IV. Nuclear Structure

Topics to be covered include:
- Collective rotational model
- Collective vibrational model
- Shell model
- Advanced shell models
- Hartree-Fock

General References:
1) deShalit and Fesbach, Theoretical Nuclear Physics, Volume I: Nuclear Structure, Chapter VI
Collective rotational model:

Previously I presented the excitation spectra for nuclei which display level spacings characteristic of a rigid rotor. These rotational bands occur in most nuclei between closed shells where the electric quadrupole moments are large. We also observe rotational energy level spacings built on states with non-zero angular momentum. The driving force for the intrinsic deformation away from a spherical shape is the non-central tensor force in the N-N interaction. Below are examples for even-even and even-odd nuclei:

Empirical fit: \[ E(J) = AJ(J+1) + BJ^2(J+1)^2 \]
\[ A \approx 0.01 \text{ to } 0.02 \text{ MeV}; \quad B \approx 10^{-6} \text{ to } 10^{-5} \text{ MeV} \text{ (very small)} \Rightarrow \text{Rigid rotor} \]
Collective rotational model:

Qualitative restriction for rotational collective motion: *the motion of the nucleons which define the deformed shape should be rapid compared with the rotation of the overall shape.*

\[
KE_{\text{nucleon}} \approx 20 \text{ MeV} = \frac{1}{2} mv^2 \text{ (Non - Rel.)}
\]

\[
\frac{v}{c} = \frac{\sqrt{40 \text{ MeV}}}{\sqrt{940 \text{ MeV}}} = 0.2
\]

Overall rotational frequency of the intrinsic, deformed shape

\[
\omega \ll \frac{0.2c}{2r_0A^{1/3}}, \quad r_0 = 1.2 \text{ fm}, \quad (\text{frequency of nucleon motion})
\]

\[
\hbar\omega \ll \frac{\hbar c}{10r_0A^{1/3}} = \frac{16 \text{ MeV}}{A^{1/3}}
\]

For \( A = 180 \), \( \hbar\omega \ll 2.8 \text{ MeV} \), where typical energies are \( \sim 0.01 \text{ MeV} \)
Collective rotational model:

Consider the Hamiltonian for a many-body system with overall rotation:

For particles $i = 1, 2, \ldots A$

\[
\begin{align*}
  x'_i &= x_i \cos \theta + y_i \sin \theta \\
  y'_i &= -x_i \sin \theta + y_i \cos \theta \\
  x_i &= x'_i \cos \theta - y'_i \sin \theta \\
  y_i &= x'_i \sin \theta + y'_i \cos \theta
\end{align*}
\]

From symmetry, $\sum_{i=1}^{A} x'_i y'_i = 0$

however in the Lab frame $\sum_{i=1}^{A} x_i y_i \neq 0$

In general, $\theta = \frac{1}{2} \arctan \left[ \frac{2 \sum x_i y_i}{\sum (x_i^2 - y_i^2)} \right]$ and the Hamiltonian in the Lab frame cannot be separated into internal (intrinsic) coordinates and the external coordinate $\theta$, where

\[
H_{Lab}(x_i, y_i)_{i=1,2,\ldots A} \neq H_1(\theta) + H_2(x'_i, y'_i)_{i=1,2,\ldots A}
\]

but in general must have the form

\[
H_{Lab}(x_i, y_i)_{i=1,2,\ldots A} = H_1(\theta) + H_2(x'_i, y'_i)_{i=1,2,\ldots A} + H_3(\theta, x'_i, y'_i)_{i=1,2,\ldots A}
\]

Note that the cross term appears, unlike in the analogous case where the C.M. and internal coordiantes can be separated in the Hamiltonian.
Collective rotational model:

**Born-Oppenheimer Approximation:**
If the body rotational frequency is small compared with the internal nucleon frequencies, then the orientation $\theta$ can be treated as a parameter, rather than dynamical, and the wave function for internal coordinates can be approximated by

$$[H_2(\vec{r}''_i) + H_3(\theta_i, \vec{r}''_i)]\chi(\vec{r}''_i) = E(\theta)\chi(\vec{r}''_i),$$

where $\vec{r}''_i$ represents the 3D intrinsic coordinates and

$$[H_1(\theta) + E(\theta)]\phi(\theta) = E(\theta)\phi(\theta)$$

where $E(\theta)$ is the energy eigenvalue of the system,

$$H\Psi = [H_1(\theta) + H_2(\vec{r}''_i) + H_3(\theta, \vec{r}''_i)]\Psi = E\Psi$$

and

$$\Psi \approx \chi(\vec{r}''_i)\Phi(\theta_i),$$

$\theta_i$ are the 3D angles of the body-fixed system in the Lab, e.g. Euler angles.

$H_3(\theta, \vec{r}''_i)$ couples intrinsic and collective motion and may be treated as a perturbation, thus simplifying the Hamiltonian to

$$H(\vec{r}''_i, \theta_i) \approx H_1(\theta_i) + H_2(\vec{r}''_i) \equiv H_{\text{int}}(\vec{r}''_i) + T_{\text{rot}}(\theta_i)$$

Define the angular momentum operator $\vec{R}$ which acts on the body-fixed coordinates $\theta_i$

$$T_{\text{rot}} = \frac{\hbar^2}{2J_x'}R_x^2 + \frac{\hbar^2}{2J_y'}R_y^2 + \frac{\hbar^2}{2J_z'}R_z^2$$

where $J_{x'}, J_{y'}, J_{z'}$ and moments of interia wrt the principal axes in the body-fixed coordinate system.
Collective rotational model:

Define the angular momentum operator $\vec{J}$ which acts on the intrinsic nucleon coordinates $\vec{r}_i'$, angular momentum operator $\vec{I}$ which acts on the lab coordinates $\vec{r}_i$, and operator $\vec{R}$ which acts on the body-fixed frame but does not affect the particles. Rotation of lab coordinates by $\delta\alpha$ about arbitrary axis $\hat{n}$, $e^{-i\delta\alpha\hat{n}\cdot\vec{I}} \chi(\vec{r}_i') = \chi(\vec{r}_i')$ doesn't affect $\chi(\vec{r}_i')$ where $\vec{I}\chi(\vec{r}_i') = 0$.

\[ e^{-i\delta\alpha\hat{n}\cdot\vec{R}} \chi(\vec{r}_i')\Phi(\theta_k) = e^{-i(-\delta\alpha)\hat{n}\cdot\vec{J}} \chi(\vec{r}_i')\Phi(\theta_k) \]

which gives $(\vec{R} + \vec{J})\chi(\vec{r}_i')\Phi(\theta_k) = 0 \Rightarrow \vec{I} = \vec{R} + \vec{J}$
Collective rotational model:

Operators \( \tilde{I} \), \( I^2 \) and \( I_z \) are the only physical angular momentum operators in this discussion; operators \( \tilde{R} \) and \( \tilde{J} \) are unphysical. For this discussion I will also assume that the intrinsic particle distribution in the body-fixed coordinate system is axially symmetric (some nuclei are not however). The moments of inertia are:

\[
J_x' = J_y' = J
\]

\[
T_{rot} = \frac{\hbar^2}{2J} \left( R_x'^2 + R_y'^2 \right) + \frac{\hbar^2}{2J} R_z'^2 = \frac{\hbar^2}{2J} R^2 + \left( \frac{\hbar^2}{2J'} - \frac{\hbar^2}{2J} \right) R_z'^2
\]

\[
= \frac{\hbar^2}{2J} \left( I^2 + J^2 - 2\tilde{I} \cdot \tilde{J} \right) + \left( \frac{\hbar^2}{2J'} - \frac{\hbar^2}{2J} \right) \left( I_z' - J_z' \right)^2
\]

where the axially symmetric, intrinsic wave function is an eigenvalue of \( J_z' \)

\[
J_z' \chi_\Omega (\vec{r}_i') = \Omega \chi_\Omega (\vec{r}_i')
\]

and \( \Phi(\theta_k) \) is an eigenstate of \( T_{rot} \), specifically that of a 3D-symmetric top represented by the Wigner rotation \( D \)-matrices:

\[
I^2 D_{MK}^{I*} (\theta_k) = I(I+1) D_{MK}^{I*} (\theta_k)
\]

\[
I_z D_{MK}^{I*} (\theta_k) = MD_{MK}^{I*} (\theta_k)
\]

\[
I^{\prime} z D_{MK}^{I*} (\theta_k) = KD_{MK}^{I*} (\theta_k)
\]

where (spherical harmonic) \( Y_{IM} (\hat{r}) = \sum_K D_{MK}^{I*} (\theta) Y_{IK} (\hat{r}') \)
Collective rotational model:

The Hamiltonian becomes:

\[
H = \left[ H_{\text{int}} + \frac{\hbar^2}{2 \mathcal{J}} J^2 \right] + \frac{\hbar^2}{2 \mathcal{J}} \left( I^2 - 2 I_z J_z' \right) + \left( \frac{\hbar^2}{2 \mathcal{J}} - \frac{\hbar^2}{2 \mathcal{J}} \right) \left( I_z' - J_z' \right)^2 \\
+ \left[ H_{\text{coup}} + \frac{\hbar^2}{\mathcal{J}} \left( I'_{+} J'_{-} + I'_{-} J'_{+} \right) \right]
\]

where \( I'_{\pm} = \mp \frac{1}{\sqrt{2}} \left( I_{x'} \pm i I_{y'} \right) \), \( J'_{\pm} = \mp \frac{1}{\sqrt{2}} \left( J_{x'} \pm i J_{y'} \right) \)

and the coupling and Coriolis terms can be treated as a small perturbation. The lowest-order Hamiltonian is

\[
H_0 = H'_{\text{int}} + \frac{\hbar^2}{2 \mathcal{J}} \left( I^2 - 2 I_z J_z' \right) + \left( \frac{\hbar^2}{2 \mathcal{J}} - \frac{\hbar^2}{2 \mathcal{J}} \right) \left( I_z' - J_z' \right)^2
\]

with normalized eigenfunctions given by

\[
\Psi = \sqrt{\frac{2I+1}{8\pi^2}} D_{MK}^* (\theta_k) \chi_\Omega (\vec{r}')
\]
Collective rotational model:

The angular momentum vector operators and their z-projections are represented as

Rotation of the body coordinates cannot change the internal wave function or its z-component of angular momentum. Therefore $R_z \chi = 0$, which requires $\vec{R} \perp z'$ and therefore $K = \Omega$

This embodies the requirement of the rotational model that the internal nucleon motion is independent of the overall body-fixed rotation.
Collective rotational model:

The intrinsic wave function is symmetric wrt reflections about the $x'$, $y'$ plane, or wrt to $180^\circ$ rotations about the $x'$ or $y'$ axes. This symmetry requires that

$$e^{-i\pi R_y} \Psi = \Psi$$

where $R_y$ acts on the body coordinates, rotating about the $y'$ axis by $\pi$.

Replace the body-fixed operator with the combination of intrinsic and lab coordinates and work out the result for the body-fixed coordinates first:

$$e^{-i\pi R_y} D^{I^*}_{MK}(\theta_k) = e^{-i\pi (I_y J_y)} D^{I^*}_{MK}(\theta_k),$$

where $J_y$ does not operate on $\theta_k$

$$= e^{-i\pi J_y} D^{I^*}_{MK}(\theta_k) = (-1)^{I+K} D^{I^*}_{M,-K}(\theta_k)$$

Then work out the result for the intrinsic coordinates

$$e^{-i\pi R_y} \chi_\Omega(\vec{r}_i) = e^{i\pi J_y} \chi_\Omega(\vec{r}_i') = e^{i\pi J_y} \sum_j a_j \chi^J_\Omega(\vec{r}_i')$$

where in the last step a multipole expansion of the internal nucleon wave function is introduced. This gives

$$e^{i\pi J_y} \sum_j a_j \chi^J_\Omega(\vec{r}_i') = \sum_j a_j (-1)^{J+\Omega} \chi^J_{-\Omega}(\vec{r}_i')$$
Collective rotational model:

Combining these operations we get

\[ e^{-i\pi r_y} \Psi = \sqrt{\frac{2I+1}{8\pi^2}} \sum_{J} a_J (-1)^{I+K+J+\Omega} D^I_{M,-K} (\theta_k) \chi^J_{-\Omega} (\vec{r}_i') \]

Simplify the phase by noting that \( J + \Omega \) is an integer when \( J \) and \( \Omega \) are either integer or half-integer, and therefore \( 2(J + \Omega) \) is an even integer. The phase can therefore be simplified to

\[ (-1)^{I+K+J+\Omega} = (-1)^{I+K+J+\Omega-2(J+\Omega)} = (-1)^{I+K-J-\Omega} = (-1)^{-J}, \text{ using } K = \Omega. \]

The reflection, or rotation of \( \Psi \) by \( \pi \) gives

\[ \sqrt{\frac{2I+1}{8\pi^2}} (-1)^{-J} D^I_{M,-K} (\theta_k) \chi^J_{-\Omega} (\vec{r}_i') \]

for each multipole. To ensure reflection symmetry the normal and reflected wave functions must be added, resulting in

\[ \Psi(IKM) = \sqrt{\frac{2I+1}{16\pi^2}} \sum_{J} a_J \left\{ D^I_{MK} (\theta_k) \chi^J_{K} (\vec{r}_i') + (-1)^{I-J} D^I_{M,-K} (\theta_k) \chi^J_{-K} (\vec{r}_i') \right\} \]

where \( K \geq 0 \).
Collective rotational model:

Consider the special case when \( J = 0 \), then \( K = \Omega = 0 \), and the w.f. is

\[
\Psi(I,0,M) = \sqrt{\frac{2I + 1}{16\pi^2}} (1 + (-1)^I) D_{M0}^{I*} (\theta_k) \chi_0^0 (\vec{r}_i)
\]

Only states with even, total angular momentum \( I = 0, 2, 4 \cdots \) exist.

The energy spectrum is

\[
E_{ikm} = E_{\text{int}} + \frac{\hbar^2}{2\mathcal{J}} [I(I+1) - 2K^2]
\]

where

\[
(I_{z'} - J_{z'})^2 \Psi = (I_{z'} - J_{z'})(I_{z'} - J_{z'}) \Psi = (K - \Omega)^2 \Psi = 0
\]

If the intrinsic state \( K \neq 0 \), then the spectrum goes like \( I = |K|, |K|+1, |K|+2, \cdots \)

where the excited state rotational spectrum is built on the intrinsic state \( \chi_K \)

For even - even nuclei, \( K = 0 \), and the excitation spectrum is well described by \( E = (\hbar^2 / 2\mathcal{J})I(I+1) \), where the moment of inertia \( \mathcal{J} \) is the only fit parameter.

For even - odd nuclei rotational bands may appear for several values of \( K \) corresponding to different, excited internal states \( \chi_K^I \). For \(^{177}\)Lu rotational bands appear for \( K = \frac{3}{2}^+, \frac{5}{2}^-, \frac{5}{2}^+ \) and all the energy levels are roughly fitted with one parameter

\[
(\hbar^2 / 2\mathcal{J}) = 0.013 \text{ MeV}
\]
Collective rotational model:

Three rotational bands in $^{177}$Lu built on three intrinsic states with $K = \frac{7}{2}^+, \frac{9}{2}^-, \frac{5}{2}^+$
Collective rotational model:

Next we will consider estimates of the moments of inertia and the relation between the shape deformation and the electric quadrupole moments discussed in Chapter 2. In the body-fixed reference frame the radius parameter may be expressed as

\[ R = R_0 \left[ 1 + \sum_{\mu} \beta_{2\mu} Y_{2\mu}(\theta, \phi) \right] \]

and with axial symmetry this reduces to

\[ R(\theta) = R_0 [1 + \beta Y_{20}(\theta)] \]

\[ R(\theta = 0, \pi) = R_0 \left[ 1 + \beta \sqrt{\frac{5}{4\pi}} \right], \quad R(\theta = \pi / 2) = R_0 \left[ 1 - \beta \sqrt{\frac{5}{16\pi}} \right] \]

the deformation parameter is \[ \delta = \frac{\Delta R}{R_0} = \frac{3}{2} \sqrt{\frac{5}{4\pi}} \beta = 0.946 \beta \]

For a rigid rotor with this spheroidal shape and uniform density

\[ J_{\text{rig}} = \frac{2}{5} M_N A R_0^2 [1 + 0.31 \beta] + \cdots \quad \text{where } M_N \text{ is nucleon mass} \]

and \( A \) is nucleon number. The corresponding electric quadrupole moment is

\[ Q_0 = \frac{3}{\sqrt{5\pi}} Z R_0^2 \beta [1 + 0.16 \beta] \]

Note that \( Q_0 \rightarrow 0 \) as \( \beta \rightarrow 0 \), but \( J_{\text{rig}} \xrightarrow{\beta \rightarrow 0} J_{\text{sphere}} \)
Collective rotational model:

For $^{178}$Hf $Q_0 = 8.1 \times 10^{-24}$ cm$^2 \Rightarrow \beta \approx 0.3$ assuming $R_0 = 1.2A^{1/3}$ fm

The resulting moment of inertia gives

$$\frac{\hbar^2}{2J_{\text{rig}}} = 3 \text{ KeV} \quad \text{where the empirical value is} \quad \frac{\hbar^2}{2J_{\text{exp}}} = 15.5 \text{ KeV}$$

which means that the rigid rotor moment of inertia is too large.

Another limiting model is the irrotational flow model where a spherical “core” does not rotate and only the outer “bulge” flows around the core.

For rare earth nuclei
Collective rotational model:

Single-particle model in a deformed binding potential – a 3D axially symmetric harmonic oscillator:

\[
H_{\text{int}} = -\sum_i \frac{\hbar^2}{2M} \nabla_i^2 + \frac{M}{2} \sum_i \left[ \omega_x^2 (x_i^2 + y_i^2) + \omega_z^2 z_i^2 \right]
\]

To reproduce the shell-model energy levels in the $\beta \to 0$ limit requires additional terms; an $\ell^2$ potential mimicks the effects of the Woods-Saxon surface shape and a $\ell \cdot s$ spin-orbit potential ensures the proper $(\ell, j)$ level splittings. The result is the Nilsson Hamiltonian (Dan. Mat. Fys. Medd. 29, No. 16 (1955))

\[
H_{\text{int}} = -\sum_i \frac{\hbar^2}{2M} \nabla_i^2 + \frac{M}{2} \sum_i \left[ \omega_x^2 (x_i^2 + y_i^2) + \omega_z^2 z_i^2 \right] + C \sum_i \ell_i \cdot s_i + D \sum_i \ell_i^2
\]

where

\[
\omega_z^2 = \omega_0^2 (1 - \frac{4}{3} \delta), \quad \omega_x^2 = \omega_y^2 = \omega_0^2 (1 + \frac{2}{3} \delta)
\]

and requiring constant volume gives the constraint

\[
\omega_0^2 \left(1 - \frac{4}{3} \delta - \frac{1}{27} \delta^3 \right)^{1/6} = \text{const.} \Rightarrow \omega_0 (\delta)
\]

The single-particle, Hamiltonian with deformed binding potential defined by Nilsson is

\[
H = -\frac{\hbar^2}{2M} \nabla^2 + \frac{1}{2} M \omega_0^2 r^2 - M \omega_0^2 r^2 \delta \frac{4}{3} \sqrt{\frac{\pi}{5}} Y_{20}(\theta) + C \ell \cdot s + D \ell^2
\]
Collective rotational model:

Eigenfunct ions of the spherical, central - interaction H.O. Hamiltonian

\[ H_0 = -\frac{\hbar^2}{2M} \nabla r^2 + \frac{1}{2} M \omega_r^2 r'^2 \]

have the following eigenvalue s

\[ H_0 |N\ell\Lambda\Sigma \rangle = \left(N + \frac{3}{2}\right) \hbar \omega_0 |N\ell\Lambda\Sigma \rangle \]

\[ \ell_z |N\ell\Lambda\Sigma \rangle = \Lambda |N\ell\Lambda\Sigma \rangle \]

\[ \ell^2 |N\ell\Lambda\Sigma \rangle = \ell(\ell + 1) |N\ell\Lambda\Sigma \rangle \]

\[ s_z |N\ell\Lambda\Sigma \rangle = \Sigma |N\ell\Lambda\Sigma \rangle \]

and will serve as basis states for expansions of the full eigenfunct ions.

The non - spherical, spin - orbit and \( D\ell^2 \) components couple these basis states and the solution involves coupled equations. Couplings between different principal q.n. (\( N \)) are neglected. The total angular momentum \( z \) - component commutes with the full Nilsson Hamiltonian where

\[ j_z = \ell_z + s_z \text{ with eigenvalue } \Omega = \Lambda + \Sigma. \]

Eigenfunct ion expansions are constructed for states with fixed \( N, \Omega \)

\[ \chi_{N\Omega} = \sum_{\ell, \Lambda} a_{\ell\Lambda}^{\Omega} |N\ell\Lambda, \Sigma = \Omega - \Lambda \rangle \]
Collective rotational model:

Diagonalizing the coupled-equations gives the single-particle energy levels to the right and on the next slide for nuclei with $8 < (Z,N) < 20$ as a function of deformation where the $x$-axis parameter $\eta$ is defined by

$$\eta = 2\hbar \omega_0 (\delta) \frac{\delta}{C}$$

Positive (negative) values of $\eta$ correspond to prolate (oblate) quadrupole deformations.

Deformations alter the energy level ordering and hence the ground-state spin-parities and the excited-state spectrum of the intrinsic state upon which rotational bands are built.
Collective rotational model:

Nilsson states
Collective rotational model:

A better understanding of the nuclear moments of inertia is attained by including residual pairing interactions via the so-called “cranking” model.


D. R. Inglis [Phys. Rev. 96, 1059 (1954); 97, 701 (1955)] worked out the problem of a self-consistent, mean field potential, which determines single-particle orbitals, being externally “cranked,” either rotationally or vibrationally.

The rotational energy is calculated as the extra energy the nucleons require to follow the slowly rotating self-consistent potential field.

Nilsson and Prior [Mat. Fys. Medd. Dan. Vid. Selsk. 32, no.16 (1961)] applied this model to rotational spectra and calculated nuclear moments of inertia, showing that pairing interactions are quite capable of explaining these moments.
Collective rotational model:

Nilsson and Prior, define single particle states in a deformed potential with deformation parameter $\delta$ determined by the electric Quad. moment:

$$|\nu\rangle = \sum_j c_j^\nu |\chi^j_k\rangle$$ (e.g. superposition of H.O. states)

$$|\nu\rangle = a^+_\nu |0\rangle$$ where $a^+_\nu$ is a single-particle creation operator.

The Hamiltonian with pairing interactions is of the form

$$H = \sum_{\nu} \epsilon_\nu \left( a^+_\nu a_\nu + a^+_\nu a^+_\nu \right) - G \sum_{\nu,\nu'} a^+_\nu a^+_\nu a^-_{\nu'} a^-_{\nu'}$$

In the BCS formalism using the Bogoliubov - Valatin quasi-particle transformation

$$a^+_\nu = U_\nu \alpha^+_\nu + V_\nu \alpha^-_{\nu}$$

$$a^-_{\nu} = U_\nu \alpha^-_{\nu} - V_\nu \alpha^+_\nu \quad U_\nu^2 + V_\nu^2 = 1,$$

the moment of inertia is

$$\mathcal{J} = 2\hbar^2 \sum_{\nu,\nu'} \frac{|\langle \nu | j_x | \nu' \rangle|^2}{E_\nu + E_{\nu'}} \left(U_\nu V_{\nu'} - V_\nu U_{\nu'}\right)^2 \propto \Delta$$

where

$$U_\nu^2 = \frac{1}{2} \left(1 + \frac{\epsilon_\nu - \lambda}{E_\nu}\right), \quad V_\nu^2 = \frac{1}{2} \left(1 - \frac{\epsilon_\nu - \lambda}{E_\nu}\right), \quad E_\nu = \sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2}.$$

where the gap energy $\Delta = G \sum_\nu U_\nu V_{\nu'}$, (from Fermi energy level $\lambda$ to unoccupied states)

is determined by fitting the odd - even nuclear mass splitting.
Collective rotational model:

From Nilsson and Prior:

(cases A and B correspond to minor adjustments in the single-particle basis states)
Collective vibrational model:

The other, major type of collective nuclear excitation is vibrational modes corresponding to quantized phonon excitations in the nucleon motion. The dominant modes are the $\lambda = 0, 1, 2, \text{ and } 3$ multipoles corresponding to monopole (expansion – contraction) or the so-called “breathing” mode, dipole oscillations between protons and neutrons, quadrupole oscillations and octupole oscillations. Each is illustrated below:
Collective vibrational model:

- $\lambda = 0$ monopole vibration or “breathing” mode; these states tend to be at higher excitation energies due to the large, nuclear compressibility.

- $\lambda = 1$ dipole vibration between protons and neutrons – Giant Dipole state

- $\lambda = 2$ quadrupole vibrations, both isoscalar ($\Delta I = 0$) and isovector ($\Delta I = 1$) or the Giant Quadrupole, corresponding to protons and neutrons oscillating out-of-phase.

Vibrational excitations of deformed nuclei also occur, where the protons and neutrons oscillate out-of-phase in a so-called “scissors mode” as shown to the right.

Experiments: $^{64}$Mo (N = 52) ... $^{100}$Mo (N = 58)
Collective vibrational model:

Vibrational excitations of deformed nuclei also occur, where rotational bands build on top of vibrating, deformed nuclei.

$\beta$ – vibration

$\gamma$ – vibration
Collective vibrational model:
We invoke the same assumptions used to model rotational motion wherein the vibrational frequencies are much smaller than the characteristic nucleon crossing frequencies, i.e. the Born – Oppenheimer approximation.

I will only discuss the most common isoscalar quadrupole and octupole vibrations of approximately spherical nuclei. The model was proposed by Aage Bohr (Niels’son) in 1952.

Bohr Hamiltonian:
We start with the idea that the binding potential radius will depend on angle and time,

\[ R = R_0 \left[ 1 + \sum_{\lambda \mu} \alpha_{\lambda \mu} Y_{\lambda \mu} (\theta, \phi) \right] \]

where \( \alpha_{\lambda \mu} \) is time-dependent (oscillatory). The (classical) Hamiltonian of the collective, vibrational motion contains kinetic and potential energy terms, where

\[ H_{vib} = \frac{1}{2} B \sum_{\lambda \mu} |\dot{\alpha}_{\lambda \mu}|^2 + \frac{1}{2} C \sum_{\lambda \mu} |\alpha_{\lambda \mu}|^2 \]

In order that \( R \) is real we require that \( \alpha_{\lambda \mu} \) transform under rotations as \( Y_{\lambda \mu}^* \), where

\[ \sum_{\mu} Y_{\lambda \mu}^* Y_{\lambda \mu} \propto Y_{\lambda 0} \]

a scalar using the addition theorem, and

\[ \alpha_{\lambda \mu}^* = (-1)^\mu \alpha_{\lambda,-\mu} \]

The above classical Hamiltonian is that of a harmonic oscillator with frequency

\[ \omega = \sqrt{C / B} \]
Collective vibrational model:

Quantizing $H_{vib}$ replaces $\alpha_{\lambda\mu}$ with phonon creation and annihilation operators $a_{\lambda\mu}^+, a_{\lambda\mu}$ where

$$[a_{\lambda\mu}, a_{\lambda\nu}^+] = \delta_{\mu\nu}, \quad [a_{\lambda\mu}, a_{\lambda\nu}] = [a_{\lambda\mu}^+, a_{\lambda\nu}^+] = 0$$

the latter expressing the symmetry for integer spin ($\lambda$) boson states. The phonon number operator is

$$\hat{n}_{\lambda\mu} = a_{\lambda\mu}^+ a_{\lambda\mu}$$

for phonons with angular momentum $\lambda$, and $z$-component $\mu$, and parity $(-1)^{\lambda}$, where

$$a_{\lambda\mu} |0\rangle = 0 \quad \text{where} \ |0\rangle \text{ is the no-phonon vacuum state}$$

$$a_{\lambda\mu}^+ |0\rangle = |1, \lambda\mu\rangle \quad \text{where} \ |1, \lambda\mu\rangle \text{ is a 1-phonon state}$$

$$a_{\lambda\mu} |n_\mu, \lambda\mu\rangle = \sqrt{n_\mu} |n_\mu - 1, \lambda\mu\rangle$$

$$a_{\lambda\mu}^+ |n_\mu, \lambda\mu\rangle = \sqrt{n_\mu + 1} |n_\mu + 1, \lambda\mu\rangle$$

The 2-phonon state $a_{\lambda\mu_1}^+ a_{\lambda\mu_2}^+ |0\rangle$ with angular momentum $|I, M\rangle$ and the proper Bose-symmetry is

$$|I, M\rangle_{2-phonon} = \sum_{\lambda\mu_1, \lambda\mu_2} (\lambda\mu_1 \lambda\mu_2 | IM) a_{\lambda\mu_1}^+ a_{\lambda\mu_2}^+ |0\rangle$$

For Bose statistics interchanging labels $1 \leftrightarrow 2$ does not change the sign. From the symmetry for Clebsch-Gordon coefficients

$$(\lambda\mu_1 \lambda\mu_2 | IM) = (-1)^{\lambda_1 + \lambda_2 - I} (\lambda\mu_2 \lambda\mu_1 | IM)$$

we find that $I$ is even-only. For quadrupole vibrations the 2-phonon states have $I^p = 0^+, 2^+, 4^+$ and for octupole vibrations the 2-phonon states are $I^p = 0^+, 2^+, 4^+, 6^+$

For combined 2-phonon quadrupole & octupole vibrations the states are $I^p = 1^-$ to $5^-$
Collective vibrational model:

The energy levels for \( n_\lambda \) phonons of multipole \( \lambda \) is

\[
E_{\lambda n} = \hbar \omega \sum_\mu \left( \hat{n}_\mu + \frac{1}{2} \right) = \hbar \omega \left( \frac{2\lambda + 1}{2} + n_\mu \right)
\]

which are degenerate for all the \(|IM\rangle_{n_\lambda\text{-phonons}}\)

\[\begin{align*}
\hbar \omega & : 0^+, 2^+, 4^+ \\
\hbar \omega & : 2^+ \\
\hbar \omega & : 0^+_{gs} \\
\hbar \omega & : 0^+_{gs}
\end{align*}\]

\( \lambda = 2 \) quadrupole  
\( \lambda = 3 \) octupole
Collective vibrational model:

Examples of $\lambda=2$
1- and 2-phonon states

Anharmonic interactions break the $0^+, 2^+, 4^+$ degeneracy

The picture for $\lambda=3$
1- and 2-phonon states is messy.
The next slide shows the excited state spectrum for $^{208}$Pb which has a very strong $3^-\text{ state}$. 

FIGURE 5-11 The lowest-energy states of various spherical even-even nuclei. Excitation energies (in MeV) are given at the right, and $I^e$ are shown at the left. Note that in all cases the ground state is $0^+$, the first excited state is $2^+$, and there are three states at about twice its excitation energy with $I^e = 0^+$, $2^+$, and $4^+$, not necessarily in that order. In some of these nuclei, all three of the latter group are not yet known experimentally.
Collective vibrational model:

1\textsuperscript{st} excited states is a 3\textsuperscript{−} at 2.6 MeV

Several 2\textsuperscript{−}, 3\textsuperscript{−}, 4\textsuperscript{−}, 5\textsuperscript{−} (but no 1\textsuperscript{−}) states which may have $\lambda = 2\&3$ 2-phonon mixtures

Several 0\textsuperscript{+}, 2\textsuperscript{+}, 4\textsuperscript{+}, 6\textsuperscript{+} states at about twice the energy of the 3\textsuperscript{−} (MeV)

$^{208}\text{Pb}$ – the messy real world!
Shell Model Calculations

In conventional shell model calculations the lower, closed shell states (core) are treated as inert and valence nucleons populate the higher energy levels in multiple configurations as determined by the two-body effective interaction. Each configuration contributes to the nuclear $J^\pi$ state. We will calculate basis states with which to expand the full wave function, then diagonalize to find the shell-model states and energies.

If the 2 neutrons do not interact, then they both go into the lowest energy 1d5/2 state.

If they interact (scatter) then all 6 combinations of 2 neutrons in the 3 levels of the “s-d” shell may be populated with some probability.
Shell Model Calculations

The total Hamiltonian of the nucleus is given by

\[ H = \sum_{i=1}^{A} T_i + \sum_{i<j} v_{ij} = H_0 + V_C \]

where \( T_i \) is the KE of nucleon \( i \), \( v_{ij} \) is the N-N potential,

\[ \langle H_0 \rangle_{gs}, \langle V_C \rangle_{gs} \] are the total KE and PE of the nuclear ground state.

Recall that in Brueckner theory (Chapter 3) the g.s. PE is approximated by the \( g \)-matrix

\[ \langle V_C \rangle_{gs} \approx \sum_{i<j} \langle ij | G_{B,ij} | ij \rangle A = \sum_{i<j} g_{ij} \]

The shell-model basis states should be as similar to the real states as practical in order that the wave function expansions converge with a reasonable number of components.

To achieve this we will add/subtract an effective, one-body potential to the Hamiltonian which estimates the effective mean-field interaction between one nucleon and the other (A-1) nucleons, and include this potential term in the Hamiltonian of the basis states.

\[ H = \sum_{i=1}^{A} T_i + \sum_{i=1}^{A} U_i + \sum_{i<j} v_{ij} - \sum_{i=1}^{A} U_i \]

Next, separate the "core" and "valence" nucleon contributions, with \( a, b \) core and valence nucleons \( (A = a + b) \)

\[ H = \sum_{i=1}^{a} T_{i,core} + \sum_{i=1}^{b} T_{i,val} + \sum_{i=1}^{a} U_{i,core} + \sum_{i=1}^{b} U_{i,val} + \sum_{i<j=1}^{a} v_{ij,core} + \sum_{i=1}^{a} \sum_{j=1}^{b} v_{ij,core-val} + \sum_{i<j=1}^{b} v_{ij,val} - \sum_{i=1}^{a} U_{i,core} - \sum_{i=1}^{b} U_{i,val} \]
Shell Model Calculations

\[ H = H_{\text{core}} + \sum_{i=1}^{b} T_{i,\text{val}} + \sum_{i=1}^{b} U_{i,\text{val}} + \sum_{i=1}^{a} \sum_{j=1}^{b} v_{ij,\text{core-val}} + \sum_{i=1}^{b} v_{ij,\text{val}} - \sum_{i=1}^{b} U'_{i,\text{val}} - \sum_{i=1}^{b} U''_{i,\text{val}} \]

where terms involving only the core nucleons are collected into \( H_{\text{core}} \) and the one - body potential for the valence nucleons are separated into two parts which scale with the number of core \( (U') \) and valence \( (U'') \) nucleons. For this discussion I will neglect the residual core + valence interaction terms

\[ \sum_{i=1}^{a} \sum_{j=1}^{b} v_{ij,\text{core-val}} - \sum_{i=1}^{b} U'_{i,\text{val}} \]

but realistic shell model calculations include these effects. The shell - model Hamiltonian is

\[ H_{\text{SM}} = H_{\text{core}} + \sum_{i=1}^{b} T_{i,\text{val}} + \sum_{i=1}^{b} U_{i,\text{val}} + \sum_{i=1}^{b} v_{ij,\text{val}} - \sum_{i=1}^{b} U'_{i,\text{val}} \]

\[ \approx H_{\text{core}} + \sum_{i=1}^{b} T_{i,\text{val}} + \sum_{i=1}^{b} U_{i,\text{val}} + \left[ \sum_{i<j}^{b} g_{ij,\text{val}} - \sum_{i=1}^{b} U''_{i,\text{val}} \right] \equiv H_{\text{core}} + \sum_{i=1}^{b} T_{i,\text{val}} + \sum_{i=1}^{b} U_{i,\text{val}} + \sum_{i<j}^{b} v_{ij,\text{val}} \]

\[ \equiv H_{\text{core}} + H_{\text{val}} \]

where we assume that the Brueckner theory result,

\[ \left< \sum_{i<j} v_{ij} \right>_{\text{gs}} \approx \sum_{i<j} g_{ij} \] is also valid for other, low - lying state matrix elements.
Shell Model Calculations

With the neglect of core + valence interactions the wave function may be written as

\[ \Psi = \chi_{\text{core}}\psi_{\text{val}} \]

where

\[ H_{SM}\Psi = (H_{\text{core}} + H_{\text{val}})\chi_{\text{core}}\psi_{\text{val}} = E\chi_{\text{core}}\psi_{\text{val}} \]

\[ H_{\text{core}}\chi_{\text{core}} = E_{\text{core}}\chi_{\text{core}} \]

\[ H_{SM}\Psi = (H_{\text{val}} + E_{\text{core}})\chi_{\text{core}}\psi_{\text{val}} = (E_{\text{val}} + E_{\text{core}})\chi_{\text{core}}\psi_{\text{val}} \]

and we must solve for the valence part

\[ H_{\text{val}}\psi_{\text{val}} = E_{\text{val}}\psi_{\text{val}} \]

Consider the $^{18}$O example with an inert $^{16}$O core and allow the 2 valence neutrons to occupy any of the three levels in the s - d shell. Calculate the $0^+$ ground state which requires the 2n basis states to be only those combinations which couple to $0^+$, for neutrons 1 & 2:

\[ |\phi_1\rangle = [1d_{5/2}\rangle_1 \otimes 1d_{5/2}\rangle_2]_{0^+}, \quad |\phi_2\rangle = [2s_{1/2}\rangle_1 \otimes 2s_{1/2}\rangle_2]_{0^+}, \quad |\phi_3\rangle = [1d_{3/2}\rangle_1 \otimes 1d_{3/2}\rangle_2]_{0^+} \]
Shell Model Calculations

The eigenvalue of the basis states are determined by
$$\left(T_{1,\text{val}} + T_{2,\text{val}} + U_{1,\text{val}} + U_{2,\text{val}}\right)|\phi_i\rangle = H_{\text{val}}^0|\phi_i\rangle = \epsilon_i|\phi_i\rangle$$

and the total wave function is expanded as
$$|\psi_{J^\pi}\rangle = \sum_i c_i|\phi_i\rangle$$

The Schrödinger Eq. for the valence nucleons is then
$$\left(H_{\text{val}}^0 + \sum_{i < j = 1}^2 v_{ij,\text{val}}^{\text{eff}}\right)|\psi_{J^\pi}\rangle = \left(H_{\text{val}}^0 + \sum_{i < j = 1}^2 v_{ij,\text{val}}^{\text{eff}}\right)\sum_k c_k|\phi_k\rangle = E_{J^\pi}\sum_k c_k|\phi_k\rangle$$

Project arbitrary basis state $|\phi_m\rangle$ and obtain
$$\epsilon_m c_m + \sum_k c_k\langle\phi_m|\sum_{i < j = 1}^2 v_{ij,\text{val}}^{\text{eff}}|\phi_k\rangle = E_{J^\pi} c_m \text{ and define the matrix element } v_{mk}^{\text{eff}} \equiv \langle\phi_m|\sum_{i < j = 1}^2 v_{ij,\text{val}}^{\text{eff}}|\phi_k\rangle$$

The matrix equation
$$\begin{pmatrix} v_{11}^{\text{eff}} & v_{12}^{\text{eff}} & v_{13}^{\text{eff}} \\ v_{21}^{\text{eff}} & v_{22}^{\text{eff}} & v_{23}^{\text{eff}} \\ v_{31}^{\text{eff}} & v_{32}^{\text{eff}} & v_{33}^{\text{eff}} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} E_{J^\pi} - \epsilon_1 & 0 & 0 \\ 0 & E_{J^\pi} - \epsilon_2 & 0 \\ 0 & 0 & E_{J^\pi} - \epsilon_3 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

is solved for three $0^+$ eigenvalues and eigenstates corresponding to three sets of expansion coefficients.
Shell Model Calculations

State-of-the-art shell model calculations attempt to improve the effective interactions, the mean potential used to determine the basis states, the estimates of core-valence interactions, and to minimize the size of the core, including “no-core” shell models, and to expand the set of basis states.

Modern calculations use harmonic oscillator basis states in order to greatly speed up the calculation of the effective interaction matrix elements. However, the H.O. states are rather poor estimates of the nominal Woods-Saxon potential eigenstate basis, so many H.O. levels are required to obtain realistic results.

Including sufficient H.O. levels and all the accompanying total, orbital, and z-component angular momentum states, plus the total and z-component iso-spin states, and then including all the n-body valence nucleon configurations which may contribute to the set of nuclear $J^\pi$ states to be described requires of order $10^9$ basis states and must be done on dedicated super-computers.
Shell Model Calculations

Vintage shell-model calculations:

Fig. 7-3 Comparison of the theoretical level energies and spins with the experimental data. The levels indicated by bold lines were used in the fitting process. The vertical axis represents the excitation energy relative to the binding energy of the $^{32}$Si core, with the Coulomb energy of the outer particles subtracted. Hatching indicates areas of high level density (Glaudemans et al. 18).
FIG. 1. Calculated energy levels for $^{134}$Nd and compared with experimental data [45,46]. Following Ref. [46], we use notations (H) and (I) for the $4^-$ bands.

Includes up to 10 quasi-particle basis states.
FIG. 1. The calculated energy levels (left columns) (in MeV) for $^{124}$Sn and $^{124}$Te compared to experiment (right columns).
Advanced Shell Model Calculations  
(as used in $2\nu-\beta\beta$ and $0\nu-\beta\beta$ decay transitions)

The calculation of nuclear transition matrix elements for use in 2-neutrino and 0-neutrino double-beta decay is a topic of present day research. See for example: Horoi and Neacsu, Phys. Rev. C 93, 024308 (2016). Because the relevant nuclear isotopes for these studies are neither light, nor closed-shell, nor ideal collective nuclei which rotate or vibrate, the nuclear structure aspects of these transitions is complex. Multiple approaches are given in the literature. The above paper lists the following general categories with several references for each. These include:

- Interacting Shell Model (ISM)
- Quasi-particle Random Phase Approximation (QRPA)
- Interacting Boson Model (IBM-2)
- Projected Hartree-Fock Bogoliubov (PHFB)
- Energy Density Functional (EDF) – not discussed
- Relativistic Energy Density Functional (REDF) – not discussed

The ISM calculations seem to be regular shell model calculations as described in the previous slides but with varying cores, shell configurations and effective interactions.

For the other models I will only describe those approaches in general terms.
Advanced Shell Model Calculations

A basic difference in the nuclear transition matrix elements for 0ν–ββ and 2ν–ββ involves the role of intermediate nuclear states. For 0ν–ββ the “closure” approximation (see below) suffices [see, Mustonen & Engel, PRC 87, 064302 (2013) and Pantis and Vergados, Phys. Lett. B 242, 1 (1990)] while for 2ν–ββ intermediate nuclear states must be summed explicitly. The importance of intermediate states in 2ν–ββ prevents using measured 2ν–ββ rates to determine the NME for 0ν–ββ.

\[ \mathcal{M}^{2\nu-\beta\beta} \approx \sum_{n} \frac{\langle f | \sum_{a} \tilde{\sigma}_{a} \tau_{a}^{+} | n \rangle \cdot \langle n | \sum_{b} \tilde{\sigma}_{b} \tau_{b}^{+} | i \rangle}{E_{n} - (M_{i} + M_{f})/2} \]

for GT dominated transitions,

\[ \tilde{\sigma}_{a,b} \text{ and } \tau_{a,b}^{+} \text{ are spin/isospin operators for nucleons } a,b. \]

In the closure approximation, \[ \sum_{n} |n\langle n| = 1, \]

and the numerator simplifies to

\[ \mathcal{M}^{0\nu-\beta\beta}_{\text{closure}} \rightarrow \langle f | \sum_{a,b} \tilde{\sigma}_{a} \cdot \tilde{\sigma}_{b} \tau_{a}^{+} \tau_{b}^{+} | i \rangle \]

Intermediate states in \(^{150}\text{Pm}\) populated in 2ν–ββ

This difference applies to all methods.
Advanced Shell Model Calculations

**ISM: Interacting Shell Model**

$^{48}\text{Ca}$ to $^{48}\text{Ti}$ double-beta decay

Kuo & Brown effective interaction
Richter (RVJB) effective interaction

8 neutrons in $1f_{7/2} - 2p_{1/2}$ valence levels

$^{40}\text{Ca}$ core

FIG. 7.2. Approximate level pattern for protons. The spin-orbit splitting is adjusted in such a way that the empirical level sequence is represented. For convenience the oscillator-level grouping and the parities of these groups are indicated at the left side of Fig. 7.2. Round brackets (2), (4), etc. and square brackets [2], [6], etc. indicate the level degeneracies and the total occupation numbers. In the $6\hbar\omega$ oscillator group the splittings are not drawn in a proper scale, the $3d$ splitting is too large. A more accurate drawing would have confused the picture too much. [Taken from Mayer and Jensen (55)].
Advanced Shell Model Calculations

ISM:
Caurier et al. PRL 100, 052503 (2008)
A = 76, 82 with \{2p_{3/2}, 1f_{5/2}, 2p_{1/2}, 1g_{9/2}\} valence basis states; $^{56}\text{Ni}$ core.

G-matrix effective interaction; $v_{\text{eff}}$ tuned to fit the low-lying spectrum in each isotope

A = 124, 128, 130, 136 with \{1g_{7/2}, 2d_{5/2}, 2d_{3/2}, 3s_{1/2}, 1h_{11/2}\} basis

Of order $10^{10}$ dimensional matrix!

FIG. 7.2. Approximate level pattern for protons. The spin-orbit splitting is adjusted in such a way that the empirical level sequence is represented. For convenience the oscillator-level grouping and the parities of these groups are indicated at the left side of Fig. 7.2. Round brackets (2), (4), etc. and square brackets [2], [6], etc. indicate the level degeneracies and the total occupation numbers. In the $6\hbar\omega$ oscillator group the splittings are not drawn in a proper scale, the 3d splitting is too large. A more accurate drawing would have confused the picture too much. [Taken from Mayer and Jensen (55)].
Advanced Shell Model Calculations – Quasi-particle Random Phase Approximation

In the random phase approximation (RPA) 2p-2h matrix elements are simplified; simultaneous 2p-2h excitations are neglected and are reduced to sums of 1p-1h “active” excitations times “inert” ground-state averages of the other particle-hole excitation in the pair. An arbitrary 2p-2h excitation is driven by effective interactions containing the operator $a_p^+ a_q^+ a_r a_s$ which excites 2 nucleons from orbitals $r,s$ to $p,q$ as in the diagram. The essence of the RPA is to write this operator as:

$$a_p^+ a_q^+ a_r a_s \rightarrow \langle a_q^+ a_r \rangle a_p^+ a_s - \langle a_q^+ a_s \rangle a_p^+ a_r - \langle a_p^+ a_r \rangle a_q^+ a_s + \langle a_p^+ a_s \rangle a_q^+ a_r$$

where the $\langle a_q^+ a_r \rangle$, etc. are ground-state matrix elements.

Mustonen and Engel, PRC 87, 064302 (2013) is a deformed, self-consistent, Skyrme QRPA applied to $^{76}$Ge, $^{130}$Te, $^{136}$Xe, $^{150}$Nd: deformed HF basis, Skyrme contact $v^{eff}$
**Advanced Shell Model Calculations** – Interacting Boson Model (IBM)

In the IBM valence protons and neutrons in even-even nuclei are paired (pp and nn) into integer spin objects (bosons) which are, in turn, allowed to interact and excite into boson plus boson-hole states. Lower energy levels are treated as an inert core as in the SM. For example, $^{128}\text{Xe}$ ($Z = 54$, $N = 74$) is near closed shells 50 and 82 with 4 valence protons forming 2 pp bosons and 8 valence neutron holes forming 4 nn bosons. The bosons are assumed to be in either $L = 0$ (s) or 2 (d) states only.

The IBM Hamiltonian using s-boson and d-boson creation and annihilation operators contains 9 terms with corresponding fitting parameters and is given by

$$
H = \varepsilon_s (s^+ s) + \varepsilon_d (d^+ \tilde{d}) + \sum_{L=0,2,4} \frac{\sqrt{2L+1} C_L}{2} \left[ (d^+ \otimes d^+) L \otimes (\tilde{d} \otimes \tilde{d}) L \right]^0 \\
+ \frac{V_2}{\sqrt{2}} \left[ (d^+ \otimes d^+) (2) \otimes (\tilde{d} \otimes s) (2) + (d^+ \otimes s^+) (2) \otimes (\tilde{d} \otimes \tilde{d}) (2) \right]^0 \\
+ \frac{V_0}{2} \left[ (d^+ \otimes d^+) (0) \otimes (s \otimes s) (0) + (s^+ \otimes s^+) (0) \otimes (\tilde{d} \otimes \tilde{d}) (0) \right]^0 \\
+ U_2 \left[ (d^+ \otimes s^+) (2) \otimes (\tilde{d} \otimes s) (2) \right]^0 + \frac{U_0}{2} \left[ (s^+ \otimes s^+) (0) \otimes (s \otimes s) (0) \right]^0
$$

where $\tilde{d}_\mu = (-1)^\mu d_{-\mu}$.

With a fixed set of parameters the solutions, as a function nuclear $Z,N$, range from rotational to vibrational.
Advanced Shell Model Calculations – Interacting Boson Model (IBM)

For example, Barea and Iachello, PRC 79, 044301 (2009) apply the IBM to \(0\nu-\beta\beta\) NME for \(^{76}\text{Ge},\ ^{82}\text{Se},\ ^{100}\text{Mo},\ ^{128}\text{Te},\ ^{130}\text{Te},\ ^{136}\text{Xe},\ ^{150}\text{Nd},\ ^{154}\text{Sm}\)

![Graph showing neutrinoless double-beta decay matrix elements](image)

**Fig. 2.** (Color online) Neutrinoless double-\(\beta\) decay matrix elements in the formulation of Šimkovic et al. [10] for IBM-2, Set I (this work), QRPA with \(g_A = 1.25\) and Jastrow SRC [20], and SM [8].
Advanced Shell Model Calculations -- Projected Hartree-Fock Bogoliubov

See e.g. Rath et al., PRC 88, 064322 (2013); PRC 82, 064310 (2010) applied to $^{94,96}$Zr, $^{98,100}$Mo, $^{104}$Ru, $^{110}$Pd, $^{128,130}$Te, and $^{150}$Nd

Hartree-Fock models will be discussed later. In a nutshell HF solutions are self-consistent solutions of the many-body Hamiltonian with effective interactions in which the potentials are determined by the effective two-body interactions folded with the single-particle states, and the states are determined by solving the Sch.Eq. with those potentials. HF requires an iterative solution. Brueckner HF uses the g-matrix interaction; HF Bogoliubov uses quasi-particle basis states. The PHFB uses deformed basis states with $\lambda = 0, 2, 4$ multipole components of the effective two-body interaction. The PHFB Hamiltonian is

$$H = H_{sp} + V_{pairing} + V_{quad} + V_{hexadecupole}$$

$H_{sp}$ (single - particle) includes the KE and single - particle potentials $U_i$

The multipole interactions for 2p - 2h excitations are

$$V(\lambda \lambda) = C_\lambda \sum_{\alpha \beta \gamma \delta} \sum_v (-1)^v \langle \alpha | q_{\lambda v} | \gamma \rangle \langle \beta | q_{\lambda, -v} | \delta \rangle a_\alpha^+ a_\beta^+ a_\delta a_\gamma$$

for $\lambda = 2, 4$ where $C_\lambda$ is a coupling parameter and

$$q_{\lambda v} = r^\lambda Y_{\lambda v}(\theta, \phi)$$
Hartree-Fock Models

The basic idea is to find a method to optimize the single particle states and single-particle binding potential such that the effects of the two-body interactions on the nuclear eigenstates are accounted for with a simple, single particle model. Start with a simple, product form for the A-body wave function where anti-symmetrization is ignored. This will give the Hartree potential.

\[ \Phi_\alpha (1, 2, \cdots A) = \phi_{\alpha_1} (1) \phi_{\alpha_2} (2) \cdots \phi_{\alpha_A} (A) \]  

where \( \int \phi_\alpha^* \phi_\alpha d^3 r = 1 \), \( \alpha \) denotes an eigenstate of the A-body system and single particle states \( \phi_{\alpha_i} \) fill up the lowest orbitals corresponding to many-body state \( \alpha \).

Then construct

\[ \langle \Phi_\alpha | H | \Phi_\alpha \rangle = \langle \Phi_\alpha | \sum_{i=1}^{A} T_i + \sum_{i<j} v_{ij} | \Phi_\alpha \rangle \]

and find the best set of \( \phi_\alpha \) such that \( \langle \Phi_\alpha | H | \Phi_\alpha \rangle \) is stationary with respect to variations in \( \phi_\alpha \) while maintaining the above normalization requirements. When stationarity is achieved the above matrix element corresponds to the eigenvalue of \( H \) in state \( \alpha \). Use Lagrange multipliers to write the variational condition, with normalization constraint:

\[ \delta \left\{ \int \phi_{\alpha_1}^* (1) \cdots \phi_{\alpha_A}^* (A) \left[ \sum_{i=1}^{A} T_i + \frac{1}{2} \sum_{i\neq j} v_{ij} \right] \phi_{\alpha_1} (1) \cdots \phi_{\alpha_A} (A) d^3 r_1 \cdots d^3 r_A - \sum_{k=1}^{A} \lambda_{\alpha_k} \int \phi_{\alpha_k}^* (\vec{r}_k) \phi_{\alpha_k} (\vec{r}_k) d^3 r_k \right\} = 0 \]
Hartree-Fock Models

Consider variation of one specific state, that for \( i = A \), then the preceding eqn. reduces to

\[
\int \phi^*_a \cdots \phi^*_{\alpha_{A-1}} (A-1) \delta \phi^*_a (A) \left[ \sum_{i=1}^{A} T_i + \frac{1}{2} \sum_{i \neq j} v_{ij} \right] \phi_a \cdots \phi_{\alpha_{A-1}} (A-1) \phi_a (A) d^3 r_1 \cdots d^3 r_A
\]

\[ - \lambda_A \int \delta \phi^*_a (\vec{r}_A) \phi_a (\vec{r}_A) d^3 r_A = 0 \]

where variation of a single state-function only requires one Lagrange multiplier constraint and variations of \( \phi^*_a \) and \( \phi_a \) are considered independent. The same results are obtained if we vary \( \phi_a \).

For the above eqn. to be valid for arbitrary variations \( \delta \phi^*_a (A) \) requires that its multiplicative factor be zero.

\[
\int \phi^*_a \cdots \phi^*_{\alpha_{A-1}} (A-1) \delta \phi^*_a (A) \left[ \sum_{i=1}^{A-1} T_i + T_A + \frac{1}{2} \sum_{i \neq j} v_{ij} + \sum_{j=1}^{A-1} v_{Aj} \right] \phi_a \cdots \phi_{\alpha_{A-1}} (A-1) \phi_a (A) d^3 r_1 \cdots d^3 r_A
\]

\[ - \lambda_A \int \delta \phi^*_a (\vec{r}_A) \phi_a (\vec{r}_A) d^3 r_A = 0 \]

\[
= \int \phi^*_a \cdots \phi^*_{\alpha_{A-1}} (A-1) \left[ \sum_{i=1}^{A-1} T_i + \frac{1}{2} \sum_{i \neq j} v_{ij} \right] \phi_a \cdots \phi_{\alpha_{A-1}} (A-1) \phi_a (A) d^3 r_1 \cdots d^3 r_{A-1} \int \delta \phi^*_a (A) \phi_a (A) d^3 r_A
\]

\[ + \int \delta \phi^* (A) T_A \phi_a (A) d^3 r_A + \int \phi^*_a \cdots \phi^*_{\alpha_{A-1}} (A-1) \delta \phi^*_a (A) \sum_{j=1}^{A-1} v_{Aj} \phi_a (A) d^3 r_1 \cdots d^3 r_A \]

\[ - \lambda_A \int \delta \phi^*_a (\vec{r}_A) \phi_a (\vec{r}_A) d^3 r_A = 0 \]

which is of the form: \( \int \delta \phi^*_a (\vec{r}_A) d^3 r_A [X] = 0 \) where we require \([X] = 0\), where this factor is on the next slide.
Hartree-Fock Models

\[
T_A + \int \phi_{\alpha_1}^*(1) \cdots \phi_{\alpha_{A-1}}^*(A-1) \left( \sum_{j=1}^{A-1} v_{Aj} \right) \phi_{\alpha_1}(1) \cdots \phi_{\alpha_{A-1}}(A-1) d^3 r_1 \cdots d^3 r_{A-1} - \lambda_{\alpha A} \\
+ \int \phi_{\alpha_1}^*(1) \cdots \phi_{\alpha_{A-1}}^*(A-1) \left( \sum_{i=1}^{A-1} T_i + \frac{1}{2} \sum_{i \neq j=1}^{A-1} v_{ij} \right) \phi_{\alpha_1}(1) \cdots \phi_{\alpha_{A-1}}(A-1) d^3 r_1 \cdots d^3 r_{A-1} \right] \phi_{\alpha A}(\vec{r}_A) = 0
\]

The second integral does not depend on nucleon \# A and can be replaced by a constant and combined with \( \lambda_{\alpha A} \), resulting in

\[
T_A + \int \phi_{\alpha_1}^*(1) \cdots \phi_{\alpha_{A-1}}^*(A-1) \left( \sum_{j=1}^{A-1} v_{Aj} \right) \phi_{\alpha_1}(1) \cdots \phi_{\alpha_{A-1}}(A-1) d^3 r_1 \cdots d^3 r_{A-1} - \varepsilon_{\alpha A} \right] \phi_{\alpha A}(\vec{r}_A) = 0
\]

\[\equiv (T_A + U_{\alpha A} - \varepsilon_{\alpha A}) \phi_{\alpha A}(\vec{r}_A) = 0\]

The same Sch. eq. results for all \( \{1, 2, \cdots, A\} \) nucleons. The potential \( U_{\alpha i}(\vec{r}_i) \) is that seen by nucleon \( i \) interacting with all other \( (A-1) \) nucleons.

The procedure followed is to guess the single particle potential \( U_{\alpha i}(\vec{r}_i) \), solve the Sch. eq. for \( \phi_{\alpha i} \), calculate a new potential, and then a new \( \phi_{\alpha i} \) and so on until the results converge. Since each single particle state is an eigenstate of a different Hamiltonian these states are not orthogonal.

The resulting A-body wavefunction and energy,

\[
E_{\alpha} = \sum_{i=1}^{A} \varepsilon_{\alpha i}
\]

is the Hartree solution. Next, we will consider antisymmetric wave functions and find that orthogonality is restored.
Hartree-Fock Models

For a many-body wave function of identical fermions, antisymmetrization requirements can be satisfied with a Slater determinant form given by

\[ \Phi_0(1,2,\cdots A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_\alpha(1) & \phi_\alpha(2) & \cdots & \phi_\alpha(A) \\ \phi_\beta(1) & \phi_\beta(2) & \cdots & \phi_\beta(A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_\omega(1) & \phi_\omega(2) & \cdots & \phi_\omega(A) \end{vmatrix} \]

where subscripts \( \alpha \) represent all quantum numbers, e.g. \( N, \ell, j, m_j, \tau_3 \) and \( \{1,2\cdots A\} \) are nucleon labels. The variational condition applied to arbitrary orbital \( \lambda \) is given by

\[ \int \delta_\lambda \Phi_0^*(1,2\cdots A) \left[ \sum_{i=1}^{A} T_i + \frac{1}{2} \sum_{i \neq j} v_{ij} \right] \Phi_0(1,2,\cdots A) d^3r_1 \cdots d^3r_A - \lambda \int \delta \phi_\lambda^* \phi_\lambda d^3r = 0 \]

where

\[ \delta_\beta \Phi_0(1,2,\cdots A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_\alpha(1) & \phi_\alpha(2) & \cdots & \phi_\alpha(A) \\ \delta \phi_\beta(1) & \delta \phi_\beta(2) & \cdots & \delta \phi_\beta(A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_\omega(1) & \phi_\omega(2) & \cdots & \phi_\omega(A) \end{vmatrix} \]
Hartree-Fock Models

Work out the KE term, doing the $A = 2$ case as an example

$$
\langle \delta_\alpha \Phi_0(1,2) \left| (T_1 + T_2) \right| \Phi_0(1,2) \rangle = \frac{1}{2!} \left\langle \delta \phi_\alpha(1) \phi_\beta(2) - \phi_\beta(1) \delta \phi_\alpha(2) \left| (T_1 + T_2) \right| \phi_\alpha(1) \phi_\beta(2) - \phi_\beta(1) \phi_\alpha(2) \right\rangle
$$

$$
= \left\langle \delta \phi_\alpha(1) \left| T_1 \right| \phi_\alpha(1) \right\rangle + \left\langle \delta \phi_\alpha(1) \left| \phi_\alpha(1) \right\rangle \left\langle \phi_\beta(2) \right| T_2 \left| \phi_\beta(2) \right\rangle \right\rangle \text{ where nucleon labels are arbitrary.}
$$

For $A > 2$ this is

$$
\langle \delta_\lambda \Phi_0 \sum_{i=1}^{A} T_i \left| \Phi_0 \right\rangle = \langle \delta \phi_\lambda(1) \left| T_1 \right| \phi_\lambda(1) \right\rangle + \sum_{\mu=\alpha, \neq \lambda} \langle \delta \phi_\lambda(1) \left| \phi_\lambda(1) \right\rangle \left\langle \phi_\mu(2) \right| T_2 \left| \phi_\mu(2) \right\rangle
$$

Similarly, work out the interaction term starting with the $A = 2$ example

$$
\langle \delta_\alpha \Phi_0(1,2) \left| v_{12} \right| \Phi_0(1,2) \rangle = \frac{1}{2!} \left\langle \delta \phi_\alpha(1) \phi_\beta(2) - \phi_\beta(1) \delta \phi_\alpha(2) \left| v_{12} \right| \phi_\alpha(1) \phi_\beta(2) - \phi_\beta(1) \phi_\alpha(2) \right\rangle
$$

$$
= \frac{1}{2} \left[ \langle \delta \phi_\alpha(1) \phi_\beta(2) \left| v_{12} \right| \phi_\alpha(1) \phi_\beta(2) \rangle + \langle \phi_\beta(1) \delta \phi_\alpha(2) \left| v_{12} \right| \phi_\beta(1) \phi_\alpha(2) \rangle \right]
$$

$$
- \langle \delta \phi_\alpha(1) \phi_\beta(2) \left| v_{12} \right| \phi_\beta(1) \phi_\alpha(2) \rangle - \langle \phi_\beta(1) \delta \phi_\alpha(2) \left| v_{12} \right| \phi_\alpha(1) \phi_\beta(2) \rangle \right]
$$

Exchange labels $1 \leftrightarrow 2$ in the second term, which does not change the sign of the energy and note that the interaction is symmetric, $v_{12} = v_{21}$, and obtain

$$
\langle \phi_\beta(1) \delta \phi_\alpha(2) \left| v_{12} \right| \phi_\beta(1) \phi_\alpha(2) \rangle = \langle \phi_\beta(1) \delta \phi_\alpha(1) \left| v_{21} \right| \phi_\beta(2) \phi_\alpha(1) \rangle = \langle \phi_\beta(2) \delta \phi_\alpha(1) \left| v_{12} \right| \phi_\beta(2) \phi_\alpha(1) \rangle
$$

$$
= \langle \delta \phi_\alpha(1) \phi_\beta(2) \left| v_{12} \right| \phi_\alpha(1) \phi_\beta(2) \rangle \text{ which is the first term above. The 3rd and 4th terms are similarly equal.}$$
Hartree-Fock Models

Therefore

\[ \langle \delta_\alpha \Phi_0 (1,2) | v_{12} | \Phi_0 (1,2) \rangle = \langle \delta \phi_1 (1) \phi_\beta (2) | v_{12} | \phi_\alpha (1) \phi_\beta (2) \rangle - \langle \delta \phi_1 (1) \phi_\beta (2) | v_{12} | \phi_\beta (1) \phi_\alpha (2) \rangle \]

and in general we get

\[ \langle \delta \lambda \Phi_0 | \sum_{i<j} v_{ij} | \Phi_0 \rangle = \sum_{\mu=\alpha}^\omega \left[ \langle \delta \phi_\lambda (1) \phi_\mu (2) | v_{12} | \phi_\lambda (1) \phi_\mu (2) \rangle - \langle \delta \phi_\lambda (1) \phi_\mu (2) | v_{12} | \phi_\mu (1) \phi_\lambda (2) \rangle \right] \]

We may add/subtract the \( \mu = \lambda \) term, \( \langle \delta \phi_\lambda (1) \phi_\lambda (2) | v_{12} | \phi_\lambda (1) \phi_\lambda (2) \rangle \) which removes the \( \mu \neq \lambda \) restriction, resulting in

\[ \langle \delta \lambda \Phi_0 | \sum_{i<j} v_{ij} | \Phi_0 \rangle = \sum_{\mu=\alpha}^\omega \left[ \langle \delta \phi_\lambda (1) \phi_\mu (2) | v_{12} | \phi_\lambda (1) \phi_\mu (2) \rangle - \langle \delta \phi_\lambda (1) \phi_\mu (2) | v_{12} | \phi_\mu (1) \phi_\lambda (2) \rangle \right] \]

Combing all terms gives

\[ \langle \delta \phi_\lambda (1) | T_1 | \phi_\lambda (1) \rangle + \sum_{\mu=\alpha}^\omega \langle \delta \phi_\lambda (1) | \phi_\lambda (1) \rangle \langle \phi_\mu (2) | T_2 | \phi_\mu (2) \rangle \]

\[ + \sum_{\mu=\alpha}^\omega \left[ \langle \delta \phi_\lambda (1) \phi_\mu (2) | v_{12} | \phi_\lambda (1) \phi_\mu (2) \rangle - \langle \delta \phi_\lambda (1) \phi_\mu (2) | v_{12} | \phi_\mu (1) \phi_\lambda (2) \rangle \right] - \lambda \lambda \langle \delta \phi_\lambda (1) | \phi_\lambda (1) \rangle = 0 \]

The summation in the second term does not involve the varied wave function \( \phi_\lambda \) and can be replaced with a constant and combined with the Lagrange multiplier as before. Setting the multiplicative factor which acts on \( \langle \delta \phi_\lambda (1) \rangle \) to zero results in the coupled - channels Schrodinger equation

\[ T_1 | \phi_\lambda (1) \rangle + \sum_{\mu=\alpha}^\omega \langle \phi_\mu (2) | v_{12} | \phi_\mu (2) \rangle | \phi_\lambda (1) \rangle - \sum_{\mu=\alpha}^\omega \langle \phi_\mu (2) | v_{12} | \phi_\lambda (2) \rangle | \phi_\mu (1) \rangle = \epsilon_\lambda | \phi_\lambda (1) \rangle \]

The 2nd term is the "direct" potential and 3rd is the "exchange" potential, a consequence of antisymmetry.
Hartree-Fock Models

A self-consistent solution is obtained as above where an initial guess for the direct and exchange potentials and solution of the coupled-equations gives the initial, trial set of single particle states. Then new potentials are calculated from the matrix elements, a new set of states is obtained and so on.

Typical, effective interactions for the direct and exchange terms are shown here, from Negele, Phys. Rev. C1, 1260 (1970).

Fig. 3. The short-range direct interaction $V_s$, the long-range direct interaction $V_{dir}$, and the long-range exchange interaction $V_{ex}$. The solid lines, short dashes, and long dashes correspond to the average, unlike, and like interactions, respectively. Note that the scale for $V_s$ is contracted by a factor of 20.
Hartree-Fock Models

Example Hartree-Fock charge densities calculated by Negele, PRC 1, 1260 (1970) are shown below.

![Graph showing Hartree-Fock Models with data and Hartree-Fock lines with different isotopes labeled O, Ca, Zr, and Pb.](image-url)

Fig. 6. Theoretical (dashed lines) and empirical (solid lines) charge-density distributions, including proton size and c.m. motion corrections. The empirical distributions for O, Ca, and Pb are from Refs. 72, 69, and 73, respectively.
This concludes Chapter IV: Nuclear Structure