PART II
1. THE HAMILTONIAN

1.1 Quasiparticle Treatment of the Shell-Model Hamiltonian:

In the second-quantised form, the usual shell-model hamiltonian $\mathcal{H}$ is given by

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}}$$

where

$$\mathcal{H}_0 = \sum_\alpha \varepsilon_\alpha c_\alpha \dagger c_\alpha$$

and

$$\mathcal{H}_{\text{int}} = \frac{1}{4} \sum_{\alpha \beta \gamma \delta} \langle \psi_\beta | \psi_\gamma \rangle \mathcal{A}_{\alpha \beta} c_\alpha \dagger c_\beta \dagger c_\delta c_\gamma$$

Here the Greek subscripts $(\alpha)$ designate all the quantum numbers $n, l, j, m$ of a single-particle shell-model states, while the Latin subscripts $(a)$ denote all the quantum numbers except the angular momentum projection quantum number $m$. Very frequently we shall also use $a, b, \text{etc.}$, to denote only the angular momentum quantum numbers, and the corresponding Greek letters $\alpha, \beta, \text{etc.}$, to denote only the respective projection quantum numbers. The occurrence of these symbols in phase factors, in dimension factors, or in angular momentum coupling coefficients will make it obvious wherever such practice is being adhered to. $c_\alpha \dagger$ and $c_\alpha$ are the single-particle creation and annihilation operators, respectively, and obey the usual fermion anticommutation rules

$$[c_\alpha \dagger, c_\beta]_+ = \delta_{\alpha \beta} c_\alpha \dagger c_\beta + c_\beta c_\alpha \dagger = 6 \delta_{\alpha \beta} ; [c_\alpha \dagger, c_\beta \dagger]_+ = [c_\alpha, c_\beta]_+ = 0$$
These operators are defined relative to the true (particle) vacuum \(|0_p\rangle\) which generally represents the ground-state of the closed shell nucleus such that

\[ C_\alpha |0_p\rangle = 0 \quad \text{for all } \alpha, \quad (1.3) \]

\(H_0\) is the sum of single-particle energies \(\epsilon_\alpha\), \(H_\text{int}\) is the residual two-body interaction, \(v\) is the two-body potential, and the label \(A\) denotes matrix elements with respect to antisymmetric states.

In spherical nuclei with partially filled shells, the most important effect of the two-body force is to produce pairing correlations. In order to take into account pairing correlations in the ground-state, the following transformation\(^3\) (known as Bogoliubov-Valatin transformation) is introduced by defining a new set of (quasiparticle) creation and annihilation operators as

\[ \alpha_\alpha^+ = U_\alpha C_\alpha^+ - S_\alpha V_\alpha C_\alpha, \quad (1.4a) \]

\[ \alpha_\alpha = U_\alpha C_\alpha - S_\alpha V_\alpha C_\alpha^+, \quad (1.4b) \]

where \(S_\alpha = (-1)^{\sigma_\alpha}\), and \(-\alpha\) is obtained by changing the sign of the magnetic quantum number of the state \(\alpha\). The transformation coefficients \(U_\alpha\) and \(V_\alpha\) are real and independent of the projection quantum number due to spherical symmetry and satisfy

\[ U_\alpha^2 + V_\alpha^2 = 1. \quad (1.5) \]

This follows from the requirement that the quasiparticle operators \(\alpha\)'s must satisfy the same fermion anticommutation relations (1.2)
as the operators \( C \)'s, \( \nu \) and \( \omega \) physically represent the occupancy and nonoccupancy probabilities for the state \( \alpha \). For a level far above the Fermi level, \( U_\alpha \approx 1, \nu_\alpha \approx 0 \) and the quasiparticle is the same as a particle. For a level far below the Fermi level \( U_\alpha \approx 0, \nu_\alpha \approx 1 \) and the quasiparticle is a hole. But for levels in the neighbourhood of the Fermi level, a quasiparticle is partly particle and partly hole and their admixture is determined by the coefficients \( U \) and \( V \).

These new operators are defined with respect to the new (quasi) vacuum, also known as the BCS ground-state \( \langle \phi \rangle \), such that

\[
\langle \alpha | \phi \rangle = 0 \quad \text{for all } \alpha.
\]  

(1.6)

In view of (1.5), the transformation (1.4a, 1.4b) is orthogonal, and hence the converse relations are

\[
\begin{align*}
C_\alpha &= U_\alpha \alpha_\alpha + S_\alpha \nu_\alpha \alpha_\alpha^\dagger \\
C_\alpha &= U_\alpha \alpha_\alpha + S_\alpha \nu_\alpha \alpha_\alpha^\dagger.
\end{align*}
\]

(1.7a, 1.7b)

Since the quasiparticle transformation (1.4) does not conserve the number of particles, the solutions obtained by the present method will not be normally applicable to any particular nucleus. Therefore, we have to introduce a chemical potential (Fermi-energy parameter) \( \lambda \) and instead of diagonalising \( H \), we diagonalise \( H \)

\[
H = H - \lambda N.
\]

(1.8)

The chemical potential has been introduced in view of this fact, and its value is fixed to make the expectation value of the total
Particle number operator \( \langle \phi | \mathcal{N} | \phi \rangle = \langle \phi | \sum_{\alpha} c_\alpha^+ c_\alpha | \phi \rangle \) equal to the number of nucleons (neutrons or protons) \( N \) in the unfilled major shell, we are dealing with. Thus \( \lambda \) enables us to apply this theory to the calculation of specific nucleus in an average sense.

The Hamiltonian \( H \) can be expressed in terms of quasiparticle operators in a straightforward way. The transformed Hamiltonian (after eliminating the dangerous terms) then becomes

\[
H = \mathcal{U} + \overline{H}_0 + \overline{H}_{\text{int}},
\]

where

\[
\mathcal{U} = \sum_{\alpha} \left[ \epsilon_\alpha - \lambda + \frac{1}{4} \sum_{\beta} \langle \psi_{\alpha}^{\dagger} | \psi_{\beta} \rangle A_{\alpha} \right] \overline{V}_{\alpha}
\]

\[
+ \frac{1}{4} \sum_{\alpha, \beta} \langle \psi_{\alpha}^{\dagger} | \psi_{\beta} \rangle \overline{V}_{\alpha} \overline{V}_{\beta}
\]

is the ground-state energy, and

\[
\overline{H}_0 = \sum_{\alpha} E_\alpha \mathcal{A}_\alpha^{\dagger} \mathcal{A}_\alpha
\]

is the independent quasiparticle Hamiltonian, while

\[
\overline{H}_{\text{int}} = \sum_{\alpha, \beta} \langle \psi_{\alpha}^{\dagger} | \gamma_{\beta} \rangle A_{\alpha} \mathcal{A}_\beta^{\dagger} \mathcal{A}_\gamma
\]

represents the residual interaction between quasiparticles. The symbol : denotes normal product of the fermion operators.

The quasiparticle energy \( E_\alpha \) appearing in Eq. (1.11) is given by

\[
E_\alpha = \left[ (\hat{\epsilon}_\alpha - \lambda)^2 + \Delta_\alpha \right] \overline{V}_{\alpha}
\]
where
\[ \hat{\varepsilon}_a = \varepsilon_a + \mu_a \]
is the single-particle shell-model energy corrected for the self-energy (or Hartree-Fock potential) \( \mu_a \)

\[ \mu_a = \sum \langle \alpha \beta | V | \alpha \beta \rangle A^a_b \tag{1.14} \]

the sum of the interaction energies of particle 'a' with all the others. The chemical potential \( \lambda \) and the energy gap parameters \( \Delta_a \) are obtained by solving the set of simultaneous equations (1.15) for all the single-particle states 'a':

\[ \Delta_a = \frac{1}{2} \sum \frac{[b]}{[a]} G(aabb\alpha) \frac{\Delta b}{E_b} \tag{1.15} \]
together with the number Eq.(1.16):

\[ N = \frac{1}{2} \sum [a] \left[ 1 - \frac{\hat{\varepsilon}_a - \lambda}{E_a} \right] \tag{1.16} \]

Here \([a]\) stands for \(2a + 1\) and \(G(abcdJ)\) is the antisymmetric two-body matrix element of \(\nu\) between angular momentum coupled states \(\langle ab|J\rangle\) and \(\langle cd|J\rangle\) and satisfies the following symmetry relations

\[ G(aabcdJ) = G(cdabJ) = -(-1)^{a+b-J} G(bacdJ) \]
\[ = (-1)^{c+d-J} G(abdcJ) = (-1)^{a+b+c+d} G(badcJ). \tag{1.17} \]

The coefficients \(U_a\) and \(V_a\) of Eq.(1.4) are obtained from

\[ U_a^2 = \frac{1}{2} \left[ 1 + \frac{\hat{\varepsilon}_a - \lambda}{E_a} \right] \tag{1.18a} \]
The values of \( \lambda, \Delta'5, E'5, \) and \( \sqrt{2}S \) for even Ni-isotopes corresponding to different effective interactions are already given in Table III of Part IB of this thesis.

The Eq. (1.16), strictly speaking, applies to an even number of nucleons, as the right hand side is the expectation value of the total number operator in a state of no quasiparticles (i.e., BCS vacuum). For an odd-mass nucleus, the expectation value has to be taken in the state of single quasiparticles. As a result the right hand side of Eq. (1.16) has an extra term

\[
\frac{\hat{1}_b - \lambda}{E_b} \tag{1.19}
\]

where \( b \) is the single quasiparticle state under consideration. The resultant solutions for \( \lambda \) and \( \Delta'5 \) will thus depend on the quasiparticle states. It has been seen by actual numerical computation in the case of odd-mass Ni isotopes that the effect of this extra term makes a very small difference in \( \lambda \) and \( \Delta'5 \).

1.2 Independent Quasiparticle Hamiltonian:

In the independent quasiparticle approximation, i.e., neglecting \( \hat{H}_{\text{int}} \) completely, each excited state is specified by what
quasiparticles it contains, and its excitation energy is the sum of the corresponding E's. It appears from the nature of the Bogoliubov-Valatin transformation, however, that a system containing an even number of particles can only contain an even number of quasiparticles, and similarly odd particle numbers go with odd quasiparticle numbers. So the ground-state of an even nucleus is the quasi-vacuum; the excited states are obtained by exciting 2, 4, ..., etc. quasiparticles. The minimum energy for two quasiparticles will be $2 \Delta$. To get these excited correctly one has to diagonalise $\hat{H}_{\text{int}}$ in the space of 2, 4, ..., etc., quasiparticles. To obtain the collective one-phonon state one diagonalises $\hat{H}_{\text{int}}$ in the space of two quasiparticles, while for two-phonon states one has to diagonalise $\hat{H}_{\text{int}}$ in the space of two and four quasiparticles; the mixing of one- and two-phonon states can be interpreted as an anharmonicity of the nuclear vibration. The details of the vibrational calculation will be done in the following sections.

On the other hand, the ground-state of an odd-mass nucleus contains one quasiparticle. As there are a large number of low-lying one quasiparticle states, for all of them the minimum energy is $\Delta$, and hence such nuclei should not show an energy gap. This is in conformity with experimental results. The gap represents the energy necessary to break one of the condensed pairs, and an odd-mass nucleus has one unpaired particle. Higher excited states are given by three quasiparticle states. Once again to get these excited
states correctly one would be required to diagonalise $H_{\text{int}}$ in the space of one and three quasiparticles. The details of this part of the work has not been included in this thesis and are contained in the recent publication by the author.

1.3 The Pairing Force

The calculations are made specially simple by the use of the pairing force. It is written as

$$G(abcdj) = -\delta a \delta b \delta c \delta d \delta j \delta \overline{a} \overline{d} \overline{j} G_{p}.$$  \hspace{1cm} (1.20)

In other words, it acts only between pairs of total angular momentum zero. $-G_{p}$ is the attractive strength of the pairing force and is taken to be a constant in the particular major shell we are working with. In this case $\Lambda$ and $\Delta$ ($\Delta$ will no longer depend on the level) for a given nucleus are obtained by solving the following two equations

$$I = \frac{1}{4} G_{p} \sum_{b} \frac{1}{\left[\left(\hat{E}_{b} - \lambda\right)^{2} + \Delta^{2}\right] V_{b}} \hspace{1cm} (1.21)$$

and

$$N = \frac{1}{2} \sum_{\alpha} \left[ \frac{\left(\hat{E}_{\alpha} - \lambda\right)}{\left[\left(\hat{E}_{\alpha} - \lambda\right)^{2} + \Delta^{2}\right] V_{\alpha}} \right]. \hspace{1cm} (1.22)$$

The pairing plus quadrupole interaction has been extensively used in the quasiparticle calculation. We have also used this interaction in our MTDA calculation and the results of even Ni and Sn isotopes are presented in Sec.6 of this part of the thesis.
1.4 BCS Ground-State $|o\rangle$ Wave Function

The criterion that the BCS ground-state $|o\rangle$ is such that

$$a_\alpha |o\rangle = 0; \quad \forall \alpha,$$

which follows from the definition of an annihilation operator, is used in the construction of the BCS ground-state $|o\rangle$. One can verify by using the definition of $a_\alpha$ in terms of $C_\alpha^+$ and $C_\alpha^-$ that the above condition is satisfied by

$$|o\rangle = \prod_{\alpha} \left\{ U_\alpha - S_\alpha V_\alpha C_\alpha^+ C_\alpha^- \right\} |0_p\rangle. \quad (1.23)$$

One can see from Eq. (1.23) that $|o\rangle$ corresponds to a superposition of states with different even number of nucleons and therefore, it describes average ground-state properties of neighboring even nuclei. It is possible to project out the part of the wave function from Eq. (1.23) which corresponds to the required number of nucleons under consideration, and then use this projected (suitably normalised) wave function in the calculation of the ground-state nuclear properties. In Part IB of this thesis, we have projected out the part of the wave function from Eq. (1.23) that contains four particles corresponding to Ni$^{60}$, and then taken the overlap of this projected (normalised) BCS wave function with the exact shell-model ground-state wave function of Ni$^{60}$.

One quasiparticle state, two quasiparticle state, ......... are obtained by creating one quasiparticle, two quasiparticles, ......
1.5 Expressing \( \tilde{H}_{\text{int}} \) in Terms of Quasiparticle Operators:

\( \tilde{H}_{\text{int}} \) of Eq. (1.12) can be written in terms of \( \alpha \) operators, involving sixteen terms. These terms can be grouped into the following parts depending on the number of quasiparticle creation and annihilation operators contained in it, i.e.,

\[
\tilde{H}_{\text{int}} = H_{40} + H_{04} + H_{31} + H_{13} + H_{12} \tag{1.25}
\]

where the two numbers used as labels denote the number of quasiparticle creation and annihilation operators, respectively.

Let us introduce the angular momentum coupled pair creation and annihilation operators (normalised) \( \mathcal{A}^+, \mathcal{A} \) and the number operator \( \hat{N} \), for quasiparticles, each coupled to angular momentum \( J \) with projection \( M \), defined as

\[
\mathcal{A}^+(abJM) = N(ab) \mathcal{A}^+(abJM),
\]

\[
\mathcal{A}(abJM) = \left[ \mathcal{A}^+(abJM) \right]^+ = N(ab) \mathcal{A}(abJM),
\]

and

\[
\hat{N}(abJM) = -\mathcal{A}^+abJM + \mathcal{A}^+(abJM) = \sum_{\alpha \beta} \left[ \begin{array}{c c c}
\alpha \\
\beta \\
J \\
M
\end{array} \right] \mathcal{A}_\alpha^{\dag} \mathcal{A}_\beta \tag{1.26}
\]

where the unnormalised operators \( \mathcal{A}^* \) and \( \mathcal{A} \) are defined as
\( A(\alpha \beta \gamma \delta) = -c_{-i}^{-a+b-j} A^\dagger(\beta \alpha \gamma \delta) = \sum_{a \beta} \left[ \begin{array}{ccc} a & b & j \\ \rho & \mu \end{array} \right] d_{\alpha a}^\dagger d_{\rho \beta}, \)  

\( A(\alpha \beta \gamma \delta) = -c_{+i}^{a+b-j} A^\dagger(\gamma \delta \alpha \beta) = \sum_{a \rho} \left[ \begin{array}{ccc} a & b & j \\ \rho & \mu \end{array} \right] a_{\rho} a_{\alpha}, \)

and \( N(\alpha \beta) \) is the normalisation factor of \( A \)-operators in the sense that

\[ \langle 0 | A(\alpha \beta \gamma \delta) A^\dagger(\alpha \beta \gamma \delta) \mid 0 \rangle = 1, \]

One then finds

\[ N(\alpha \beta) = \frac{1}{\sqrt{14 \delta_{\alpha \beta}}}. \]

The operators \( \tilde{A}^\dagger \) and \( \tilde{A} \) form an orthonormal and nonredundant set in the two-quasiparticle space with the restriction \( a \leq b \).

In terms of the above defined operators the quantities on the right hand side of Eq. (1.25) are written as

\[ H_{40} = H_{04} = -\frac{1}{8} \sum_{\alpha \beta \gamma \delta} c_{-i}^{j+m} (U_{\alpha} U_{\beta} V_{\gamma} V_{\delta} + V_{\alpha} V_{\beta} U_{\gamma} U_{\delta}) \]

\[ \times G(\alpha \beta \gamma \delta) \tilde{A}^\dagger(\alpha \beta \gamma \delta) A^\dagger(\gamma \delta \alpha \beta), \]

\[ H_{31} = H_{13} = -\frac{1}{8} \sum_{\alpha \beta \gamma \delta} c_{-i}^{j+m} (U_{\alpha} U_{\beta} V_{\gamma} U_{\delta} - V_{\alpha} V_{\beta} U_{\gamma} U_{\delta}) \]

\[ \times G(\alpha \beta \gamma \delta) \tilde{A}^\dagger(\alpha \beta \gamma \delta) N(\gamma \delta \alpha \beta), \]
H_{22} = \frac{1}{4} \sum_{abcd} \left[ (U_{ab} U_{bc} U_{cd} + V_{ab} V_{bc} V_{cd}) G_{abcd} \right]
+ (U_{ab} U_{bc} U_{cd} + V_{ab} V_{bc} V_{cd}) F_{abcd} - \epsilon_{1}^{a+b-J} (U_{ab} V_{bc} V_{cd})
+ V_{ab} U_{bc} V_{cd} F_{bacd} \right] A_{aj}^{(abjm)} A_{cdjm}.

Here \( F_{abcd} \) is the hole-particle matrix element, related to \( G \) through a Racah coefficient by the relation

\[ F_{abcd} = -\sum_{j'} \omega_{ij} \omega_{abcdj'} G_{abcdj'}, \]

and satisfies

\[ F_{abcd} = F_{cdab} = \epsilon_{1}^{a+b+c+d} F_{badc}. \]