0} + \frac{1}{E-H_0}QV + \frac{1}{E-H_0}QV\frac{1}{E-H_0}QV + \cdots$$

$$VQ\frac{1}{E-H_0-QV}QV = VQ\frac{1}{E-H_0}QV + VQ\frac{1}{E-H_0}QV\frac{1}{E-H_0}QV$$

$$+ VQ\frac{1}{E-H_0}QV\frac{1}{E-H_0}QV\frac{1}{E-H_0}QV + \cdots$$

$$= VQ\sum_{n=1}^{\infty}\left(\frac{1}{E-H_0}QV\right)^n$$

$$V_{eff} = V + VQ \sum_{n=1}^{\infty} \left(\frac{1}{E - H_0} QV \right)^n \qquad (1)$$

Furthermore, since H_0 is diagonal in the basis states we have chosen,

$$H_0 |\Psi_i\rangle = \sum_r \epsilon_r |\Psi_i\rangle$$

ϵ_r : single particle energies

r : over all occupied single particle states in $|\Psi\rangle$

H_0 may be replaced by $\sum_s \epsilon_r$ in the denominator of (1)

i- There is however, no known proof that the series is actually convergent.

ii- Furthermore, in principle it is not easy to carry out the calculation beyond the third order or so in a nontrivial P-space.

However, V_{eff} obtained by using (1) to roughly second-order produces results in agreement with the experimental data.

The procedure outlined above to find V_{eff} in a shell model space is also known as a renormalization procedure, since it normalizes an int. (V) for complete Hilbert space $\xrightarrow{\text{to}}$ one suitable for the truncated space.

6-9 Deformed Shell Model:

Deformed single particle States:

So far we have assumed:

Single-particle states are generated by a spherical pot. well (made of average int. of a nucleon with all other nucleons)

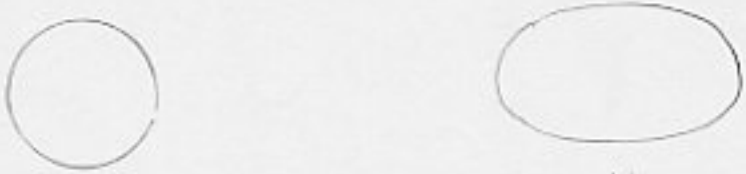
This is reasonable assumption if the equilibirium shape of the nucleus is spherical.

But for many nuclei a deformed shape is more stable,

⟶ A deformed average pot. well is a more reasonable one to generate the basis single particle basis.

i) In the first case self-consistat pot. = spherical.

ii) " " second " " " " = deformed



(i) The nucl. shape (ii)

Let us again assume axial symmetry ($\omega_1 = \omega_2 \neq \omega_3$).

$$h(r_i) = -\frac{\hbar^2}{2\mu_i}\nabla_i^2 + \frac{1}{2}\mu_i\omega_0^2 r_i^2 + a\,s\cdot l$$

is now replaced by $\longrightarrow$ $h = h_0 + h_s + a\,s\cdot l + b\,l^2$

(Nilsson Pot.)

This pot. applies in medium and heavy nuclei.

where $h_0(r_i) = -\frac{\hbar^2}{2\mu_i}\nabla_i^2 + V(r_i) = -\frac{\hbar^2}{2\mu_i}\nabla_i^2 + \frac{1}{2}\mu_i\omega_0^2 r^2$

$$h_{osc} = \frac{\mu}{2}\left(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2\right)$$

$s\cdot l$: spin orbit term

l^2: lowers the energy of one particle state at large values l.
(to give proper ordering of single particle states in the spherical limit)

We assume axial symmetry ($\omega_1 = \omega_2 \neq \omega_3$).

If the volume of nucleus remains = const.

$\longrightarrow$ We can describe the shape by only one deformation parameter (δ).

$$\omega_1^2 = \omega_2^2 \equiv \omega_\perp^2 = \omega_0^2\left(1 + \frac{2}{3}\delta\right) \qquad \omega_3^2 = \omega_0^2\left(1 - \frac{4}{3}\delta\right)$$

$$\omega_\perp \simeq \omega_0\left(1 + \frac{1}{3}\delta\right) \qquad \omega_3 \simeq \omega_0\left(1 - \frac{2}{3}\delta\right)$$

From the constancy of volume $\longrightarrow \frac{1}{V} \sim \omega_1 \omega_2 \omega_3 = \text{const.}$

$$\longrightarrow \omega_0 \equiv \omega_0(\delta) = \omega_0(0)\left(1-\frac{4}{3}\delta^2-\frac{16}{27}\delta^3\right)^{-1/6}$$

Note: For large deformation we can ignore S.l and l^2 terms.

$$\delta = \frac{\omega_\perp - \omega_3}{\omega_0}$$

$$\omega_0 = \frac{1}{3}(\omega_1+\omega_2+\omega_3) = \frac{1}{3}(2\omega_\perp+\omega_3)$$

ω_0 may be taken to be the same as the harmonic osc. frequency in the spherical limit.

Now,

$$h_{osc} = \frac{\mu}{2}(\omega_1^2 x^2+\omega_2^2 y^2+\omega_3^2 z^2) = (\omega_\perp^2(x^2+y^2)+\omega_3^2 z^2)$$

$$= \frac{\mu\omega_0^2}{2}\left[\left(1+\frac{2}{3}\delta\right)(x^2+y^2)+\left(1-\frac{4}{3}\delta\right)z^2\right]$$

$$= \frac{\mu\omega_0^2}{2}\left[(x^2+y^2+z^2)-\frac{4}{3}\delta\left(z^2-\frac{1}{2}(x^2+y^2)\right)\right]$$

$$= \frac{\mu\omega_0^2}{2}\left[r^2-\frac{4}{3}\delta\sqrt{\frac{4\pi}{5}}r^2Y_{20}\right] = h_{\omega_0}+h\delta$$

where $Y_{20} = \sqrt{\frac{5}{4\pi}}\left(\frac{3}{2}\cos^2\theta-\frac{1}{2}\right) = \sqrt{\frac{5}{4\pi}}\left(z^2-\frac{1}{2}(x^2+y^2)\right)$

$$\longrightarrow h\delta = -\frac{2}{3}\sqrt{\frac{4\pi}{5}}\delta\,\mu_i\omega_0^2 r^2 Y_{20}(\hat{r})$$

$$h\omega_0 = \frac{1}{2}\mu_i\omega_0^2 r^2$$

Introducing dimensionless coord.;

$$r' = \sqrt{\frac{\mu_i \omega_0}{\hbar}}\, r$$

$$H \Psi_{\alpha r} = \mathcal{E}_{\alpha r} \Psi_{\alpha r}$$

$$H = \tfrac{1}{2}\hbar\omega_0(-\nabla^2 + r'^2) - \hbar\omega_0 B r'^2 Y_{20} + a\, l\cdot s + b l^2$$

The sol. of $H_0 = \tfrac{1}{2}\hbar\omega_0(-\nabla^2 + r'^2)$, the spherical Harmonic op.;

$$|N, \ell, \Lambda, \Sigma\rangle = N_0 (-)^n r'^{\ell} e^{-\frac{1}{2}r'^2} {}_1F_1(-n, \ell+\tfrac{3}{2}, r^2) Y_{1\Lambda} X_\Sigma$$

(X_Σ: spin func.)

where $N_0 = \dfrac{[2\Gamma(n+\ell+\frac{3}{2})]^{1/2}}{(n!)^{1/2}\,\Gamma(\ell+\frac{3}{2})}$

$$E_{N\ell} = \hbar\omega_0 (N + \tfrac{3}{2}) \qquad N = 2n + \ell \quad (n = 0, 1, 2, \ldots)$$

$$\left(H_0 |N, \ell, \Lambda, \Sigma\rangle = E_{N\ell} |N, \ell, \Lambda, \Sigma\rangle \right)$$

$${}_A^{}F_B^{}[(a), (b), z] = {}_AF_B[a_1, a_2 \cdots a_A; b_1, b_2, \cdots b_B; z]$$

$$= \sum_{n=0}^{\infty} \frac{((a)_A)_n\, z^n}{((b)_B)_n\, n!} \qquad \left((a)_m = a(a+1)(a+2)\cdots(a+m-1) \right)$$

$$= 1 + \frac{a_1 a_2 \cdots a_A\, z}{b_1 b_2 \cdots b_B\, 1!} + \frac{a_1(a_1+1)\, a_2(a_2+1)\cdots a_A(a_A+1)\, z^2}{b_1(b_1+1)\, b_2(b_2+1)\cdots b_B(b_B+1)\, 2!} + \cdots$$

generalized hypergeometric func.

The sols $\psi_{\alpha K}$ of H are obtained by diagonalization of H in this basis.

In general the quadrupole field $\beta r^2 Y_{20}$ mixes the quantum numbers N. However, where β ranges from 0.15 to 0.35, this mixing is small and usually neglected.

⟶ N can be used for classification of the deformed states.

Ω: the projection of J on the body-fixed quantization axis (the 3-axis) (good quantum number for axially symmetric nuclei)

Note:

$$[J^2, H] \neq 0 \quad [l^2, H] \neq 0 \quad [l_z, H] \neq 0$$

$$[S_z, H] \neq 0 \quad \text{but} \quad [J_z, H] = 0$$

$\hat{z}$: symmetry axis of the field

Also $[H_0, H] \neq 0$

$$J_z |N \Omega \alpha\rangle = \Omega |N, \Omega, \alpha\rangle$$

$$H|N,\Omega,\alpha\rangle = \mathcal{E}_{N\Omega\alpha}\,|N,\Omega,\alpha\rangle$$

$$|N,\Omega,\alpha\rangle = \sum_{\ell,\Lambda} C_{\ell\Lambda}^{N\alpha}\,|N,\ell,\Lambda,\Sigma\rangle \qquad (\Sigma=\Omega-\Lambda)$$

Λ: Projection of the orbital angular momentum along the sym. axis.

Σ: " " " spin " " " " "

α: other quantum numbers.

The superposition coeffs. $C_{\ell\Lambda}^{N\alpha}(\delta)$, which are normalized so that;

$$\sum_{\ell\Lambda} |C_{\ell\Lambda}^{N\alpha}(\delta)|^2 = 1$$

are determined simultaneously with the energy eigenvalues in the numerical diagonalization of the H matrix.

$\delta > 0 \longrightarrow$ nucleus is prolate

$\delta < 0 \longrightarrow$ " " oblate

$\langle N', \ell', \Lambda', \Sigma' | H | N, \ell, \Lambda, \Sigma \rangle$ is <u>not</u> diagonal in any of the quantum numbers N, ℓ, Λ, and Σ, but it is <u>easily</u> calculated in this representation.

$$\langle N', \ell', \Lambda', \Sigma' | \ell \cdot S | N, \ell, \Lambda, \Sigma \rangle = \frac{1}{2} \delta_{NN'} \delta_{\ell\ell'}$$

$$\times \left\{ \sqrt{(\ell \mp \Lambda)(\ell \pm \Lambda + 1)}\ \delta_{\Lambda', \Lambda \pm 1} \delta_{\Sigma', -\Sigma} \pm \Lambda \delta_{\Lambda\Lambda'} \delta_{\Sigma\Sigma'} \right\}$$

$$\langle N', \ell', \Lambda', \Sigma' | r^2 Y_{20} | N, \ell, \Lambda \Sigma \rangle = \langle N', \ell' | r^2 | N\ell \rangle \langle \Lambda' | Y_{20} | \Lambda \rangle \delta_{\Sigma\Sigma'}$$

$$\langle N'\ell' | r^2 | N\ell \rangle = \delta_{N', N-2} \left\{ \frac{1}{2} \sqrt{(N+\ell+1)(N+1-1)}\ \delta_{\ell', \ell-2} \right.$$

$$\left. + \frac{1}{2} \sqrt{(N-\ell)(N+\ell+1)}\ \delta_{\ell\ell'} + \frac{1}{2} \sqrt{(N-\ell)(N-\ell-2)}\ \delta_{\ell', \ell+2} \right\}$$

$$+ \delta_{N'N} \left\{ \sqrt{(N-\ell+2)(N+\ell+1)}\ \delta_{\ell', \ell-2} + (N + \tfrac{3}{2}) \delta_{\ell'\ell} \right.$$

$$\left. + \sqrt{(N-\ell)(N+\ell+3)}\ \delta_{\ell', \ell+2} \right\}$$

$$+ \delta_{N', N+2} \left\{ \frac{1}{2} \sqrt{(N+\ell+1)(N+\ell+3)}\ \delta_{\ell', \ell-2} \right.$$

$$+ \frac{1}{2} \sqrt{(N-\ell+2)(N+\ell+3)}\ \delta_{\ell'\ell}$$

$$\left. + \frac{1}{2} \sqrt{(N-\ell)(N-\ell+2)}\ \delta_{\ell', \ell+2} \right\}$$

Alternative expression;

$$\langle N'\ell'|r^n|N\ell\rangle = \left[\frac{\Gamma\left(\frac{N-\ell+2}{2}\right)\Gamma\left(\frac{N'-\ell'+2}{2}\right)}{\Gamma\left(\frac{N+\ell+3}{2}\right)\Gamma\left(\frac{N'+\ell'+3}{2}\right)}\right]^{1/2}\left(\frac{\ell-\ell'+n}{2}\right)!\left(\frac{\ell'-\ell+n}{2}\right)!$$

$$\times \sum_\alpha \frac{\Gamma\left(\frac{\ell+\ell'+n+3}{2}+\alpha\right)}{\alpha!\left(\frac{N-\ell}{2}-\alpha\right)!\left(\frac{N'-\ell'}{2}-\alpha\right)!\left(\frac{\ell'+n-N}{2}+\alpha\right)!\left(\frac{\ell+n-N'}{2}+\alpha\right)!}$$

(using the $\varphi_{N\ell}$ of P140)

$\langle \ell'\Lambda'|Y_{20}|\ell\Lambda\rangle$ can be obtained from;

$$\int d\hat{r}\, Y^*_{\ell m}(\hat{n})\, Y_{\ell_1 m_1}(\hat{n})\, Y_{\ell_2 m_2}(\hat{n}) = \sqrt{\frac{(2\ell_1+1)(2\ell_2+1)}{4\pi(2\ell+1)}}\,(\ell_1 0, \ell_2 0|\ell 0)\cdot(\ell_1 m_1, \ell_2 m_2|\ell m)$$

or

$$\langle \ell'\Lambda'|Y_{20}|\ell\Lambda\rangle = (-)^{\ell'-\Lambda'}\begin{pmatrix}\ell' & 2 & \ell\\ -\Lambda' & 0 & \Lambda\end{pmatrix}\left[(2\ell'+1)(2\ell+1)\right]^{1/2}$$

$\langle \ell'\Lambda'|Y_{20}|\ell\Lambda\rangle \neq 0$ if $\ell+\ell'+2 =$ even