Chapter 3

Theoretical Framework

3.1 Introduction

The atomic nucleus is a many-body quantum system made up of strongly interacting fermions. The properties of nucleus are shaped by the interplay of electromagnetic, weak and strong forces. The nucleus exhibits both the single and the collective degrees of freedom. The interplay of the single particle and collective motion of the nucleons inside the nucleus is responsible for giving the different shapes and structure to the nucleus at higher excitation and angular momentum. The study of the nucleus presents many aspects which challenge our understanding, ranging from many-body manifestations of nuclear properties to the forces between nucleons in the nuclear medium and their relationship to the underlying fundamental interactions. For predicting the shapes of the nucleus, a number of theories are developed over the years using different approximations of the nuclear potential. But the most successful among them are the ones based on the mean field approximation of the nuclear potential. In this approximation, nucleons are assumed to move in a mean field produced by the rest of the nucleons within the nucleus.

The two main theory or model which predict shape of the nucleus are the microscopic Hartree-Fock theory and the Total Routhian Surface (TRS) calculations. In the microscopic Hartree-Fock model, the calculation are done by changing the contributions of the individuals wave functions to find out the minimum of the potential energy. While in case of TRS calculations the total Routhians are calculated for different shapes of the nuclear potential and the shape of the nucleus corresponds to the minimum of the TRS.
3.2 Microscopic Hartree-Fock Model

Thus in the first case the wave-functions are changed to find out the minimum of the potential energy, while in the second case the shape of potential is changed to find out the minimum of the total Routhians. Both these models do predict the nuclear shapes in a self-consistent manner. The basic difference in the calculations done with these approaches is evident by the fact that the first (HIF) is treating the system in a fixed frame, while the second approach (TRS) treats it in the rotating frame. This chapter presents a brief description of both these models.

3.2 Microscopic Hartree-Fock Model

This model provides the mean field, microscopically by taking into account the nucleon-nucleon interaction. At its fundamental level, it starts with a shell structure and two-body interaction among the nucleons. So the nuclear Hamiltonian is of the following form [1,2],

$$H = H_0 + V_{\text{residual}},$$  \hspace{1cm} (3.1)

where $H_0$ is the shell model Hamiltonian and $V_{\text{residual}}$ two body residual interactions among nucleons in the shell model orbits. A number of attempts were made over the years to find the residual interaction starting from realistic two-nucleon interaction in free space [3-6] and sometimes taking into account the core polarization effect also. In practice phenomenological interactions, such as pairing and quadrupole interaction [5-7], surface delta interaction [8,9] finite range interactions [1] are found to give a more adequate description of the deformation and the nuclear properties of the nuclei in different mass regions. Out of these interactions, the surface delta interaction is an important and effective interaction among the particles near the Fermi surface. This is because of the fact, that in a nucleus, most of the collisions occur at the nuclear surface where the Pauli principle loses its importance and the nucleons feel the strong attractive interaction [10]. On the other hand, well inside the nucleus the nucleons move almost independently while outside the nucleus the nuclear wave functions have exponentially decaying tails, indicating negligible probability of finding the nucleons outside the nuclear volume. For this reason the surface delta interaction is considered in the present calculations.
The Hartree-Fock wave functions are the nuclear wave functions for which the overall nuclear energy is minimum. Such wave function can be written as in terms of the orthonormal setup of known single particle wave function. The single particle state $|I\rangle$ which in $(jm)$ representation is of the following form:

$$|I\rangle = |nljm\tau\rangle,$$

with $\tau$ as the isospin index. The nuclear Hamiltonian can be written as

$$H = T + V = \sum_{ij} \langle i|T|j\rangle \, a_i^\dagger \, a_j^{} + \frac{1}{4} \sum_{ijkl} \langle ij|V|kl\rangle \, a_i^\dagger \, a_j^{} \, a_k^\dagger \, a_l^{},$$

where the first part is the matrix element for the kinetic energy operator and the second part is the anti-symmetric matrix element of the two body interaction. The operator $a_i$ and $a_i^\dagger$ are the annihilation and creation operator associated with a single particle state $|I\rangle$, and it satisfies the fermion anti commutation relations.

The total nuclear wave function for a nucleus with $n$ particles is supposed to be a later determinant of single particle orbits $\lambda_1, \lambda_2, \lambda_3, \lambda_4, ..., \lambda_n$. Thus the HF wave-function can be written as

$$\psi = \prod_{i=1}^{n} b_i^\dagger \lambda_\lambda_1 \lambda_\lambda_2 \lambda_\lambda_3 \lambda_\lambda_4 \ldots \lambda_\lambda_n |0\rangle,$$

where $b_i^\dagger$ is the creation operator for a single particle state $\lambda$ and $|0\rangle$ is the vacuum state.

The single particle orbits are chosen in such a way so as to minimize the HF energy

$$E_{HF} = \langle \phi|H|\phi\rangle = \sum_{\lambda\phi} \langle \lambda|T|\lambda\rangle + (1/2) \sum_{\lambda\mu\phi} \langle \lambda\mu|V|\lambda\mu\rangle.$$

Now in order to find the orbits $\lambda$ they are to be expanded in terms of complete orthonormal set of known single particle wave functions $|i\rangle$, i.e.,

$$|\lambda\rangle = \sum_i c_i^\lambda |i\rangle$$

and

$$b_i^\dagger = \sum_i c_i^\lambda a_i$$

The condition of Hartree-Fock energy minimization can be expressed as

$$\frac{\delta}{\delta c_i^\lambda} [E_{HF} - e_\lambda (\sum_j |c_j^\lambda|^2 - 1)] = 0,$$
where $e_a$ is a Lagrange multiplier. Putting the value of $E_{HF}$ from (3.5), in the equation above, we get
\[
\sum_j \langle i|T|j \rangle + \sum_{\lambda \phi} \langle i|V|j \lambda \rangle |c_j^\lambda|^2 = e_a |c_i^\lambda|^2.
\] (3.9)

Equation above is equivalent to an eigen value problem and the HF orbits are the eigen functions of the Hamiltonian $H$
\[
H|\lambda\rangle = e_\lambda |\lambda\rangle,
\] (3.10)

Where $H$ is given by
\[
\langle i|H|j \rangle = \langle i|T|j \rangle + \sum_{\lambda \phi} \langle i|V|j \lambda \rangle.
\] (3.11)

### 3.2.1 The Angular Momentum Projection

A given deformed intrinsic Hartree-Fock state $|\Psi_K\rangle$ is a superposition of various good angular momentum ($J$) states
\[
|\Psi_K\rangle = \sum_{j} \alpha_j^K |\Psi_{JK}\rangle,
\] (3.12)

where $|\Psi_{JK}\rangle$ are the states with good angular momentum ($J$) and are projected out using the projection operator, given by
\[
P_{JM} = \frac{2J+1}{8\pi^2} \int d\Omega \ R_{JK}^M (\Omega) R(\Omega).
\] (3.13)

Here $R(\Omega)$ is the rotation operator ($e^{-iaJ_z}e^{-ibJ_y}e^{-icJ_x}$) and $\Omega$ stands for the Euler angles $(\alpha, \beta, \gamma)$. For intrinsic states with axial symmetry, two of the Euler angles $\alpha, \gamma$ are integrated out and we are left with the integrals for the kernels of Euler angle $\beta$.

The projection operator has the following properties
\[
P_{KM}^J P_{JM}^K = P_{MK}^J P_{JM}^K = P_{JK}^J.
\] (3.14)

For axial symmetry, we can evaluate the matrix elements overlap of various tensor operators (one body operators) such as quadrupole moment, angular momentum operators and the two body operator $V$, using the wave functions obtained by the projection operator. For the Hamiltonian the overlap is
\[
H_{K_1K_2}^J = \langle \Psi_{K_2}^J|H|\Psi_{K_1}^J \rangle = \frac{2J+1}{2} \frac{1}{(N_{K_1K_1}^J N_{K_2K_2}^J)^{1/2}} I_1,
\] (3.15)
where

$$I_1 = \int_0^\pi d\beta \sin \beta d^J_{iK_1K_2}(\beta) < \Phi_{K_1} | H e^{-i\beta J_1} | \Phi_{K_2} >$$  \quad (3.16)$$

and

$$N_{K_1K_2}^J = \frac{2J + 1}{2} \int_0^\pi d\beta \sin \beta d^J_{iK_1K_2}(\beta) < \Phi_{K_1} | e^{-i\beta J_1} | \Phi_{K_2} >$$  \quad (3.17)$$
is the amplitude overlap for angular momentum \(J\). For the tensor operator \(T^L\) of rank \(L\),

Figure 3.1: The prolate deformed Hartree-Fock orbits for protons and neutrons of \(^{122}\text{Cs}\).
3.3 The Cranked Hartree-Fock Bogoliubov Model (CHFB)

the reduced matrix elements are given by

\[ < \Psi_{K_1}^{j_1} | T^L | \Psi_{K_2}^{j_2} > = \frac{1}{2} \frac{(2j_2 + 1)(2j_1 + 1)^{1/2}}{(N_{K_1}^{j_1}, N_{K_2}^{j_2})^{1/2}} \sum_{\mu \nu} C_{\mu \nu}^{j_1 j_2} I, \]  

(3.18)

where

\[ I = \int \limits_0^\pi \sin(\beta) d_\mu d_{\nu K_2} \langle \beta \rangle < \Psi_{K_1} | T^L e^{-i\beta j_s} | \Psi_{K_2} > \]  

(3.19)

with \( T^L \) as the symbol of electromagnetic operators \( E2, M1 \) etc. and \( K_1, K_2 \), the axial quantum numbers.

The Hamiltonian and kernels of various quantities are calculated with 64-points Gauss-Legendre quadrature formula. In general, two states \( | \Psi_1^{JM} > \) and \( | \Psi_2^{JM} > \), projected from two intrinsic configurations \( | \Phi_{K_1} > \) and \( | \Phi_{K_2} > \) are not orthogonal to each other. So wherever necessary, we orthonormalise them and then diagonalised using the equation

\[ \sum_{K'} (H_{KK'}^J - EN_{K'}^J) C_{K'}^J = 0. \]  

(3.20)

Here \( C_{K'}^J \) is the orthonormalised amplitude, which can be identified as the bandmixing amplitudes. As a typical example the prolate HF orbits for protons and neutrons of \( ^{122}\text{Cs} \) (27 active protons and 39 neutrons) of are shown in figure 3.1. Intrinsic configurations with the odd proton and neutron were considered and the rest of the active 26 protons and 38 neutrons are in the lowest time-reversal symmetric proton and neutron orbits. The calculations are performed with all these active nucleons.

3.3 The Cranked Hartree-Fock Bogoliubov Model (CHFB)

Among the theoretical models used to describe the high spin states in nuclei, the Cranked Hartree-Fock Bogoliubov Model is most widely used model in present nuclear structure research which is based on the cranked shell model (CSM), given by D. Inglis in 1954 [11, 12]. The CSM model is already discussed in chapter 1. The total Hamiltonian is given by

\[ H = H_{\text{cranking}} + H_{\text{residual}}, \]  

(3.21)
where $H_{\text{cranking}}$ is the cranking Hamiltonian i.e. the single particle Hamiltonian in the rotating frame and $H_{\text{residual}}$ is the Hamiltonian of the two body residual interaction.

In terms of second quantization the cranking Hamiltonian takes the following form

$$H = \sum_{ij} [(|i\rangle|H_0(j)\rangle a_i^+ a_j - \omega(|i\rangle|J_0(j)\rangle a_i^+ a_j)],$$  \hspace{1cm} (3.22)

where the operators $a_i^+$ and $a_i$ are the creation and annihilation operators respectively and the summation runs over all the basis states (eigen states) of $H_0$. The $H_{\text{residual}}$, on the other hand includes the individual nucleon-nucleon interaction. Here this two body interaction is considered as the pairing interaction between the nucleons. The strength of this pairing interaction between the nucleons is strongest when the two nucleons are exactly in the time-reversed orbits. This situation is called monopole pairing [13] and is the most common type of pairing found in the nuclei. Therefore monopole pairing is taken in this model. The Hamiltonian corresponding to this interaction is

$$H_{\text{residual}} = H_{\text{pair}} = -G \sum_{ij} a_i^+ a_i a_j a_j^+, \hspace{1cm} (3.23)$$

where $a_i a_j$ annihilates a pair of particles in the time reversed states $|j\rangle$ coupled to $J = 0$ and $|j^-\rangle$ and $a_i a_i^+$ creates a pair of particles in the time-reversed states $|i\rangle$ and $|i^-\rangle$ coupled to $J = 0$. The constant $G$ indicates the strength of the monopole pairing and is positive. The magnitude of $G$ is larger for high-$j$ orbitals and it depends on the spatial overlap of the two nucleons. Its strength decreases with mass as in heavier nuclei the outer nucleons are further apart. The strength is also lower for protons than for the neutrons because of the Coulomb repulsion between the paired particles. For protons and neutrons its strength can be estimated [14] from

$$G_p = \frac{17.9 + 0.176 (N - Z)}{A} \text{MeV}, \hspace{1cm} G_n = \frac{18.95 - 0.078 (N - Z)}{A} \text{MeV}. \hspace{1cm} (3.24)$$

The process of annihilation of pair of particles in one state and their creation in another state involves a change of energy, which must be included in the Hamiltonian. If the energy increase per particle is denoted by $\lambda$ (also called chemical potential), and $\hat{N}$ is the
3.3 The Cranked Hartree-Fock Bogoliubov Model (CHFB)

particle number operator, then

\[ H_{\text{residual}} = H_{\text{pair}} - \lambda \hat{N}. \]  

(3.25)

Now, the kind of two body interaction given by (3.23) can not be used straightway along with one body wave functions obtained by solving the cranking Hamiltonian. Therefore the above two-body interaction Hamiltonian has to be reduced to one body Hamiltonian [15]. This is approximated in the following way

\[ H_{\text{residual}} = H_{\text{pair}} \approx - \Delta \sum_i (P_i^+ + P_i), \]  

(3.26)

where,

\[ \Delta = G(\langle 0|P|0 \rangle) \]  

(3.27)

is the pairing gap parameter, while \(|0\rangle\) is the quasi-particle vacuum or ground state. In this approximation \(H_{\text{pair}}\) contains the product of two creation and two annihilation operators which are treated separately. This is contrary to the exact case where the pair annihilation and creation is treated simultaneously. So as a consequence of this approximation, the particle number is not conserved corresponding to particle transfer from one state to another. In the calculations this particle number conservation is achieved with the help of chemical potential. For doing this, the chemical potential is treated as a Lagrange multiplier (- \(\lambda\)), and is varied in such a way so that the particle number operator equals the correct particle number, i.e.,

\[ \langle \tilde{0}|\hat{N}|\tilde{0} \rangle = N. \]  

(3.28)

Thus the total Cranked Hartree Fock Bogoliubov Hamiltonian can be written as

\[ H = H_0 - \omega J_x - \Delta(P^+ + P) - \lambda N \]  

(3.29)

which on expansion in terms of matrix elements, takes the form as below

\[ \begin{pmatrix} 
<i|\hat{h}_0|j> - \lambda \delta_{ij} - \omega <i|\hat{J}_x|j> & \Delta <i|P^+ + P|j> \delta_{ij} \\
\Delta <i|P^+ + P|j> \delta_{ij} & - <i|\hat{h}_0|j> + \omega \delta_{ij} + \lambda <i|\hat{J}_x|j> 
\end{pmatrix}. \]  

(3.30)

Here the dimension of the matrix is doubled as after the inclusion of pairing, the hole states also come in picture along with the particle states. In the calculation process...
pairing gap parameter $\Delta$ and the particle number $N$ are obtained self consistently by iteration process at every rotational frequency. In the above Hamiltonian matrix, each matrix element is found separately and once all the matrix elements of HFBC Hamiltonian are calculated then one can diagonalize the matrix to find eigen values as well as the eigen functions of the system. The eigen values so obtained will be the Routhians for the given value of the rotational frequencies.

### 3.4 The Quantities obtained

From these calculations the following physical quantities are obtained:

1. Quasi-particle Routhian
2. Single particle alignments and total alignments
3. Total Routhian Surface

#### 3.4.1 Quasi-particle Routhian

The eigen values of HFBC Hamiltonian for a given deformation are known as quasi-particle Routhians. The experimental Routhians are calculated from the experimental data and compared with them so as to finalize which configuration is actually responsible for the band found experimentally. The quasi-particle Routhians for proton and neutron calculated for $^{122}$Cs nucleus are shown in figure 3.2.

#### 3.4.2 Particle alignments

As defined in chapter 1 the total cranking Hamiltonian can be extended for all of the independent particles of the system and is given as

$$H_{HFBC} = H_0 - \hbar \omega J_z. \quad (3.31)$$

The eigen values of the cranking Hamiltonian, which are also called the total Routhians, can be defined as

$$e_\nu = \langle \nu' | H'' | \nu'' > = \langle \nu' | H_{int} | \nu'' > - \omega \langle \nu' | J_z | \nu'' > (3.32)$$
Figure 3.2: Single quasi-particles Routhians as a function of the rotational frequency calculated at the shape parameters obtained from the TRS calculation ($\beta_2 = 0.27, \beta_4 = 0$ and $\gamma = 0$), appropriate for $^{122}$Cs, (a) for protons and (b) neutrons. The parity and the signature ($\pi, \alpha$) of the levels are solid lines (+, +1/2), dotted lines (+, -1/2), dashed lines (-, -1/2), dot-dashed lines (-, +1/2). Here quasiparticle levels A, B, C etc. for protons and a, b, c etc. for neutrons.
which implies that
\[
\frac{de}{d\omega} = -\langle \nu^x J_x | \nu^x \rangle = i_\omega
\] (3.33)
i.e. the slope of the single particle Routhian is the alignment of given orbital \(i_x\). Any change in the alignment of one or more of the orbitals will lead to change in the aligned angular momentum of the system.

### 3.4.3 Total Routhian Surfaces

A certain type of theoretical calculations can predict energy of the nucleus as a function of the deformation parameters, the rotational frequencies, the parity of the single-particle configuration and signature (additional quantum number). Such calculations are called Total Routhian Surface (TRS) calculations [16-18]. In these calculations, the total energy for a given nucleus and configuration is calculated for a range of \(J_32\) and \(J_7\) using,

\[
E_{\text{total}}(Z, N, J_\beta) = E_{\text{macro}}(Z, N, J_\beta) + E_{\text{micro}}(Z, N, J_\beta),
\] (3.34)

where \(J_\beta\) denotes the deformation parameters \((J_32, J_7)\) required to completely define the nuclear surface and \(E_{\text{macro}}(Z, N, J_\beta)\) is the energy of the nucleus calculated using Liquid Drop Model with original parameters, while the microscopic part of the energy, \(E_{\text{micro}}\), depends on the single-particle motion of individual nucleons near the Fermi surface and is formed of two parts. One part is the shell correction energy in the absence of a residual pairing interaction, \(E_{\text{shell}}\), while the other part is the pairing energy, \(E_{\text{pair}}\). Both \(E_{\text{shell}}\) and \(E_{\text{pair}}\) depend strongly on the number of quasi-particles. The shell correction energy is calculated by Strutinsky method [19] (section 3.4.4) using deformed Wood-Saxon single particle potential [20] while the pairing energy is calculated using BCS formalism, taking into consideration the monopole pairing interaction whose strength is determined using the average gap method [21]. Once all these energies are obtained, the total energy is minimized with respect to the deformation parameters \(J_\beta\) and the equilibrium deformation corresponding to the minimum energy is obtained. The TRS calculated by this procedure for a set up of \(J_32\) and \(J_7\) values in a \(J_3 - J_7\) plane would tell the minima of TRS values which correspond to the stable shapes of the nucleus. As an example, figure 3.3 displays a TRS plot for ground state band in \(^{127}\)Cs nucleus at a rotational frequency of 0.0 MeV.
3.4 The Quantities obtained

Figure 3.3: The TRS plot for $^{122}$Cs nucleus, calculated at a rotational frequency $\hbar\omega = 0.0$ MeV.

The TRS values calculated for large number of points in a $\beta - \gamma$ plane are thus used to form a contour plot.

3.4.4 The Shell corrections

The Liquid Drop Model (LDM) describes the bulk properties of nuclei by taking account of the volume, Coulomb repulsion, surface area, symmetry (neutron to proton ratio) and pairing. However, although this empirical model can reproduce the average properties of most nuclei, there are significant deviations from this near closed shells where the LDM underestimates the binding energy. It is therefore necessary to include a correction that takes account of this phenomenon in order to accurately calculate, for instance, ground-state masses as the differences can be more than 10 MeV. Near a closed shell the level density at the Fermi surface is very low and this leads to extra binding energy. Qualitatively this is because the nucleons are occupying 'deeper' orbitals. The shell effects can therefore be thought of as arising from fluctuations in the level density around the
Fermi surface. The method for incorporating these effects is called the Strutinsky shell correction [18]. The shell correction energy to the LDM energy in (3.34) is

$$E_{\text{shell\text{-}correction}} = -2 \int_{-\infty}^{\mu} g(\varepsilon) \varepsilon d\varepsilon$$

(3.35)

Where $g(\varepsilon)$ is the mean energy density of the single-particle states at energy $\varepsilon$ and given by

$$g(\varepsilon) = \sum_i \delta(\varepsilon - \varepsilon_i).$$

(3.36)

Here $\delta(\varepsilon - \varepsilon_i)$ is the Dirac $\delta$-function.

The Fermi energy, $\mu$, corresponding to $g(\varepsilon)$ is determined from

$$n = 2 \int_{-\infty}^{\mu} g(\varepsilon) d\varepsilon$$

(3.37)

such that the total number of particles, $n$, is conserved [18].

3.5 Conclusion

In this chapter, the two theoretical models based on the mean field approximation of the nuclear potential have been discussed. Both these models have been used to getting the structural information of the nuclei considered in the present work. The various nuclear structure quantities calculated with both the models have been discussed along with their description.
Bibliography


