Chapter 3

Theoretical Models

3.1 Introduction

As we have discussed in Chapter 1 that the nucleus is a many-body system of interacting fermions and therefore, an exact description of the nucleus is not possible. Among different approximations successful for developing a model for nucleus, the mean field approximation is the most popular one. Here each nucleon is treated to be independently moving under a potential which is an average interaction generated by all other nucleons in the nucleus. The shell model dwells upon this approximation and this one has been successful in explaining the extra-stability of some nuclei having magic numbers of protons and/or neutrons. Moreover, this model continues to be the most popular for the description of nuclei close to the shell closures. As we will be dealing with the nuclei near the $N = Z = 28$ shell gap, we would like to describe this model in somewhat detail in the next section.

However, as one looks at the nuclei away from the shell gap, the valence nucleons outside the magic core collaborate in a coherent fashion to generate a collective motion in nuclei, such as nuclear rotation, which has been already described in Chapter 1. To describe the nuclei of this (rotational) type, a phenomenological model was first proposed by Nilsson [1], where he calculated the single particle energies in a deformed harmonic oscillator potential well. These calculations have been modified in recent years [2] by including hexadecapole deformation, pairing and Coulomb term and using different forms of potential energy, e.g., the deformed Woods-Saxon
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potential. Therefore, in the subsequent chapters we would also like to describe the Cranked Shell Model (CSM) - one of the collective models, which has been used to interpret the results of the data during the course of this work.

3.2 The Shell-Model

3.2.1 Theory of Shell-Model

The shell-model approach played a fundamental role in early understanding of atoms and nuclei; in nuclear physics in particular, it has provided us with our best understanding of the sd shell nuclei. To this day, it still remains a fundamental approach in nuclear physics and is considered a fundamental theoretical starting point in the derivation of most models applying to larger nuclei. The basic assumption of the nuclear shell-model relies on the point that each nucleon in a nucleus moves in an independent fashion under an average potential. This is indicative of the fact that the nucleons could move in an unperturbed orbit due to the Pauli exclusion principle. Each quantum state is then defined by a radial quantum number \( n \), orbital quantum number \( l \), and total angular momentum quantum number \( j \). To calculate the various properties of the nucleus in any of its allowed states, one should obtain the wavefunctions of the states, which are the eigenfunctions of many-body Shroedinger equation:

\[
H \Psi(r) = E \Psi(r) \tag{3.1}
\]

where, \( \Psi \) are the solutions of the Schroedinger one-body equation, and the Hamiltonian of this system is given by:

\[
H = \sum_i T_i + \sum_{i<j} V_{ij} \tag{3.2}
\]

where, \( T_i \) and \( V_{ij} \) are, respectively, the kinetic energy of the \( (i)th \) nucleon and \( n-n \) two-body potential energy for all the possible pairs of nucleon. This Hamiltonian is shown to be equivalent to a sum of one-body potential \( (H_o) \) and a residual interaction \( (H_{res}) \):

\[
H = H_o + H_{res} \tag{3.3}
\]
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Here $H_0$ acts as an average potential wherein all the nucleons move independently. The Harmonic oscillator or Woods-Saxon potential is taken into consideration for $H_0$, whereas for the residual part ($H_{\text{res}}$) it is the perturbation on the system of independent motion in the average field. There also exist a spin-orbit term ($\hat{I} \cdot \hat{s}$) and an $(\hat{I}^2)$ term in $H_0$. The eigenvalue ($E_0$) of the unperturbed Hamiltonian ($H_0$) is then defined by:

$$H_0 \Psi(r) = E_0 \Psi(r) \quad (3.4)$$

and

$$E_0 = \sum_i \epsilon_i \quad (3.5)$$

where, the single particle energy, $\epsilon$, is the eigenvalue of the Schroedinger equation:

$$(T + V_0)\Psi(r) = \epsilon \Psi(r) \quad (3.6)$$

The presence of the residual interaction then brings the mixing of the unperturbed wavefunctions, which in terms, gives a correction term in the total unperturbed energy. This is obtained by diagonalizing the matrix of some dimension, depending on the number of the single-particle levels in the calculation, which brings the limit in computing capability.

In the calculation one assumes that the valence nucleons occupy a selected set of single particle orbitals (called a model space), outside a closed and inert core. Assuming that all the properties of the nucleus are governed by the valence nucleons only, one then diagonalises the Hamiltonian with a suitable choice of two-body residual interaction. The results of the shell-model calculations are crucially dependent on the model space and the choice of the form of the two-body interaction. Generally, there are several ways for an appropriate choice of residual interaction. One of them, which we used during our calculations, is based on the schematic assumption that the residual two-body interaction is of simple radial form [3]. The often used potentials are the Yukawa or the Gaussian type. The main advantage of this is that it leads to a rather simple calculation to compute the effective interactions. Further, the strengths and the ranges of these potentials could be adjusted to produce a best fit to the experimental information. The choice of Delta or the Modified Surface Delta (MSD) interaction are often used for this type of interaction.
3.2.2 Shell-Model Code: OXBASH

The present day shell model calculations are an extension of the original shell model by Mayer and Jensen, which assumed a single configuration for single nuclear level, corresponding to a nucleon in a single particle orbit. The modern calculations are based on many or all of the multinucleon configurations, assuming the valence nucleons occupy the available orbits outside the inert core. There are three approaches for such a calculation:

1. ***j-scheme*** has the multiparticle basis vectors, which are constructed to satisfy a good total angular momentum, \( \vec{J} \), and isospin, \( \vec{T} \). This has the demerit of complex angular-momentum-coupling algebra associated with it.

2. ***m-scheme*** has an algorithm of the basis, using 1 or 0, to represent an occupied or unoccupied orbit. It has the advantage of not performing any complex angular-momentum algebra, but has the disadvantage of increasing dimension of the matrices with the increase of particle number.

3. **Projection Scheme** builds the basis states in the m-scheme and then uses j-scheme to compute the Hamiltonian matrix. The major disadvantage of this scheme is the difficulty in transition from m-scheme to j-scheme.

The flow chart of the OXBASH (Oxford-Buenos Aires Shell Model) code is shown in Fig. 3.1, which is based on the projection scheme. It generates the basis states in m-scheme and then computes the matrix in the j scheme. Therefore, it bypasses the complication of the angular momentum algebra in \( j - j \) coupled basis and also avoids the huge matrix dimension generated during m-scheme. The OXBASH code consists of seven main programs and some supporting codes, which we would briefly mention here.

- **BASIS** generates an m-scheme Slater determinant-basis for a particular number of nucleons and for a particular \( J_z \) and \( T_z \). The data file with an extension \'.sps' contains already the information of the single particle states, from which the multi-particle basis are generated with the use of Slater determinants and occupation number.
Figure 3.1: The schematic of the sequence in which the OXBASH code run. The extension of the files are given which are required to run the computer code immediately after the previous one. The '.sps' file is needed by all the programs, therefore, not being mentioned in the diagram.

- **PREDICT** is used to produce a subset out of the multi-basis states generated by the BASIS.

- **PROJ** runs to generate basis states of good spin and isospin quantum number. Here a set of orthonormal basis vectors are then produced out of good spin and isospin vectors.

- **MATRIX** then constructs the Hamiltonian matrix taking outputs from the PROJ and for this matrix formation an operator file ('*.op') is required containing the single-particle energies and the two-body $m$-scheme matrix elements. OPER program generates this file.
• **LANCZOS** is then used to diagonalize the Hamiltonian, which gives some lowest eigenvalues and eigenvectors.

• **MVEC** program then converts the eigenvectors in terms of \( m \)-scheme basis. Different spectroscopic factors are then easily calculated, after one gets the eigenvalues and eigenvectors.

• **TRAMP** is needed to calculate percentage amplitudes, one- and two-body transition densities.

• **TRANS** could also be used just after **MVEC** to calculate electromagnetic moments, transition rates, occupation number etc.

• **SHELL** is the program which formulates a batch file to correctly run all the programs and to make an appropriate connectivity between the type of interaction and the model space.

### 3.2.3 Calculation with OXBASH

The orbits involved near \(^{56}\text{Ni}\) are the \(1f_{7/2}\) orbit below and the \(2p_{3/2}, 1f_{5/2}, 2p_{1/2},\) and \(1g_{9/2}\) (upper \(fp\) shell) orbital above the \(N, Z = 28\) shell gap. For this so-called full \(fp\) model space several parameter sets exist, namely the **FPPN**, **FPVPN** and the **A80PN** [3]. We used the **A80PN** [3] parameter set for the two-body residual interaction. Here the matrix-elements were obtained from the modified surface delta interaction (MSDI) and from a least squares fit to experimental binding and excitation energies (ASDI). Employing the rapidly increasing computer power, many nuclei could recently be well explained by the large-scale full \(fp\) shell-model calculations [4, 5, 6].

There exists two mechanism for the generation of the observed higher angular momentum states in these nuclei, which we have described in the earlier chapter. For that a shell-model space with large basis states are not feasible due to large dimensionality of the matrices. Unfortunately, the current computational limit for calculations in the full \(fp\) configuration space are mass \(A = 52\) nuclei [7] with basis dimensions in excess of 100 million states. Therefore, the configuration space for
calculations in the vicinity of $^{56}\text{Ni}$ must be truncated at present [8]. However, it should be mentioned that more recent developments try to make a detour around the problems associated with such large dimensions in the model space by tracing the most significant components via Monte-Carlo methods, such as, Shell-Model Monte-Carlo (SMMC) [9], and Quantum Monte-Carlo Diagonalization (QMCD) [10, 11]. Due to this computational difficulties, we have performed the calculations within a truncated model space.

Before we setup our truncation scheme, we define a partition, which is eventually a set of occupancies for the orbits under consideration. For $^{62}\text{Cu}$, for example, taking $^{56}\text{Ni}$ as an inert core, we can define a partition in the $A80PN$ model space as

$$P = \{ \pi\{(f_{5/2})^0, (p_{3/2})^0, (p_{1/2})^0, (g_{9/2})^1\}; \nu\{(f_{5/2})^2, (p_{3/2})^1, (p_{1/2})^1, (g_{9/2})^1\} \}$$

where we restrict the valence proton and one valence neutron in the $g_{9/2}$ orbital, and so on.

When the calculations are performed within this large model space, large number of partition (i.e. configurations) may arise as a result of all possible distribution within different orbitals. Such unrestricted calculations lead to the restriction on the computational capability, as it requires huge memory in computer for diagonalizing the matrix. Therefore, the model space could internally be truncated including only those configurations, which contribute dominantly in the calculations. If we could make a correct guess of the dominant configurations, then it would substantially reduce the computing time, thereby, also differing slightly from the unrestricted calculations. Here our truncation scheme is very similar to the one devised by Kabadiyaski et al. [12], except the fact that the number of partitions chosen are mainly governed by the existing computational limitations. The main advantage of this scheme is that since we choose only the most dominant configurations for a particular state, we need not renormalize the two-body residual interaction to include the effect of the avoided configurations, which are small with respect to the dominant ones. The only demerit of this scheme is that we may have to initially guess the most dominant configurations.
3.3 Cranked Shell Model

In order to describe the rotational behavior of a deformed nucleus, one has to modify the Nilsson model Hamiltonian to a deformed rotating potential. This is achieved in the Cranked Shell Model (CSM) through the inclusion of a term of the form $\omega j_x$ in the Hamiltonian which rotates a deformed symmetric nucleus with a frequency $\omega$ perpendicular to its symmetry axis (generally the assumed $z$-axis). This term is the well known expression in classical mechanics for the inertial forces, the Coriolis and the Centrifugal. Under the influence of these inertial forces, the time reversal symmetry is broken as the wavefunction of a particle is different depending on whether it is moving in the direction or in the counter direction of rotation of the nucleus. Therefore, for a rotating deformed nucleus, all the degeneracy of the single particle are removed. The parity still continues to be a good quantum number which is related to the reflection symmetry of the nuclear potential. One more symmetry is, however, related to the invariance of nuclear potential under a rotation of $\pi$ around an axis perpendicular to the symmetry axis. This constant of motion is called the signature ($\alpha$) and is defined as:

$$e^{-i\pi j_x} |\pi \alpha \rangle = e^{-i\pi \alpha} |\pi \alpha \rangle$$  \hspace{1cm} (3.7)

The rotation of $2\pi$ gives a $-ve$ sign to the wavefunction, therefore,

$$e^{-i2\pi \alpha} = -1 = e^{\pm i\pi}$$  \hspace{1cm} (3.8)

and therefore, $\alpha = \pm 1/2$. As the system has a $4\pi$ symmetry, states having a total angular momentum differing by $2\hbar$ have the same signature. That means, for odd-$A$ nuclei $\alpha = 1/2$ corresponds to states with spin, $I = 1/2, 5/2, 9/2, \ldots$ and $\alpha = -1/2$ corresponds to $I = 3/2, 7/2, 11/2, \ldots$ while for even-even or odd-odd nuclei $\alpha = 0$ corresponds to states with $I = 0, 2, 4, \ldots$ and $\alpha = 1$ for $I = 1, 3, 5, \ldots$. The inertial forces, therefore, group the states in two signature partners depending on the values of their angular momenta.

However, experimentally it is the total angular momentum ($\bar{I}$) and not the frequency $\omega$ which is measured. Therefore, the connection between the observables, $E, I$, and $\omega$ can be established following the Fig. 3.2, which shows a vector diagram
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Figure 3.2: The schematic of the angular momentum coupling of a rotationally aligned nucleon having angular momentum \( j \), in an axially symmetric nucleus rotating with angular momentum \( \bar{R} \) about an axis (X) perpendicular to the symmetry axis.

illustrating the angular momentum coupling of a rotationally aligned nucleon with angular momentum \( \vec{j} \) in an axially symmetric nucleus. Here \( i_x \) is the component of the total angular momentum along the rotational axis (also known as aligned angular momentum) and \( \Omega \) is the projection of \( \vec{j} \) on the symmetry axis. the algebraic sum of \( \Omega \)'s (for more than one aligned nucleons) is defined as \( K \). The aligned angular momentum is then defined as:

\[
I_x(I) = \sqrt{(I + 1/2)^2 - K^2}
\]  
(3.9)

The frequency of rotation about x-axis is classically given by:

\[
\omega = \frac{dE}{dI_x}
\]  
(3.10)

following which the frequency of the nuclear rotation is given by:

\[
\hbar \omega = \frac{E(I + 1) - E(I - 1)}{I_x(I + 1) - I_x(I - 1)}
\]  
(3.11)
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It should be noted that for quadrupole transitions with \( \Delta I = 2 \) and \( K \) small compared to \( I \), the above equation reduces to \( \hbar \omega = E_\gamma / 2 \), where the gamma ray energy \( E_\gamma = E(I + 1) - E(I - 1) \).

The rotational spectrum of a deformed nucleus also allows the evaluation of the moments of inertia of the nucleus. The kinematical moment of inertia is defined by:

\[
J^{(1)} = \frac{I_x}{\omega}
\]  
(3.12)

and the dynamic moment of inertia by:

\[
J^{(2)} = \frac{dI_x}{d\omega}
\]  
(3.13)

These quantities are evaluated from the level scheme in the following way:

\[
J^{(1)}(\omega) = \frac{(2I - 1)}{E_\gamma(I \rightarrow I - 2)}
\]  
(3.14)

\[
J^{(2)}(\omega) = \frac{4}{\{E_\gamma(I \rightarrow I - 2) - E_\gamma(I - 2 \rightarrow I - 4)\}}
\]  
(3.15)

### 3.3.1 CSM Formalism

The Cranked Shell Model (CSM) is the most widely used phenomenological model for a rotating nucleus, which is described in the literature [13] in detail. Therefore, we will briefly survey the basic features of this model before we start showing how to use it with experimental data for comparison. This model describes independent particle motions in a rotating nucleus with both static deformation and pairing fields. The calculations are performed in the body-fixed frame of the nucleus which is a rotating frame of reference. Therefore, the inertial forces are present in the body-fixed frame which influence the nucleonic motion. The formalism of the model used in the present work is given by Bengston and Fraundorf [13]. The Hamiltonian for an axially symmetric nucleus in a rotating body fixed frame is given by:

\[
H = H_o - \omega J_x
\]  
(3.16)

where \( H_o \) is the single particle Hamiltonian which is the Woods-Saxon potential [2] in the present model. Here \( X \)- and \( Z \)-axis are the rotation and symmetry axis, respectively, thus ensuring the collective rotation.
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Since the single particle wavefunctions are not eigenfunctions of $J_z$, the rotation leads to a mixing of the single particle states. However, the signature and parity remain good quantum numbers. The eigenvalues of $H$ can be defined as:

$$e = \langle \mu | H | \mu \rangle = \langle \mu | H_0 | \mu \rangle - \omega \langle \mu | J_x | \mu \rangle \quad (3.17)$$

which implies that

$$\frac{de}{d\omega} = - \langle \mu | J_x | \mu \rangle \quad (3.18)$$

This means that the slope of the single particle energies as a function of rotational frequency is a measure of aligned angular momentum in the body fixed frame. The pairing correlation can be introduced by including an additional term in the Hamiltonian. In terms of creation and annihilation operators, the new Hamiltonian stands like:

$$H' = \sum_{ij} \{ H_0 a_i^+ a_j - \omega J_z a_i^+ a_j \} - \sum_{i > j} G a_i^+ a_j^+ a^*_j a^*_i \quad (3.19)$$

where $G$ is the pairing strength. The summation runs over all the considered basis states for the first and the second term but for the last term runs only over one half (indicated by $>$) of the energetically degenerate time reversed states. The pairing term is linearized as:

$$H_{pair} = -G < P > \sum_{i > j} (a_i^+ a_j^+ + a_i a_j) / 2 \quad (3.20)$$

where it is assumed that

$$< a_i^+ a_j^+ > = < P >= < a_j a_i > \quad (3.21)$$

The parameter $\Delta = \frac{G < P >}{2}$ is extracted from the experimental odd-even mass difference.

It should be noted here that the pairing Hamiltonian consists of two terms, which have a different structure than the one body terms in the Hamiltonian (3.19). To way out this problem, the nucleus is described by a double dimensional space which simultaneously contains both particle and hole states. To every particle state with energy $E_\mu$, there is a conjugate hole state with energy ($-E_\mu$) on the opposite side of the Fermi surface and if the particle state is occupied the hole state must
be unoccupied. The Fermi surface is defined for a vacuum configuration where all the hole states are filled. In this representation, a particle annihilation operator is equivalent to a hole creation operator and vice versa. Moreover, now the particles and holes will not be treated separately and will be collectively known as the quasiparticles and the quasiparticle energy as a function of rotational frequency will be termed as routhians.

Since the pairing term does not conserve the particle number, the Fermi energy ($\lambda$) term is introduced in the CSM Hamiltonian as a Lagrangian multiplier to the particle number $N$, thereby the complete look of the Hamiltonian becomes:

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

(3.22)

The eigenvalue problem is then formulated as:

$$ H|\alpha\mu> = E_{\alpha\mu}|\alpha\mu> $$

(3.23)

The solution is obtained numerically and the lowest eigenstate of $H(\omega)$ corresponds to the yrast state.

### 3.3.2 Calculation with CSM

In the present model, the absolute energy is not calculated, rather the energy is calculated with respect to a reference configuration. For example, for an even-even nucleus the reference configuration may correspond to the ground state band. At higher frequencies, where the +ve and -ve energy levels cross each other, the reference structure is considered as the continuation of the previous structure because its intrinsic structure is assumed to be changing smoothly in the crossing region. The prediction of this model can not be directly compared with experimental data as experimentally the energy of each state is obtained as a function of its angular momentum, whereas the CSM predicts the energy in the rotating frame with respect to a reference configuration as a function of rotational frequency. For deducing the experimental Routhian it is defined as:

$$ E'(I) = \frac{1}{2} [E(I + 1) + E(I - 1)] - \omega(I)I_x(I) $$

(3.24)
After transforming the variable from \( I \) to \( \omega \), the relative energy is defined as:

\[
e'(\omega) = E'(\omega) - E'_0(\omega)
\]  \hspace{1cm} (3.25)

where \( E'_0 \) is the reference configuration (normally defined as the ground state band of the nearest even-even nucleus). Similarly, the relative aligned angular momentum is defined as:

\[
i(\omega) = I_x(\omega) - I^*_0(\omega)
\]  \hspace{1cm} (3.26)

The ground state bands of even-even nuclei which are used as reference configurations, are often established for a limited frequency region and therefore, an extrapolation to higher frequencies is required. This is generally accomplished by fitting the moment of inertia of the low spin members of the ground state band to Harris formula [14].

\[
J = J_o + J_1 \omega^2
\]  \hspace{1cm} (3.27)

where \( J_o \) and \( J_1 \) are constants. Then,

\[
I^*_0(\omega) = (\omega J_o + \omega^3 J_1)
\]  \hspace{1cm} (3.28)

Since the reference configuration has only collective excitation, the relative quantities \( e' \) and \( i \) denote the quasiparticle energy and quasiparticle aligned angular momentum. With this background an experimental level scheme can be compared with the CSM predictions.

### 3.4 Conclusion

To conclude this chapter, we have discussed here the basic postulates of two models, which have been used to interpret our experimental data. The Shell-Model code **OXBASH** has been described in a way we have used it to interpret the nuclei nearby the double magic nucleus \(^{56}\text{Ni}\). The Cranked Shell Model is also described, prediction of which has been used for a direct or indirect comparison with observed level scheme.
Bibliography