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ABSTRACT

A generalized quasiparticle transformation is presented which includes n-n,p-p, and n-p (T = 0 and T = 1) pairing correlations. The quasiparticle co-ordinates are required to be complex. The resulting gap equations for N = Z even-even nuclei are solved for the nuclei in the sd shell. To permit interaction between the Hartree-Fock (HF) and pair potentials, the Hartree-Fock-Bogoliubov (HFB) equations, including both T = 0 and T = 1 pairing, are also solved for these nuclei.

Although T = 1 pairing correlations are not significant, T = 0 pairing correlations play a very important role, rectifying many of the failures of the HF theory in this region. T = 0 pairing restores axial symmetry to the equilibrium shapes of Mg^{24} and S^{32} and explains the vibrational nature of Ar^{36}. These conclusions are reproduced by the following nucleon-nucleon interactions: the Yale t -matrix (s-p-sd), the Nestor-Davies-Krieger-Baranger effective interaction (s-p-sd and s-p-sd-pf), and the Rosenfeld effective interaction (sd).

Evaluation of various approximations to HFB is facilitated by deriving the canonical form of the density matrix and the pairing tensor for generalized isospin pairing. The general quasiparticle transformation is equivalent to the product of three transformations: (1) an isospin-conserving rotation in particle space (canonical

basis), (2) an isospin-generalized "special" quasiparticle transformation, (3) a rotation in quasiparticle space.

The canonical basis often bears no resemblance to the corresponding HF basis. The third transformation may not be approximated by the unit transformation, nor is the pair potential diagonal in the canonical basis. The BCS approximation of neglecting elements of the pair potential connecting different spatial orbitals is therefore unjustified. Iterating between the HF and the BCS equations in an attempt to permit both degrees of freedom to interact with one another is an even worse approximation to HFB than merely solving the BCS equations with the trivial HF basis.

The HFB equations are derived by a variational principle. The self-consistent symmetries of the HFB solutions are discussed. Usage of the same effective interaction in both the HF and the pair potential is justified.

INTRODUCTION

A satisfactory theory of nuclear structure should explain the properties of nuclei in terms of the interactions between their constituent particles. It is convenient to neglect relativistic effects and the possible existence of many-body forces. The Schroedinger equation with two body interactions should then provide a fundamental description of a many nucleon system. The first order description one should arrive at is the shell model.

The nuclear shell model of Mayer and Jensen (1950) was the first successful attempt to explain some elementary properties of nuclear structure in terms of an independent particle model. Each nucleon moves in a stationary orbit determined by a central potential which is assumed to represent an average effect of the actual internucleon forces. As these forces are short-ranged and strong, it is not evident that they give rise to such an independent particle description. The early shell model makes no attempt to derive the average potential from the real forces.

The Brueckner-Goldstone theory of nuclear matter supplies this fundamental justification of the shell model for an infinitely large nucleus containing an equal number of uniformly distributed protons

and neutrons. The Coulomb force is ignored. The value in considering such a system is that the single particle wave functions are known to be plane waves. Unfortunately real nuclei are finite. Obtaining the wave function becomes a formidable part of the theory.

Hartree-Fock (HF) theory is a good first approximation in our attempt to justify an independent particle model. It has the advantage of providing a self-consistent potential. An independent particle description of nuclei did not seem plausible before the Mayer-Jensen shell model and the Brueckner-Goldstone theory. It is for this reason that HF was first applied to nuclei (1963) so long after it had been successful in determining the wave functions of atomic electrons (1930). It has been most extensively applied to nuclei in the 2s-1d shell. The intrinsic state properties (deformation, moments of inertia) of many nuclei in this shell are not correctly predicted by HF theory.

The shell model or HF potential does not account for all effects of the actual inter-nucleon forces. Residual components of these forces introduce additional correlations into the wave functions. One such correlation is the pairing effect. Two nucleons in time-reversed degenerate orbitals have a large spatial overlap and therefore form a pair with an increment in binding energy. A theory of pairing correlations was obtained when the Bardeen-Cooper-Schrieffer (BCS) - Bogoliubov

theory of superconductivity was adapted to nuclei by A. Bohr, B.R. Mottleson, and D. Pines and by S. Belyaev. The independent modes of the system are no longer particles but quasiparticles (a linear combination of particle and hole). In the most familiar form only proton-proton (p-p) and neutron-neutron (n-n) pairing are considered. We find that such correlations are not important in the 2s-1d shell, and therefore do not explain the failure of HF.

There are compelling physical arguments to demonstrate the likelihood of neutron-proton (n-p) pairing being an important correlation in N = Z even-even nuclei. The neglect of n-p pairing cannot be justified. We present a generalized quasiparticle transformation which includes p-p, n-n, and n-p (T = 0 and T = 1) pairing correlations. A simple set of generalized gap equations are derived for N = Z even-even nuclei. These gap equations were first derived by Goswami and Chen with the Green's function rather than the quasiparticle formalism.

The BCS theory has the defect that the pairing correlations are not permitted to alter the underlying single particle basis (HF degrees of freedom). A satisfactory theory should allow HF and pairing degrees of freedom to interact with each other in a self-consistent fashion. The general quasiparticle transformation provides the appropriate formalism:

Hartree-Fock-Bogoliubov (HFB) theory.

The general quasiparticle transformation is expressed in terms of the isospin-generalized "special" quasiparticle transformation to demonstrate the relationship between HFB and the various approximations to HFB: HF-BCS, iterating between Hartree-Bogoliubov (HB) and BCS, and iterating between approximate HB (a modified HF) and BCS. We examine the conditions for which each of these approximations is valid.

The effective interaction appropriate for the HF potential is the τ-matrix. Pairing correlations alter the τ-matrix in a fairly obvious fashion. A more perplexing problem is whether the τ-matrix may be used as the effective interaction in the pairing potential.

The HFB equations, including T = 0 and T = 1 pairing, are solved for the N = Z even-even nuclei in the 2s-1d shell. T = 0 pairing correlations dominate over T = 1 pairing correlations in all cases of physical interest. Many of the discrepancies of HF are resolved. T = 0 pairing restores axial symmetry to the equilibrium shapes of Mg^{24} and S^{32} and indicates a vibrational, rather than rotational, structure for Ar^{36}.

I. THE HAMILTONIAN

1. Schroedinger's Equation

A fundamental theory of nuclear structure should explain the properties of nuclei in terms of the interactions between their constituent particles. A bound nucleon has a binding energy of 5 to 10 Mev and a kinetic energy of about 25 Mev. Since the nucleon mass is about 1000 Mev, and the π - meson mass (lightest particle exchanged between nucleons) is 137 Mev, it may be assumed that a non-relativistic description is a good approximation. Inter-nucleon interactions may then be represented by a potential. The possible existence of many-body forces is neglected. The Schroedinger equation with two body interactions is therefore chosen as the fundamental equation.

$$H|\Psi\rangle = E|\Psi\rangle \tag{1.1a}$$

$$H = T + V = \sum_{i=1}^{A} T_i + \sum_{i<j=1}^{A} v_{ij} \tag{1.1b}$$

The techniques developed to solve (1.1) are not sufficiently refined to determine the validity of our assumptions.[1]

2. Model Spaces and Effective Hamiltonians

It is customary to derive the Hartree-Fock (HF) equations beginning with the Hamiltonian (1.1b). The HF potential is then described in terms of matrix elements in a shell-model basis.

$$\langle \phi_i(1)\, \phi_j(2) \,|\, v_{12} \,|\, \phi_k(1)\, \phi_\ell(2) \rangle$$

One then observes that if the interaction v_{12} has a hard core, the matrix elements diverge, rendering the HF equations meaningless. Brueckner theory is then invoked to justify the replacement of v by the reaction matrix K (which has well-defined matrix elements).

When HF is generalized to Hartree-Fock-Bogoliubov (HFB) to include the effects of pairing correlations, we encounter a variety of contradictory prescriptions for obtaining the effective interaction:

(a) The same K-matrix used in HF may be used in both the HF and pair potentials in HFB. [2]

(b) The effective force to use in HFB is the K-matrix renormalized to account for the smearing of the Fermi surface by pairing correlations. [3]

(c) The effective force to be used in the pair potential is not related to the K-matrix. [4]

We follow a procedure which removes these ambiguities. [5] Every nuclear structure calculation begins with a truncation of the space of basis states. This requires

the replacement of H by an effective Hamiltonian H^{eff}. With certain approximations the effective interaction reduces to the reaction matrix. Depending upon how we choose the truncated (model) space, we arrive at different definitions for the reaction matrix, and different conclusions concerning the justifiability of using the reaction matrix in the pair renormalized HF potential and in the pair potential. For an appropriate choice of the model space, various nuclear structure theories (HF, BCS, HFB, RPA) should be considered as successive approximations to the eigenfunctions of H^{eff}. After determining H^{eff} we shall consider these theories.

The Schroedinger equation for a many-body system with two-body interactions was given in (1.1). A single particle potential

$$U = \sum_{i=1}^{A} U_i \tag{1.2}$$

is introduced. It is chosen to absorb the major effects of the two-body interactions v_{ij} . The Hamiltonian is separated into two parts.

$$H = H_0 + H_1 \tag{1.3}$$

where Ho contains only single particle operators

$$H_0 = T + U = \sum_{i=1}^{A} (T_i + U_i) \tag{1.4}$$

and H_1 contains the residual interactions unaccounted for by U .

$$H_1 = V - U = \sum_{i<j=1}^{A} v_{ij} - \sum_{i=1}^{A} U_i \tag{1.5}$$

Of course H is independent of the choice of U. However the wave-function $|\Psi\rangle$ and energy E will be determined through a perturbation expansion in powers of H_1. A judicious choice for U can ensure a faster convergence of the perturbation series.

The single particle eigenfunctions of H_0 satisfy

$$(T_i + U_i)|\phi(i)\rangle = \epsilon_\phi |\phi(i)\rangle \cdot \tag{1.6}$$

The set $\{|\phi\rangle\}$ form a complete orthonormal basis of single particle states. Many-particle eigenstates of H_0 are A-dimensional Slater determinants constructed from different combinations of the one particle states.

$$|\Phi_i\rangle = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_a(1) & \phi_b(1) & \phi_c(1) & \cdots & \phi_z(1) \\ \phi_a(2) & \phi_b(2) & \phi_c(2) & \cdots & \phi_z(2) \\ \phi_a(3) & \phi_b(3) & \phi_c(3) & \cdots & \phi_z(3) \\ \vdots & \vdots & \vdots & & \vdots \\ \phi_a(A) & \phi_b(A) & \phi_c(A) & \cdots & \phi_z(A) \end{vmatrix} \tag{1.7a}$$

$$H_0 |\Phi_i\rangle = E_i |\Phi_i\rangle \tag{1.7b}$$

where E_i is simply the sum of the single particle energies of the occupied states.

$$E_i = \sum_{\phi \text{ occupied}} \epsilon_\phi \tag{1.8}$$

The unperturbed ground-state wave function $|\Phi_0\rangle$ and ground state energy E_0 are obtained by filling the A lowest energy orbitals.

The set $\{|\Phi_i\rangle\}$ form a complete orthonormal basis of A-particle states, so that

$$|\Psi\rangle = \sum_i a_i |\Phi_i\rangle \tag{1.9}$$

Substitute (1.3) and (1.9) into (1.1a) and form the scalar product with $\langle \Phi_i|$.

$$\sum_j \langle \Phi_i|H_0+H_1|\Phi_j\rangle a_j = \sum_j \langle \Phi_i|E|\Phi_j\rangle a_j \tag{1.10}$$

or

$$\sum_j \{E_i\delta_{ij} + \langle \Phi_i|H_1|\Phi_j\rangle\} a_j = E a_i \tag{1.11}$$

We have simply rewritten the Schroedinger equation as

$$[H_0 + H_1]\,\underline{a} = E\,\underline{a}\,. \tag{1.12}$$

Before proceeding we must note two difficulties:

(a) The expansion (1.9) is over an infinite number of basis states, clearly making our Schroedinger equation (1.12) somewhat intractable.

(b) The matrix elements $\langle \Phi_i|H_1|\Phi_j\rangle$ may be expressed in terms of the two body matrix elements

$$\langle \phi_i(1)\ \phi_j(2)\,|\,v_{12}\,|\,\phi_k(1)\ \phi_\ell(2)\rangle\,.$$

The nucleon-nucleon interaction v_{12} , which is determined from two nucleon scattering data, becomes strongly

repulsive at small particle separations. This short range repulsion is often approximated by a hard core. A schematic representation of the potential is given in Figure (1.1).

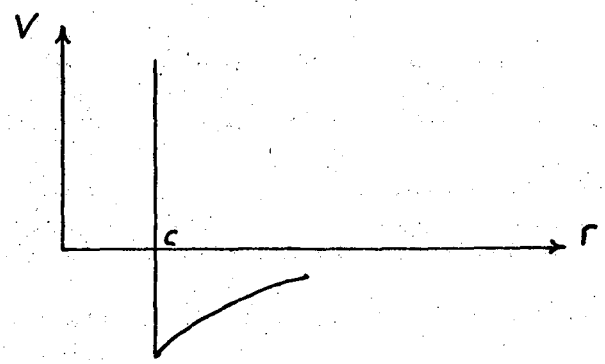


Figure (1.1)

r is the separation distance. The core radius C is about 0.4 fm. The presence of this repulsive core ensures that nuclei maintain a finite size. The wave-functions $|\phi\rangle$ are commonly expressed as linear combinations of harmonic oscillator wave-functions, which may have non-zero overlap near r=0. Therefore the hard core also ensures that the two body matrix elements of v_{ij} will diverge. This is unfortunate, for it not only renders the Schroedinger equation (1.12) useless, but it also threatens to make a perturbation expansion in terms of H_1 meaningless (since each term in the expansion diverges).

These are certainly formidable difficulties. Yet they may be circumvented.

The concept of a "model space" is introduced to alleviate the difficulty of solving an infinite dimensional eigenvalue problem. The states not included in the model

space will renormalize the interaction so that V is replaced by an "effective interaction" V^{eff}. Matrix elements of V^{eff} will generally be well-behaved, even though V contains singularities. The eigenvalue of the effective Hamiltonian, $H^{eff} = T + V^{eff}$ is E, the true ground state energy of the system of interacting particles. The eigenvector of H^{eff} is the "model wave-function", which exactly reproduces the component of $|\Psi\rangle$ inside the model space. The component of $|\Psi\rangle$ outside the model space can also be retrieved. The technique is very powerful, and its results are implicit in all nuclear structure calculations.

Denote by D the space spanned by the set $\{|\Phi_i\rangle\}$. Select a number N_d of this set to form a N_d dimensional model space d. The operator P projects onto d.

$$P = \sum_{i \in d} |\Phi_i\rangle\langle\Phi_i| \tag{1.13}$$

The operator Q projects out of d.

$$Q = \sum_{i \notin d} |\Phi_i\rangle\langle\Phi_i| \tag{1.14}$$

Clearly

$$Q + P = I . \tag{1.15}$$

The model wave-function is defined by

$$|\Psi_d\rangle = P|\Psi\rangle = \sum_{i \in d} a_i |\Phi_i\rangle . \tag{1.16}$$

Define the Green function

$$G = \frac{Q}{E-H_0} = \sum_{i \notin d} \frac{|\Phi_i\rangle\langle\Phi_i|}{E-E_i} \,. \tag{1.17}$$

The wave function $|\Psi\rangle$ may be re-expressed.

$$|\Psi\rangle = (P+Q)|\Psi\rangle = |\Psi_d\rangle + \sum_{i \notin d} a_i \, |\Phi_i\rangle \tag{1.18}$$

Rewriting (1.11)

$$\langle\Phi_i|H_1|\Psi\rangle = (E-E_i)\, a_i \,. \tag{1.19}$$

Solving (1.19) for a_i and substituting into (1.18)

$$|\Psi\rangle = |\Psi_d\rangle + \sum_{i \notin d} \frac{|\Phi_i\rangle\langle\Phi_i|H_1|\Psi\rangle}{E-E_i}$$

$$= |\Psi_d\rangle + G H_1 |\Psi\rangle \,. \tag{1.20}$$

Define the effective interaction H_1^{eff}.

$$H_1^{eff}|\Psi_d\rangle = H_1|\Psi\rangle \tag{1.21}$$

Substitute into (1.20).

$$|\Psi\rangle = |\Psi_d\rangle + G H_1^{eff} |\Psi_d\rangle \tag{1.22}$$

Substitute (1.22) into (1.21).

$$H_1^{eff}|\Psi_d\rangle = H_1|\Psi_d\rangle + H_1 G H_1^{eff} |\Psi_d\rangle \tag{1.23}$$

The effective interaction H_1^{eff} is therefore determined by

$$H_1^{eff}(E) = H_1 + H_1 G H_1^{eff}(E) \tag{1.24}$$

where the E dependence of the effective interaction (through the energy denominator in G) has been explicitly noted. The matrix representation of H_1^{eff} is

$$\langle \Phi_i | H_1^{eff}(E) | \Phi_j \rangle = \langle \Phi_i | H_1 | \Phi_j \rangle + \sum_{k \notin d} \frac{\langle \Phi_i | H_1 | \Phi_k \rangle \langle \Phi_k | H_1^{eff}(E) | \Phi_j \rangle}{E - E_k} \tag{1.25}$$

To obtain the counterpart of (1.11) for the model space, substitute (1.21) into (1.19).

$$\langle \Phi_i | H_1^{eff}(E) | \Psi_d \rangle = (E - E_i) a_i \tag{1.26}$$

Expanding $|\Psi_d\rangle$ as in (1.16) provides the eigenvalue equation for the model space.

$$\sum_{j \in d} \{ E_i \delta_{ij} + \langle \Phi_i | H_1^{eff}(E) | \Phi_j \rangle \} a_j = E a_i \tag{1.27}$$

This equation is valid for all i, not just for $i \in d$. Consider the set of equations in (1.27) for which $i \in d$. They constitute an N_d dimensional eigenvalue equation.

$$[H_0 + H_1^{eff}(E)]_d \underline{a} = E \underline{a} \tag{1.28}$$

One of the eigenvalues of

$$H^{eff}(E) = H_0 + H_1^{eff}(E) \tag{1.29}$$

is the exact ground state energy of the system of interacting particles. The corresponding eigenvector of H^{eff} exactly reproduces the component of $|\Psi\rangle$ in d. (1.25) and (1.27) are coupled through the E dependence of H_1^{eff}. One must first guess E, then solve (1.25) for H_1^{eff}. Solving (1.28) determines a new value for E which is used to re-calculate H_1^{eff}. The procedure is continued until the results are the same on two successive iterations. Selecting $i \in d$, $j \in d$, (1.25) and (1.27) are solved for E and the component of $|\Psi\rangle$ in d. Then choosing $i \notin d$, $j \in d$, (1.25) and (1.27) may be solved for the component of $|\Psi\rangle$ outside of d. Equations (1.25) and (1.27) therefore constitute a restatement of the Schroedinger equation (1.11). No information has been lost nor have any approximations been made.

Unfortunately, since H^{eff} is a function of E, the eigenvectors of H^{eff} will in general not be orthogonal. (Even though the various solutions $|\Psi\rangle$ are orthogonal, their projections onto the model space might not be orthogonal.)

Choose the model wave function to be normalized to unity.

$$\langle \Psi_d | \Psi_d \rangle = 1 \tag{1.30}$$

Then

$$\langle \Psi | \Psi_d \rangle = 1. \tag{1.31}$$

By iterating (1.24) we obtain an equivalent expression for H_1^{eff}.

$$H_1^{eff}(E) = H_1 \sum_{m=0}^{\infty} (G H_1)^m \tag{1.32}$$

Define the effective interaction V^{eff} by

$$H^{eff}(E) = T + V^{eff}(E) \,. \tag{1.33}$$

Combining (1.4), (1.29), and (1.33)

$$V^{eff}(E) = H_1^{eff}(E) + U \,. \tag{1.34}$$

Equation (1.33) is a natural starting point for nuclear structure calculations. If the choice of the model space is such that its dimensionality is too large to permit exact diagonalization of H^{eff}, then other methods must be considered to obtain approximate eigenfunctions of H^{eff}. HF, BCS, HFB, RPA may then be interpreted as successive approximations to an exact diagonalization of H^{eff}. There is an alternative interpretation of these theories. To be more explicit we consider various choices for the model space.

A. The model space d is equivalent to the entire space D.

From (1.16), $|\Psi_d\rangle = |\Psi\rangle$. From (1.17) G = 0 so that $H_1^{eff} = H_1$ (1.24), and (1.27) is equivalent to the Schroedinger equation (1.11).

B. The dimensionality of d is finite but greater than unity.

For example, let U be the harmonic oscillator(HO) potential.

$$U = U_{HO} \equiv U(r) + \alpha_{\ell \cdot s}\, \underline{\ell} \cdot \underline{s} + \alpha_{\ell^2}\, \underline{\ell}^2 \tag{1.35}$$

Then $H_0 = T + U_{HO}$ has eigenfunctions

$$H_0 | N l j m \tau \rangle = \epsilon_{Nlj} \, | N l j m \tau \rangle \tag{1.36}$$

where N = principal quantum number

l = orbital angular momentum

j = total angular momentum

m = projection of j on body-fixed Z axis

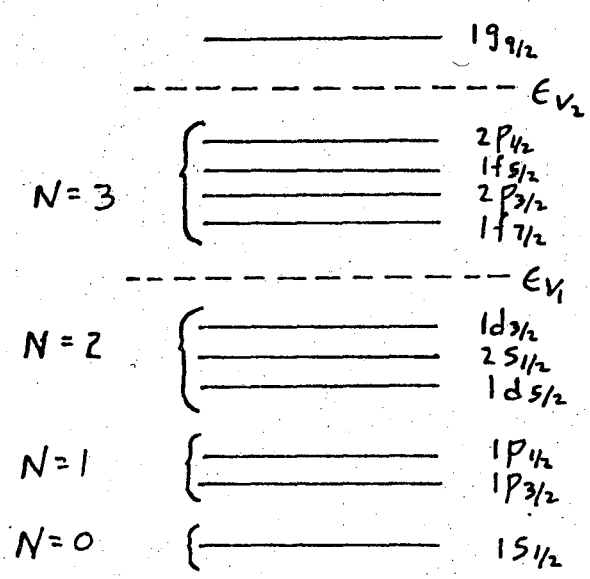
τ = isospin projection ($+\frac{1}{2}$ for proton, $-\frac{1}{2}$ for neutron).

Number the orbitals in the order of increasing energy: $\epsilon_1, \epsilon_2, \cdots \epsilon_A, \cdots$. Choose an energy

$$\epsilon_v > \epsilon_A \, . \tag{1.37}$$

Choose the model space to consist of all A dimensional Slater determinants where the single particle orbitals are HO states with $\epsilon_i \leq \epsilon_v$.

The HO spectrum is presented in Figure (1.2).



Figure(1.2)

For nuclei filling the 2s-1d shell the dashed lines in Figure (1.2) are two reasonable choices for ϵ_V . Suppose we choose $\epsilon_V = \epsilon_{V_1}$. The number of proton states with $\epsilon_i \leq \epsilon_V$ is 20 . Mg^{24} has 12 protons. The number of ways of putting A indistinguishable particles in N states is

$$\frac{N!}{(N-A)!\,A!} .$$

The number of possibilities for 12 protons in 20 states is 125,970. Similarly for the neutrons, so that the total number of configurations is $(125,970)^2$. If we choose $\epsilon_V = \epsilon_{V_2}$, the number of neutron or proton states is 40, giving rise to $(4,116,628,880)^2$ configurations. Even considering Mg^{24} as an inert O^{16} core with 8 particles in the 2s-1d shell leaves 4 protons (neutrons) in 12 states, with $(495)^2 = 245,025$ configurations. Clearly we have exceeded the bounds of even the most sophisticated computer. Methods for obtaining approximate eigenfunctions of H^{eff} are developed in the following chapters.

The effective interaction must now be determined. For a suitable set of approximations it can be reduced to the reaction matrix. Expand equation (1.32), recalling that $H_1 = V - U$.

$$\begin{aligned} H_1^{eff}(E) &= \{ V + VGV + VGVGV + \cdots - U \} + \cdots \\ &= \{ V \sum_{m=0}^{\infty} (GV)^m - U \} + \cdots \end{aligned} \tag{1.38}$$

The terms outside the bracket contain at least one U

factor. If they are neglected

$$H_1^{eff}(E) = V \sum_{m=0}^{\infty} (GV)^m - U . \qquad \text{(approximation)} \quad (1.39)$$

Combining (1.33),(1.39)

$$V^{eff}(E) = V \sum_{m=0}^{\infty} (GV)^m \qquad (1.40)$$

or

$$V^{eff}(E) = V + VGV^{eff}(E) . \qquad (1.41)$$

To obtain the reaction matrix it is assumed that the only important intermediate states consist of multiple scatterings between two particles. More precisely, it is assumed that

$$Q = Q_{2p} \qquad \text{(approximation)} \quad (1.42)$$

where $Q_{2p} = \sum_{K(2p)} |\Phi_{K(2p)}\rangle\langle\Phi_{K(2p)}| .$ (1.43)

The state $|\Phi_{K(2p)}\rangle$ has two particles in states $|m\rangle$, $|n\rangle$ with $\epsilon_m, \epsilon_n > \epsilon_\nu$, the remaining particles having $\epsilon_i \leq \epsilon_\nu$. It is also assumed that all particles except the pair under consideration remain inert. The matrix element $\langle\Phi_i|V^{eff}(E)|\Phi_j\rangle$ then reduces to the two body matrix element

$$\langle \phi_i(1)\ \phi_j(2)\ |\ v_{12}\ |\ \phi_K(1)\ \ \phi_\ell(2)\ \rangle$$

if particles 3,4,...A have identical states in configurations $|\Phi_i\rangle, |\Phi_j\rangle$. Otherwise $\langle\Phi_i|V^{eff}|\Phi_j\rangle = 0$.

Q_{2p} then reduces to

$$Q_{2p} = \sum_{\epsilon_m, \epsilon_n > \epsilon_v}' |mn\rangle\langle mn| . \qquad \text{(approximation)} \quad (1.44)$$

With these approximations V^{eff} becomes the reaction matrix.

$$K(E) = v + v \frac{Q_{2p}}{E - H_0} K(E) \qquad (1.45)$$

The reaction matrix is a two-body effective interaction. Even though $Q = Q_{2p}$, if we had not required that all particles remain inert except the pair undergoing multiple scattering, then the effective interaction would contain many-body terms. The two-body interaction v_{ij} can therefore give rise to many body effective interactions $v^{eff}_{ijk\ldots}$.

K (E) has the matrix representation

$$\langle ij|K(E)|kl\rangle = \langle ij|v|kl\rangle + \sum_{\epsilon_m, \epsilon_n > \epsilon_v}' \frac{\langle ij|v|mn\rangle\langle mn|K(E)|kl\rangle}{E - H_0} . \qquad (1.46)$$

Actually this representation of K is deceptive. The energy denominator $1/(E - H_0)$ depends not only on the active particle states $|m\rangle$, $|n\rangle$ and the passive hole states $|k\rangle$, $|l\rangle$. It also depends upon the energies of all the passive particles.

$$\frac{1}{E - H_0} = \frac{1}{E - E_i + \epsilon_k + \epsilon_l - \epsilon_m - \epsilon_n}$$

where E_i is the energy of the state $|\Phi_i\rangle$ from which $|\Phi_i(2p)\rangle$ is derived. Therefore K depends not only on E. It is also a function of the configuration $|\Phi_i\rangle$. For each $|\Phi_i\rangle$ there is a different K (E). This is a very undesirable feature. If the variation in E_i is small compared to typical values of $(\epsilon_K+\epsilon_\ell-\epsilon_m-\epsilon_n)$, then K (E) will be configuration independent. (This effect should be distinguished from the state, or E, dependence of K.)

In the following example the physical processes which contribute to K will be more thoroughly discussed.

C. The dimensionality of the model space is unity.

The model space contains a single configuration $|\Phi_0\rangle$.

$$H_0|\Phi_0\rangle = E_0|\Phi_0\rangle \tag{1.47}$$

The model space eigenvalue equation (1.28) is simply

$$E_0 + \langle\Phi_0|H_1^{eff}(E)|\Phi_0\rangle = E \tag{1.48}$$

or $$\Delta E = E - E_0 = \langle\Phi_0|H_1^{eff}(E)|\Phi_0\rangle. \tag{1.49}$$

Inserting (1.32)

$$\Delta E = \sum_{m=0}^{\infty} \langle\Phi_0|H_1\left\{\frac{Q}{E-H_0}H_1\right\}^m|\Phi_0\rangle \tag{1.50}$$

where $$Q = \sum_{i\neq 0}|\Phi_i\rangle\langle\Phi_i|. \tag{1.51}$$

This is just the result of Brillouin-Wigner (BW) perturbation theory. As in (1.38) - (1.41), we drop all terms in H_1^{eff} which contain U except the term - U. Then the energy added to the system through the interactions

v_{ij} is $\langle \Phi_0 | V^{eff}(E) | \Phi_0 \rangle$

where V^{eff} is defined in (1.41).

As a particular example choose U to be the HF potential.

$$U = U_{HF}$$

$$(T + U_{HF})_i \, |\phi(i)\rangle = \epsilon_\phi \, |\phi(i)\rangle$$

$$(T + U_{HF}) \, |\Phi_{HF}\rangle = E_{HF} \, |\Phi_{HF}\rangle \qquad (1.52)$$

$$E_{HF} = \sum_{i=1}^{A} \epsilon_i$$

(E_{HF} has the meaning assigned in (1.8),rather than its more familiar sense.) $|\Phi_{HF}\rangle$ is an A - dimensional Slater determinant. Each single particle orbital $|\phi\rangle$ is a linear combination of HO orbitals. The A lowest energy states are filled. Define a Fermi energy.

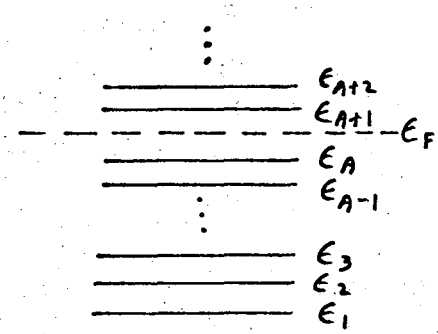


Figure (1.3)

Replace Q by Q_{2p}, which now has the form

$$Q_{2p} = \sum_{\epsilon_m, \epsilon_n > \epsilon_F} |mn\rangle\langle mn| \qquad (1.53)$$

(Compare with (1.44).) The energy denominator $1/(E - H_0)$

has the value $1/(E-E_{HF}+\epsilon_K+\epsilon_\ell-\epsilon_m-\epsilon_n)$, where $|K\rangle$ and $|\ell\rangle$ are the hole states. K then has the matrix representation

$$\langle ij|K(E)|K\ell\rangle = \langle ij|v|K\ell\rangle + \sum_{\epsilon_m,\epsilon_n>\epsilon_F} \frac{\langle ij|v|mn\rangle\langle mn|K(E)|K\ell\rangle}{E-E_{HF}+\epsilon_K+\epsilon_\ell-\epsilon_m-\epsilon_n} \cdot \tag{1.54}$$

Since d consists of only one configuration, the problem of K(E) being configuration dependent does not arise.

It is now appropriate to note the inconvenience of calculating E in terms of an infinite series in which each component contains E. Goldstone's linked cluster theorem provides a solution to this difficulty. If we include contributions to E corresponding to linked diagrams only then the perturbation energy is

$$\Delta E = \sum_{m=0}^{\infty} \langle \Phi_0 | H_1 \left\{ \frac{Q}{E_0-H_0} H_1 \right\}^m | \Phi_0 \rangle_L \cdot \tag{1.55}$$

(A linked diagram is one that can not be separated into two parts without cutting any lines.) Comparing with (1.50), note that the energy denominator $1/(E - H_0)$ has been replaced by $1/(E_0 - H_0)$. This feature is especially desirable for large systems, since

$$\frac{1}{E-H_0} = \frac{1}{\Delta E + (E_0-H_0)} \approx \frac{1}{\Delta E}$$

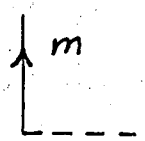
which vanishes as A increases. That is, terms in the BW expansion past first order yield negligible contributions to ΔE for a large system. The BW series converges extremely slowly. The factor $1/(E_0 - H_0)$, however, is of

order one for all A.

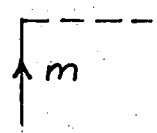
For our example, $E_0 = E_{HF}$. The reaction matrix (1.54) then assumes its most familiar form.

$$\langle ij|K|k\ell\rangle = \langle ij|v|k\ell\rangle + \sum_{\epsilon_m,\epsilon_n>\epsilon_F} \frac{\langle ij|v|mn\rangle\langle mn|K|k\ell\rangle}{\epsilon_k+\epsilon_\ell-\epsilon_m-\epsilon_n} \tag{1.56}$$

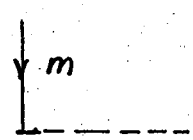
Description of the physical processes contributing to the reaction matrix is aided by the following diagrams.



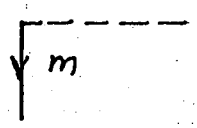
creation of a particle in state $|m\rangle$ where $\epsilon_m > \epsilon_F$



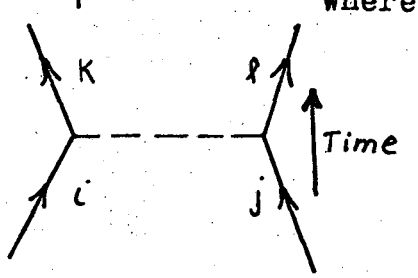
destruction of a particle in state $|m\rangle$ where $\epsilon_m > \epsilon_F$



destruction of a particle in state $|m\rangle$ where $\epsilon_m < \epsilon_F$ (creation of a hole)



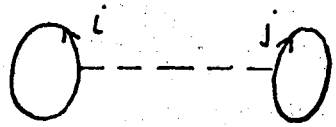
creation of a particle in state $|m\rangle$ where $\epsilon_m < \epsilon_F$ (destruction of a hole)



particles in states $|i\rangle, |j\rangle$ scatter into states $|K\rangle, |\ell\rangle$

Consider the process whereby particles in occupied states $|i\rangle, |j\rangle$ forward scatter, remaining in $|i\rangle, |j\rangle$.

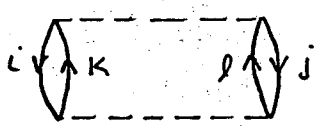
The energy contribution is $\langle ij|v|ij\rangle$. Summing over distinct pairs



$$= \frac{1}{2} \sum_{\epsilon_i, \epsilon_j < \epsilon_F} \langle ij|v|ij\rangle . \tag{1.57}$$

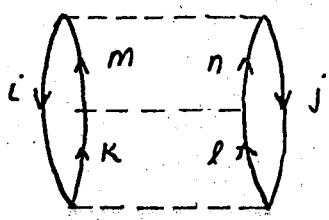
Let particles in occupied states $|i\rangle$, $|j\rangle$ scatter into unoccupied states $|k\rangle$, $|\ell\rangle$. (Thereby creating holes in $|i\rangle$, $|j\rangle$. At a later time the particles in $|k\rangle$, $|\ell\rangle$ may scatter back to their original states (annihilating the holes). This is a second order process with intermediate state energy

$E_0 - H_0$ = (sum of hole energies) - (sum of particle energies).



$$= \frac{1}{2} \sum_{\substack{\epsilon_i, \epsilon_j < \epsilon_F \\ \epsilon_k, \epsilon_\ell > \epsilon_F}} \frac{\langle ij|v|k\ell\rangle\langle k\ell|v|ij\rangle}{\epsilon_i + \epsilon_j - \epsilon_k - \epsilon_\ell} \tag{1.58}$$

The third order process is



$$= \frac{1}{2} \sum_{\substack{\epsilon_i, \epsilon_j < \epsilon_F \\ \epsilon_k, \epsilon_\ell, \epsilon_m, \epsilon_n > \epsilon_F}} \frac{\langle ij|v|mn\rangle\langle mn|v|k\ell\rangle\langle k\ell|v|ij\rangle}{(\epsilon_i + \epsilon_j - \epsilon_m - \epsilon_n)(\epsilon_i + \epsilon_j - \epsilon_k - \epsilon_\ell)} , \tag{1.59}$$

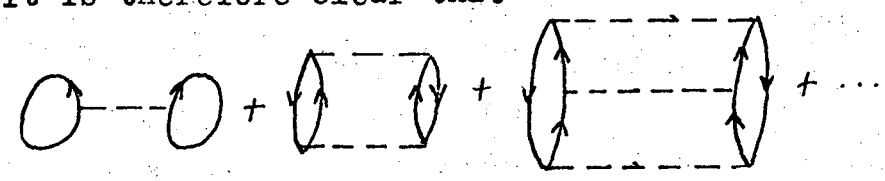
and so on.

Returning to our expression for the reaction matrix (1.56), let i = k, j = l, and iterate.

$$\langle ij|K|ij\rangle = \langle ij|v|ij\rangle + \sum_{\epsilon_k,\epsilon_\ell>\epsilon_F} \frac{\langle ij|v|k\ell\rangle\langle k\ell|v|ij\rangle}{\epsilon_i+\epsilon_j-\epsilon_k-\epsilon_\ell}$$

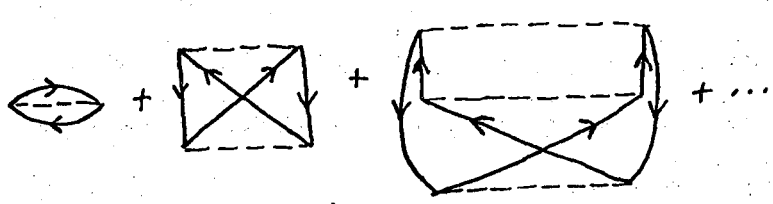
$$+ \sum_{\epsilon_k,\epsilon_\ell,\epsilon_m,\epsilon_n>\epsilon_F} \frac{\langle ij|v|mn\rangle\langle mn|v|k\ell\rangle\langle k\ell|v|ij\rangle}{(\epsilon_i+\epsilon_j-\epsilon_m-\epsilon_n)(\epsilon_i+\epsilon_j-\epsilon_k-\epsilon_\ell)} + \cdots \tag{1.60}$$

It is therefore clear that



$$= \frac{1}{2} \sum_{\epsilon_i,\epsilon_j<\epsilon_F} \langle ij|K|ij\rangle \cdot \tag{1.61}$$

Similarly the exchange terms may be evaluated.



$$= -\frac{1}{2} \sum_{\epsilon_i,\epsilon_j<\epsilon_F} \langle ij|K|ji\rangle \tag{1.62}$$

The total interaction energy obtained from this class of intermediate states is

$$\tfrac{1}{2} \sum_{\epsilon_i,\epsilon_j<\epsilon_F} \{\langle ij|K|ij\rangle - \langle ij|K|ji\rangle\} \cdot \tag{1.63}$$

This constitutes the Brueckner ladder approximation. A pair of particles are permitted to scatter against each other any number of times. The two holes and all other particles remain inert during this process.

Actually this interpretation is strictly true only if $U = 0$. By choosing $U = U_{HF}$, we use $\epsilon_i = (T + U_{HF})_i$. U_i^{HF} includes interactions between the particle in state $|i\rangle$ and all other particles in states $|K\rangle$, $\epsilon_K < \epsilon_F$. Including U_i^{HF} in the energy denominator means that the pair of particles undergoing multiple scattering are still bound in the effective potential created by their interactions with all other particles. Furthermore, choosing $U = U_{HF}$ ensures that in the Goldstone expansion (1.55) the terms past first order with U interactions cancel the corresponding terms containing interactions with passive unexcited states (lollipops and bubbles). This explains the approximation made in (1.39).

Even though $\langle ij|v|k\ell\rangle$ diverges for an interaction with a hard core, $\langle ij|K|k\ell\rangle$ may be well-behaved. This remarkable feature may be easily demonstrated. Consider the matrix element $\langle i\bar{i}|v|j\bar{j}\rangle$, where the bar denotes time-reversal. Assume a separate potential.

$$\langle i\bar{i}|v|j\bar{j}\rangle = \lambda v_i v_j \tag{1.64}$$

(All other matrix elements are assumed to be zero.) Substituting into (1.56)

$$\langle i\bar{i}|K|j\bar{j}\rangle = \lambda v_i v_j + \sum_{\epsilon_m > \epsilon_F} \frac{\lambda v_i v_m \langle m\bar{m}|K|j\bar{j}\rangle}{2(\epsilon_j - \epsilon_m)} \tag{1.65}$$

since $\epsilon_{\bar{i}} = \epsilon_i$. Therefore

$$\langle i\bar{i}|K|j\bar{j}\rangle = \lambda \mathcal{N}_i K_j \tag{1.66}$$

where

$$K_j = \mathcal{N}_j + \sum_{\epsilon_m > \epsilon_F} \frac{\lambda \mathcal{N}_m^2 K_j}{2(\epsilon_j - \epsilon_m)} . \tag{1.67}$$

Solving for K_j

$$K_j = \frac{\mathcal{N}_j}{1 + \frac{\lambda}{2} \sum_{\epsilon_m > \epsilon_F} \frac{\mathcal{N}_m^2}{(\epsilon_m - \epsilon_j)}} . \tag{1.68}$$

Substituting into (1.66)

$$\langle i\bar{i}|K|j\bar{j}\rangle = \frac{\mathcal{N}_i \mathcal{N}_j}{\frac{1}{\lambda} + \frac{1}{2} \sum_{\epsilon_m > \epsilon_F} \frac{\mathcal{N}_m^2}{(\epsilon_m - \epsilon_j)}} . \tag{1.69}$$

As the strength of the interaction λ become infinite, the matrix elements of K remain well-defined.

The last two choices for the model space may be compared:

B. The model space contains all configurations formed from HO states with energy below ϵ_V . The effective force may be approximated by the reaction matrix (1.46). The intermediate states have HO energies $\epsilon_m, \epsilon_n > \epsilon_V$. K is calcualted in a HO basis with HO energies in the

energy denominator. The number of configurations in the model space will generally be too large to permit exact diagonalization of H^{eff}. HF, BCS, HFB, RPA should be considered as successive approximations to exact diagonalization. The same reaction matrix is to be used in all these theories. In particular, it is to be used in HFB to calculate the pair-renormalized HF potential and the pair potential.

C. The model space contains one configuration $|\Phi_0\rangle$. If $|\Phi_0\rangle$ is $|\Phi_{HF}\rangle$, the effective interaction may be approximated by the reaction matrix (1.56). The intermediate states have HF energies $\epsilon_m, \epsilon_n > \epsilon_F$. K is calculated in a HF basis with HF single particle energies in the energy denominator. The effective interaction contains the projection operator

$$Q = \sum_{i \neq 0} |\Phi_i\rangle\langle\Phi_i| = 1 - |\Phi_0\rangle\langle\Phi_0| . \tag{1.70}$$

If $|\Phi_0\rangle$ is altered from $|\Phi_{HF}\rangle$ to $|\Phi_{BCS}\rangle$, $|\Phi_{HFB}\rangle$, or $|\Phi_{RPA}\rangle$, the operator Q obviously changes, so that V^{eff} must be altered. In particular, the form of the reaction matrix changes when pairing correlations are included. And it may not be possible to justify using any form of the reaction matrix in the pair potential.

3. Wick's Theorem and Quasiparticle Hamiltonians

The original Hamiltonian (1.1) containing kinetic energy and two-body interactions has been replaced by an effective Hamiltonian (1.34) containing kinetic energy and effective n-body interactions (n = 2,3,...). The effective Hamiltonian operates in a model space d, which is obtained by an appropriate truncation of the entire space. If the effective n-body interactions for n > 2 can be neglected, the reduced Schroedinger equation is

$$H^{eff}(E)\,|\Psi_d\rangle = E\,|\Psi_d\rangle \tag{1.71}$$

where

$$H^{eff}(E) = T + V^{eff}(E) = \sum_{i=1}^{A} T_i + \sum_{i<j=1}^{A} v_{ij}^{eff}(E). \tag{1.72}$$

The superscript "eff" and the E dependence will no longer be explicitly indicated. Unless otherwise mentioned H, V, v_{ij}, should be understood to mean $H^{eff}(E)$, $V^{eff}(E)$, $v_{ij}^{eff}(E)$.

It is assumed that exact diagonalization of the effective Hamiltonian in the model space is impractical. We now consider methods for obtaining approximate eigenfunctions.

A description of the ground state and low-lying excited states of the system is required. Although the

effective interaction is not singular, as is the true interaction, it still results in strong interactions between the particles. It is often possible to find a canonical transformation of particle co-ordinates such that the particles in the new co-ordinates are approximately non-interacting. These transformed particles are called "quasiparticles."

The ground state of the interacting system is described as a "quasiparticle" vacuum. Low lying excitations are described by "quasiparticle" excitations. When many "quasiparticles" are present their interactions may not be neglected, and the independent "quasiparticle" description breaks down.

In HF the "quasiparticles" are particles whose properties are renormalized by forward and exchange scatterings with all other particles. In BCS and HFB the "quasiparticles"are Bogoliubov quasiparticles, which are linear combinations of particles and holes (or to be more precise, HF "quasiparticles" and "quasiholes"). In RPA the "quasiparticles"are phonons, which are described in terms of HF particles and holes or Bogoliubov quasiparticles.

The goal, therefore, is to express the effective Hamiltonian as

$$H = E_0 + H_{q.p.} + H_{q.p.-int.} \tag{1.73}$$

where E_0 is the ground state energy of the system of interacting particles, $H_{q.p.}$ describes the elementary excitations ("quasiparticles") and $H_{q.p.-int.}$ is the (hopefully) weak interaction between the "quasiparticles."

The Hamiltonian may be expressed in the notation of second quantization

$$H = \sum_{ij} \langle i | T | j \rangle a_i^\dagger a_j + \frac{1}{4} \sum_{ijkl} \langle ij | v | kl \rangle_A a_i^\dagger a_j^\dagger a_l a_k \quad (1.74)$$

where $\{|i\rangle\}$ form a complete orthonormal single particle basis and

$$\langle ij | v | kl \rangle_A = \langle ij | v | kl \rangle - \langle ij | v | lk \rangle . \quad (1.75)$$

$a_i^\dagger$ creates and a_i annihilates a particle in state $|i\rangle$. Since they are Fermion operators they satisfy the anticommutation relations.

$$\begin{aligned} [a_i, a_j]_+ &= [a_i^\dagger, a_j^\dagger]_+ = 0 \\ [a_i^\dagger, a_j]_+ &= \delta_{ij} \end{aligned} \quad (1.76)$$

where

$$[A, B]_\pm = AB \pm BA . \quad (1.77)$$

A system with particles in states $|K_1\rangle$, $|K_2\rangle$, ... $|K_A\rangle$ is represented by

$$|\Phi\rangle = a_{K_1}^\dagger a_{K_2}^\dagger \cdots a_{K_A}^\dagger |0\rangle \quad (1.78)$$

where $|0\rangle$ signifies the vacuum state. The wave function is anti-symmetrized, so that it may also be represented by the Slater determinant

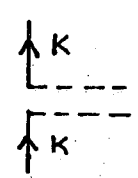
$$\Phi = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_{K_1}(1) & \phi_{K_2}(1) & \cdots & \phi_{K_A}(1) \\ \phi_{K_1}(2) & \phi_{K_2}(2) & \cdots & \phi_{K_A}(2) \\ \vdots & \vdots & & \vdots \\ \phi_{K_1}(A) & \phi_{K_2}(A) & \cdots & \phi_{K_A}(A) \end{vmatrix} . \qquad (1.79)$$

With the aid of Wick's theorem we are able to express the Hamiltonian (1.74) in the form of equation (1.73). This will be very useful in deriving the various self-consistent field formalisms.

We introduce a reference state, the choice of which is arbitrary. A convenient choice is the ground state of the system. Define new operators b^+, b such that if a state $|K\rangle$ is unoccupied in the reference state then

$b_k^+ = a_k^+$ creates a "particle"

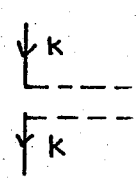
$b_k = a_k$ annihilates a "particle"



and if the state $|K\rangle$ is occupied then

$b_k^+ = a_k$ creates a hole

$b_k = a_k^+$ annihilates a hole



The normal product of a number of creation operators b_k^+ and annihilation operators b_k is defined as the product of these operators rearranged so that the

creation operators are to the left of the annihilation operators. A minus sign is included if an odd number of operator permutations is required to achieve this ordering. Denote the normal product of ABC... by N[ABC...]. (A,B,C... are linear combinations of b^+,b.) For example

$$N[b_i b_j^\dagger] = -b_j^\dagger b_i$$

$$N[b_i b_j^\dagger b_k^\dagger b_\ell] = b_j^\dagger b_k^\dagger b_i b_\ell .$$

The reference state expectation value of a normal product is zero.

$$\langle \Phi_0 | N[ABC\cdots] | \Phi_0 \rangle = 0 \tag{1.80}$$

The annihilation operators are at the right and act directly on $|\Phi_0\rangle$. b_k annihilates a "particle"or a hole. Since, by definition, $|\Phi_0\rangle$ contains no "particles" or holes, $b_i|\Phi_0\rangle = 0$.

The contraction of two operators is defined by

$$\overbrace{AB} \equiv \langle AB \rangle = \langle \Phi_0 | AB | \Phi_0 \rangle . \tag{1.81}$$

In particular

$$\langle b_i^+ b_j \rangle = \langle b_i^+ b_j^+ \rangle = \langle b_i b_j \rangle = 0 \tag{1.82}$$

$$\langle b_i b_j^\dagger \rangle = \delta_{ij} .$$

A normal product may contain pairs of contracted operators. The contracted pair may be removed from the normal product by permuting operators so that the contracted operators are side by side, introducing a change of sign if the number of permutations is odd. For example

$$N[\overbrace{ABCD}] = -\overbrace{AC}\, N[BD]$$

$$N[\overbrace{A\overbrace{BC}D}E F] = -\overbrace{AC}\,\overbrace{BD}\, N[EF].$$

Wick's theorem states that the product of operators ABC... is equal to the normal product of the operators, plus the sum of all normal products with one pair contracted, plus the sum of all normal products with two pairs contracted, and so on. For example

$$AB = N[AB] + \overbrace{AB}$$

$$\begin{aligned} ABCD = {} & N[ABCD] + \overbrace{AB}\, N[CD] - \overbrace{AC}\, N[BD] \\ & + \overbrace{AD}\, N[BC] + \overbrace{BC}\, N[AD] - \overbrace{BD}\, N[AC] \\ & + \overbrace{CD}\, N[AB] + \overbrace{AB}\,\overbrace{CD} - \overbrace{AC}\,\overbrace{BD} + \overbrace{AD}\,\overbrace{BC}. \end{aligned}$$

These two examples of Wick's theorem enable us to rewrite the Hamiltonian (1.74) as

$$H = H_0 + H_2 + H_4 \tag{1.83}$$

where H_n is the sum of all terms with n uncontracted operators.

$$H_0 = \sum_{ij} \langle i|T|j\rangle \langle a^\dagger_i a_j\rangle +$$

$$1/2 \sum_{ijkl} \langle ij|v|kl\rangle_A \langle a^\dagger_i a_k\rangle \langle a^\dagger_j a_l\rangle +$$

$$1/4 \sum_{ijkl} \langle ij|v|kl\rangle_A \langle a^\dagger_i a_j\rangle \langle a_l a_k\rangle \tag{1.84}$$

$$H_2 = \sum_{ij} \langle i|T|j\rangle N[a^\dagger_i a_j] +$$

$$\sum_{ijkl} \langle ij|v|kl\rangle_A \langle a^\dagger_j a_l\rangle N[a^\dagger_i a_k] +$$

$$\frac{1}{4} \sum_{ijkl} \langle ij|v|kl\rangle_A \langle a^\dagger_i a^\dagger_j\rangle N[a_l a_k] +$$

$$\frac{1}{4} \sum_{ijkl} \langle ij|v|kl\rangle_A \langle a_l a_k\rangle N[a^\dagger_i a^\dagger_j] \tag{1.85}$$

$$H_4 = \frac{1}{4} \sum_{ijkl} \langle ij|v|kl\rangle_A N[a^\dagger_i a^\dagger_j a_l a_k] \tag{1.86}$$

It has been assumed that

$$\langle ij|v|kl\rangle_A = \langle kl|v|ij\rangle_A = \langle ji|v|lk\rangle_A .$$

Define a density matrix ρ .

$$\rho_{ji} = \langle a^\dagger_i a_j\rangle \tag{1.87a}$$

ρ is clearly Hermitian.

$$\rho^\dagger = \rho \tag{1.87b}$$

Define a pairing tensor τ .

$$\tau_{ji} = \langle a_i a_j \rangle \tag{1.88a}$$

$$\tau^*_{ji} = \langle a^\dagger_j a^\dagger_i \rangle \tag{1.88b}$$

Recalling the anti-commutation relation (1.76) it is apparent that τ is anti-symmetric.

$$\tilde{\tau} = -\tau \tag{1.88c}$$

Define a HF potential Γ .

$$\Gamma_{ij} = \sum_{Kl} \langle iK | v | jl \rangle_A \, \rho_{lK} \tag{1.89a}$$

Using the Hermiticity of ρ it is easy to demonstrate that Γ is Hermitian.

$$\Gamma^\dagger = \Gamma \tag{1.89b}$$

Define a HF Hamiltonian $\mathcal{H}$.

$$\mathcal{H}_{ij} = T_{ij} + \Gamma_{ij} \tag{1.90a}$$

$\mathcal{H}$ is Hermitian.

$$\mathcal{H}^\dagger = \mathcal{H} \tag{1.90b}$$

Define a pair potential Δ .

$$\Delta_{ij} = \frac{1}{2} \sum_{Kl} \langle ij | v | Kl \rangle_A \, \tau_{Kl} \tag{1.91a}$$

$$\Delta^*_{ij} = \frac{1}{2} \sum_{Kl} \langle Kl | v | ij \rangle_A \, \tau^*_{Kl} \tag{1.91b}$$

Since $\langle ij|v|kl\rangle_A = -\langle ji|v|kl\rangle_A$, Δ is anti-symmetric.

$$\tilde{\Delta} = -\Delta \tag{1.91c}$$

H_0 and H_2 may be more simply expressed.

$$H_0 = \sum_{ij} \{ T_{ij} + \tfrac{1}{2} \Gamma_{ij} \} \rho_{ji} + \tfrac{1}{2} \sum_{ij} \Delta_{ij} \Gamma^*_{ij} \tag{1.92}$$

$$H_2 = \sum_{ij} \mathcal{H}_{ij} N[a^+_i a_j] + \tfrac{1}{2} \sum_{ij} \Delta_{ij} N[a^+_i a^+_j] + \tfrac{1}{2} \sum_{ij} \Delta^+_{ij} N[a_i a_j] \tag{1.93}$$

Since $\langle \Phi_0 | N[\cdots] | \Phi_0 \rangle = 0$,

$\langle \Phi_0 | H_2 | \Phi_0 \rangle = \langle \Phi_0 | H_4 | \Phi_0 \rangle = 0$,

and $\langle \Phi_0 | H | \Phi_0 \rangle = H_0$. If the reference state $|\Phi_0\rangle$ is chosen to be the ground state, then H_0 is E_0 , the ground state energy of the system. Then for the HF, BCS, and HFB theories H_2 is $H_{q.p.}$, the independent "quasiparticle" terms; and H_4 is $H_{q.p.-int.}$, the interactions between the "quasiparticles."

The physical significance of the quantities involved in this representation of H will become evident as we use this formulation to derive the various self-consistent field theories.

References to Chapter 1

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4. E.M.Henley and L. Wilets, Phys. Rev. 133, B1118 (1964).

5. M.H. Macfarlane, The Reaction Matrix in Nuclear Shell Theory, Lectures given at the International School of Physics "Enrico Fermi," XL Course (Nuclear Structure and Nuclear Reactions), Varenna, 1967.
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II. HARTREE - FOCK THEORY

1. Introduction

Hartree - Fock (HF) theory [1] is the first order approximation in a many - body theory of nuclei. It determines a one - particle self - consistent potential, and therefore supports an independent particle description of finite nuclei. It is instructive to present the HF formalism, since pairing theory in its most satisfactory form (HFB) may be derived as a generalization of HF.

For a given nucleus the HF equations typically have many solutions. The usual criterion for selecting one of them as the ground state solution is to choose the wave function which provides maximum binding energy. This seems to us to be not altogether satisfactory. The various minima often vary in $\langle H \rangle_{HF}$ by only a few Mev. Corrections to the binding energy from higher order diagrams, for rotational energy, and for zero-point fluctuation energy are considerably greater than these variations in $\langle H \rangle_{HF}$. Furthermore, the wave function which does minimize $\langle H \rangle_{HF}$ generally has a large gap between the last filled orbital and the first empty orbital. It is therefore fairly stable against particle - hole admixtures and pairing correlations. The other wave functions often have small gaps, so that introducing pairing correlations might be expected to lower the

energy of these states. These correlations will also increase the energy of the lowest elementary excitations, thereby stabilizing these wave functions.

For these reasons we do not consider the "minimum $\langle H \rangle_{HF}$ criterion" to be reliable. Instead the HF wave functions are here regarded as single particle bases which are useful for introducing additional correlations, such as pairing. The selection of the ground state wave function can be made only after correlations have been included and the energy is calculated to all significant orders. Alternatively one may consider the experimental data to choose the wave function which is most physically meaningful.

We shall demonstrate that, with the exception of Ne^{20}, HF theory fails to explain the properties of $N = Z$ even-even nuclei in the 2s-1d shell.

2. Derivation of the HF Equations

The HF approximation restricts the wave function to a single Slater determinant.

$$|\Phi_0\rangle = a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \cdots a^\dagger_{\alpha_A} |0\rangle \tag{2.1}$$

Each single particle state is a linear combination of basis states.

$$a^\dagger_\alpha = \sum_k D^\alpha_k \, a^\dagger_k \tag{2.2a}$$

or

$$|\alpha\rangle = \sum_k D^\alpha_k \, |k\rangle \tag{2.2b}$$

The transformation coefficients are chosen to be real. For a system with time - reversal degeneracy, no generality is lost with this phase convention. The inverse transformation ($D^{-1} = \tilde{D}$) is

$$a^\dagger_k = \sum_\alpha D^\alpha_k \, a^\dagger_\alpha \, . \tag{2.3}$$

The unitarity conditions are

$$\sum_k D^{\alpha_1}_k D^{\alpha_2}_k = \delta_{\alpha_1 \alpha_2} \tag{2.4a}$$

$$\sum_\alpha D^\alpha_{k_1} D^\alpha_{k_2} = \delta_{k_1 k_2} \, . \tag{2.4b}$$

(2.4) may also be derived by requiring that

$$[a^\dagger_{\alpha_1}, a_{\alpha_2}]_+ = \delta_{\alpha_1 \alpha_2} \, .$$

The density matrix has a simple form in the $|\alpha\rangle$ representation.

$$\rho_{\alpha_2\alpha_1} = \langle a^\dagger_{\alpha_1} a_{\alpha_2}\rangle = \begin{cases} \delta_{\alpha_1\alpha_2} & \text{if } |\alpha_1\rangle \text{ is occupied} \\ 0 & \text{if } |\alpha_1\rangle \text{ is unoccupied} \end{cases} \tag{2.5}$$

$\rho_{\alpha\alpha}$ is simply the probability that the state $|\alpha\rangle$ is occupied in $|\Phi_0\rangle$.

The HF potential (1.89a) and Hamiltonian (1.90a) are

$$\Gamma_{ij} = \sum_{\alpha \text{ occupied}} \langle i\alpha | v | j\alpha\rangle_A \tag{2.6}$$

$$\mathcal{H}_{ij} = T_{ij} + \Gamma_{ij} \ . \tag{2.7}$$

They are symmetric.

The operator $a_i\ a_j$ has non-zero matrix elements only when the final and initial states differ by two particles.

$\langle A' | a_i a_j | A\rangle = 0$ unless $A' = A - 2$.

Since the HF wave function is a single A particle determinant, the pairing tensor (1.88) vanishes. Consequently the pair potential (1.91) is zero. Alternatively, we may say the HF approximation consists in ignoring the abnormal contractions.

The ground state energy (1.84) is

$$E_0 = \sum_{\alpha \text{ occ.}} \langle\alpha | T | \alpha\rangle + \tfrac{1}{2} \sum_{\alpha\beta \text{ occ.}} \langle\alpha\beta | v | \alpha\beta\rangle_A \ . \tag{2.8}$$

It contains the kinetic energy of each particle and the interaction energy from the forward and exchange scattering of each pair of particles. (The factor $\frac{1}{2}$ compensates for the double counting of each pair in the summation.)

H_2 (1.93) has the simple form

$$H_2 = \sum_{ij} \mathcal{H}_{ij} N [a^+_i a_j] \cdot \tag{2.9}$$

The HF equations may be derived from a variational principle or by the equation of motion method. We present both techniques.

The variational principle consists in choosing the occupied orbitals $|\alpha\rangle$ such that the ground state energy is an extremum. The matrix elements of T and v in the $|\alpha\rangle$ basis may be expanded.

$$\langle \alpha_1 | T | \alpha_2 \rangle = \sum_{K_1 K_2} D^{\alpha_1}_{K_1} D^{\alpha_2}_{K_2} \langle K_1 | T | K_2 \rangle \tag{2.10}$$

$$\langle \alpha_1 \alpha_2 | v | \alpha_3 \alpha_4 \rangle_A = \sum_{K_1 K_2 K_3 K_4} D^{\alpha_1}_{K_1} D^{\alpha_2}_{K_2} D^{\alpha_3}_{K_3} D^{\alpha_4}_{K_4} \langle K_1 K_2 | v | K_3 K_4 \rangle_A \tag{2.11}$$

Substituting into (2.8)

$$E_0 = \sum_{\substack{\alpha \text{ occ.} \\ ij}} D^{\alpha}_i D^{\alpha}_j \langle i | T | j \rangle + \frac{1}{2} \sum_{\substack{\alpha\beta \text{ occ.} \\ ijkl}} D^{\alpha}_i D^{\beta}_j D^{\alpha}_k D^{\beta}_l \langle ij | v | kl \rangle_A \cdot \tag{2.12}$$

Alternatively the density matrix may be evaluated in the $|K\rangle$ basis. Using (2.3)

$$\langle a^{+}_{i} a_{j} \rangle = \sum_{\alpha\beta} D^{\alpha}_{i} D^{\beta}_{j} \langle a^{+}_{\alpha} a_{\beta} \rangle$$

Noting (2.5) we obtain

$$\rho_{ji} = \langle a^{+}_{i} a_{j} \rangle = \sum_{\alpha\, occ.} D^{\alpha}_{i} D^{\alpha}_{j} \,. \tag{2.13}$$

Substituting (2.13) into (1.84), we arrive at (2.12). E_0 should be stationary with respect to arbitrary variations in each coefficient D^{α}_{i}. A constraint is that the wave functions $|\alpha\rangle$ remain normalized.

$$\langle \alpha | \alpha \rangle = \sum_{i} |D^{\alpha}_{i}|^{2} = 1 \tag{2.14}$$

The variational principle is

$$\frac{\partial}{\partial D^{\alpha}_{i}} \left\{ E_0 - \epsilon_\alpha \left(\sum_{j} |D^{\alpha}_{j}|^{2} - 1 \right) \right\} = 0 \,. \tag{2.15}$$

ϵ_α is a Lagrange multiplier. Substituting (2.12) into (2.15) provides the HF equations.

$$\sum_{j} \left\{ \langle i | T | j \rangle + \sum_{\beta\, occ.} \langle i\beta | v | j\beta \rangle_{A} \right\} D^{\alpha}_{j} = \epsilon_\alpha D^{\alpha}_{i} \tag{2.16}$$

or

$$\sum_{j} \mathcal{H}_{ij} D^{\alpha}_{j} = \epsilon_\alpha D^{\alpha}_{i} \,. \tag{2.17a}$$

The HF equations present an eigenvalue problem.

$$\mathcal{H} \underline{D}^{\alpha} = \epsilon_\alpha \underline{D}^{\alpha} \tag{2.17b}$$

or

$$\mathcal{H} |\alpha\rangle = \epsilon_\alpha |\alpha\rangle \,. \tag{2.17c}$$

The eigenvectors $\underline{D}^{\alpha}$ provide the orbitals $|\alpha\rangle$ for which the binding energy is an extremum. In this basis H is diagonal with elements ϵ_α .

$$\epsilon_\alpha = \langle\alpha|T|\alpha\rangle + \sum_{\beta\ occ.}{}' \langle\alpha\beta|v|\alpha\beta\rangle_A \tag{2.18}$$

ϵ_α , the single particle energy, contains the kinetic energy and the energy acquired through forward and exchange scattering of a particle in state $|\alpha\rangle$ with particles in all occupied states $|\beta\rangle$.

The HF Hamiltonian is a function of the occupied orbitals $|\alpha\rangle$. These orbitals, in turn, are determined by H. This is the source of the self - consistency feature of the HF potential. The HF equations must be solved by an iterative procedure. An initial guess is made for the orbitals. $\mathcal{H}_{ij}$ may then be calculated. Diagonalizing $\mathcal{H}$ yields a new set of orbits. They are used to re-calculate $\mathcal{H}_{ij}$. This procedure is continued until successive interations produce identical orbits.

Since $\mathcal{H}$ is a function of the set $\{|\alpha\rangle\}_{occupied}$ there may be different solutions corresponding to different HF Hamiltonians. Therefore, the various solutions $|\Phi_0\rangle$ are, in general, not orthogonal.

The HF equations may also be derived by the equation of motion method. We want to reduce the effective Hamiltonian, which contains strong interactions between particles, to an independent particle Hamiltonian, for

which the eigenmodes of the system are approximately non-interacting. H has been expressed as

$$H = H_0 + H_2 + H_4 \cdot$$

If there is a basis in which H_2 has the form

$$H_2 = \sum_\alpha \epsilon_\alpha \, N[a^\dagger_\alpha a_\alpha] \tag{2.19}$$

then

$$H = E_0 + \sum_\alpha \epsilon_\alpha N[a^\dagger_\alpha a_\alpha] + H_4 \cdot$$

The HF ground state has one particle in each of the A lowest energy states.

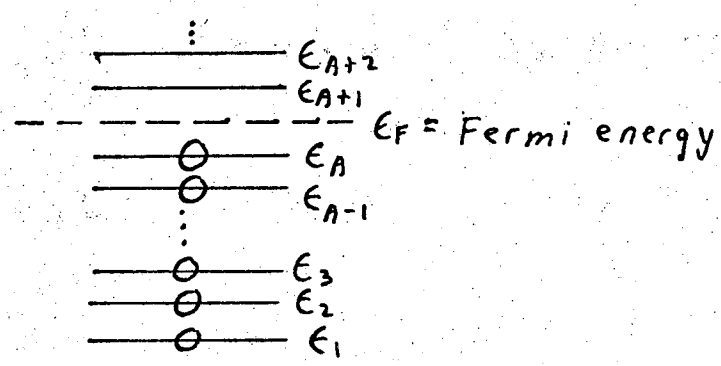


Figure (2.1)

The ground state contains no "particles" or holes. Therefore

$$N[a^\dagger_\alpha a_\alpha] = a^\dagger_\alpha a_\alpha \qquad \epsilon_\alpha > \epsilon_F \quad (a^\dagger_\alpha \text{ creates a "particle"})$$

$$N[a^\dagger_\alpha a_\alpha] = -a_\alpha a^\dagger_\alpha \qquad \epsilon_\alpha < \epsilon_F \quad (a_\alpha \text{ creates a hole}) \tag{2.20}$$

and

$$H = E_0 + \sum_{\epsilon_\alpha > \epsilon_F} \epsilon_\alpha a^\dagger_\alpha a_\alpha - \sum_{\epsilon_\alpha < \epsilon_F} \epsilon_\alpha a_\alpha a^\dagger_\alpha$$
$$+ 1/4 \sum_{\alpha_1\alpha_2\alpha_3\alpha_4} \langle \alpha_1 \alpha_2 | v | \alpha_3 \alpha_4 \rangle_A N[a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} a_{\alpha_4} a_{\alpha_3}]. \tag{2.21}$$

H_4 has zero matrix elements between states with zero or one particle or hole. It represents the residual interaction between "particles," between holes , and betweeen "particles" and holes. If H_4 is neglected, H assumes the form of an independent particle Hamiltonian.

$$H \approx E_0 + \sum_{\epsilon_\alpha > \epsilon_F} \epsilon_\alpha a^\dagger_\alpha a_\alpha - \sum_{\epsilon_\alpha < \epsilon_F} \epsilon_\alpha a_\alpha a^\dagger_\alpha \tag{2.22}$$

To determine the orbitals $|\alpha\rangle$ consider the commutator $[H_2, a^\dagger_\alpha]_-$. Substituting (2.19)

$$[H_2, a^\dagger_\alpha]_- = \epsilon_\alpha a^\dagger_\alpha \tag{2.23}$$

or

$$[H_2, a^\dagger_\alpha]_- = \epsilon_\alpha \sum_i D^\alpha_i a^\dagger_i . \tag{2.24}$$

The commutator may also be evaluated using (2.9).

$$[H_2, a^\dagger_\alpha]_- = \sum_i \left(\sum_j H_{ij} D^\alpha_j \right) a^\dagger_i \tag{2.25}$$

Equating coefficients of a_i^+ in the last two equations

$$\sum_j \mathcal{H}_{ij} D_j^\alpha = \epsilon_\alpha D_i^\alpha$$

which are the HF equations. Of course, this result is obtained more directly by simply noting that diagonalizing $\mathcal{H}$ puts H_2 (2.9) in the desired form. The equation of motion method is presented, however, as it will provide a natural generalization of the HF equations to include pairing (HFB).

3. Symmetries of the HF Solutions

The nucleon - nucleon interaction v_{ij} is invariant under time - reversal and parity and is a scalar under rotations. Since the HF Hamiltonian does not equal the true Hamiltonian, $\mathcal{H}$ may not have the same symmetry properties as H.

For each symmetry type s there corresponds an operator S. If s is a symmetry of the Hamiltonian H, then

$$[H, S]_- = 0 \quad . \tag{2.26}$$

If the set of occupied orbitals remains invariant under one of these symmetry operations

$$S\{|\alpha\rangle\}_{occ.} = \{|\alpha\rangle\}_{occ.} \tag{2.27a}$$

or

$$[\rho, S]_- = 0 \tag{2.27b}$$

then the HF Hamiltonian also commutes with S

$$[\mathcal{H}, S]_- = 0 \tag{2.28}$$

and s is termed a "self-consistent symmetry."

Consider the definition of $\mathcal{H}$.

$$\mathcal{H}_{ij} = \langle i|T|j\rangle + \sum_{kl} \langle ik|v|jl\rangle_A \rho_{lk}$$

If a self-consistent symmetry is introduced into the density matrix, then $\mathcal{H}$ will reflect that symmetry. Consequently ρ of the following iteration will possess it. Therefore, if the trial density matrix contains a self-consistent symmetry, then so will the

density matrix of the final self-consistent solution.

Harmonic oscillator wave - functions are chosen as the basis states.

$$|\alpha\rangle = \sum_k D_k^\alpha \, |N\ell JmT\rangle_k \tag{2.29}$$

For the present we choose $|\alpha\rangle$ to have a definite isospin.

$$|\alpha\rangle = \sum_k D_k^\alpha \, |N\ell Jm T_\alpha\rangle_k \tag{2.30}$$

Then

$$T_z \{ |\alpha\rangle \}_{occ.} = \{ |\alpha\rangle \}_{occ.} \tag{2.31a}$$

or

$$T_z \, |\Phi_0\rangle = |\Phi_0\rangle \tag{2.31b}$$

(except for a constant of normalization) and isospin projection provides a self-consistent symmetry. ρ has the block form

$$\rho = \begin{bmatrix} \rho_{pp} & 0 \\ 0 & \rho_{nn} \end{bmatrix} . \tag{2.32a}$$

Since the two - body interaction conserves isospin projection, if k and l have the same value of τ ; then so do i and j. Therefore $\mathcal{H}$ also has the form

$$\mathcal{H} = \begin{bmatrix} \mathcal{H}_{pp} & 0 \\ 0 & \mathcal{H}_{nn} \end{bmatrix} \tag{2.32b}$$

By the same argument, if we choose $|\alpha\rangle$ to have a definite parity, then

$$P\,|\Phi_0\rangle = |\Phi_0\rangle \tag{2.33}$$

and ρ and $\mathcal{H}$ have the form

$$\rho = \begin{bmatrix} \rho_{++} & 0 \\ 0 & \rho_{--} \end{bmatrix} \qquad \mathcal{H} = \begin{bmatrix} \mathcal{H}_{++} & 0 \\ 0 & \mathcal{H}_{--} \end{bmatrix}. \tag{2.34}$$

For nuclei with even numbers of neutrons and protons, the orbitals can be ensured to occur in time - reversed, degenerate pairs: $|\alpha\rangle$, $|\bar{\alpha}\rangle$. The time-reversal operator acting on a harmonic oscillator state gives

$$\mathcal{T}\,|N\ell Jm\rangle \equiv |\overline{N\ell Jm}\rangle = (-1)^{J-m+\ell}\,|N\ell J-m\rangle. \tag{2.35}$$

(We choose $\langle \underline{r}\,|\,\ell m_\ell\rangle = Y_{\ell m_\ell}$. For the choice $\langle \underline{r}\,|\,\ell m_\ell\rangle = i^{\ell}\,Y_{\ell m_\ell}$, $\mathcal{T}\,|Jm\rangle = (-1)^{J-m}\,|J-m\rangle$.)

If $|\alpha\rangle$ is given by (2.30), then $|\bar{\alpha}\rangle$ is

$$|\bar{\alpha}\rangle = \sum_{K} D_{\bar{K}}^{\bar{\alpha}} \, |\overline{N\ell J m \tau_\alpha}\rangle_K = \sum_{K} D_K^{\alpha} (-1)^{J-m+\ell} \, |N\ell J - m \tau_\alpha\rangle_K . \quad (2.36)$$

Phases are chosen so that $D_{\bar{K}}^{\bar{\alpha}} = D_K^{\alpha}$. Since

$$\mathcal{J}|\alpha\rangle = |\bar{\alpha}\rangle \quad \text{and} \quad \mathcal{J}|\bar{\alpha}\rangle = -|\alpha\rangle \quad (2.37)$$

we have

$$\mathcal{J}|\Phi_0\rangle = |\Phi_0\rangle \quad (2.38)$$

so that

$$[\mathcal{H}, \mathcal{J}]_- = 0 \quad (2.39)$$

and time - reversal is a self - consistent symmetry.

Since the rotation operator $R_y(\pi)$ is equivalent to $\mathcal{J}P$ (within a phase)

$$R_y(\pi)|\Phi_0\rangle = |\Phi_0\rangle \quad (2.40)$$

and

$$[\mathcal{H}, R_y(\pi)]_- = 0 \quad (2.41)$$

so that rotation by π about the y axis is a self-consistent symmetry.

The body - fixed axes may be chosen to be the principal axes. That is, the wave function may be chosen to have ellipsoidal symmetry with respect to the body fixed axes (reflection symmetry through xy, xz, yz planes). This will be achieved if the components of $|\alpha\rangle$ are required to have $m - \frac{1}{2}$ = even integer, and those of $|\bar{\alpha}\rangle$ therefore have $m - \frac{1}{2}$ = odd integer. More specifically, $|\alpha\rangle$ contains the set of states $\{|jm\rangle\}_1$ with

$$m = \cdots -7/2, -3/2, 1/2, 5/2, \cdots \quad (|\alpha\rangle) \tag{2.42a}$$

and $|\bar{\alpha}\rangle$ is composed of the set $\{|jm\rangle\}_2 = \mathcal{T}\{|jm\rangle\}_1$. $|\bar{\alpha}\rangle$ has components with

$$m = \cdots -5/2, -1/2, 3/2, 7/2, \cdots \quad (|\bar{\alpha}\rangle) \tag{2.42b}$$

This choice diagonalizes the inertia tensor.[2]

Consider the rotation operator $R_z(\theta)$.

$$R_z(\theta)|jm\rangle = e^{-im\theta}|jm\rangle \tag{2.43}$$

so that

$$R_z(\pi)|jm\rangle = \begin{cases} -i\,|jm\rangle & (m-1/2) \text{ even} \\ +i\,|jm\rangle & (m-1/2) \text{ odd} \end{cases} \tag{2.44}$$

Noting the restriction (2.42)

$$R_z(\pi)\,|\alpha\rangle = -i\,|\alpha\rangle \tag{2.45a}$$

$$R_z(\pi)\,|\bar{\alpha}\rangle = +i\,|\bar{\alpha}\rangle\,. \tag{2.45b}$$

Therefore

$$R_z(\pi)\,|\Phi_0\rangle = |\Phi_0\rangle \tag{2.46}$$

and

$$[\mathcal{H}, R_z(\pi)]_- = 0\,. \tag{2.47}$$

Rotation by π about the z axis is a self-consistent symmetry.

For all nuclei (not just even-even ones), if the orbitals are divided into two sets in accordance with (2.42), then ρ connects states with m - $\frac{1}{2}$ even, and it connects states with m - $\frac{1}{2}$ odd.

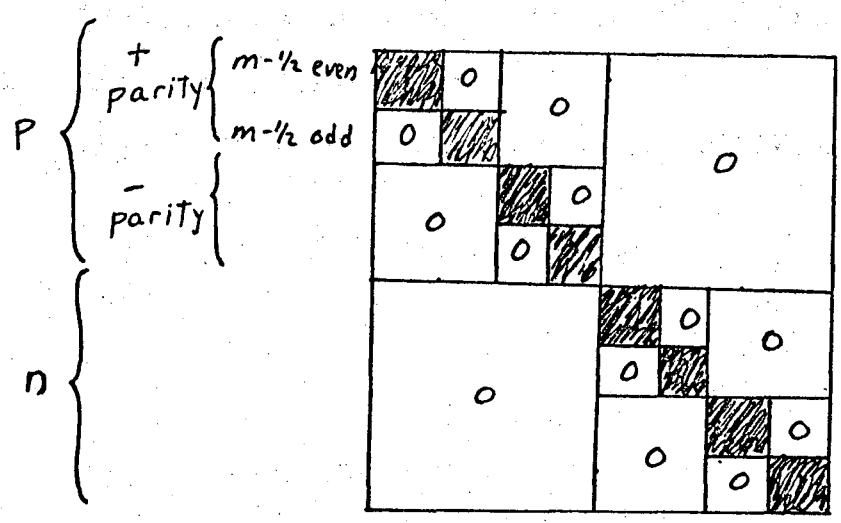
$$\rho = \begin{array}{cc} \begin{array}{cc} m-\frac{1}{2}\ \text{even} & m-\frac{1}{2}\ \text{odd} \end{array} & \\ \begin{bmatrix} \rho & 0 \\ 0 & \bar{\rho} \end{bmatrix} & \begin{array}{l} m-\frac{1}{2}\ \text{even} \\ m-\frac{1}{2}\ \text{odd} \end{array} \end{array} \tag{2.48}$$

where $\bar{\rho}_{ji} = \rho_{\bar{j}\bar{i}}$. Since the two-body interaction conserves angular momentum projection ($M = m_i + m_k = m_j + m_l$), $\mathcal{H}$ has the same form.

$$\mathcal{H} = \begin{array}{cc} \begin{array}{cc} m-\tfrac{1}{2} \text{ even} & m-\tfrac{1}{2} \text{ odd} \end{array} & \\ \begin{bmatrix} \mathcal{H} & 0 \\ 0 & \bar{\mathcal{H}} \end{bmatrix} & \begin{array}{l} m-\tfrac{1}{2} \text{ even} \\ m-\tfrac{1}{2} \text{ odd} \end{array} \end{array} \tag{2.49}$$

where $\bar{\mathcal{H}}_{ij} = \mathcal{H}_{\bar{i}\bar{j}}$. For even-even nuclei with time-reversal degeneracy $\bar{\rho} = \rho$ and $\bar{\mathcal{H}} = \mathcal{H}$.

By requiring the occupied orbitals to have good isotopic spin projection and parity and to be time - reversal invariant, ρ and $\mathcal{H}$ have been reduced to the block form:



(2.50)

The dimension of the required matrix diagonalization is therefore considerably reduced.

Axial symmetry about the z axis requires

$$R_z(\theta)\,|\Phi_0\rangle = |\Phi_0\rangle \quad \text{for all } \theta . \tag{2.51}$$

If $R_z(\theta)|\alpha\rangle = |\alpha\rangle$ for all θ, then (2.43) indicates that all components of $|\alpha\rangle$ must have the same $|m\rangle$.

$$|\alpha\rangle = \sum_K D_K^\alpha \, |N \ell J m_\alpha \tau_\alpha\rangle_K \tag{2.52}$$

Then

$$[\mathcal{H}, R_z(\theta)]_- = 0 \qquad \text{for all } \theta \tag{2.53}$$

and axial symmetry is a self-consistent symmetry. ρ and $\mathcal{H}$ will connect only states with the same m.

Spherical symmetry requires that $|\alpha\rangle$ be an eigenstate of $\underline{J}^2$ and J_z. Then only radial mixing is permitted.

$$|\alpha\rangle = \sum_K D_K^\alpha \, |N \ell_\alpha J_\alpha m_\alpha \tau_\alpha\rangle \tag{2.54}$$

$\underline{J}\{|\alpha\rangle\}$ occ. = $\{|\alpha\rangle\}$occ. is satisfied only if all m states for a given J are equally occupied (but not necessarily full). Then ρ and $\mathcal{H}$ connect states with all quantum numbers identical except N, and spherical symmetry is a self - consistent symmetry.

4. Separation of Core and Valence Particles

Choose the model space to consist of all configurations with A_c particles filling a closed core and the remaining A_v particles ($A = A_c + A_v$) distributed in the valence shell. Then the ground state wave function is

$$|\Phi_0\rangle = |\Phi_v\rangle\,|\Phi_c\rangle \,. \tag{2.55}$$

Let $|K\rangle$ represent a HO state ($|K\rangle = |Nljm\tau\rangle$). Then the core component of $|\Phi_0\rangle$ is

$$|\Phi_c\rangle = a^\dagger_{K_1} a^\dagger_{K_2} \cdots a^\dagger_{K_{A_c}} \,|0\rangle \,. \tag{2.56}$$

For nuclei in the 2s - 1d shell, $|\Phi_c\rangle$ may be chosen as the spherical O^{16} wave function (1s and 1p orbitals fully occupied), and $|\Phi_v\rangle$ may be restricted to have components within the 2s - 1d shell. Deviations of the true core wave function from (2.56) (radial mixing, core deformation, correlations) and interactions between the core and valence particles (other than those contained in the HF potential) should properly be accounted for in the effective interaction.

The separation of core and valence particles is attained by choosing $|\Phi_c\rangle$ as the reference state in the Hamiltonian (1.83 - 1.86). (The selection of

reference state is quite arbitrary. It need not be the ground state of the A particle system, nor need it have A particles.) H_0 is then given by (2.8). It may be referred to as the core energy.

$$E_c = \sum_{k \in core} \langle k|T|k\rangle + \frac{1}{2} \sum_{k_1 k_2 \in core} \langle k_1 k_2 | v | k_1 k_2 \rangle_A \qquad (2.57)$$

If the core consists of filled $(N\ell J)$ orbitals, then the core energy is

$$E_c = \sum_{(N\ell J) \in core} 2(2J+1) \langle (N\ell J) m | T | (N\ell J) m \rangle +$$

$$\frac{1}{2} \sum_{\substack{JT \\ (N\ell J)_1 (N\ell J)_2 \in core}} (2J+1)(2T+1) \langle (N\ell J)_1 (N\ell J)_2 JT | v | (N\ell J)_1 (N\ell J)_2 JT \rangle_A \qquad (2.58)$$

H_2 is given by (2.19).

$$H_2 = \sum_k e_k N[a^\dagger_k a_k] \qquad (2.59)$$

The normal ordering is with respect to $|\Phi_c\rangle$, so that

$$H_2 = \sum_{k \in valence} e_k a^\dagger_k a_k - \sum_{k \in core} e_k a_k a^\dagger_k . \qquad (2.60)$$

The single particle energy is given by (2.18).

$$e_k = \langle k|T|k\rangle + \sum_{k' \in core} \langle kk'|v|kk'\rangle_A \qquad (2.61)$$

or $$e_{N\ell J} = \langle (N\ell J)\, m \,|\, T \,|\, (N\ell J)\, m \rangle +$$

$$\frac{1}{2(2J+1)} \sum_{\substack{JT \\ (N'\ell'J') \in core}}' (2J+1)(2T+1) \langle (N\ell J)(N'\ell'J')\, JT | v | (N\ell J)(N'\ell'J')\, JT \rangle_A \,. \tag{2.62}$$

H_4 is given by (1.86). The Hamiltonian then has the form

$$H = E_c + \sum_{k \in valence}' e_k a_k^\dagger a_k - \sum_{k \in core}' e_k a_k a_k^\dagger$$

$$+ \tfrac{1}{4} \sum_{k_1 k_2 k_3 k_4}' \langle k_1 k_2 | v | k_3 k_4 \rangle_A N [a_{k_1}^\dagger a_{k_2}^\dagger a_{k_4} a_{k_3}] \,. \tag{2.63}$$

This representation has the advantage of reducing the dimensionality of the eigenvalue problem. Furthermore, experimental values may be used for the single particle energies e_{Nlj}. The early self-consistent field calculations used a central interaction, which can not produce a spin - orbit spliting between the $d_{5/2}$ and $d_{3/2}$ orbitals. Using the experimental single particle energies corrected this defect.

We have arrived at this representation by choosing $|\Phi_c\rangle$ (2.56) as the reference state. If the wave function $|\Phi_0\rangle$ is then restricted to the form (2.55), there can be no holes, and the Hamiltonian is simplified.

$$H = E_c + \sum_{K \in \text{valence}} e_K a^\dagger_K a_K$$
$$+ 1/4 \sum_{K_1 K_2 K_3 K_4} \langle K_1 K_2 | v | K_3 K_4 \rangle_A a^\dagger_{K_1} a^\dagger_{K_2} a_{K_4} a_{K_3} \quad (2.64)$$

Restricting the model wave function in this fashion is not, of course, an approximation, as all configurations outside the model space are to be accounted for in the effective interaction.

Wick's theorem may be applied a second time. The reference state is $|\Phi_0\rangle$. The Hamiltonian (2.64) has the representation

$$H = E_c + E_V + H_2 + H_4 \quad (2.65)$$

where E_V, H_2, and H_4 are given by (1.84 - 1.86), the summations being restricted to states in the valence shell, and the expectation values and normal products are now with respect to $|\Phi_0\rangle$.

In the HF approximation the ground state wave function is

$$|\Phi_0\rangle = a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \cdots a^\dagger_{\alpha_{A_V}} |\Phi_c\rangle \quad (2.66)$$

with

$$|\alpha\rangle = \sum_{K \in \text{valence}} D^\alpha_K |K\rangle . \quad (2.67)$$

The ground state energy is

$$E_{HF} = E_C + E_V$$

where E_V is given by (2.8), the summations being restricted to the valence particles.

$$E_V = \sum_{\alpha=1}^{A_V} \langle \alpha | \tau | \alpha \rangle + 1/2 \sum_{\alpha,\beta=1}^{A_V} \langle \alpha\beta | v | \alpha\beta \rangle_A \tag{2.68}$$

with

$$\langle jm\tau | \tau | j'm'\tau' \rangle = e_j \, \delta_{jj'} \, \delta_{mm'} \, \delta_{\tau\tau'} \, . \tag{2.69}$$

The HF Hamiltonian is

$$\mathcal{H}_{ij} = \langle i | \tau | j \rangle + \sum_{\alpha=1}^{A_V} \langle i\alpha | v | j\alpha \rangle_A \, . \tag{2.70}$$

The eigenvalue equation

$$\mathcal{H} \underline{D}^{\alpha} = \epsilon_{\alpha} \underline{D}^{\alpha} \tag{2.71}$$

is restricted to the space of valence orbitals.

5. Nuclear Deformations

The various self-consistent field formalisms provide a microscopic description of nuclear deformations. The many particle wave functions may be characterized by their multipole moments.

$$Q_{LM} = r^L Y_{LM} \tag{2.72}$$

In second quantized notation

$$Q_{LM} = \sum_{ij} \langle i | Q_{LM} | j \rangle a^{+}_{i} a_j \tag{2.73}$$

so that

$$\langle Q_{LM} \rangle = \sum_{ij} \langle i | Q_{LM} | j \rangle \rho_{ji} \tag{2.74}$$

In HF theory

$$\langle Q_{LM} \rangle = \sum_{\alpha \text{ occupied}} \langle \alpha | Q_{LM} | \alpha \rangle \tag{2.75}$$

If the wave function displays time-reversal degeneracy, $\langle Q_{LM} \rangle = \langle Q_{L-M} \rangle$ and $\langle Q_{LM} \rangle = 0$ for odd M due to reflection symmetry. We calculate $\langle Q_{LM} \rangle$ for L = 2 and 4 and M $\leq$ L. The units are fm^L.

The deformation parameter β is related to $\langle Q_{20} \rangle$ by

$$\beta = \frac{4\pi}{5A} \cdot \frac{\langle Q_{20} \rangle}{\langle r^2 \rangle} \tag{2.76}$$

where

$$\langle r^L \rangle = \frac{1}{A} \sum_{ij}' \langle i | r^L | j \rangle \rho_{ji} \cdot \tag{2.77}$$

The RMS radius of the nucleus is

$$R_{RMS} = \sqrt{\langle r^2 \rangle} \cdot \tag{2.78}$$

The moment of inertia is calculated from the microscopic wave function by the cranking method. Details of the derivation are available elsewhere.[3] The result for the HF wave function is

$$\mathcal{J}_x = 2 \sum_{\substack{\alpha \text{ occ.} \\ \beta \text{ unocc.}}}' \frac{|\langle \alpha | J_x | \beta \rangle|^2}{\epsilon_\beta - \epsilon_\alpha} \tag{2.79}$$

with similar relations for $\mathcal{J}_y$ and $\mathcal{J}_z$. For axial symmetry, $\mathcal{J}_x = \mathcal{J}_y$ and $\mathcal{J}_z = 0$.

If a nucleus is a good axial rotator its energy levels follow

$$E_I = (\hbar^2/2\mathcal{J})\, I\,(I+1) \cdot \tag{2.80}$$

The experimental spectrum may be characterized by the energy ratios

$$R_I = (E_I - E_0)/(E_2 - E_0) \quad . \tag{2.81}$$

For a good rotator

$$R_4 = 3\,1/3 \text{ and } R_6 = 7.$$

The experimental value of the inertial parameter $A = (\hbar^2/2\mathcal{J})$ (Mev) may be obtained from the spacing between any two rotational levels.

$$A_{I_2 - I_1} = \frac{E_{I_2} - E_{I_1}}{I_2(I_2+1) - I_1(I_1+1)} \tag{2.82}$$

In particular

$$A_{2-0} = (E_2 - E_0)/6 \quad \text{and} \quad A_{4-2} = (E_4 - E_2)/14 \quad .$$

6. Effective Nucleon - Nucleon Interactions

To determine the dependence on the choice of force of the results in this and succeeding chapters, all calculations are performed with three different forces.

a) Rosenfeld interaction: This effective force has been widely used to study the nuclei in the 2s - 1d shell. It is a central interaction with a Yukawa radial dependence.

$$V = V_0 \frac{e^{-r/a}}{r/a} \underline{\tau}_1 \cdot \underline{\tau}_2 \, (0.3 + 0.7 \, \underline{\sigma}_1 \cdot \underline{\sigma}_2)$$

$$V_0 = 50 \text{ Mev} \qquad a = 1.35 \text{ fm.}$$

The oscillator parameter is $b = 1.65$ fm. (The radial wave function is $R_{nl} \sim e^{-\frac{1}{2}(r/b)^2}$, where $b^2 = \hbar/m\omega_0$ Also $\nu = 1/b^2$.)

O^{16} is assumed to form an inert core, so that the single particle operator in the Hamiltonian becomes

$$\langle i | \tau | j \rangle = e_i \, \delta_{ij}$$

where $|i\rangle$, $|j\rangle$ are HO orbitals. A realistic force contains a $\underline{L}.\underline{S}$ component. Therefore different nuclei within the same shell should have different spacings between $|l \; j + \frac{1}{2}\rangle$ and $|l \; j - \frac{1}{2}\rangle$. The absence of the $\underline{L}.\underline{S}$ component in the Rosenfeld force may be compensated by altering the single particle energies e_i for the various nuclei. Also the core polarization changes for each

nucleus, so that it is proper to choose different e_i for different nuclei. Two sets of single particle energies have been used.

Rosenfeld 1 : Kelson and Bar - Touv single particle energies.

$$e_{1d_{5/2}} = -7.0 \text{ Mev} \quad e_{2s_{\frac{1}{2}}} = -4.2 \text{ Mev} \quad e_{1d_{3/2}} = 0.0 \text{ Mev}$$

Rosenfeld 2 : O^{17} single particle energies.

$$e_{1d_{5/2}} = -4.142 \text{ Mev} \quad e_{2s_{\frac{1}{2}}} = -3.172 \text{ Mev} \quad e_{1d_{3/2}} = +\ 0.94 \text{ Mev}$$

b) Yale t - matrix: The Yale potential was determined by fitting nucleon-nucleon scattering data.[4] It contains central, tensor, spin - orbit, and quadratic spin - orbit components. Since a hard core is included, one must use the t - matrix elements of the potential in nuclear structure calculations.[5] As is customary, the dependence of the t - matrix on the single particle wave functions and energies (double self - consistency) is ignored. The single particle basis includes the 1s, 1p, 2s, and 1d orbitals. The oscillator parameter is $b^2 = 3.1 \text{ fm}^2$.

c) Nestor-Davies-Krieger-Baranger (NDKB) effective potential: This potential was designed for HF calculations. Accordingly, in fitting the force parameters primary emphasis was given to reproducing

the binding energy and density of nuclear matter. Less emphasis was given to fitting the scattering data. There is no hard core, and second order contributions to the binding energy of nuclear matter are small. It contains central, tensor, spin - orbit, and repulsive velocity - dependent components. Explicitly, the interaction used is

$$U_j = (\hbar^2/m)\{V_j^c(r) + [(p^2/\hbar^2)\omega_j(r) + \omega_j(r)(p^2/\hbar^2)] + V_j^T(r)\, S_{12} + V_j^{LS}(r)\, \underline{L}\cdot\underline{S}\}$$

where m is the nucleon mass. The tensor operator is

$$S_{12} = [3(\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\underline{r}) - r^2(\underline{\sigma}_1\cdot\underline{\sigma}_2)]/r^2,$$

the orbital and spin angular momentum operators are

$$L = (\underline{r}\times\underline{p})/\hbar$$

$$S = \tfrac{1}{2}(\underline{\sigma}_1 + \underline{\sigma}_2),$$

$\underline{r}$ and $\underline{p}$ are the relative co-ordinate and relative momentum

$$\underline{r} = \underline{r}_1 - \underline{r}_2$$

$$\underline{p} = \tfrac{1}{2}(\underline{p}_1 - \underline{p}_2) = -i\hbar\nabla_r .$$

The subscript j denotes the components of the interaction: singlet - even (SE), singlet - odd (SO), triplet-even (TE), and triplet-odd (TO). The functions $V_j(r)$ and $\omega_j(r)$ have a Gaussian shape.

$$V_j(r) = -A_j \exp(-\tfrac{1}{2} r^2/\alpha_j^2)$$

$$\omega_j(r) = B_j \exp(-\tfrac{1}{2} r^2/\beta_j^2)$$

with the exception of the tensor part $V_j^T(r)$.

$$V_j^T(r) = -A_j(\tfrac{1}{2} r^2/\alpha_j^2) \exp(-\tfrac{1}{2} r^2/\alpha_j^2)$$

For attractive $V_j(r)$, $A_j > 0$ and for repulsive $\omega_j(r)$, $B_j > 0$. A_j has units of fm^{-2}, while B_j is dimensionless. $\hbar^2/m = 41.47 Mev \cdot fm^2$. We choose the set of parameters denoted by NDKB as mixture 2. (See table 2.1)
The oscillator parameter is b = 1.70fm. To study the effects of space truncation, all calculations with the NDKB force were performed for two different single particle bases.

NDKB1. 1s,1p,2s,1d

NDKB2. 1s,1p,2s,1d,2p,1f

7. HF in the 2s - 1d Shell

We confine our attention to N = Z even - even nuclei. Then time - reversal and (if the Coulomb force is neglected) proton - neutron exchange are self-consistent symmetries. The calculation and interpretation of wave functions are thereby simplified. Parity has been assumed to be a good symmetry. No attempt has been made to obtain triaxial solutions with the NDKB force.

The experimental and calculated binding energies of these nuclei are presented in Table 2.2. For the spherical nuclei, O^{16} and Ca^{40}, addition of the p - f shell resulted in a small increment in binding. This is caused by radial mixing of the 1p and 2p orbitals. For the strongly deformed nuclei the increment in binding is greater, as an increase in deformation energy contributes to the increment as well as the radial mixing. Without the p - f shell, the 12 particles in the 1p orbital must maintain spherical symmetry. Admixtures of the 2p - 1f states into the 1p states permits these particles to have a deformation. Inclusion of the p-f shell generally increases the deformation parameter β of the nucleus by about 50%.[21] The HF gap is also considerably increased.

The observed spectra are in Figures 2.3 - 2.7. The

solutions to the HF equations are listed in Table 2.15.

O^{16}

The ground state is spherical. Only radial mixing is permitted. The experimental and calculated single particle energies are in Table 2.3. The experimental single particle energies are obtained[1] from the mass differences

$$O^{16} + n - O^{17} = 4.142 \text{ Mev}$$
$$O^{15} + n - O^{16} = 5.669 \text{ Mev}$$

and the experimental spectra of O^{15} and O^{17}.

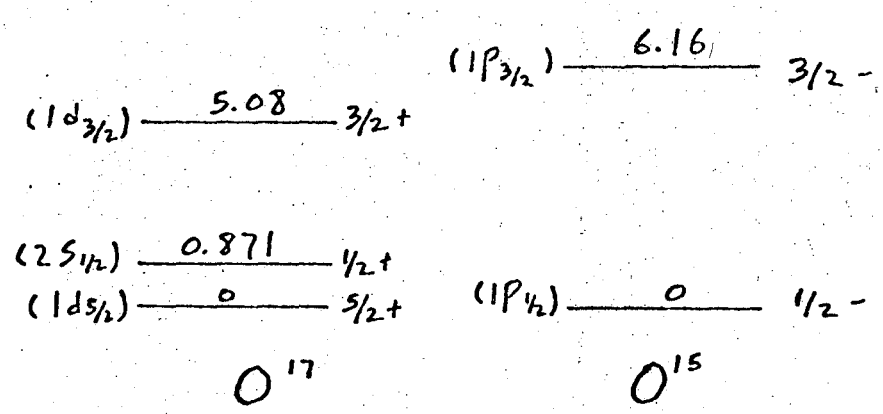


Figure 2.2: The lowest positive parity levels in O^{17} and the lowest negative parity levels in O^{15}.

Whereas the experimental value of the gap between 1p and 2s-1d shells is 11.5 Mev, the calculated value is $\sim$ 16 Mev for both the Yale and the NDKB forces.

Ne^{20}

The "rotational" levels have energy ratios

$$R_4 = 2.61 \qquad R_6 = 5.45.$$

Since a rotator should have $R_4 = 3\ ^1/_3$ and $R_6 = 7$, Ne^{20} is not a good example of a rotator. (The rare earth nuclei fit the model considerably better. Hf^{172}, for instance, has $R_4 = 3.26$ and $R_6 = 6.63$.) The inertial parameters are

$$A_{2-0} = 0.272 \text{ Mev} \qquad A_{4-2} = 0.187 \text{ Mev}.$$

Their average will be considered as the experimental value of A.

$$A_{exp.} = 0.230 \text{ Mev}$$

For all forces, the lowest HF minimum is prolate with an $\Omega = \frac{1}{2}+$ occupied orbital. The properties of this state are fairly insensitive to the choice of force. (See Table 2.4.) Angular momentum projection on this intrinsic state yields an energy spectrum in very good agreement with the experimental values.[7] HF theory therefore provides an adequate explanation for the Ne^{20} energy spectrum.

Mg^{24}

The 0^+, 2^+ and 4^+ levels have the energy ratio

$$R_4 = 3.00.$$

The average of the inertial parameters

$$A_{2-0} = 0.228 \text{ Mev} \qquad A_{4-2} = 0.196 \text{ Mev}$$

is taken as the experimental value.

$$A_{exp} = 0.212 \text{ Mev}$$

The large number of HF solutions should be noted. Their variation in binding energy is small. As the asymmetric solution is the lowest minimum and has a large gap, it has been considered as the intrinsic wave function corresponding to the ground state. This interpretation is no longer tenable.

Giraud and Sauer [8] have performed the angular momentum projection calculation on the asymmetric wave function. (The force was a Rosenfeld mixture with Gaussian radial dependence, oscillator length b = 1.65 fm, strength V_0 = 53.2 Mev, and O^{17} single particle energies.) The calculated excitation energies are (experimental values in parentheses) : 1.36 (1.37) Mev for the first 2^+ state, 2.48 (4.12) Mev and 2.54 (4.23) Mev for the 4^+ - 2^+ doublet, and 3.85 (5.22) Mev for the 3^+ state. The agreement is not very satisfactory. Except for the

first 2^+ state, the remainder of the spectrum is much too compressed. Variation of the strength V_0 from 40 to 60 Mev and increasing the $\underline{l}\cdot\underline{s}$ splittings by a factor of two did not achieve better agreement.

Experimental data on stripping spectroscopic factors [9] and the γ branching ratio [10] of Mg^{25} favor an axially symmetric rather than an asymmetric shape for the Mg^{24} even-even core. Parikh [11] concludes that the "prolate 1 solution (Rosenfeld 1, sd) is in best agreement with experiments. The triaxial solution is unable to account for the structure of the wave functions in spite of the fact that it is the lowest in energy."

Clearly the asymmetric HF solution can no longer be considered as the intrinsic wave function corresponding to the ground state and low lying excited states.

The static quadrupole moment of the first 2^+ state has been measured through the reorientation effect in Coulomb excitation.

$$Q_{2+} = -0.26 \pm 0.08b \qquad \text{(Ref. 12)}$$

$$Q_{2+} = -0.243 \pm 0.035b \qquad \text{(Ref. 13)}$$

A negative static quadrupole moment implies a prolate deformation in the intrinsic state.

Parikh's findings and the measurement of Q_{2+} lead us to a re-consideration of the prolate HF solution with $\Omega = \frac{1}{2}, {}^3/_2$ occupied orbitals. (See tables 2.5 - 2.9.) The various forces produce similar wave functions for

this state. They exhibit several deficiencies. The HF gap is small (0.463 Mev for the Yale force), so that this HF wave function is not stable against p-h admixtures. The binding energy is 3 - 4 Mev less than that obtained with the asymmetric wave function. The inertial parameter is considerably smaller than the experimental value. Introducing pairing correlations may eliminate these objections. The small HF gap is desirable for obtaining strong pairing with little loss of HF energy. The pairing will create a gap for elementary excitations, thereby stabilizing the wave function. The gain in pairing energy will more than compensate for loss of HF energy, so that total binding may increase by several Mev. Finally, pairing may alter the inertial parameter by as much as an order of magnitude.

Si^{28}

Bar - Touv and Goswami [14] have suggested that the first excited 0^+ state corresponds to a spherical intrinsic state. The ground state 0^+ is lowered to its observed position by interaction with the excited 0^+ state. The experimental value of A should therefore be determined from the $2^+ - 4^+$ spacing.

$R_2 = 2.59$

$A_{2-0} = 0.299$ Mev

$A_{4-2} = 0.202$ Mev

$A_{exp.} = 0.202$ Mev

Coulomb excitation of the first 2^+ state yielded a static quadrupole moment of

$$Q_{2+} = 0.177 \pm 0.070 \text{ b} \qquad \text{(Ref. 15)}$$

thereby confirming the oblate deformation of the intrinsic wave function. Tewari and Grillot [16] have projected states of good J from the oblate and prolate Yale wave functions. The calculated spectrum is in poor agreement with experiment. Unfortunately all low lying oblate HF solutions have large HF gaps. One would not expect to be able to introduce pairing correlations into these wave functions.

S^{32}

The S^{32} spectrum does not seem to have a ready explanation, being neither a good rotational nor vibrational spectrum. The 0^+ state at 3.78 Mev might correspond to the spherical intrinsic state.[14] It will then interact with the ground state 0^+, so that the experimental value of A should be taken from the $2^+ - 4^+$ spacing.

$R_2 = 2.00$

$A_{2-0} = 0.374$ Mev

$A_{4-2} = 0.161$ Mev

$A_{exp} = 0.161$ Mev

The lowest HF minimum is asymmetric with a large gap. The Rosenfeld force favors oblate shapes, while the NDKB and Yale forces prefer prolate. Several of the axially symmetric solutions have small HF gaps, and are good bases in which to include pairing. The lowest prolate and oblate states are presented in Tables 2.10, 2.11.

Ar^{36}

The energy spectrum is characteristic of an anharmonic vibrator. The lowest HF maximum is oblate with deformation $\beta = -0.10$ to -0.15 and inertial parameter A = 0.20 to 0.28 Mev. These values are representative of a strongly deformed nucleus. All

other HF solutions have small gaps. HF theory, therefore, can not explain the vibrational nature of Ar^{36}. It might be expected that introducing pairing into the prolate HF wave function will yield a stable and only slightly deformed wave function. If the resulting inertial parameter is large, then the excitation energy of the rotational states will be greater than that of the vibrational states. Characteristic wave functions for the prolate solution are in Tables 2.12, 2.13. The other forces yield somewhat different wave functions, but the level orderings are similar, the empty orbital always having $\Omega = 3/2$.

Ca^{40}

The ground state is spherical. Single particle energies are in Table 2.11.

We may conclude that, with the exception of Ne^{20}, HF theory fails to explain the properties of N = Z even - even nuclei in the 2s - 1d shell.

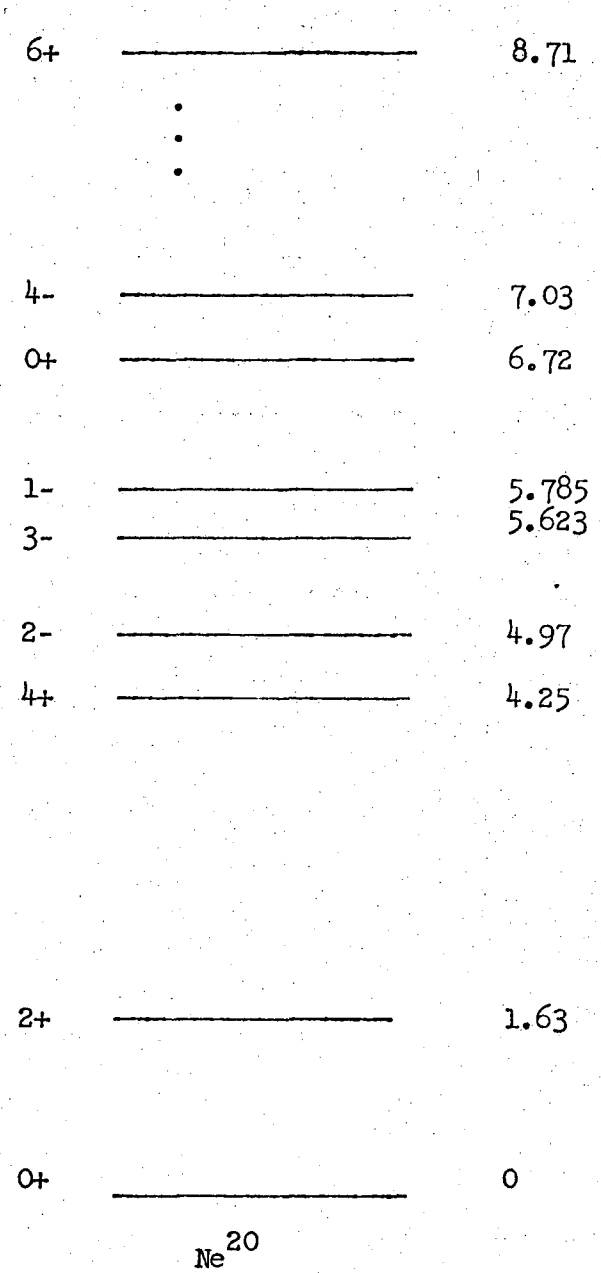


Fig. 2.3 Ne^{20} energy level diagram (Ref. 18)

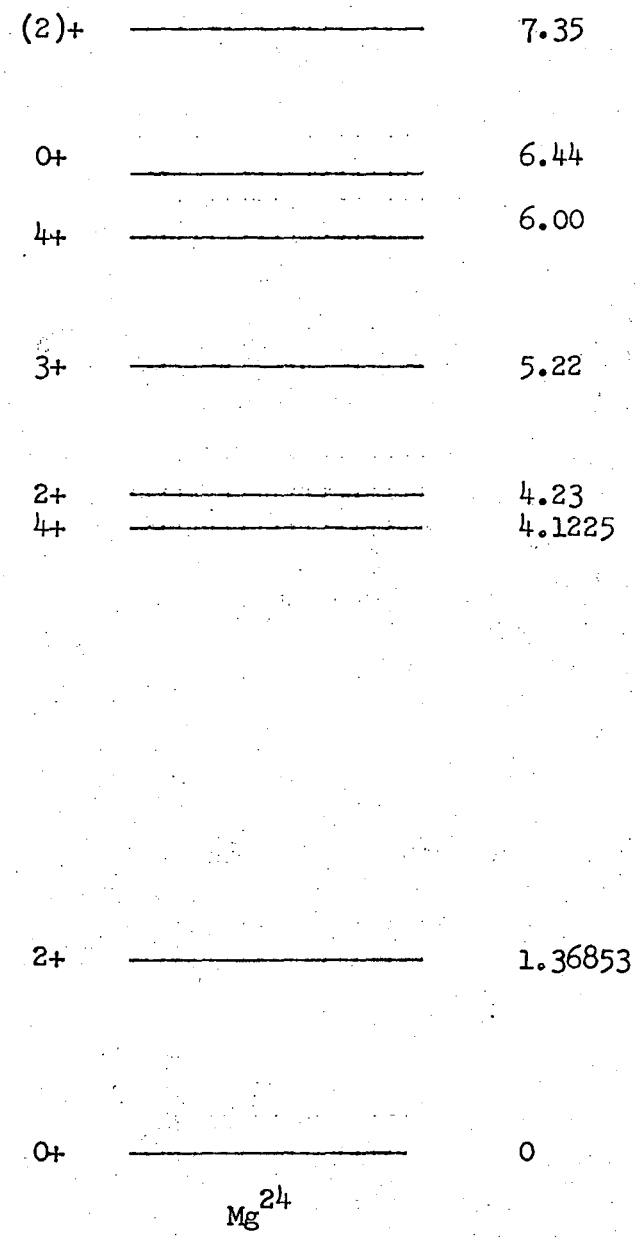


Fig. 2.4 Mg^{24} energy level diagram (Ref. 18)

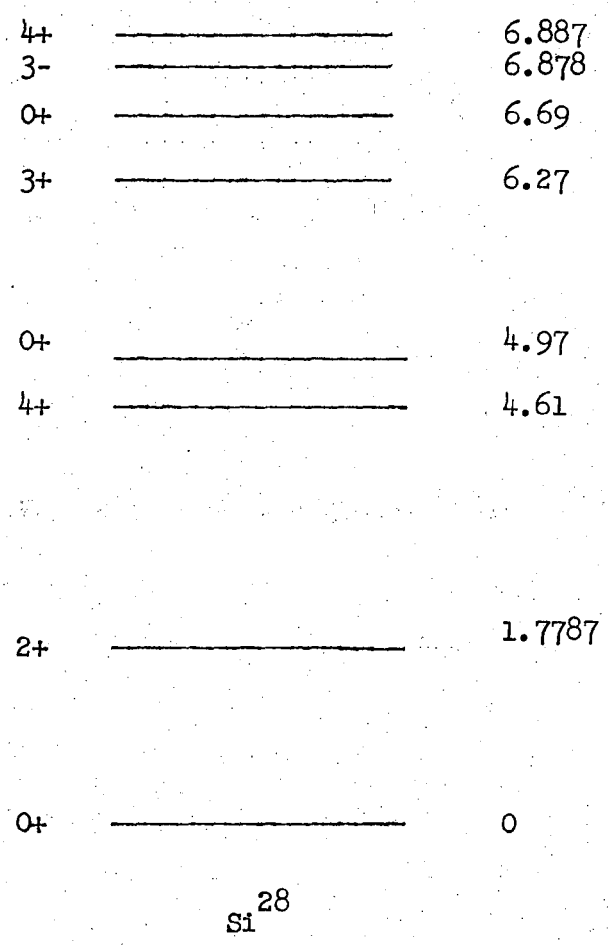


Fig. 2.5 Si^{28} energy level diagram (Ref. 19)

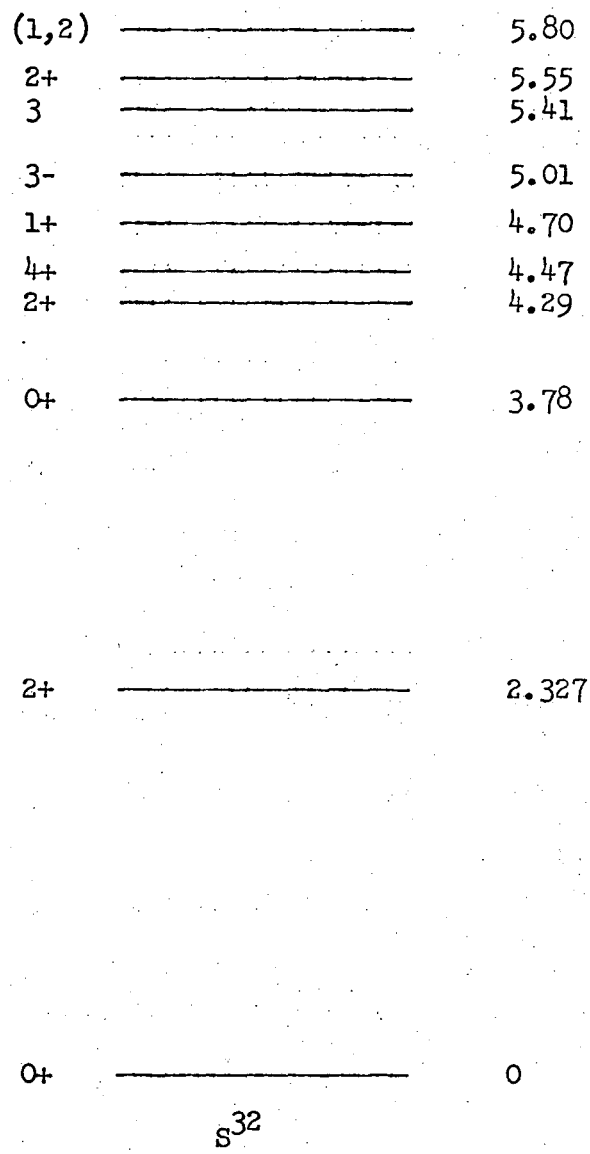


Fig. 2.6 S^{32} energy level diagram (Ref. 19,20)

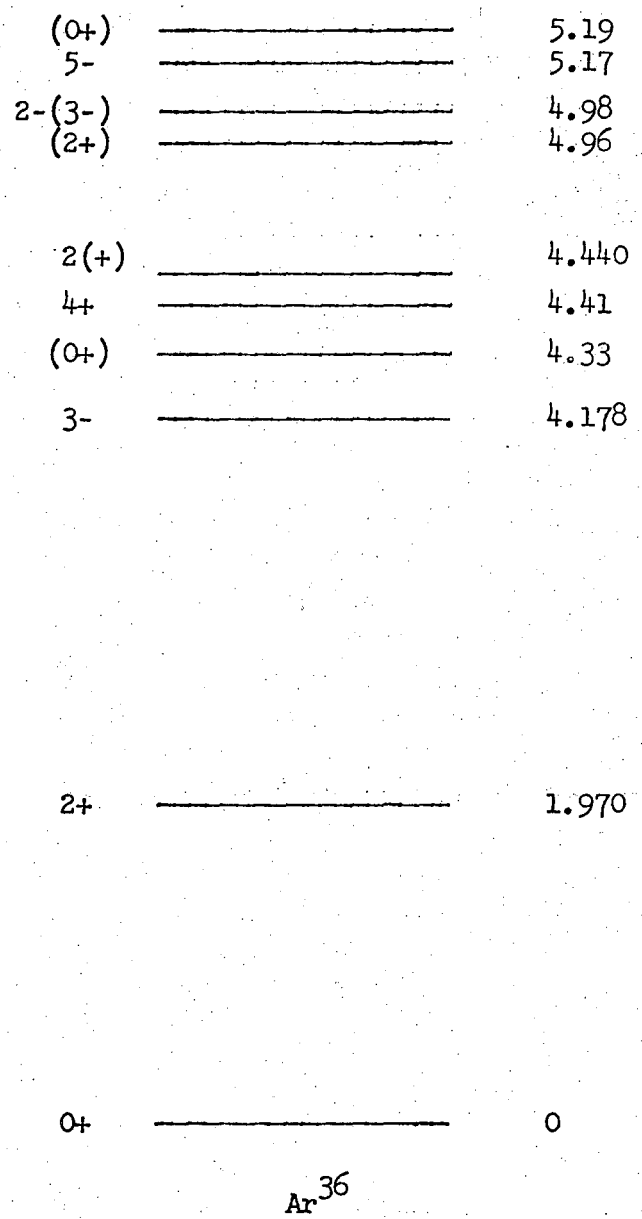


Fig. 2.7 Ar^{36} energy level diagram (Ref. 19)

Table 2.1: NDKB Force Parameters

	A_c	α_c	B	β	A_T	α_T	A_{LS}	α_{LS}
TE	7.227	0.575	1.0	0.575	0.490	1.20		
SE	2.127	0.903	0.6	0.903				
TO	0.219	1.40	0.128	1.40	-0.35	1.0	1.40	0.8
SO	-0.128	1.40	0.307	1.40				

Table 2.2: Binding Energy per Particle (Mev)

	Expt.	Yale	NDKB 1	NDKB 2
O^{16}	8.72	5.08	4.75	4.83
Ne^{20}	8.96	5.07	4.37	4.62
Mg^{24}	9.36	5.55	4.51	4.78
Si^{28}	9.71	6.35	5.11	5.35
S^{32}	9.92	7.11	5.58	5.67
Ar^{36}	10.10	8.08	6.28	6.35
Ca^{40}	10.27	8.87	6.97	6.97

The "experimental binding energies" are obtained by subtracting the Coulomb energy from the observed binding energies. (Ref. 17)

Table 2.3: Single Particle Energies in O^{16} (Mev)

	Expt.	Yale	NDKB 1	NDKB 2
$1s_{1/2}$	~-35	-46.34	-47.81	-50.61
$1p_{3/2}$	-21.83	-20.40	-20.85	-21.89
$1p_{1/2}$	-15.669	-16.23	-14.86	-15.41
$1d_{5/2}$	-4.142	-0.39	0.61	0.60
$2s_{1/2}$	-3.271	0.09	3.49	3.54
$1d_{3/2}$	+0.94	4.78	8.23	8.80
$2p_{3/2}$				17.58
$1f_{7/2}$				16.56
$2p_{1/2}$				25.16
$1f_{5/2}$				19.16

Table 2.4 : Occupied $\Omega = 1/2 +$ Level in Prolate Ne^{20}

	$1s_{1/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
Rosenfeld 1	-	0.821	-0.428	-0.378
Rosenfeld 2	-	0.715	-0.581	-0.389
Yale	0.038	0.732	-0.567	-0.375
NDKB 1	0.015	-0.831	0.431	0.353
NDKB 2	0.016	-0.803	0.474	0.362

Table 2.5: Prolate Mg^{24} (Prolate 1, Rosenfeld 1)

ϵ_α	Ω_α	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
-19.382	1/2	.851	-.464	-.247
-15.054	3/2	.974	0	.225
-11.991	1/2	.463	.439	.770
-10.156	5/2	1.000	0	0
- 6.169	1/2	.249	.770	-.588
- 4.054	3/2	-.225	0	.974

Table 2.6: Prolate Mg^{24} (Prolate 2, Rosenfeld 2)

ϵ_α	Ω_α	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
-17.974	1/2	.718	-.626	-.303
-12.216	3/2	.964	0	.267
-10.735	1/2	.610	.358	.706
- 6.901	5/2	1.000	0	0
- 5.030	1/2	.334	.692	-.640
- 2.624	3/2	-.267	0	.964

Table 2.7: Prolate Mg^{24} (Yale)

ϵ_α	Ω_α	$1s_{1/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
-14.982	1/2	.021	.713	-.595	-.370
- 9.505	3/2	0	.951	0	.310
- 9.042	1/2	.036	-.612	-.271	-.742
- 4.970	5/2	0	1.000	0	0
- 4.247	1/2	.143	-.337	-.745	.557
- 1.835	3/2	0	-.310	0	.951

Energies are in Mev.

Table 2.8: Prolate Mg^{24} (NDKB 1)

ϵ_α	Ω_α	$1s_{1/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
-11.619	1/2	.036	-.826	.469	.310
- 7.415	3/2	0	.965	0	.261
- 5.780	1/2	.012	-.505	-.379	-.775
- 3.852	5/2	0	1.000	0	0
-0.546	1/2	.096	-.241	-.795	.548
1.650	3/2	0	-.261	0	.965

Table 2.9: Prolate Mg^{24} (NDKB 2)

ϵ_α	Ω_α	$1s_{1/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
-13.543	1/2	.043	-.795	.518	.312
- 8.031	3/2	0	.958	0	.288
- 5.920	1/2	.013	- .527	-.341	-.788
- 2.457	5/2	0	1.000	0	0
0.753	1/2	.123	-.289	-.780	.540
3.484	3/2	0	-.288	0	.958

Energies are in Mev.

Table 2.10: Prolate S^{32} (NDKB 2)

ϵ_α	Ω_α	$1s_{1/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
-19.683	1/2	.031	-.904	.420	.078
-17.738	3/2	0	.961	0	.277
-13.121	1/2	.010	.251	.373	.893
-11.622	5/2	0	1.000	0	0
-7.421	3/2	0	-.277	0	.961
-6.727	1/2	.052	-.344	-.827	.441

Table 2.11 : Oblate S^{32} (NDKB 2)

ϵ_α	Ω_α	$1s_{1/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
-16.633	5/2	0	1.000	0	0
-15.937	1/2	.010	-.827	-.423	.370
-13.646	3/2	0	.836	0	-.549
-11.317	1/2	.091	.408	-.900	-.120
-9.803	3/2	0	.549	0	.836
-7.595	1/2	.015	-.386	-.051	-.921

Energies are in Mev.

Table 2.12: Prolate Ar^{36} (Rosenfeld 2)

ϵ_α	Ω_α	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
-23.648	1/2	.730	-.676	-.104
-22.008	3/2	.980	0	.199
-21.549	1/2	.683	.715	.150
-18.352	5/2	1.000	0	0
-17.530	1/2	-.027	-.180	.983
-14.892	3/2	-.199	0	.980

Table 2.13: Prolate Ar^{36} (NDKB 2)

ϵ_α	Ω_α	$1s_{1/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
-21.477	1/2	.010	-.943	.328	.053
-20.085	3/2	0	.984	0	.180
-16.960	5/2	0	1.000	0	0
-14.982	1/2	.044	-.301	-.778	-.550
-13.472	1/2	.050	-.138	-.533	.833
-12.402	3/2	0	-.180	0	.984

Energies are in Mev.

Table 2.14: Single Particle Energies in Ca^{40} (Mev)

	Rosenfeld 1	Rosenfeld 2	Yale	NDKB 1	NDKB 2
$1s_{1/2}$			-79.874	-83.418	-83.144
$1p_{3/2}$			-52.443	-51.641	-51.468
$1p_{1/2}$			-48.181	-45.134	-45.118
$1d_{5/2}$	-27.771	-24.913	-27.791	-24.868	-24.835
$2s_{1/2}$	-25.278	-24.349	-24.307	-18.016	-18.059
$1d_{3/2}$	-20.771	-19.831	-21.181	-15.108	-15.164
$1f_{7/2}$					- 1.940
$2p_{3/2}$					5.355
$1f_{5/2}$					9.738
$2p_{1/2}$					10.142

Table 2.15: HF in the 2s - 1d Shell

Nucleus	Force	Shape	E_{HF}	HF Gap	Q_{2M}	Q_{4M}	A	β	R_{rms}
Ne^{20}	Rosenfeld 1	Prolate 1	-46.049	8.325	12.7	82.6	0.27		
		Asymmetric	-43.044	6.055	-6.6	16.2	0.48		
					0	0	0.48		
						-68.8	0.15		
		Oblate	-39.439	1.995	-6.9	18.8	0.11		
		Spherical	-39.237	6.447	0	0	∞		
		Prolate 2	-37.989	0.743	2.6	-67.5	0.02		
	Rosenfeld 2	Prolate 1	-37.714	9.390	13.5	70.5	0.34		
		Spherical	-35.521	8.376	0	0	∞		
		Asymmetric	-32.989	6.335	-6.7	17.3	0.52		
					0	0	0.52		
						-73.0	0.16		
		Oblate	-28.007	1.609	-6.9	18.8	0.10		
		Prolate 2	-26.839	0.529	2.8	-69.6	0.02		
	Yale	Prolate	-101.482	5.810	16.3	92.2	0.22	0.269	2.756
		Asymmetric	-96.006	2.945	4.0	-87.3	0.30	0.067	2.756
					4.9	69.5	0.08		
						0.4	0.30		
		Spherical	-94.337	2.365	0	0	∞	0	2.784
	NDKB 1	Prolate	-87.523	4.414	13.9	90.6	0.15	0.246	2.666
	NDKB 2	Prolate	-92.305	6.212	18.8	107.8	0.21		

For axial shapes: $Q_{2M} = Q_{20}$ and $Q_{22} = 0$. $Q_{4M} = Q_{40}$ and $Q_{42} = Q_{44} = 0$. $A = A_x = A_y$ and $A_z = \infty$.
For asymmetric shapes: $Q_{2M} = (Q_{20}, Q_{22})$. $Q_{4M} = (Q_{40}, Q_{42}, Q_{44})$. $A = (A_x, A_y, A_z)$.
Energies are in Mev. R_{rms} has units of fm. Q_{LM} has units of fm^L.

Table 2.15 (continued)

Nucleus	Force	Shape	E_{HF}	HF Gap	Q_{2M}	Q_{4M}	A	β	R_{rms}
Mg^{24}	Rosenfeld 1	Asymmetric	-97.586	7.324	15.6	-5.5	0.23		
					-4.0	-66.8	0.21		
						3.9	0.54		
		Prolate 1	-94.105	3.063	15.2	-4.1	0.15		
		Prolate 2	-93.505	5.334	7.6	-118.4	0.16		
		Oblate 1	-92.181	2.795	-13.3	62.7	0.12		
		Oblate 2	-91.248	2.308	-2.1	116.2	0.07		
		Prolate 3	-90.224	4.856	6.8	97.8	0.18		
		Oblate 3	-89.588	2.070	-10.8	10.9	0.09		
	Rosenfeld 2	Asymmetric	-80.661	8.339	15.2	-23.2	0.21		
					-4.8	-68.2	0.26		
						3.2	0.54		
		Prolate 1	-76.427	6.035	6.8	104.2	0.19		
		Oblate 1	-75.085	2.031	-13.3	43.0	0.13		
		Prolate 2	-74.605	1.480	16.2	-12.3	0.10		
		Prolate 3	-73.467	6.284	7.1	-135.7	0.14		
		Oblate 2	-69.798	2.643	-12.8	28.8	0.17		
	Yale	Asymmetric	-133.144	5.376	19.8	-11.6	0.18	0.254	2.855
					4.8	77.9	0.17		
						1.2	0.40		
		Prolate	-129.568	0.463	20.0	-6.3	0.05	0.257	2.853
		Oblate 1	-126.307	0.102	-16.6	63.2	0.01	-0.211	2.864
		Oblate 2	-124.828	0.915	-15.4	38.1	0.10	-0.197	2.858
	NDKB 1	Prolate	-108.615	1.635	17.3	2.3	0.10	0.237	2.760
		Oblate	-104.821	0.770	- 13.0	19.2	0.05	-0.178	2.771
	NDKB 2	Prolate	-114.810	2.110	23.2	-1.6	0.14	0.327	2.727
		Oblate	-108.876	1.249	- 17.5	27.0	0.09	-0.242	2.751

Table 2.15 (continued)

Nucleus	Force	Shape	E_{HF}	HF Gap	Q_{2m}	Q_{4M}	A	β	R_{rms}
Si^{28}	Rosenfeld 1	Oblate 1	-154.717	7.659	-18.7	76.0	0.21		
		Prolate	-153.244	5.701	19.0	-88.9	0.20		
		Asymmetric	-151.723	7.000	7.0	29.2	0.242		
					-3.1	-67.1	0.235		
						-57.3	0.19		
		Oblate 2	-149.930	5.290	-0.5	-95.4	0.25		
		Spherical	-148.600	5.719	0	0	∞		
		Oblate 3	-146.242	2.147	-0.3	117.5	0.07		
	Rosenfeld 2	Oblate 1	-129.798	8.310	-20.0	69.8	0.23		
		Prolate	-128.927	7.515	18.6	-100.9	0.19		
		Oblate 2	-121.053	1.757	-0.2	123.5	0.07		
		Oblate 3	-118.095	3.395	-0.4	-113.9	0.17		
		Spherical	-114.304	3.801	0	0	∞		
	Yale	Oblate	-177.941	7.170	-23.8	88.9	0.19	-0.249	2.927
		Prolate	-174.925	4.040	23.7	- 111.4	0.15	0.248	2.923
		Spherical	-154.723	-	0	0	-	0	2.922
	NDKB 1	Oblate 1	-143.007	6.553	-20.3	82.1	0.17	-0.228	2.827
		Prolate	-138.220	0.916	21.6	-87.6	0.15	0.243	2.826
		Oblate 2	-136.110	2.093	- 0.3	-119.5	0.12	-0.004	2.834
		Spherical	-133.166	0.762	0	0	∞	0	2.832
	NDKB 2	Oblate 1	-149.805	8.504	-25.9	92.9	0.22		
		Prolate	-146.411	3.413	28.7	-109.6	0.20		
		Oblate 2	-138.111	2.615	-0.3	-140.7	0.14	-0.004	2.800
		Spherical	-134.582	1.384	0	0	∞	0	2.785

Table 2.15 (continued)

Nucleus	Force	Shape	E_{HF}	HF Gap	Q_{2M}	Q_{4M}	A	β	R_{rms}
S^{32}	Rosenfeld 1	Asymmetric	-214.883	6.584	-14.1	+3.4	0.21		
					-4.2	-72.0	0.25		
						-6.6	0.40		
		Oblate 1	-212.850	5.316	-1.5	-95.3	0.25		
		Oblate 2	-212.608	5.279	-4.7	109.3	0.19		
		Spherical	-211.500	5.719	0	0	∞		
		Oblate 3	-207.552	3.145	-6.9	- 83.2	0.20		
	Rosenfeld 2	Asymmetric	-182.220	7.520	-15.4	-5.8	0.19		
					-3.8	-74.7	0.27		
						-4.3	0.47		
		Oblate 1	-179.248	6.357	-6.3	134.8	0.14		
		Oblate 2	-177.293	3.409	-1.2	-113.6	0.17		
		Prolate	-173.852	2.428	13.5	-35.3	0.25		
		Spherical	-173.488	3.801	0	0	∞		
		Oblate 3	-171.612	3.644	-6.9	-99.1	0.20		
	Yale	Asymmetric	-227.737	4.487	15.7	-71.5	0.16	0.139	2.977
					9.3	-42.1	0.29		
						54.1	0.21		
		Prolate	-222.485	1.775	16.1	-78.4	0.15	0.143	2.974
	NDKB 1	Prolate	-178.658	3.807	14.0	-47.2	0.19	0.133	2.878
		Oblate	-172.666	1.222	-4.6	119.2	0.11	-0.044	2.882
		Spherical	-170.287	0.329	0	0	∞	0	2.882
	NDKB 2	Prolate	-181.933	4.200	18.1	-63.2	0.24	0.174	2.864
		Oblate	-174.698	1.514	-6.4	147.6	0.12	-0.061	2.865
		Spherical	-171.520	0.559	0	0	∞	0	2.852

Table 2.15 (continued)

Nucleus	Force	Shape	E_{HF}	HF Gap	Q_{2M}	Q_{4M}	A	β	R_{rms}
Ar^{36}	Rosenfeld 1	Oblate	-280.582	7.392	-12.0	-79.7	0.28		
		Asymmetric	-278.189	4.605	- 3.2	57.3	0.41		
					- 3.9	-45.3	0.23		
						0.03	0.41		
		Prolate	-276.817	2.442	5.9	-10.2	0.20		
		Spherical	-271.988	4.739	0	0	∞		
	Rosenfeld 2	Oblate	-240.955	8.348	-12.1	-90.1	0.26		
		Asymmetric	-238.606	5.858	-3.3	67.0	0.49		
					-4.1	-52.9	0.18		
						7.8	0.49		
		Prolate	-235.284	2.638	6.2	-12.4	0.22		
		Spherical	-230.172	4.728	0	0	∞		
	Yale	Oblate	-291.071	5.721	-15.3	-100.6	0.20	-0.117	3.017
		Prolate	-285.959	1.459	7.3	-18.7	0.14	0.056	3.021
		Spherical	-281.901	1.150	0	0	∞	0	3.016
	NDKB 1	Oblate	-225.964	4.508	-13.6	-70.8	0.21	-0.112	2.914
		Prolate	-222.270	0.647	6.3	-11.8	0.06	0.052	2.917
		Spherical	-221.833	2.795	0	0	∞	0	2.927
	NDKB 2	Oblate	-228.610	6.340	-17.0	-86.7	0.26		
		Prolate	-223.192	1.070	8.1	-15.6	0.11	0.067	2.909
		Spherical	-222.078	3.171	0	0	∞	0	

Energies are in Mev. R_{rms} has units of fm.

Q_{LM} has units of fm^L.

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Including the orbitals from $1g_{9/2}$ to $1i_{13/2}$ has a small effect on the binding energy and RMS radius, but Q_{20} is increased by 40% for sd shell nuclei.

III. THE SPECIAL QUASIPARTICLE TRANSFORMATION

1. Pairing in Nuclei

The HF potential does not account for all effects of the effective Hamiltonian. Residual components of the effective forces may introduce correlations into the presently uncorrelated (except for Pauli "correlations") HF wave function. We shall now consider in detail "pairing correlations". Pairs of nucleons in time - reversed degenerate orbitals may have correlated wave functions, resulting in an increment in binding energy. It is energetically favorable for two like nucleons to pair to $J = 0$ since this configuration provides maximum spatial overlap. The ground state angular momentum of an odd nucleus is determined by the J of the odd unpaired nucleon.

The HF potential accounts for forward and exchange scatterings between all pairs of particles. The relevant matrix elements are

$$\langle \alpha(1)\ \beta(2) \mid v \mid \alpha(1)\ \beta(2) \rangle_A \ .$$

For energies well below the Fermi surface, all orbitals are occupied. The exclusion principle therefore ensures that the HF potential accounts for all important scatterings below the surface of the nucleus. Near the surface, however, orbitals are available for other than forward and exchange

scattering.

Pairing theory accounts for the scattering of pairs of particles between different pairs of time - reversed degenerate orbitals. The corresponding matrix elements are

$$\langle \alpha(1)\ \bar{\alpha}(2) \mid v \mid \beta(1)\ \bar{\beta}(2) \rangle_A .$$

The sharp Fermi surface of the HF theory is replaced by a diffuse Fermi surface (in particle space).

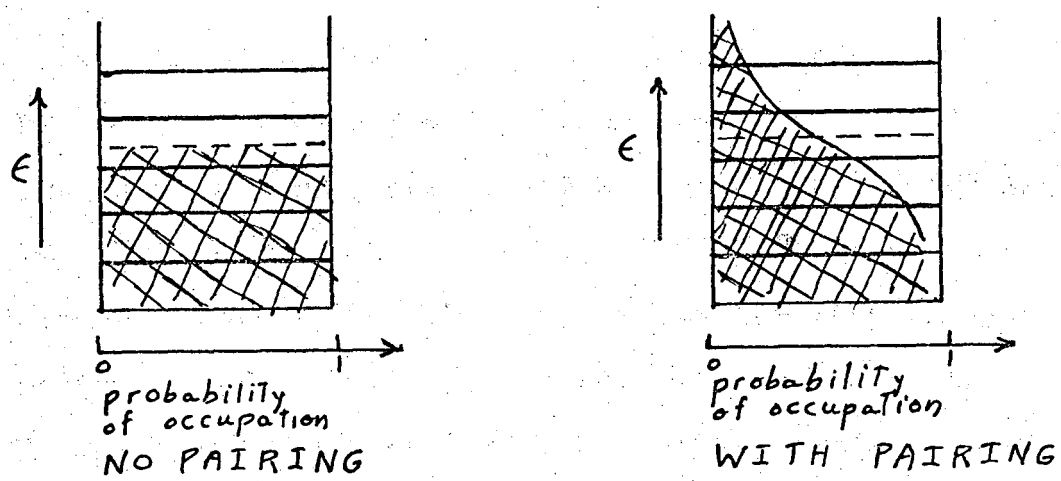

Figure (3.1)

Although this pair scattering produces rearrangements only in the neighbourhood of the surface, resulting in only a small increment in total binding energy, we shall see that macroscopic nuclear properties such as deformations and moments of inertia may be drastically altered. The spectrum of low - lying excitations is fundamentally changed. Even the underlying single particle basis may be significantly modified by the pairing correlations.

2. Bogoliubov Quasiparticles

Although the existence of pairing in nuclei has long been recognized, a systematic theory was not developed until the BCS theory of superconductivity (1957) was applied to nuclei (1959).[1,2] The Bogoliubov quasiparticle method is equivalent to the BCS formulation.

The properties of the special Bogoliubov quasiparticle transformation will be worked out in considereable detail. This is desirable because:

a) The essential features of pairing theory are most easily demonstrated by the special transformation.

b) $|T_z| = 1$ pairing can be directly studied with the special transformation.

c) Familiarity with the special transformation will enable us to generalize the pairing theory to include $T = 0$ and $T = 1$ pairing.

d) The most desirable form of the pairing theory (HFB) is derived from the general Bogoliubov quasiparticle transformation. The general transformation may always be described in terms of the special transformation in an appropriate single particle basis. This is true even if $T = 0$ and $T = 1$ pairing co-exist. The ground state wave function may always be given in the form of the familiar BCS wave function.

In I.3 we introduced the notion of "quasiparticles" as the elementary excitations of the system. The ground state is therefore a "quasiparticle" vacuum. In the HF description the "quasiparticles" are "particles"

$$b^{\dagger}_{\alpha} = a^{\dagger}_{\alpha} \qquad (\epsilon_{\alpha} > \epsilon_F) \tag{3.1a}$$

or holes.

$$b^{\dagger}_{\alpha} = a_{\alpha} \qquad (\epsilon_{\alpha} < \epsilon_F) \tag{3.1b}$$

If the state $|\alpha\rangle$ is paired with the time reversed degenerate state $|\bar{\alpha}\rangle$, the qppropriate generalization is the special Bogoliubov quasiparticle transformation.

$$b^{\dagger}_{\alpha} = u_{\alpha} a^{\dagger}_{\alpha} - v_{\alpha} a_{\bar{\alpha}} \tag{3.2a}$$

$$b_{\alpha} = u^{*}_{\alpha} a_{\alpha} - v^{*}_{\alpha} a^{\dagger}_{\bar{\alpha}} \tag{3.2b}$$

$$b^{\dagger}_{\bar{\alpha}} = u_{\bar{\alpha}} a^{\dagger}_{\bar{\alpha}} - v_{\bar{\alpha}} a_{\alpha} \tag{3.2c}$$

$$b_{\bar{\alpha}} = u^{*}_{\bar{\alpha}} a_{\bar{\alpha}} - v^{*}_{\bar{\alpha}} a^{\dagger}_{\alpha} \tag{3.2d}$$

We shall see that $|v_{\alpha}|^2$ is the probability that the orbits $|\alpha\rangle$, $|\bar{\alpha}\rangle$ are occupied.

The quasiparticles are Fermions and must satisfy the anti-commutation relations.

$$[b^{+}_{\alpha}, b^{+}_{\beta}]_{+} = [b_{\alpha}, b_{\beta}]_{+} = 0 \tag{3.3a}$$

$$[b^{+}_{\alpha}, b_{\beta}]_{+} = \delta_{\alpha\beta} \tag{3.3b}$$

In particular

$$[b^{+}_{\alpha}, b_{\alpha}]_{+} = 1$$

$$[b_{\alpha}, b_{\bar{\alpha}}]_{+} = 0 \, .$$

These commutators may be evaluated with (1.76) and (3.2).

$$|u_{\alpha}|^{2} + |v_{\alpha}|^{2} = 1 \tag{3.4a}$$

$$u_{\alpha} v_{\bar{\alpha}} + u_{\bar{\alpha}} v_{\alpha} = 0 \tag{3.4b}$$

It is therefore required that

$$|u_{\alpha}| = |u_{\bar{\alpha}}| \tag{3.5a}$$

$$|v_{\alpha}| = |v_{\bar{\alpha}}| \tag{3.5b}$$

We choose the pairing parameters to be real, with the phase convention

$$u_{\bar{\alpha}} = u_{\alpha} \tag{3.6a}$$

$$v_{\bar{\alpha}} = -v_{\alpha} \, . \tag{3.6b}$$

Rewriting (3.2)

$$b^{+}_{\alpha} = u_{\alpha} a^{+}_{\alpha} - v_{\alpha} a_{\bar{\alpha}} \tag{3.7a}$$

$$b_{\alpha} = u_{\alpha} a_{\alpha} - v_{\alpha} a^{+}_{\bar{\alpha}} \tag{3.7b}$$

$$b^{+}_{\bar{\alpha}} = u_{\alpha} a^{+}_{\bar{\alpha}} + v_{\alpha} a_{\alpha} \tag{3.7c}$$

$$b_{\bar{\alpha}} = u_{\alpha} a_{\bar{\alpha}} + v_{\alpha} a^{+}_{\alpha} \, . \tag{3.7d}$$

The conditions (3.4) may also be obtained by requiring the transformation

$$\begin{bmatrix} b^{+}_{\alpha} \\ b_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} u_{\alpha} & -v_{\alpha} \\ -v^{*}_{\bar{\alpha}} & u^{*}_{\bar{\alpha}} \end{bmatrix} \begin{bmatrix} a^{+}_{\alpha} \\ a_{\bar{\alpha}} \end{bmatrix} \tag{3.8}$$

to be unitary ($U^{+} \; U = I$) and real so that

$$\begin{bmatrix} b^{+}_{\alpha} \\ b_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} u_{\alpha} & -v_{\alpha} \\ v_{\alpha} & u_{\alpha} \end{bmatrix} \begin{bmatrix} a^{+}_{\alpha} \\ a_{\bar{\alpha}} \end{bmatrix} . \tag{3.9}$$

The inverse of this orthogonal transformation ($o^{-1} = \tilde{o}$) is

$$|\Phi_0\rangle = \prod_{\alpha>0} (u_\alpha + v_\alpha a^+_\alpha a^+_{\bar{\alpha}})|0\rangle \cdot \qquad (3.14)$$

This wave function has the unfortunate property of not being an eigenstate of the particle number operator.

$$N = \sum_\alpha a^+_\alpha a_\alpha \qquad (3.15)$$

We require that the average number of particles in the ground state equals the true particle number N_o .

$$\langle \Phi_0 | N | \Phi_0 \rangle = N_0 \qquad (3.16)$$

The Hamiltonian H is replaced by H - λ N

$$H \longrightarrow H' = H - \lambda N \qquad (3.17)$$

where λ is a Lagrange multiplier which is adjusted so that the constraint (3.16) is satisfied. H' is obtained from H simply be replacing T with T - λ .

4. The Hamiltonian

With the aid of (3.11) the density matrix (1.87a) may be evaluated.

$$\rho_{\alpha\beta} = \langle a^{\dagger}_{\beta} a_{\alpha} \rangle$$
$$= \langle \Phi_0 | (u_\beta b^{\dagger}_{\beta} + v_\beta b_{\bar{\beta}})(u_\alpha b_\alpha + v_\alpha b^{\dagger}_{\bar{\alpha}}) | \Phi_0 \rangle \tag{3.18}$$

Utilizing (3.12) and $\langle \Phi_0 | b^{\dagger}_{\alpha} b^{\dagger}_{\beta} | \Phi_0 \rangle = 0$

$$\rho_{\alpha\beta} = v_\beta v_\alpha \langle \Phi_0 | b_{\bar{\beta}} b^{\dagger}_{\bar{\alpha}} | \Phi_0 \rangle .$$

Using $b_{\bar{\beta}} b^{\dagger}_{\bar{\alpha}} = \delta_{\beta\alpha} - b^{\dagger}_{\bar{\alpha}} b_{\bar{\beta}}$ and (3.12)

$$\rho_{\alpha\beta} = v_\alpha^2 \delta_{\alpha\beta} . \tag{3.19}$$

The occupation probability is v_α^2 .

The number conservation constraint (3.17) is simply

$$\mathrm{Tr}\, \rho = N_0 \tag{3.20}$$

or

$$2 \sum_{\alpha > 0} v_\alpha^2 = N_0 . \tag{3.21}$$

The pairing tensor (1.88a) may be similarly determined.

$$t_{\alpha\beta} = \langle a_\beta a_\alpha \rangle \tag{3.22}$$

Let $\alpha, \beta > 0$ and use (3.11b,d).

$$\tau_{\alpha\beta} = \tau_{\bar{\alpha}\bar{\beta}} = 0 \tag{3.23a}$$

$$\tau_{\alpha\bar{\beta}} = \langle a_{\bar{\beta}}\, a_{\alpha} \rangle = u_{\alpha} v_{\alpha}\, \delta_{\alpha\beta} \tag{3.23b}$$

$$\tau_{\bar{\alpha}\beta} = \langle a_{\beta}\, a_{\bar{\alpha}} \rangle = -u_{\alpha} v_{\alpha}\, \delta_{\alpha\beta} \tag{3.23c}$$

The adjoint of the pairing tensor (1.88b)

$$\tau^{*}_{\alpha\beta} = \langle a^{+}_{\alpha}\, a^{+}_{\beta} \rangle \tag{3.24}$$

may be obtained directly from (3.23). For $\alpha, \beta > 0$

$$\tau^{*}_{\alpha\beta} = \tau^{*}_{\bar{\alpha}\bar{\beta}} = 0 \tag{3.25a}$$

$$\tau^{*}_{\alpha\bar{\beta}} = \langle a^{+}_{\alpha}\, a^{+}_{\bar{\beta}} \rangle = u_{\alpha} v_{\alpha}\, \delta_{\alpha\beta} \tag{3.25b}$$

$$\tau^{*}_{\bar{\alpha}\beta} = \langle a^{+}_{\bar{\alpha}}\, a_{\beta} \rangle = -u_{\alpha} v_{\alpha}\, \delta_{\alpha\beta} \,. \tag{3.25c}$$

The HF potential in the $|\alpha\rangle$ basis is

$$\Gamma_{\alpha_1\alpha_2} = \sum_{\beta > 0} \langle \alpha_1 \beta | v | \alpha_2 \beta \rangle_A\, v_{\beta}^{2} \,. \tag{3.26}$$

It should be noted that this potential differs from the one used in HF theory (2.6) through the occupation probability

N_β^2. Since $\langle \alpha_1 \beta | v | \alpha_2 \beta \rangle_A = \langle \alpha_2 \beta | v | \alpha_1 \beta \rangle_A$, Γ is symmetric.

$$\Gamma_{\alpha_1 \alpha_2} = \Gamma_{\alpha_2 \alpha_1} \tag{3.27}$$

The HF Hamiltonian is

$$\mathcal{H}_{\alpha_1 \alpha_2} = T_{\alpha_1 \alpha_2} + \Gamma_{\alpha_1 \alpha_2} . \tag{3.28}$$

It is also symmetric.

$$\mathcal{H}_{\alpha_1 \alpha_2} = \mathcal{H}_{\alpha_2 \alpha_1} \tag{3.29}$$

For any system with time - reversal symmetry the expression for the pair potential (1.91a)

$$\Delta_{ij} = \frac{1}{2} \sum_{kl} \langle ij | v | kl \rangle_A t_{kl}$$

may be simplified. Assume $t_{kl} = 0$ for $k,l > 0$ or $k,l < 0$.

$$\Delta_{ij} = \frac{1}{2} \sum_{kl>0} \langle ij | v | k\bar{l} \rangle_A t_{k\bar{l}} + \frac{1}{2} \sum_{kl>0} \langle ij | v | \bar{k}l \rangle_A t_{\bar{k}l}$$

Since t is anti-symmetric and $\langle ij | v | \bar{k}l \rangle_A = - \langle ij | v | l\bar{k} \rangle_A$, the second sum equals the first sum, and

$$\Delta_{ij} = \sum_{kl>0} \langle ij | v | k\bar{l} \rangle_A t_{k\bar{l}} .$$

For i, j > 0 or i, j < 0, the matrix element $\langle i j | v | k \bar{l} \rangle_A$ vanishes (by angular momentum projection conservation), so that non-vanishing elements of Δ have $i > 0$, $j < 0$ or $i < 0$, $j > 0$.

$$\Delta_{i\bar{j}} = \sum_{k l > 0} \langle i \bar{j} | v | k \bar{l} \rangle_A \, \zeta_{k\bar{l}} \tag{3.30}$$

This result is not restricted to the special transformation.

The pair potential for the special transformation is

$$\Delta_{\alpha_1 \bar{\alpha}_2} = \sum_{\beta > 0} \langle \alpha_1 \bar{\alpha}_2 | v | \beta \bar{\beta} \rangle_A \, u_\beta v_\beta \, . \tag{3.31}$$

Although Δ is antisymmetric, so that

$$\Delta_{\alpha_1 \bar{\alpha}_2} = - \Delta_{\bar{\alpha}_2 \alpha_1} \tag{3.32}$$

it is not true that $\Delta_{\alpha_1 \bar{\alpha}_2} = - \Delta_{\alpha_2 \bar{\alpha}_1}$. Since $\langle \alpha_1 \bar{\alpha}_2 | v | \beta \bar{\beta} \rangle_A = \langle \bar{\alpha}_1 \alpha_2 | v | \bar{\beta} \beta \rangle_A = \langle \alpha_2 \bar{\alpha}_1 | v | \beta \bar{\beta} \rangle_A$, the correct symmetry relation is

$$\Delta_{\alpha_1 \bar{\alpha}_2} = \Delta_{\alpha_2 \bar{\alpha}_1} \, . \tag{3.33}$$

The Hamiltonian

$$H' = H_0' + H_2' + H_4' \tag{3.34}$$

is now completely determined. (See 1.86, 1.92, 1.93, 3.17.) Before explicitly writing H', we present simplifications in the form of H_o' and H_2' which are valid whenever the system has time-reversal symmetry. Consider the pairing energy in the ground state.

$$E_{pair} = \frac{1}{2} \sum_{ij} \Delta_{ij} t^*_{ij} \tag{3.35}$$

Assume $\Delta_{ij} = t^*_{ij} = 0$ for $i,j > 0$ or $i,j < 0$.

$$E_{pair} = \frac{1}{2} \sum_{i,j>0} \Delta_{ij} t^*_{ij} + \frac{1}{2} \sum_{i,j<0} \Delta_{ij} t^*_{ij}$$

Since Δ and t are both anti-symmetric, the second sum equals the first sum, and

$$E_{pair} = \sum_{ij>0} \Delta_{ij} t^*_{ij} . \tag{3.36}$$

Similarly

$$\frac{1}{2} \sum_{ij} \Delta_{ij} N[a^+_i a^+_j] = \sum_{ij>0} \Delta_{ij} N[a^+_i a^+_j] . \tag{3.37}$$

For a system with time-reversal symmetry H' has the representation

$$H_o' = E_o - \lambda N_o = \sum_{ij} (T - \lambda + \tfrac{1}{2}\Gamma)_{ij} \rho_{ji} + \sum_{ij>0} \Delta_{ij} t^*_{ij} \tag{3.38a}$$

or

$$H_0' = E_0 - \lambda N_0 = \sum_{ij}' \langle i | T - \lambda | j \rangle \rho_{ji} + \frac{1}{2} \sum_{ijkl}' \langle ij | v | kl \rangle_A \rho_{ki} \rho_{lj} + \sum_{ijkl>0}' \langle i\bar{j} | v | k\bar{l} \rangle_A \kappa^*_{i\bar{j}} \kappa_{k\bar{l}} \tag{3.38b}$$

$$H_2' = \sum_{ij}' (\mathcal{H} - \lambda)_{ij} N[a^\dagger_i a_j] + \sum_{ij>0}' \Delta_{i\bar{j}} N[a^\dagger_i a^\dagger_{\bar{j}}] + \sum_{ij>0}' \Delta^*_{i\bar{j}} N[a_{\bar{j}} a_i] \tag{3.39}$$

$$H_4' = \frac{1}{4} \sum_{ijkl}' \langle ij | v | kl \rangle_A N[a^\dagger_i a^\dagger_j a_l a_k] . \tag{3.40}$$

For the special quasiparticle transformation (that is, when (3.14) is the reference state) H' has the representation

$$H_0' = E_0 - \lambda N_0 = \sum_{\alpha \gtrless 0}' (T - \lambda + \tfrac{1}{2}\Gamma)_{\alpha\alpha} \mathcal{N}_\alpha^2 + \sum_{\alpha>0}' \Delta_{\alpha\bar{\alpha}} \mathcal{U}_\alpha \mathcal{N}_\alpha \tag{3.41a}$$

or

$$H_0' = E_0 - \lambda N_0 = \sum_{\alpha \gtrless 0}' \langle \alpha | T - \lambda | \alpha \rangle \mathcal{N}_\alpha^2 + \frac{1}{2} \sum_{\alpha\beta \gtrless 0}' \langle \alpha\beta | v | \alpha\beta \rangle_A \mathcal{N}_\alpha^2 \mathcal{N}_\beta^2 + \sum_{\alpha\beta>0}' \langle \alpha\bar{\alpha} | v | \beta\bar{\beta} \rangle_A \mathcal{U}_\alpha \mathcal{N}_\alpha \mathcal{U}_\beta \mathcal{N}_\beta \tag{3.41b}$$

$$H_2' = \sum_{\alpha\beta>0}{}' (\mathcal{H}-\lambda)_{\alpha\beta}\, N[a^\dagger_\alpha a_\beta] + \sum_{\alpha\beta>0}{}' \Delta_{\alpha\bar{\beta}} \left(N[a^\dagger_\alpha a^\dagger_{\bar{\beta}}] + N[a_{\bar{\beta}} a_\alpha] \right). \tag{3.41c}$$

5. BCS Equations

The occupation probabilities V_α^2 are as yet undetermined. The equation which provides their values may be obtained by a variational principle or by the equation of motion method.

The variational principle consists in choosing the V_α^2 such that the ground state energy is minimized. The orbitals $|\alpha\rangle$ are considered as given. The normalization condition

$$u_\alpha^2 + v_\alpha^2 = 1$$

restricts the variation of V_α. The variational principle is

$$\frac{\delta H_0'}{\delta v_\alpha} = \frac{\partial H_0'}{\partial v_\alpha} + \frac{\partial H_0'}{\partial u_\alpha}\frac{\partial u_\alpha}{\partial v_\alpha} = 0 \tag{3.42a}$$

or

$$\frac{\delta H_0'}{\delta v_\alpha} = \frac{\partial H_0'}{\partial v_\alpha} - \frac{v_\alpha}{u_\alpha}\frac{\partial H_0'}{\partial u_\alpha} = 0 \tag{3.42b}$$

Substituting (3.41b) into (3.42b) leads to the BCS equations.

$$(\mathcal{H}_{\alpha\alpha} - \lambda)\, u_\alpha v_\alpha + \tfrac{1}{2}\Delta_{\alpha\bar{\alpha}}\,(u_\alpha^2 - v_\alpha^2) = 0 \tag{3.43a}$$

or

$$(\epsilon_\alpha - \lambda)\, u_\alpha v_\alpha + \tfrac{1}{2}\Delta_\alpha\,(u_\alpha^2 - v_\alpha^2) = 0 \tag{3.43b}$$

where ϵ_α denotes $\mathcal{H}_{\alpha\alpha}$ and Δ_α is $\Delta_{\alpha\bar{\alpha}}$.

$$\epsilon_\alpha = \langle\alpha|T|\alpha\rangle + \sum_{\beta>0}{}' \langle\alpha\beta|v|\alpha\beta\rangle_A\, v_\beta^2 \tag{3.44}$$

$$\Delta_\alpha = \sum_{\beta>0}{}' \langle\alpha\bar{\alpha}|v|\beta\bar{\beta}\rangle_A\, u_\beta v_\beta \tag{3.45}$$

The single particle energy ϵ_α differs from its HF counterpart (2.18) through the occupation probabilities. The BCS equations have the solution

$$u_\alpha^2 = \frac{1}{2}\left(1 + \frac{\epsilon_\alpha - \lambda}{\sqrt{(\epsilon_\alpha-\lambda)^2 + \Delta_\alpha^2}}\right) \tag{3.46a}$$

$$v_\alpha^2 = \frac{1}{2}\left(1 - \frac{\epsilon_\alpha - \lambda}{\sqrt{(\epsilon_\alpha-\lambda)^2 + \Delta_\alpha^2}}\right) . \tag{3.46b}$$

Just as the HF potential was determined self-consistently, so is the pair potential. The pair field (3.45) determines the pairing degrees of freedom (3.46), yet it is also determined by them. The solution is obtained by iteration. An initial guess is made for the set u_α, v_α and λ (consistent with number conservation). ϵ_α and Δ_α are calculated (3.44, 3.45). A new set of parameters u_α, v_α is calculated with (3.46). λ is varied so that the number conservation constraint (3.21) is satisfied. The potentials are then recalculated. The procedure is continued until the parameters remain unchanged on successive iterations.

An alternative approach is to combine the equation for the pair potential (3.45) and the BCS equations (3.46). For an attractive force Δ and ϵ have opposite signs. $U_\alpha V_\alpha$ is therefore given by

$$u_\alpha v_\alpha = -\frac{1}{2}\frac{\Delta_\alpha}{\sqrt{(\epsilon_\alpha-\lambda)^2 + \Delta_\alpha^2}} . \tag{3.47}$$

If Δ_α is negative, U_α and V_α may be chosen positive. Substituting (3.47) into (3.45)

$$\Delta_\alpha = -\frac{1}{2}\sum_{\beta>0}{}' \langle \alpha\bar{\alpha}|v|\beta\bar{\beta}\rangle_A \frac{\Delta_\beta}{\sqrt{(\epsilon_\beta-\lambda)^2+\Delta_\beta^2}}. \quad (3.48)$$

The solution is obtained by iteration.

The BCS equations may also be derived by the equation of motion method. The quasiparticles are to represent the approximately independent modes of excitation. It is therefore required that

$$H_2' = \sum_\alpha{}' E_\alpha b_\alpha^\dagger b_\alpha . \quad (3.49)$$

Then H' has the form

$$H' = E_0 - \lambda N_0 + \sum_\alpha{}' E_\alpha b_\alpha^\dagger b_\alpha + H_4' . \quad (3.50)$$

If H_4', the quasiparticle interactions, is small, then H' has the desired form of an independent quasiparticle Hamiltonian.

Assume that

$$\overline{|\langle \alpha\bar{\alpha}'|v|\beta\bar{\beta}\rangle_A|} \ll \overline{|\langle \alpha\bar{\alpha}|v|\beta\bar{\beta}\rangle_A|}. \quad (\alpha'\neq\alpha) \quad (3.51a)$$

Then $$|\Delta_{\alpha\bar{\alpha}'}| \ll |\Delta_{\alpha\bar{\alpha}}| . \quad (3.51b)$$

It should be stressed that this is a crucial approximation in the BCS theory. We shall later give examples for which it

is not justified.

It is also assumed that

$$|\mathcal{H}_{\alpha\alpha'}| << |\mathcal{H}_{\alpha\alpha}| . \qquad (\alpha \neq \alpha') \tag{3.52}$$

This assumption is satisfied, of course, if $\mathcal{H}$ is diagonal in the $|\alpha\rangle$ basis. That is, $|\alpha\rangle$ could be chosen as the eigenvectors of the pair-modified HF Hamiltonian (3.26, 3.28). These modified HF wave functions may differ from those of the original HF potential (2.6, 2.7). We shall later demonstrate that the original HF basis is more desirable than the modified HF basis. The unmodified basis is therefore used, and it is assumed that off-diagonal matrix elements of the pair-modified HF Hamiltonian in this basis are small. The justification for this seemingly inconsistent choice will later become apparent.

With assumptions (3.51, 3.52), H_2' (3.41c) has the form

$$H_2' = \sum_{\alpha>0} (\epsilon_\alpha - \lambda) N[a^+_\alpha a_\alpha] + \sum_{\alpha>0} \Delta_\alpha \left(N[a^+_\alpha a^+_{\bar{\alpha}}] + N[a_{\bar{\alpha}} a_\alpha] \right) . \tag{3.53}$$

Consider the commutator $[H_2', b^+_\alpha]_-$. Using (3.49)

$$[H_2', b^+_\alpha]_- = E_\alpha b^+_\alpha . \tag{3.54}$$

Substituting (3.7a) into (3.54)

$$[H_2', b^+_\alpha]_- = E_\alpha (u_\alpha a^+_\alpha - v_\alpha a_{\bar{\alpha}}) . \tag{3.55}$$

The commutator may also be evaluated with (3.53).

$$[H_2', b_\alpha^+]_- = \{(\epsilon_\alpha - \lambda)u_\alpha - \Delta_\alpha v_\alpha\} a_\alpha^+ + \{\Delta_\alpha u_\alpha + (\epsilon_{\bar\alpha} - \lambda) v_\alpha\} a_{\bar\alpha} \quad (\alpha > 0) \tag{3.56}$$

Equate coefficients of a_α^+ and $a_{\bar\alpha}$ in (3.55,3.56).

$$(\epsilon_\alpha - \lambda) u_\alpha - \Delta_\alpha v_\alpha = E_\alpha u_\alpha \tag{3.57a}$$

$$\Delta_\alpha u_\alpha + (\epsilon_{\bar\alpha} - \lambda) v_\alpha = -E_\alpha v_\alpha \tag{3.57b}$$

For time-reversal degeneracy $\epsilon_{\bar\alpha} = \epsilon_\alpha$. Rewrite (3.57) in matrix form.

$$\begin{bmatrix} (\epsilon_\alpha - \lambda) & \Delta_\alpha \\ \Delta_\alpha & -(\epsilon_\alpha - \lambda) \end{bmatrix} \begin{bmatrix} u_\alpha \\ -v_\alpha \end{bmatrix} = E_\alpha \begin{bmatrix} u_\alpha \\ -v_\alpha \end{bmatrix} \tag{3.58}$$

Multiplying (3.57a) by v_α and (3.57b) by u_α and adding we arrive at the BCS equation.

$$(\epsilon_\alpha - \lambda) u_\alpha v_\alpha + \tfrac{1}{2} \Delta_\alpha (u_\alpha^2 - v_\alpha^2) = 0 .$$

The quasiparticle energy E_α is determined by

$$\begin{vmatrix} (\epsilon_\alpha - \lambda) - E_\alpha & \Delta_\alpha \\ \Delta_\alpha & -(\epsilon_\alpha - \lambda) - E_\alpha \end{vmatrix} = 0 . \tag{3.59}$$

Solving for E_α

$$E_\alpha = \sqrt{(\epsilon_\alpha - \lambda)^2 + \Delta_\alpha^2} . \tag{3.60}$$

The quasiparticle energy displays the energy gap in the excitation spectrum. In the absence of pairing, the energy required to lift a particle from a level below the Fermi surface to an unoccupied level (creation of a "particle"- hole pair) is

$$\mathcal{E}_{ex} = \epsilon_{\alpha_1} - \epsilon_{\alpha_2} \cdot \quad (\epsilon_{\alpha_1} > \epsilon_F > \epsilon_{\alpha_2}) \tag{3.61}$$

$\mathcal{E}_{ex}$ may be very small if the levels in the neighbourhood of the Fermi surface are closely spaced. When pairing is present the analog of the "particle" - hole state is a two quasiparticle state with excitation energy

$$\begin{aligned} \mathcal{E}_{ex} &= E_{\alpha_1} + E_{\alpha_2} \\ &= \sqrt{(\epsilon_{\alpha_1} - \lambda)^2 + \Delta_{\alpha_1}^2} + \sqrt{(\epsilon_{\alpha_2} - \lambda)^2 + \Delta_{\alpha_2}^2} \cdot \end{aligned} \tag{3.62}$$

Even if $(\epsilon_{\alpha_1} - \lambda)$ and $(\epsilon_{\alpha_2} - \lambda)$ vanish, there is still an excitation energy

$$\mathcal{E}_{ex}^{min} = |\Delta_{\alpha_1}| + |\Delta_{\alpha_2}| \cdot \tag{3.63}$$

The pairing correlations therefore create an energy gap between the ground state and low-lying excitations.

6. Hartree - Bogoliubov Equations

There are formalisms for which no approximations are required to ensure that

$$H_2' = \sum_K E_K b_K^+ b_K .$$

More careful consideration must be given to the choice of the single particle basis. A criterion for the "best" basis must be formulated. It will be demonstrated that simply choosing the eigenvectors of the pair modified HF Hamiltonian as the single particle basis is not a consistent method for including the effects of pairing correlations on the HF degrees of freedom. Furthermore, the eigenvectors of the pair-modified HF Hmailtonian are even less desirable than are those of the original HF Hamiltonian. There is a third basis, termed the "canonical basis," which is most satisfactory. It is determined by either the Hartree - Bogoliubov [3] (HB) or the Hartree-Fock-Bogoliubov (HFB) equations.

The first derivation of the HB equations is by a variational principle. Choose the basis $|\alpha\rangle$ so that the ground state energy (with a BCS wave function) is minimized. Since

$$|\alpha\rangle = \sum_K D_K^\alpha \, |K\rangle \tag{3.64}$$

the matrix elements of T and V may be rotated .

$$\langle \alpha_1 | T | \alpha_2 \rangle = \sum_{K_1 K_2} D_{K_1}^{\alpha_1} D_{K_2}^{\alpha_2} \langle K_1 | T | K_2 \rangle \tag{3.65}$$

$$\langle \alpha_1 \alpha_2 | v | \alpha_3 \alpha_4 \rangle_A = \sum_{k_1 k_2 k_3 k_4} D^{\alpha_1}_{k_1} D^{\alpha_2}_{k_2} D^{\alpha_3}_{k_3} D^{\alpha_4}_{k_4} \langle k_1 k_2 | v | k_3 k_4 \rangle_A \tag{3.66}$$

where the D coefficients are assumed to be real. For time-reversal degeneracy the phases may be chosen so that

$$D^{\bar{\alpha}}_{\bar{k}} = D^{\alpha}_{k} \quad . \tag{3.67}$$

Substituting (3.65 - 3.67) into (3.41b)

$$H_0' = E_0 - \lambda N_0 = \sum_{\substack{\alpha > 0 \\ k_1 k_2}} D^{\alpha}_{k_1} D^{\alpha}_{k_2} v_\alpha^2 \langle k_1 | T - \lambda | k_2 \rangle +$$

$$\frac{1}{2} \sum_{\substack{\alpha_1 \alpha_2 > 0 \\ k_1 k_2 k_3 k_4}} D^{\alpha_1}_{k_1} D^{\alpha_2}_{k_2} D^{\alpha_1}_{k_3} D^{\alpha_2}_{k_4} v_{\alpha_1}^2 v_{\alpha_2}^2 \langle k_1 k_2 | v | k_3 k_4 \rangle_A + \tag{3.68}$$

$$\sum_{\substack{\alpha_1 \alpha_2 > 0 \\ k_1 k_2 k_3 k_4}} D^{\alpha_1}_{k_1} D^{\alpha_1}_{k_2} D^{\alpha_2}_{k_3} D^{\alpha_2}_{k_4} u_{\alpha_1} v_{\alpha_1} u_{\alpha_2} v_{\alpha_2} \langle k_1 \bar{k}_2 | v | k_3 \bar{k}_4 \rangle_A \, .$$

Alternatively, the density matrix and the pairing tensor may be evaluated in the $|k\rangle$ basis. Invert (3.64) ($D^{-1} = \tilde{D}$).

$$|k\rangle = \sum_{\alpha} D^{\alpha}_{k} \, |\alpha\rangle \tag{3.69}$$

Then $\langle a^{+}_{k_1} a_{k_2} \rangle = \sum_{\alpha_1 \alpha_2} D^{\alpha_1}_{k_1} D^{\alpha_2}_{k_2} \langle a^{+}_{\alpha_1} a_{\alpha_2} \rangle \, .$

Inserting (3.19)

$$\rho_{k_2 k_1} = \langle a^{+}_{k_1} a_{k_2} \rangle = \sum_{\alpha} D^{\alpha}_{k_1} D^{\alpha}_{k_2} v_\alpha^2 \tag{3.70}$$

Similarly

$$\kappa_{k_2 \bar{k}_1} = \langle a_{\bar{k}_1} a_{k_2} \rangle = \sum_{\alpha} D^{\alpha}_{k_1} D^{\alpha}_{k_2} u_\alpha v_\alpha \, . \tag{3.71}$$

(3.68) is obtained by substituting (3.70, 3.71) into (3.38b).

The pairing degrees of freedom have been varied (3.42) to minimize the ground state energy. This variational principle resulted in the BCS equations (3.43).

The variational principle for the HF degrees of freedom includes a normalization constraint.

$$\frac{\partial}{\partial D^{\alpha}_{k}} \left\{ H_0' - \epsilon_\alpha \left(\sum_j |D^{\alpha}_j|^2 - 1 \right) \right\} = 0 \tag{3.72}$$

Substituting (3.68) into (3.72) leads to

$$\sum_{k_2} \left\{ (\mathcal{H} - \lambda)_{k_1 k_2} \mathcal{N}_\alpha^2 + \Delta_{k_1 \bar{k}_2} u_\alpha \mathcal{N}_\alpha \right\} D^{\alpha}_{k_2} = \epsilon_\alpha D^{\alpha}_{k_1} \tag{3.73}$$

where $\mathcal{H}$ is defined by (3.26, 3.28) and Δ by (3.31). This is one form of the HB equations. The quantity in brackets is the HB Hamiltonian

$$\mathcal{H}^{HB}_{k_1 k_2}(\alpha) = (\mathcal{H} - \lambda)_{k_1 k_2} \mathcal{N}_\alpha^2 + \Delta_{k_1 \bar{k}_2} u_\alpha \mathcal{N}_\alpha \tag{3.74}$$

so that

$$\sum_{k_2} \mathcal{H}^{HB}_{k_1 k_2}(\alpha) D^{\alpha}_{k_2} = \epsilon_\alpha D^{\alpha}_{k_1} \cdot \tag{3.75a}$$

The HB equations present an eigenvalue problem.

$$\mathcal{H}^{HB}(\alpha) \underline{D}^{\alpha} = \epsilon_\alpha \underline{D}^{\alpha} \tag{3.75b}$$

or

$$\mathcal{H}^{HB}(\alpha) |\alpha\rangle = \epsilon_\alpha |\alpha\rangle \cdot \tag{3.75c}$$

It should be mentioned that ϵ_α is not the single particle energy.

$$\epsilon_\alpha = \langle \alpha | \mathcal{H}^{HB}(\alpha) | \alpha \rangle = (\mathcal{H}_{\alpha\alpha} - \lambda) v_\alpha^2 + \Delta_{\alpha\bar{\alpha}} u_\alpha v_\alpha \quad (3.75d)$$

As in the HF theory, the HB equations provide a self-consistency condition. The potentials are determined, in part, by the HF degrees of freedom, and vice-versa. Solution is obtained by iteration.

Since the HF and pair potentials each depend upon both HF and pair degrees of freedom, the BCS and HB equations are coupled to each other. One must iterate between them to achieve self-consistency in both HF and pair degrees of freedom.

Unfortunately $\mathcal{H}^{HB}$ is a functional of α. Since it is a state dependent operator its eigenvectors can not be obtained in the usual way. This state dependence should be distinguished from the state dependence of the HF Hamiltonian $\mathcal{H}$. Although the operator $\mathcal{H}$ is a function of the occupied orbits, for a given A particle wave function, there is a unique matrix representation $\langle i | \mathcal{H} | j \rangle$. The HB Hamiltonian, however, has a different representation $\langle i | \mathcal{H}^{HB}(\alpha) | j \rangle$ for each $|\alpha\rangle$.

$\mathcal{H}^{HB}$ differs from the pair-renormalized HF Hamiltonian through the inclusion of the pair potential. The important conclusion, therefore, is that changing the original HF Hamiltonian to its pair-modified form is not a consistent

method of accounting for the effects of pairing on the HF degrees of freedom. One might have hoped that iterating between the pair-modified HF equation and the BCS equation until consistency is achieved in HF and pairing degrees of freedom would be a consistent method, or at least more desirable than simply solving the BCS equations with the original HF basis. Although this procedure may have considerable intuitive appeal, we have demonstrated that it is not derivable from a variational principle. Furthermore, we shall numerically demonstrate that iterating between the BCS equations and the modified HF equations generally results in a wave function which has less in common with the exact (HB) wave function than does the wave function obtained merely by solving the BCS equations with the original HF basis.

The HB equations have an alternative form. Utilizing (3.75c)

$$\mathcal{H}^{HB}_{\alpha\beta}(\beta) = \langle \alpha | \mathcal{H}^{HB}(\beta) | \beta \rangle = 0 \cdot \quad (\alpha \neq \beta)$$

Since $\mathcal{H}_{ij} = \mathcal{H}_{ji}$ and $\Delta_{i\bar{j}} = \Delta_{j\bar{i}}$, $\mathcal{H}^{HB}$ is symmetric.

$$\tilde{\mathcal{H}}^{HB}(\alpha) = \mathcal{H}^{HB}(\alpha) \tag{3.76}$$

In particular, $\mathcal{H}^{HB}_{\alpha\beta}(\alpha) = \mathcal{H}^{HF}_{\beta\alpha}(\alpha) = 0 \quad (\alpha \neq \beta)$.
Therefore $\mathcal{H}^{HB}_{\alpha\beta}(\alpha) - \mathcal{H}^{HB}_{\alpha\beta}(\beta) = 0$. That is

$$(\mathcal{H}-\lambda)_{\alpha\beta}(\mathcal{N}_\alpha^2 - \mathcal{N}_\beta^2) + \Delta_{\alpha\bar{\beta}}(u_\alpha \mathcal{N}_\alpha - u_\beta \mathcal{N}_\beta) = 0. \tag{3.77}$$

These are also referred to as the HB equations.

Further, insight may be gained by expressing H_2' in terms of the quasiparticle operators. Since the reference state is chosen as a quasiparticle vacuum,

$$N[b_\alpha^\dagger b_\beta^\dagger] = b_\alpha^\dagger b_\beta^\dagger \tag{3.78a}$$

$$N[b_\alpha b_\beta] = b_\alpha b_\beta \tag{3.78b}$$

$$N[b_\alpha^\dagger b_\beta] = b_\alpha^\dagger b_\beta \tag{3.78c}$$

$$N[b_\alpha b_\beta^\dagger] = -b_\beta^\dagger b_\alpha . \tag{3.78d}$$

Substituting the inverse transformation (3.11) into H_2' (3.41c), and using (3.78), we may express H_2' as

$$H_2' = H_{11}' + H_{20}' + H_{02}' \tag{3.79}$$

where H_{mn}' contains terms with m quasiparticle creation operators and n annihilation operators, and

$$H_{11}' = \sum_{\alpha\beta>0}' \{ (\mathcal{H}-\lambda)_{\alpha\beta} (u_\alpha u_\beta - v_\alpha v_\beta) - \Delta_{\alpha\bar\beta} (u_\alpha v_\beta + v_\alpha u_\beta) \} (b_\alpha^\dagger b_\beta + b_{\bar\alpha}^\dagger b_{\bar\beta}) \tag{3.80}$$

$$H_{20}' + H_{02}' = \sum_{\alpha\beta>0}' \{ (\mathcal{H}-\lambda)_{\alpha\beta} (u_\alpha v_\beta + v_\alpha u_\beta) + \Delta_{\alpha\bar\beta} (u_\alpha u_\beta - v_\alpha v_\beta) \} (b_\alpha^\dagger b_{\bar\beta}^\dagger + b_{\bar\alpha} b_\beta) . \tag{3.81}$$

We have used time-reversal degeneracy

$$\mathcal{H}_{\alpha\bar\beta} = \mathcal{H}_{\bar\alpha\beta} = 0 \qquad (\alpha, \beta > 0)$$

$$\mathcal{H}_{\bar\alpha\bar\beta} = \mathcal{H}_{\alpha\beta}$$

(these relations are true even if $|\alpha\rangle$, $|\beta\rangle$ are not eigenstates of $\mathcal{H}$), and the symmetry relations

$$\mathcal{H}_{\alpha\beta} = \mathcal{H}_{\beta\alpha}$$

$$\Delta_{\alpha\bar{\beta}} = \Delta_{\beta\bar{\alpha}}$$

in deriving (3.80, 3.81).

In order that H_2' have the form

$$H_2' = \sum_k E_k b_k^+ b_k$$

$H_{20}' + H_{02}'$ clearly must vanish. It is therefore required that

$$(\mathcal{H}-\lambda)_{\alpha\beta}(U_\alpha V_\beta + V_\alpha U_\beta) + \Delta_{\alpha\bar{\beta}}(U_\alpha U_\beta - V_\alpha V_\beta) = 0 \,. \quad (3.82)$$

For $\alpha = \beta$, (3.82) reduces to the BCS equations.

$$(\mathcal{H}_{\alpha\alpha} - \lambda) U_\alpha V_\alpha + \tfrac{1}{2}\Delta_{\alpha\bar{\alpha}}(U_\alpha^2 - V_\alpha^2) = 0$$

Consider $\alpha \neq \beta$. If the BCS equations are solved without special attention to the choice of single particle basis, then $H_{20}' + H_{02}'$ vanishes only if

$$\mathcal{H}_{\alpha\beta} = \Delta_{\alpha\bar{\beta}} = 0 \,. \quad (\alpha \neq \beta) \qquad (3.83)$$

These are the assumptions we encountered (3.51, 3.52) in the derivation of the BCS equations by the equation of motion method. For a non-trivial force, however, (3.83) cannot be satisfied. If $|\alpha\rangle$ is chosen so that $\mathcal{H}_{\alpha\beta} = 0$ $(\alpha \neq \beta)$ then $\Delta_{\alpha\bar{\beta}} \neq 0$ $(\alpha \neq \beta)$.

Rather than make the assumption (3.83), we will determine the single - particle basis for which (3.82) is exactly satisfied. Multiply (3.82) by $(U_\alpha N_\alpha - U_\beta N_\beta)$. Rearranging the terms

$$\{(\mathcal{H}-\lambda)_{\alpha\beta}(N_\alpha^2 - N_\beta^2) + \Delta_{\alpha\bar{\beta}}(U_\alpha N_\alpha - U_\beta N_\beta)\}(U_\alpha U_\beta - N_\alpha N_\beta) = 0$$

In general the term in brackets must vanish.

$$(\mathcal{H}-\lambda)_{\alpha\beta}(N_\alpha^2 - N_\beta^2) + \Delta_{\alpha\bar{\beta}}(U_\alpha N_\alpha - U_\beta N_\beta) = 0$$

These are simply the HB equations.

Satisfying the BCS and HB equations therefore ensures that $H'_{20} + H'_{02} = 0$.

Finally let us consider H'_{11}.

$$H'_{11} = \sum_{\alpha\beta>0} E_{\alpha\beta}(b^+_\alpha b_\beta + b^+_{\bar{\alpha}} b_{\bar{\beta}}) \tag{3.84}$$

where

$$E_{\alpha\beta} = (\mathcal{H}-\lambda)_{\alpha\beta}(U_\alpha U_\beta - N_\alpha N_\beta) - \Delta_{\alpha\bar{\beta}}(U_\alpha N_\beta + N_\alpha U_\beta) \tag{3.85}$$

In particular

$$E_{\alpha\alpha} = (\mathcal{H}_{\alpha\alpha}-\lambda)(U_\alpha^2 - N_\alpha^2) - 2\Delta_{\alpha\bar{\alpha}} U_\alpha N_\alpha .$$

Substituting (3.46, 3.47)

$$E_{\alpha\alpha} = \sqrt{(\mathcal{H}_{\alpha\alpha}-\lambda)^2 + \Delta^2_{\alpha\bar{\alpha}}} . \tag{3.86}$$

This is the BCS result. Solving (3.82) for $\Delta_{\alpha\bar{\beta}}$ and substituting into (3.85)

$$E_{\alpha\beta} = (\mathcal{H}-\lambda)_{\alpha\beta} / (U_\alpha U_\beta - N_\alpha N_\beta) . \tag{3.87}$$

Alternatively (3.82) may be solved for $\mathcal{H}_{\alpha\beta}$, yielding

$$E_{\alpha\beta} = -\Delta_{\alpha\bar{\beta}} / (u_\alpha v_\beta + v_\alpha u_\beta) \cdot \tag{3.88}$$

Even after the BCS and HB equations are solved $E_{\alpha\beta}$, and therefore H_{11}' will generally not be diagonal. It should be emphasized that the canonical basis diagonalizes neither $\mathcal{H}$ nor Δ. A further transformation - a rotation in quasiparticle space - is required to put H_2' in the desired form. A rotation R

$$b^\dagger_\nu = \sum_\alpha R^\nu_\alpha b^\dagger_\alpha \tag{3.89}$$

is chosen to diagonalize the energy matrix $E_{\alpha\beta}$.

$$\sum_\beta E_{\alpha\beta} R^\nu_\beta = \tilde{E}_\nu R^\nu_\alpha \tag{3.90a}$$

or

$$E \underline{R}^\nu = \tilde{E}_\nu \underline{R}^\nu . \tag{3.90b}$$

Then

$$H_2' = \sum_\nu \tilde{E}_\nu b^\dagger_\nu b_\nu . \tag{3.91}$$

If $R \neq I$, then $\tilde{E}_\nu \neq E_{\nu\nu} \equiv E_\nu$.

Three transformations have been required to obtain a "quasiparticle" Hamiltonian.

U_1: Rotation in particle space

$$a^\dagger_\alpha = \sum_k D^\alpha_k a^\dagger_k \tag{3.92}$$

B_{sp}: Special Bogoliubov quasiparticle transformation

$$b^{+}_{\alpha} = u_{\alpha} a^{+}_{\alpha} - v_{\alpha} a_{\bar{\alpha}} \tag{3.93}$$

U_2: Rotation in quasiparticle space

$$b^{+}_{\nu} = \sum_{\alpha}{}' R^{\nu}_{\alpha} b^{+}_{\alpha} \tag{3.94}$$

The final Bogoliubov quasiparticle co-ordinates are given by the product of these transformations.

$$B = U_2 B_{sp} \cdot U_1 \tag{3.95}$$

The third transformation, U_2, does not, however, affect the ground state properties of the system. After the first two transformations the density matrix is

$$\rho_{\alpha\beta} = \langle a^{+}_{\beta} a_{\alpha} \rangle = v_{\alpha}^{2} \delta_{\alpha\beta}$$

and the pairing tensor is

$$\kappa_{\alpha\bar{\beta}} = \langle a_{\bar{\beta}} a_{\alpha} \rangle = u_{\alpha} v_{\alpha} \delta_{\alpha\beta} .$$

Substitute (3.93) into (3.94).

$$b^{+}_{\nu} = \sum_{\alpha}{}' (R^{\nu}_{\alpha} u_{\alpha} a^{+}_{\alpha} - R^{\nu}_{\alpha} v_{\alpha} a_{\bar{\alpha}})$$

Inverting this transformation, and recalling that the ground state is a quasiparticle vacuum, ρ and κ may be evaluated after the three transformations have been performed.

$$\langle a^{+}_{\beta} a_{\alpha} \rangle = \sum_{\nu} (R^{\nu}_{\beta} v_{\beta})(R^{\nu}_{\alpha} v_{\alpha}) = (\sum_{\nu} R^{\nu}_{\alpha} R^{\nu}_{\beta}) v_{\alpha} v_{\beta}$$

Since R is an orthogonal transformation

$$R \tilde{R} = I \quad \text{or} \quad \sum_{\nu} R^{\nu}_{\alpha} R^{\nu}_{\beta} = \delta_{\alpha\beta}$$

so that ρ is

$$\langle a^{+}_{\beta} a_{\alpha} \rangle = v_{\alpha}^{2} \delta_{\alpha\beta} .$$

Similarly

$$\langle a_{\bar{\beta}} a_{\alpha} \rangle = \sum_{\nu} (R^{\nu}_{\beta} u_{\beta})(R^{\nu}_{\alpha} v_{\alpha}) = (\sum_{\nu} R^{\nu}_{\alpha} R^{\nu}_{\beta}) u_{\beta} v_{\alpha}$$

and τ is

$$\langle a_{\bar{\beta}} a_{\alpha} \rangle = u_{\alpha} v_{\alpha} \delta_{\alpha\beta} .$$

Since the density matrix and pairing tensor are not altered by the third transformation, the ground state properties remain unaffected.

7. $|T_z| = 1$ Pairing

The conventional pairing theory permits correlations to exist only between like nucleons, that is, it accounts for p - p and n - n pairing. The appropriate formalism is obtained if, in our preceding derivations, $|\alpha\rangle$ is restricted to states of good isospin projection. So far τ has been treated on the same footing as the other quantum numbers. We now explicitly label isospin projection, so that single particle states are represented by $|\alpha\tau\rangle$.

The quasiparticle transformation is

$$b^{\dagger}_{\alpha\tau} = u_{\alpha\tau}\, a^{\dagger}_{\alpha\tau} - v_{\alpha\tau}\, a_{\bar{\alpha}\tau} \,. \tag{3.96}$$

The ground state wave function is

$$|\Phi_0\rangle = \prod_{\alpha_1>0} (u_{\alpha_1 p} + v_{\alpha_1 p}\, a^{\dagger}_{\alpha_1 p}\, a^{\dagger}_{\bar{\alpha}_1 p}) \times \prod_{\alpha_2>0} (u_{\alpha_2 n} + v_{\alpha_2 n}\, a^{\dagger}_{\alpha_2 n}\, a^{\dagger}_{\bar{\alpha}_2 n})\,|0\rangle \,. \tag{3.97}$$

Neutrons and protons need not have identical orbitals.

Since the number of neutrons and the number of protons are each to be conserved, the Hamiltonian is replaced by

$$H \longrightarrow H' = H - \lambda_p N_p - \lambda_n N_n \tag{3.98}$$

where

$$N_p = \sum_{\alpha>0} a^{\dagger}_{\alpha p}\, a_{\alpha p} \qquad N_n = \sum_{\alpha>0} a^{\dagger}_{\alpha n}\, a_{\alpha n} \tag{3.99}$$

and λ_p and λ_n are adjusted so that

$$\langle N_p \rangle = Z \qquad \langle N_n \rangle = A - Z \,. \tag{3.100}$$

This approach has the disadvantage that H' can not be obtained from H by replacing T with $T - \lambda_p - \lambda_n$. A more satisfactory method is to replace H by

$$H \longrightarrow H' = H - (\lambda_p P_p + \lambda_n P_n) N \tag{3.101}$$

where $$N = \sum_{\alpha\tau}{}' a^{\dagger}_{\alpha\tau} a_{\alpha\tau} \tag{3.102}$$

and P_τ is a projection operator

$$P_\tau = |\tau\rangle\langle\tau| \tag{3.103}$$

so that

$$P_\tau |\tau'\rangle = |\tau\rangle\langle\tau|\tau'\rangle = \delta_{\tau\tau'} |\tau\rangle . \tag{3.104}$$

H' is obtained from H by replacing T with $T - \lambda_p P_p - \lambda_n P_n$. Note that

$$N = N_p + N_n \,. \tag{3.105}$$

The density matrix is

$$\rho_{\alpha_1\tau_1, \alpha_2\tau_2} = v^2_{\alpha_1\tau_1} \delta_{\alpha_1\alpha_2} \delta_{\tau_1\tau_2} \tag{3.106}$$

so that the number conservation conditions are

$$2 \sum_{\alpha>0}{}' v^2_{\alpha p} = Z \qquad 2 \sum_{\alpha>0}{}' v^2_{\alpha n} = A - Z . \tag{3.107}$$

The pairing tensor is

$$\kappa_{\alpha_1\tau_1, \bar{\alpha}_2\tau_2} = u_{\alpha_1\tau_1} v_{\alpha_1\tau_1} \delta_{\alpha_1\alpha_2} \delta_{\tau_1\tau_2} \,. \tag{3.108}$$

The HF potential is

$$\Gamma_{\alpha_1\tau_1,\alpha_2\tau_2} = \sum_{\beta\tau}{}' \langle \alpha_1\tau_1, \beta\tau | v | \alpha_2\tau_2, \beta\tau \rangle_A \, v^2_{\beta\tau} \, . \qquad (3.109)$$

Note that $\Gamma_{\alpha_1\tau_1,\alpha_2\tau_2} = 0$ unless $\tau_1 = \tau_2$. Neutrons contribute to the proton HF potential, and viceversa.

The pair potential is

$$\Delta_{\alpha_1\tau_1,\bar{\alpha}_2\tau_2} = \sum_{\substack{\beta>0\\ \tau}}{}' \langle \alpha_1\tau_1, \bar{\alpha}_2\tau_2 | v | \beta\tau, \bar{\beta}\tau \rangle_A \, u_{\beta\tau} v_{\beta\tau} \, . \qquad (3.110)$$

The pairing matrix elements vanish unless $\tau_1 = \tau_2 = \tau$. The only non - vanishing elements of Δ are

$$\Delta_{\alpha_1\tau,\bar{\alpha}_2\tau} = \sum_{\beta>0}{}' \langle \alpha_1\tau, \bar{\alpha}_2\tau | v | \beta\tau, \bar{\beta}\tau \rangle_A \, u_{\beta\tau} v_{\beta\tau} \, . \qquad (3.111)$$

Note that only protons (neutrons) contribute to the proton (neutron) pair potential. This is a consequence of restricting the correlations to $|T_z| = 1$ pairing.

The resulting BCS equations are

$$\begin{bmatrix} (\epsilon_{\alpha\tau} - \lambda_\tau) & \Delta_{\alpha\tau} \\ \Delta_{\alpha\tau} & -(\epsilon_{\alpha\tau} - \lambda_\tau) \end{bmatrix} \begin{bmatrix} u_{\alpha\tau} \\ -v_{\alpha\tau} \end{bmatrix} = E_{\alpha\tau} \begin{bmatrix} u_{\alpha\tau} \\ -v_{\alpha\tau} \end{bmatrix} \qquad (3.112)$$

where $\epsilon_{\alpha\tau} = \mathcal{H}_{\alpha\tau,\alpha\tau}$

$$\epsilon_{\alpha\tau} = \langle \alpha | T | \alpha \rangle + \sum_{\beta\tau'}{}' \langle \alpha\tau, \beta\tau' | v | \alpha\tau, \beta\tau' \rangle_A \, v^2_{\beta\tau'} \, , \qquad (3.113)$$

and $\Delta_{\alpha\tau} = \Delta_{\alpha\tau,\bar{\alpha}\tau}$

$$\Delta_{\alpha\tau} = \sum_{\beta>0}{}' \langle \alpha\tau, \bar{\alpha}\tau | v | \beta\tau, \bar{\beta}\tau \rangle_A \, u_{\beta\tau} v_{\beta\tau} \, . \qquad (3.114)$$

The neutron and proton degrees of freedom are decoupled

except for their interdependence in $\epsilon_{\alpha T}$. Note that the single particle energies of the neutrons and protons are measured from their respective Fermi energies.

$$\hat{\epsilon}_{\alpha T} = \epsilon_{\alpha T} - \lambda_T \tag{3.115}$$

The solutions to (3.112) are

$$E_{\alpha T} = \sqrt{\hat{\epsilon}^2_{\alpha T} + \Delta^2_{\alpha T}} \tag{3.116}$$

$$U^2_{\alpha T} = 1/2\,(1 + \hat{\epsilon}_{\alpha T}/E_{\alpha T}) \tag{3117a}$$

$$V^2_{\alpha T} = 1/2\,(1 - \hat{\epsilon}_{\alpha T}/E_{\alpha T})\,. \tag{3.117b}$$

The sets of equations (3.107, 3.113 - 3.117) are coupled to each other and are solved by iteration to obtain self - consistent potentials.

8. $|T_z| = 1$ Pairing in the 2s-1d Shell

The $|T_z| = 1$ pairing equations were solved for the N = Z even-even nuclei in the the 2s-1d shell. All HF solutions reported in table 2.15 were tried as single particle bases. Since N = Z there are the symmetry relations

$$\begin{aligned} \epsilon_{\alpha p} &= \epsilon_{\alpha n} \\ u^2_{\alpha p} &= u^2_{\alpha n} \\ v^2_{\alpha p} &= v^2_{\alpha n} \\ |\Delta_{\alpha p}| &= |\Delta_{\alpha n}| \\ E_{\alpha p} &= E_{\alpha n} \\ \lambda_p &= \lambda_n \end{aligned} \tag{3.118}$$

The isotopic spin subscript will be deleted for the remainder of this section.

The moments of inertia are given by [5]

$$\mathcal{J}_x = 2 \sum_{\substack{\text{all } \alpha \\ \beta > 0}} \frac{|\langle \alpha | J_x | \beta \rangle|^2}{E_\alpha + E_\beta} \left(u_\alpha |v_\beta| - u_\beta |v_\alpha| \right)^2 \tag{3.119}$$

with similar relations for $\mathcal{J}_y$ and $\mathcal{J}_z$. The multiple moments are

$$\langle Q_{LM} \rangle = \sum_\alpha \langle \alpha | Q_{LM} | \alpha \rangle v_\alpha^2 . \tag{3.120}$$

Ne^{20}

The lowest prolate single particle basis has a large HF gap. Consequently, the BCS equations give the trivial solution (no pairing).

Similarly the asymmetric wave function is stable against $|T_z| = 1$ pairing. The Rosenfeld force yields no pairing. Although the Yale force results in a small HF gap (2.945 Mev), the pairing admixtures are small (a dispersion to orbital 6 of $V_6^2 = 0.053$ with $E_{PAIR} = -0.860$ Mev and a net gain in E_{TOTAL} of only -6 Kev).

Several of the higher lying HF wave functions with smaller HF gaps admit $|T_z| = 1$ pairing, most notably the Yale spherical wave function ($E_{PAIR} = -6.488$ Mev, $E_{TOTAL} = -95.518$ Mev). But these are not thought to have any physical significance.

Mg^{24}

The asymmetric wave function has a large HF gap, and the BCS result is the trivial one.

The prolate HF state with $\Omega = \frac{1}{2}+$. $\frac{3}{2}+$ occupied orbitals is of special concern (see tables 3.1 - 3.6). (All other prolate HF wave functions permit no pairing admixtures.) The Rosenfeld 1 and NDKB forces show very weak pairing with neglible changes in the properties of the wave function. The Rosenfeld 2 and Yale forces result in moderate pairing. The deformation parameters are only slightly altered, but the inertial parameter is considerably increased (0.10 to 0.19 Mev for Rosenfeld 2 and 0.05 to 0.17 Mev for Yale). The energy for

elementary excitations (K = 2) is substantially increased (1.48 to 3.16 Mev and 0.46 to 2.93 Mev). Since $|T_z| = 1$ pairing in this prolate state is force dependent, and since for those forces which do permit pairing the K = 2 two quasiparticle state is too low, we conclude that $|T_z| = 1$ pairing is not significant in prolate Mg^{24} wave functions.

All oblate states show $|T_z| = 1$ pairing, most notably with the Yale force ($E_{PAIR} = -4.364$ Mev, $E_{TOTAL} = -128.317$ Mev for oblate 1 and $E_{PAIR} = -4.743$ Mev, $E_{TOTAL} = -127.391$ Mev for oblate 2). However, since Mg^{24} is prolate in the intrinsic frame, these solutions are not physically relevant.

Si^{28}

The lowest oblate state has a large HF gap, so that no pairing occurs.

Similarly the lowest prolate state admits no pairing, except for the NDKB (s - p - sd) force, where the HF gap is only 0.916 Mev. However, even with such a small gap only negligible pairing results ($E_{PAIR} = -0.255$ Mev with a gain in E_{TOTAL} of -14 Kev).

For the Rosenfeld 1 force only the oblate 3 state contains pairing ($E_{PAIR} = -1.569$, $E_{TOTAL} = -146.399$). The corresponding state with the Rosenfeld 2 parameters is

oblate 2 (E_{PAIR} = -2.187, E_{TOTAL} = -121.489).

Of the remaining solutions only the spherical states have $|T_z| = 1$ pairing. (See table 3.8.) These may be of some interest, as the spherical intrinsic state has been useful in describing the experimental spectrum.[4] The HF ordering of levels is $d_{5/2}$, $d_{3/2}$, $s_{1/2}$. (The Yale force presents an exception, where the unoccupied $d_{3/2}$ lies below the filled $d_{5/2}$. The pairing calculation was not performed with this state.) The dispersion to the $d_{3/2}$ orbital is $V^2_{d_{3/2}} \sim 0.1$.

S^{32}

The asymmetric wave function admits no pairing admixtures. Nor do any of the Rosenfeld 1 wave functions.

For the prolate state the Rosenfeld 2 and the Yale forces yield non - trivial solutions (E_{PAIR} = -4.425 Mev, E_{TOTAL} = -174.091 Mev and E_{PAIR} = -3.106 Mev, E_{TOTAL} = -223.226 Mev), whereas the NDKB force does not.

In the oblate state with positive Q_{40} only the NDKB force results in a small HF gap (E_{PAIR} = -2.882 Mev, E_{TOTAL} = -173.277 Mev for s-p-sd and E_{PAIR} = -2.444 Mev, E_{TOTAL} = -174.950 Mev for s-p-sd-pf). Of the remaining oblate states (Rosenfeld 2) oblate 2 is at the pairing cutoff (E_{PAIR} = -0.021 Mev), and oblate 3 pairs (E_{PAIR} = -2.212 Mev, E_{TOTAL} = -173.876 Mev).

Ar^{36}

The oblate wave functions do not admit pairing correlations. Neither do the asymmetric states.

For the prolate state (see table 3.7) the Rosenfeld 1 force yields no pairing, while the NDKB force shows negligible pairing. Although the Rosenfeld 2 force produces little admixtures of pairing ($V_6^2 = 0.106$) the inertial parameter is increased by 50%. The Yale force creates a large dispersion ($V_{10}^2 = 0.329$) and increases A_x four-fold. Since these results are so force dependent, they do not warrant much confidence in their being physically relevant.

The spherical state (see table 3.10) contains pairing correlations only for the Rosenfeld 2 and Yale forces, although for these the dispersion is so great as to re-order the levels. The occupation probablilities are $V_{s\frac{1}{2}}^2 = 0.994$, $V_{d_{5/2}}^2 = 0.974$, $V_{d_{3/2}}^2 = 0.543$(Rosenfeld 2) and $V_{d_{5/2}}^2 = 0.956$, $V_{s\frac{1}{2}}^2 = 0.964$, $V_{d_{3/2}}^2 = 0.585$(Yale). For the Rosenfeld 2 force the $s_{\frac{1}{2}}$ single particle energy is altered from its HF position of $\epsilon_{s\frac{1}{2}} = -13$ Mev (unoccupied) to its BCS location of $\epsilon_{s\frac{1}{2}} = -22$ Mev (most occupied level). Clearly using fixed single particle energies, i.e. (2.18) rather than (3.44), as is often done, would provide very different results.

The spherical wave functions are of interest, as they have been used to explain the S^{32} spectrum.[4] (See table 3.9.) The Rosenfeld 1 force gives no pairing. The Rosenfeld 2 parameters show pair correlations, although the dispersion is not very great ($V^2_{d3/2} = 0.100$), and the gain in E_{TOTAL} is small. Although the NDKB force shows about the same pairing energy, the dispersion is considerably greater. With the pf shell the occupation probabilities are $V^2_{d\,5/2} = 0.971$, $V^2_{s\,\frac{1}{2}} = 0.509$, $V^2_{d3/2} = 0.288$. Without the pf shell, a re-ordering of levels occurs. The original HF and final BCS single particle energies are considerably different.

$$\epsilon_{d5/2} = -13.340 \rightarrow -15.099 \text{ Mev}, \quad V^2_{d5/2} = 0.972$$
$$\epsilon_{s\frac{1}{2}} = -12.377 \rightarrow -10.470 \text{ Mev}, \quad V^2_{s\frac{1}{2}} = 0.351$$
$$\epsilon_{d3/2} = -12.048 \rightarrow -10.755 \text{ Mev}, \quad V^2_{d3/2} = 0.367$$

Note that for no shape do $|T_z| = 1$ pairing correlations exist for more than three of the five force mixtures.

We may conclude that $|T_z| = 1$ pairing, as described by the special transformation, does not play a significant role in N = Z even - even nuclei in the 2s - 1d shell. In particular, it can not rectify the failure of HF theory in describing these nuclei.

Table 3.1: $|T_z| = 1$ Pairing in Prolate Mg^{24}

Force	Shape	E_{PAIR}	E_{TOTAL}	Q_{20}	Q_{40}	A_x	λ
Rosenfeld 1	Prolate 1	-0.063	-94.105	15.2	-4.0	0.16	-13.492
Rosenfeld 2	Prolate 2	-2.456	-75.325	16.0	-10.5	0.19	-11.360
Yale	Prolate	-2.463	-130.697	19.8	-4.9	0.17	-9.176
NDKB 1	Prolate	-0.457	-108.668	17.3	2.9	0.12	-6.458
NDKB 2	Prolate	-0.124	-114.814	23.2	-1.5	0.14	-6.860

Energies are in Mev. Q_{LM} has units of fm^L .

Table 3.2: Prolate Mg^{24} (Prolate 1, Rosenfeld 1)

ϵ_α	-19.385	-15.054	-11.987	-10.156	-6.173	-4.052
v_α^2	1.000	0.996	0.004	0.000	0.000	0.000
Δ_α	-0.155	-0.206	-0.194	-0.107	-0.114	-0.125
E_α	5.896	1.576	1.518	3.337	7.320	9.440

Table 3.3: Prolate Mg^{24} (Prolate 2, Rosenfeld 2)

ϵ_α	-18.008	-12.273	-10.467	-6.944	-5.205	-2.588
v_α^2	0.996	0.783	0.211	0.005	0.003	0.002
Δ_α	-0.820	-1.333	-1.262	-0.651	-0.669	-0.723
E_α	6.698	1.616	1.546	4.464	6.192	8.802

Table 3.4: Prolate Mg^{24} (Yale)

ϵ_α	-14.911	-9.982	-8.398	-5.331	-4.206	-1.568
v_α^2	0.997	0.769	0.228	0.004	0.003	0.002
Δ_α	-0.650	-1.265	-1.198	-0.487	-0.514	-0.674
E_α	5.771	1.500	1.428	3.876	5.000	7.638

All energies are in Mev.

Table 3.5: Prolate Mg^{24} (NDKB 1)

ϵ_α	-11.638	-7.536	-5.583	-3.923	-0.531	1.728
v_α^2	1.000	0.950	0.049	0.001	0.000	0.000
Δ_α	-0.196	-0.522	-0.420	-0.138	-0.183	-0.245
E_α	5.184	1.198	0.971	2.539	5.930	8.190

Table 3.6: Prolate Mg^{24} (NDKB 2)

ϵ_α	-13.547	-8.063	-5.871	-2.475	0.757	3.504
v_α^2	1.000	0.987	0.013	0.000	0.000	0.000
Δ_α	-0.096	-0.277	-0.227	-0.062	-0.072	-0.108
E_α	6.688	1.235	1.014	4.385	7.617	10.364

All energies are in Mev.

Table 3.7: $|T_z| = 1$ Pairing in Prolate Ar^{36}

Force	E_{PAIR}	E_{TOTAL}	Q_{20}	Q_{40}	A_x	λ
Rosenfeld 2	-1.535	-235.373	5.7	-11.8	0.32	-16.174
Yale	-3.667	-286.819	6.0	-19.8	0.54	-18.008
NDKB 1	-0.322	-222.277	6.0	-11.6	0.08	-13.239
NDKB 2	-0.045	-223.192	8.1	-15.6	0.12	-12.811

Energies are in Mev. Q_{LM} has units of fm^L.

Table 3.8: $|T_z| = 1$ Pairing in Spherical Si^{28}

Force	E_{PAIR}	E_{TOTAL}	λ
Rosenfeld 2	-4.462	-114.808	-12.720
NDKB 1	-3.016	-134.272	-9.206
NDKB 2	-2.444	-135.473	-9.046

Table 3.9: $|T_z| = 1$ Pairing in Spherical S^{32}

Force	E_{PAIR}	E_{TOTAL}	λ
Rosenfeld 2	-3.586	-173.875	-14.644
NDKB 1	-3.750	-172.876	-10.881
NDKB 2	-4.171	-173.487	-10.834

Table 3.10: $|T_z| = 1$ Pairing in Spherical Ar^{36}

Force	E_{PAIR}	E_{TOTAL}	λ
Rosenfeld 2	-4.077	-235.065	-16.309
Yale	-4.445	-286.324	-18.371

All energies are in Mev.

References to Chapter 3

1. A. Bohr, B.R. Mottleson, and D. Pines, Phys. Rev. 110, 936 (1958).

2. S.T. Belyaev, Mat. Fys. Medd. Dan. Vid. Selsk. 31, No.11 (1959).

3. K. Dietrich, H.J. Mang, and J. Pradal, Zeitschrift fur Physik 190, 357 (1966).

4. See reference 2.14.

5. G.E. Brown (see reference 2.3), VII.8.

IV. GENERALIZATION TO T = 0 AND T = 1 PAIRING

1. Neutron - Proton Pairing

Pairing correlations are commonly considered to exist between pairs of like nucleons (two protons or two neutrons). The failure of the conventional theory to account for the possibility of neutron - proton pairing has long been recognized.

For heavy nuclei it is often argued that since neutrons and protons are filling different shells n-p pairing correlations can not arise. This may, however, be erroneous. There are two determining factors: a) The magnitude of matrix elements connecting orbitals in different shells compared to those with all orbitals within one shell. For reasonable forces these two sets of matrix elements have similar magnitudes. Therefore one may not argue that orbitals in different shells result in small overlap integrals. b) Single particle energies. The relevant energies are not absolute energies, which may differ for neutrons and protons, but energies relative to their respective Fermi energies, which are likely to be similar. Even for heavy nuclei, therefore, one may not be justified in neglecting the possibility of n-p pairing.

For light nuclei such neglect is certainly unjustified since neutrons and protons are filling the same

shell. Furthermore, for N = Z nuclei neutrons and protons have identical single particle orbitals and relative energies (neglecting the small perturbation of the Coulomb force). In light nuclei reasonable forces have the T = 0 component stronger than the T = 1 component. This is demonstrated by the observation that all N = Z odd-odd nuclei with A < 40 (except Cl^{34}) have a T = 0 ground state. Any attempt to generalize the pairing theory by including n-p (T = 1) correlations while still neglecting n - p (T = 0) correlations is therefore highly unsatisfactory. Rather one might expect T = 0 pairing to be more important than T = 1 pairing for light N = Z nuclei.

We may anticipate a common criticism of n-p pairing theories. Since the quasiparticle vacuum does not conserve the number of pairs of particles, the ground state wave function for an even-even nucleus contains components with odd numbers of neutrons and protons. The objection is that even-even and odd-odd nuclei have intrinsically different wave functions, whereas the n-p pairing theory appears to mix them. However, even-even and odd-odd nuclei have different intrinsic structure primarily because their HF fields are essentially different. In particular, the HF field for even-even nuclei is time reversal invariant, whereas for odd-odd nuclei this is not so. But the odd-odd components of the even-even ground state

wave function are based upon the even-even HF field and therefore contain all the symmetries of even-even wave functions. The odd-odd admixtures are actually hypothetical odd-odd nuclei which display the essential symmetries of even-even rather than of odd-odd nuclei.

Some students have concluded that charge-independent pairing can not be described by the linear transformation (quasiparticle) method. Flowers and Vujicic [7] comment: "It will be recalled that Bloch and Messiah have proved that the most general type of Bogoliubov-Valatin linear canonical transformation is always equivalent to an exact and unique pairing of particles. But when forces are charge-independent it is impossible to specify uniquely for each particle its pairing partner, and this independently proves that linear transformation methods must be abandoned." This objection arises from a fundamental misunderstanding of the Bloch-Messiah theorem (reference 5.4). For isospin generalized pairing there are uniquely defined paired orbitals. However, in general, these orbitals will be linear combinations of proton and neutron basis states. The derivation of the canonical representation is presented in IV.6.

The BCS theory mixes components with different numbers of particles. The number non-conservation will not be serious if the energy is a linear function of the mass number. It is therefore required that

$$E_{N+2} - E_N \approx E_N - E_{N-2} \quad .$$

Since the experimental binding energies are discontinuous at N = Z even-even nuclei, it might appear that this requirement is violated. Consider the triplet Mg^{26}-Mg^{24}-Mg^{22}. The experimental binding energies provide

$$(E_{Mg^{26}} - E_{Mg^{24}}) - (E_{Mg^{24}} - E_{Mg^{22}}) = 11.25 \text{ Mev.}$$

This is not, however, the relevant quantity. The BCS theory mixes components of different particle number, but all components are based upon the same HF field. The (A + 2) and (A - 2) components are obtained by filling up the A particle HF field, without permitting this field to be renormalized. Now pairing correlations are significant only when the single particle levels in the vicinity of the Fermi level are closely spaced. In this case it is reasonable to expect that adding or subtracting two particles from this fixed HF field would result in similar energy increments. For $|T_z| = 1$ pairing the relevant quantity is

$$(E_{Mg^{26}} - E_{Mg^{24}}) - (E_{Mg^{24}} - E_{Mg^{22}}) = -0.976 \text{ Mev.}$$

For $T_z = 0$ pairing the relevant quantity is

$$(E_{Al^{26}} - E_{Mg^{24}}) - (E_{Mg^{24}} - E_{Na^{22}}) = -3.750 \text{ Mev.}$$

(The fixed HF field is chosen as Mg^{24} axially symmetric prolate, Yale force.) These energies are considerably smaller than the experimental value of 11.25 Mev.

Although there are many who have attempted to generalize the pairing theory,[1] we are especially indebted to A. Goswami for a T = 1 (p-p,n-n,n-p)

pairing theory (1964)[2], A. Goswami and L.S.Kisslinger for a T = 0 pairing theory (1965)[3], and H.T. Chen and A. Goswami for a completely generalized T = 0 and T = 1 pairing theory (1967)[4]. The latter was first derived with the Green's function formalism. The continuity of our argument will be served by presenting an alternative derivation employing the quasiparticle formalism.

2. Quasiparticle Transformation

The essential idea is to allow the following pairs of particles to be correlated: $|\alpha p, \bar{\alpha} p\rangle_{T=1}$, $|\alpha n, \bar{\alpha} n\rangle_{T=1}$, $|\alpha p, \bar{\alpha} n\rangle_{T=1}$, $|\alpha n, \bar{\alpha} p\rangle_{T=1}$, $|\alpha p, \bar{\alpha} n\rangle_{T=0}$, $|\alpha n, \bar{\alpha} p\rangle_{T=0}$. The conventional pairing theory permits only the first two modes. The familiar quasiparticle is a linear combination of proton (neutron) "particle" and proton (neutron) hole.

$$\begin{bmatrix} b^{+}_{\alpha} \\ b_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} u_{\alpha} & -v_{\alpha} \\ -v^{*}_{\bar{\alpha}} & u^{*}_{\bar{\alpha}} \end{bmatrix} \begin{bmatrix} a^{+}_{\alpha} \\ a_{\bar{\alpha}} \end{bmatrix} \tag{4.1}$$

Our generalization consists in having the quasiparticle be a linear combination of proton and neutron "particles" and holes. The extension is naturally obtained by letting b^{+}_{α} and a^{+}_{α} become two dimensional vectors

$$B^{+}_{\alpha} = \begin{bmatrix} b^{+}_{\alpha 1} \\ b^{+}_{\alpha 2} \end{bmatrix} \qquad A^{+}_{\alpha} = \begin{bmatrix} a^{+}_{\alpha p} \\ a^{+}_{\alpha n} \end{bmatrix} \tag{4.2}$$

and by letting u_{α} and v_{α} become two dimensional matrices.

$$U_{\alpha} = \begin{bmatrix} u_{\alpha 11} & u_{\alpha 12} \\ u_{\alpha 21} & u_{\alpha 22} \end{bmatrix} \qquad V_{\alpha} = \begin{bmatrix} v_{\alpha 11} & v_{\alpha 12} \\ v_{\alpha 21} & v_{\alpha 22} \end{bmatrix} \tag{4.3}$$

The counterpart of (4.1) is

$$\begin{bmatrix} B^{+}_{\alpha} \\ B_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} U_{\alpha} & -V_{\alpha} \\ -V^{*}_{\bar{\alpha}} & U^{*}_{\bar{\alpha}} \end{bmatrix} \begin{bmatrix} A^{+}_{\alpha} \\ A_{\bar{\alpha}} \end{bmatrix}. \tag{4.4}$$

If U_α and V_α are diagonal, the standard transformation (4.1) is recovered. The form of our transformation assumes that neutrons and protons have an identical set of single particle orbitals $\{|\alpha\rangle\}$. Consequently for $N \neq Z$ nuclei, one may not use a HF wave function for single particle states. Noting that

$$\begin{bmatrix} M_1 & M_2 \\ M_3 & M_4 \end{bmatrix}^+ = \begin{bmatrix} M_1^+ & M_3^+ \\ M_2^+ & M_4^+ \end{bmatrix}$$

the inverse transformation is

$$\begin{bmatrix} A^\dagger_\alpha \\ A_{\bar\alpha} \end{bmatrix} = \begin{bmatrix} \tilde{U}^*_\alpha & -\tilde{V}_{\bar\alpha} \\ -\tilde{V}^*_\alpha & \tilde{U}_{\bar\alpha} \end{bmatrix} \begin{bmatrix} B^\dagger_\alpha \\ B_{\bar\alpha} \end{bmatrix}. \tag{4.5}$$

The unitarity conditions are $(\mathcal{U}\,\mathcal{U}^\dagger = I)$

$$U_\alpha U_\alpha^\dagger + V_\alpha V_\alpha^\dagger = I \tag{4.6a}$$

$$U_\alpha \tilde{V}_{\bar\alpha} + V_\alpha \tilde{U}_{\bar\alpha} = 0 \tag{4.6b}$$

and $(\mathcal{U}^\dagger \mathcal{U} = I)$

$$U_\alpha^\dagger U_\alpha + (V_{\bar\alpha}^\dagger V_{\bar\alpha})^* = I \tag{4.6c}$$

$$U_\alpha^\dagger V_\alpha + (V_{\bar\alpha}^\dagger U_{\bar\alpha})^* = 0 . \tag{4.6d}$$

Some care must be taken with the choice of phases. The usual convention

$$U_{\bar\alpha} = U_\alpha \qquad V_{\bar\alpha} = -V_\alpha$$

must be rejected (for reasons which will later become apparent) and replaced by

$$U_{\bar{\alpha}} = U_{\alpha}^{*} \qquad V_{\bar{\alpha}} = -V_{\alpha}^{*} \quad . \tag{4.7}$$

We adopt this phase convention for the remainder of our discussion. (We could have chosen

$$U_{\bar{\alpha}} = \tilde{U}_{\alpha} \qquad V_{\bar{\alpha}} = -\tilde{V}_{\alpha}$$

with equivalent results.)

The unitarity conditions (4.6) become

$$U_{\alpha} U_{\alpha}^{\dagger} + V_{\alpha} V_{\alpha}^{\dagger} = I \tag{4.8a}$$

$$U_{\alpha} V_{\alpha}^{\dagger} - V_{\alpha} U_{\alpha}^{\dagger} = 0 \tag{4.8b}$$

$$U_{\alpha}^{\dagger} U_{\alpha} + V_{\alpha}^{\dagger} V_{\alpha} = 0 \tag{4.8c}$$

$$U_{\alpha}^{\dagger} V_{\alpha} - V_{\alpha}^{\dagger} U_{\alpha} = 0 \, . \tag{4.8d}$$

More explicitly

$$\sum_{\tau} (u_{\alpha\tau_1\tau} u^{*}_{\alpha\tau_2\tau} + v_{\alpha\tau_1\tau} v^{*}_{\alpha\tau_2\tau}) = \delta_{\tau_1\tau_2} \tag{4.9a}$$

$$\sum_{\tau} (u_{\alpha\tau_1\tau} v^{*}_{\alpha\tau_2\tau} - v_{\alpha\tau_1\tau} u^{*}_{\alpha\tau_2\tau}) = 0 \tag{4.9b}$$

$$\sum_{t} (u_{\alpha t\tau_1} u^{*}_{\alpha t\tau_2} + v_{\alpha t\tau_1} v^{*}_{\alpha t\tau_2}) = \delta_{\tau_1\tau_2} \tag{4.9c}$$

$$\sum_{t} (u_{\alpha t\tau_1} v^{*}_{\alpha t\tau_2} - v_{\alpha t\tau_1} u^{*}_{\alpha t\tau_2}) = 0 \, . \tag{4.9d}$$

The quasiparticle transformation simplifies .

$$\begin{bmatrix} B^{\dagger}_{\alpha} \\ B_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} U_{\alpha} & -V_{\alpha} \\ V_{\alpha} & U_{\alpha} \end{bmatrix} \begin{bmatrix} A^{\dagger}_{\alpha} \\ A_{\bar{\alpha}} \end{bmatrix} \tag{4.10a}$$

That is

$$\begin{bmatrix} b^{\dagger}_{\alpha 1} \\ b^{\dagger}_{\alpha 2} \\ b_{\bar{\alpha} 1} \\ b_{\bar{\alpha} 2} \end{bmatrix} = \begin{bmatrix} U_{\alpha 11} & U_{\alpha 12} & -V_{\alpha 11} & -V_{\alpha 12} \\ U_{\alpha 21} & U_{\alpha 22} & -V_{\alpha 21} & -V_{\alpha 22} \\ V_{\alpha 11} & V_{\alpha 12} & U_{\alpha 11} & U_{\alpha 12} \\ V_{\alpha 21} & V_{\alpha 22} & U_{\alpha 21} & U_{\alpha 22} \end{bmatrix} \begin{bmatrix} a^{\dagger}_{\alpha p} \\ a^{\dagger}_{\alpha n} \\ a_{\bar{\alpha} p} \\ a_{\bar{\alpha} n} \end{bmatrix} \tag{4.10b}$$

It will be useful to list the entire set of transformations.

$$b^{\dagger}_{\alpha \tau} = \sum_{\tau} (U_{\alpha \tau \tau} a^{\dagger}_{\alpha \tau} - V_{\alpha \tau \tau} a_{\bar{\alpha} \tau}) \tag{4.11a}$$

$$b_{\alpha \tau} = \sum_{\tau} (U^{*}_{\alpha \tau \tau} a_{\alpha \tau} - V^{*}_{\alpha \tau \tau} a^{\dagger}_{\bar{\alpha} \tau}) \tag{4.11b}$$

$$b^{\dagger}_{\bar{\alpha} \tau} = \sum_{\tau} (U^{*}_{\alpha \tau \tau} a^{\dagger}_{\bar{\alpha} \tau} + V^{*}_{\alpha \tau \tau} a_{\alpha \tau}) \tag{4.11c}$$

$$b_{\bar{\alpha} \tau} = \sum_{\tau} (U_{\alpha \tau \tau} a_{\bar{\alpha} \tau} + V_{\alpha \tau \tau} a^{\dagger}_{\alpha \tau}) \tag{4.11d}$$

The inverse transformation is

$$\begin{bmatrix} A^{\dagger}_{\alpha} \\ A_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} U^{\dagger}_{\alpha} & V^{\dagger}_{\alpha} \\ -V^{T}_{\alpha} & U^{\dagger}_{\alpha} \end{bmatrix} \begin{bmatrix} B^{\dagger}_{\alpha} \\ B_{\bar{\alpha}} \end{bmatrix}. \tag{4.12}$$

The set of all co-ordinates is given below.

$$a^{\dagger}_{\alpha \tau} = \sum_{\tau} (U^{*}_{\alpha \tau \tau} b^{\dagger}_{\alpha \tau} + V^{*}_{\alpha \tau \tau} b_{\bar{\alpha} \tau}) \tag{4.13a}$$

$$a_{\alpha \tau} = \sum_{\tau} (U_{\alpha \tau \tau} b_{\alpha \tau} + V_{\alpha \tau \tau} b^{\dagger}_{\bar{\alpha} \tau}) \tag{4.13b}$$

$$a^{\dagger}_{\bar{\alpha} \tau} = \sum_{\tau} (U_{\alpha \tau \tau} b^{\dagger}_{\bar{\alpha} \tau} - V_{\alpha \tau \tau} b_{\alpha \tau}) \tag{4.13c}$$

$$a_{\bar{\alpha} \tau} = \sum_{\tau} (U^{*}_{\alpha \tau \tau} b_{\bar{\alpha} \tau} - V^{*}_{\alpha \tau \tau} b^{\dagger}_{\alpha \tau}) \tag{4.13d}$$

The unitarity conditions (4.8) may also be derived from the commutation rules. For example, using (4.11a,b) we find

$$[b^{\dagger}_{\alpha_1 \tau_1}, b_{\alpha_2 \tau_2}]_{+} = \sum_{\tau} (U_{\alpha_1 \tau_1 \tau} U^{*}_{\alpha_1 \tau_2 \tau} + V_{\alpha_1 \tau_1 \tau} V^{*}_{\alpha_1 \tau_2 \tau}) \delta_{\alpha_1 \alpha_2}.$$

Requiring the commutator to equal $\delta_{\alpha_1\alpha_2}\,\delta_{\tau_1\tau_2}$, we have

$$\sum_{\tau}\left(U_{\alpha\tau_1\tau}\,U^{*}_{\alpha\tau_2\tau} + N_{\alpha\tau_1\tau}\,N^{*}_{\alpha\tau_2\tau}\right) = \delta_{\tau_1\tau_2}$$

which is (4.9a). The set of unitarity conditions (4.8) are obtained by requiring

$$[b^{\dagger}_{\alpha_1\tau_1}, b_{\alpha_2\tau_2}]_+ = \delta_{\alpha_1\alpha_2}\,\delta_{\tau_1\tau_2} \tag{4.14a}$$

$$[b_{\alpha_1\tau_1}, b_{\bar{\alpha}_2\tau_2}]_+ = 0 \tag{4.14b}$$

$$[a^{\dagger}_{\alpha_1\tau_1}, a_{\alpha_2\tau_2}]_+ = \delta_{\alpha_1\alpha_2}\,\delta_{\tau_1\tau_2} \tag{4.14c}$$

$$[a_{\alpha_1\tau_1}, a_{\bar{\alpha}_2\tau_2}]_+ = 0\,. \tag{4.14d}$$

3. The Hamiltonian

Recalling that the ground state is a quasiparticle vacuum the density matrix and pairing tensor are easily evaluated with the aid of the inverse transformations (4. 13).

The density matrix is $(\alpha_1, \alpha_2 > 0)$

$$\langle a^{+}_{\alpha_1\tau_1} a_{\alpha_2\tau_2} \rangle =$$

$$\langle \sum_{\tau_1} (u^{*}_{\alpha_1\tau_1\tau_1} b^{+}_{\alpha_1\tau_1} + v^{*}_{\alpha_1\tau_1\tau_1} b_{\bar{\alpha}_1\tau_1}) \sum_{\tau_2} (u_{\alpha_2\tau_2\tau_2} b_{\alpha_2\tau_2} + v_{\alpha_2\tau_2\tau_2} b^{+}_{\bar{\alpha}_2\tau_2}) \rangle =$$

$$\sum_{\tau_1\tau_2} v^{*}_{\alpha_1\tau_1\tau_1} v_{\alpha_2\tau_2\tau_2} \langle b_{\bar{\alpha}_1\tau_1} b^{+}_{\bar{\alpha}_2\tau_2} \rangle .$$

Since $\langle b_{\bar{\alpha}_1\tau_1} b^{+}_{\bar{\alpha}_2\tau_2} \rangle = \delta_{\alpha_1\alpha_2} \delta_{\tau_1\tau_2}$, the density matrix is

$$\langle a^{+}_{\alpha_1\tau_1} a_{\alpha_2\tau_2} \rangle = \sum_{\tau} v^{*}_{\alpha_1\tau\tau_1} v_{\alpha_1\tau\tau_2} \delta_{\alpha_1\alpha_2} . \qquad (4.15)$$

$$(\alpha_1, \alpha_2 > 0)$$

The non-vanishing elements are

$$\langle a^{+}_{\alpha p} a_{\alpha p} \rangle = v^{*}_{\alpha 11} v_{\alpha 11} + v^{*}_{\alpha 21} v_{\alpha 21} \qquad (4.16a)$$

$$\langle a^{+}_{\alpha n} a_{\alpha n} \rangle = v^{*}_{\alpha 12} v_{\alpha 12} + v^{*}_{\alpha 22} v_{\alpha 22} \qquad (4.16b)$$

$$\langle a^{+}_{\alpha p} a_{\alpha n} \rangle = v^{*}_{\alpha 11} v_{\alpha 12} + v^{*}_{\alpha 21} v_{\alpha 22} \qquad (4.16c)$$

$$\langle a^{+}_{\alpha n} a_{\alpha p} \rangle = v^{*}_{\alpha 12} v_{\alpha 11} + v^{*}_{\alpha 22} v_{\alpha 21} . \qquad (4.16d)$$

It is apparent that

$$\langle a^{+}_{\alpha p} a_{\alpha p} \rangle \quad \text{and} \quad \langle a^{+}_{\alpha n} a_{\alpha n} \rangle \quad \text{are real} \qquad (4.17)$$

and

$$\langle a^{+}_{\alpha p} a_{\alpha n} \rangle = \langle a^{+}_{\alpha n} a_{\alpha p} \rangle^{*} . \qquad (4.18)$$

Therefore the density matrix is Hermitian in isospin. That is, if

$$\rho_{\tau_1 \tau_2}(\alpha) = \rho_{\alpha\tau_1, \alpha\tau_2} \tag{4.19}$$

and

$$\rho(\alpha) = \begin{bmatrix} \rho_{pp}(\alpha) & \rho_{pn}(\alpha) \\ \rho_{np}(\alpha) & \rho_{nn}(\alpha) \end{bmatrix} \tag{4.20}$$

then

$$\rho^{+}(\alpha) = \rho(\alpha) . \tag{4.21}$$

The elements of ρ for $\alpha < 0$ are given by

$$\langle a^{+}_{\bar{\alpha}\tau_1} a_{\bar{\alpha}\tau_2} \rangle = \langle a^{+}_{\alpha\tau_1} a_{\alpha\tau_2} \rangle^{*} \tag{4.22}$$

resulting in the time reversal symmetry

$$\rho(\bar{\alpha}) = \rho^{*}(\alpha) . \tag{4.23}$$

The pairing tensor may be similarly evaluated. Let $\alpha_1, \alpha_2 > 0$.

$$\langle a_{\bar{\alpha}_1\tau_1} a_{\alpha_2\tau_2} \rangle =$$

$$\langle \sum_{t_1} (u^{*}_{\alpha_1 t_1 \tau_1} b_{\bar{\alpha}_1 t_1} - v^{*}_{\alpha_1 t_1 \tau_1} b^{+}_{\alpha_1 t_1}) \sum_{t_2} (u_{\alpha_2 t_2 \tau_2} b_{\alpha_2 t_2} + v_{\alpha_2 t_2 \tau_2} b^{+}_{\bar{\alpha}_2 t_2}) \rangle =$$

$$\sum_{t_1 t_2} u^{*}_{\alpha_1 t_1 \tau_1} v_{\alpha_2 t_2 \tau_2} \langle b_{\bar{\alpha}_1 t_1} b^{+}_{\bar{\alpha}_2 t_2} \rangle .$$

The pairing tensor is

$$\langle a_{\bar{\alpha}_1\tau_1} a_{\alpha_2\tau_2} \rangle = \sum_{t} u^{*}_{\alpha_1 t \tau_1} v_{\alpha_1 t \tau_2} \delta_{\alpha_1 \alpha_2} . \tag{4.24}$$

$$(\alpha_1, \alpha_2 > 0)$$

The non-vanishing elements are $(\alpha > 0)$

$$\langle a_{\bar{\alpha}p}\, a_{\alpha p} \rangle = U^*_{\alpha 11} N_{\alpha 11} + U^*_{\alpha 21} N_{\alpha 21} \tag{4.25a}$$

$$\langle a_{\bar{\alpha}n}\, a_{\alpha n} \rangle = U^*_{\alpha 12} N_{\alpha 12} + U^*_{\alpha 22} N_{\alpha 22} \tag{4.25b}$$

$$\langle a_{\bar{\alpha}p}\, a_{\alpha n} \rangle = U^*_{\alpha 11} N_{\alpha 12} + U^*_{\alpha 21} N_{\alpha 22} \tag{4.25c}$$

$$\langle a_{\bar{\alpha}n}\, a_{\alpha p} \rangle = U^*_{\alpha 12} N_{\alpha 11} + U^*_{\alpha 22} N_{\alpha 21} \,. \tag{4.25d}$$

Unitarity condition (14.9d) for $\tau_1 = \tau_2 = \tau$ is

$$U_{\alpha 1\tau} N^*_{\alpha 1\tau} + U_{\alpha 2\tau} N^*_{\alpha 2\tau} = N_{\alpha 1\tau} U^*_{\alpha 1\tau} + N_{\alpha 2\tau} U^*_{\alpha 2\tau}$$

so that $\langle a_{\bar{\alpha}\tau}\, a_{\alpha\tau} \rangle = \langle a_{\bar{\alpha}\tau}\, a_{\alpha\tau} \rangle^*$ and

$$\langle a_{\bar{\alpha}p}\, a_{\alpha p} \rangle \text{ and } \langle a_{\bar{\alpha}n}\, a_{\alpha n} \rangle \text{ are Real.} \tag{4.26}$$

For $\tau_1 = 1,\ \tau_2 = 2$

$$U_{\alpha 11} N^*_{\alpha 12} + U_{\alpha 21} N^*_{\alpha 22} = N_{\alpha 11} U^*_{\alpha 12} + N_{\alpha 21} U^*_{\alpha 22}$$

so that

$$\langle a_{\bar{\alpha}p}\, a_{\alpha n} \rangle = \langle a_{\bar{\alpha}n}\, a_{\alpha p} \rangle^* . \tag{4.27}$$

Therefore, the pairing tensor is Hermitian in isospin. If

$$\tau_{\tau_1 \tau_2}(\alpha) = \tau_{\alpha\tau_1,\, \bar{\alpha}\tau_2} \tag{4.28}$$

and

$$\tau(\alpha) = \begin{bmatrix} \tau_{pp}(\alpha) & \tau_{pn}(\alpha) \\ \tau_{np}(\alpha) & \tau_{nn}(\alpha) \end{bmatrix} \tag{4.29}$$

then

$$\tau^+(\alpha) = \tau(\alpha) \,. \tag{4.30}$$

The adjoint operation refers only to isospin co-ordinates, i.e.

$$\mathcal{L}^{\dagger}_{\tau_1\tau_2}(\alpha) = \mathcal{L}^{*}_{\alpha\tau_2,\bar{\alpha}\tau_1} \neq \mathcal{L}^{*}_{\bar{\alpha}\tau_2,\alpha\tau_1} .$$

Since the pairing tensor is anti-symmetric

$$\langle a_{\alpha\tau_1} a_{\bar{\alpha}\tau_2} \rangle = -\langle a_{\bar{\alpha}\tau_2} a_{\alpha\tau_1} \rangle \tag{4.31}$$

the time reversal symmetry is

$$\mathcal{L}(\bar{\alpha}) = -\mathcal{L}^{*}(\alpha) \tag{4.32}$$

where $\mathcal{L}_{\tau_1\tau_2}(\bar{\alpha}) = \mathcal{L}_{\bar{\alpha}\tau_1,\alpha\tau_2}$. The adjoint of the pairing tensor is

$$\langle a^{\dagger}_{\alpha_1\tau_1} a^{\dagger}_{\bar{\alpha}_2\tau_2} \rangle = \langle a_{\bar{\alpha}_2\tau_2} a_{\alpha_1\tau_1} \rangle^{*} . \tag{4.33}$$

The HF potential is

$$\Gamma_{\alpha_1\tau_1,\alpha_2\tau_2} = \sum_{\substack{\beta>0 \\ \tau_3\tau_4}} \langle \alpha_1\tau_1, \beta\tau_3 | v | \alpha_2\tau_2, \beta\tau_4 \rangle_A \langle a^{\dagger}_{\beta\tau_3} a_{\beta\tau_4} \rangle . \tag{4.34}$$

The matrix elements of v are non-zero only if $\tau_1+\tau_2 = \tau_3+\tau_4$. Therefore the diagonal - isospin elements of Γ are

$$\Gamma_{\alpha_1\tau,\alpha_2\tau} = \sum_{\substack{\beta>0 \\ \tau'}} \langle \alpha_1\tau, \beta\tau' | v | \alpha_2\tau, \beta\tau' \rangle_A \langle a^{\dagger}_{\beta\tau'} a_{\beta\tau'} \rangle . \tag{4.35}$$

There may also be off-diagonal - isospin elements.

$$\Gamma_{\alpha_1\tau,\alpha_2-\tau} = \sum_{\beta>0} \langle \alpha_1\tau, \beta-\tau | v | \alpha_2-\tau, \beta\tau \rangle_A \langle a^{\dagger}_{\beta-\tau} a_{\beta\tau} \rangle \tag{4.36}$$

The HF Hamiltonian is

$$\mathcal{H}_{\alpha_1\tau_1,\alpha_2\tau_2} = T_{\alpha_1\tau_1,\alpha_2\tau_2} + \Gamma_{\alpha_1\tau_1,\alpha_2\tau_2} . \tag{4.37}$$

Define

$$\mathcal{H}_{\tau_1\tau_2}(\alpha) = \mathcal{H}_{\alpha\tau_1,\alpha\tau_2} . \tag{4.38}$$

The matrix elements of T and v are real. Since $\rho_{\tau\tau}(\alpha)$ is real

$$\mathcal{H}_{pp}(\alpha) \quad \text{and} \quad \mathcal{H}_{nn}(\alpha) \qquad \text{are real.} \tag{4.39}$$

Since $\langle \alpha_1 p, \alpha_2 n | v | \alpha_3 n, \alpha_4 p \rangle_A = \langle \alpha_1 n, \alpha_2 p | v | \alpha_3 p, \alpha_4 n \rangle_A$
and $\rho_{pn}(\alpha) = \rho^*_{np}(\alpha)$

$$\mathcal{H}_{pn}(\alpha) = \mathcal{H}^*_{np}(\alpha) . \tag{4.40}$$

Therefore the matrix

$$\mathcal{H}(\alpha) = \begin{bmatrix} \mathcal{H}_{pp}(\alpha) & \mathcal{H}_{pn}(\alpha) \\ \mathcal{H}_{np}(\alpha) & \mathcal{H}_{nn}(\alpha) \end{bmatrix} \tag{4.41}$$

is Hermitian.

$$\mathcal{H}^\dagger(\alpha) = \mathcal{H}(\alpha) \tag{4.42}$$

Since $\rho(\bar{\alpha}) = \rho^*(\bar{\alpha})$, the time reversal symmetry is

$$\mathcal{H}(\bar{\alpha}) = \mathcal{H}^*(\alpha) . \tag{4.43}$$

The pair potential is

$$\Delta_{\alpha_1 \tau_1, \bar{\alpha}_2 \tau_2} = \sum_{\substack{\beta > 0 \\ \tau_3 \tau_4}} \langle \alpha_1 \tau_1, \bar{\alpha}_2 \tau_2 | v | \beta \tau_3, \bar{\beta} \tau_4 \rangle_A \langle a_{\bar{\beta} \tau_4} a_{\beta \tau_3} \rangle . \tag{4.44}$$

For non-zero matrix elements $\tau_1 + \tau_2 = \tau_3 + \tau_4$, so that the diagonal isospin elements are

$$\Delta_{\alpha_1 \tau, \bar{\alpha}_2 \tau} = \sum_{\beta > 0} \langle \alpha_1 \tau, \bar{\alpha}_2 \tau | v | \beta \tau, \bar{\beta} \tau \rangle_A \langle a_{\bar{\beta} \tau} a_{\beta \tau} \rangle . \tag{4.45}$$

Only protons (neutrons) contribute to the proton (neutron) pair potential. $\Delta_{\alpha_1 \tau, \bar{\alpha}_2 \tau}$ is the $|T_z| = 1$ pair potential. The $T_z = 0$ pair potential is

$$\Delta_{\alpha_1 \tau, \bar{\alpha}_2 -\tau} = \sum_{\substack{\beta > 0 \\ \tau'}} \langle \alpha_1 \tau, \bar{\alpha}_2 -\tau | v | \beta \tau', \bar{\beta} -\tau' \rangle_A \langle a_{\bar{\beta} -\tau'} a_{\beta \tau'} \rangle . \tag{4.46}$$

Define

$$\Delta_{\tau_1 \tau_2}(\alpha) = \Delta_{\alpha \tau_1, \bar{\alpha} \tau_2} . \tag{4.47}$$

Since $\langle \alpha_1 \tau, \alpha_2 \tau | v | \alpha_3 \tau, \alpha_4 \tau \rangle_A =$

$$\sum_T \langle \tfrac{1}{2} \tau \, \tfrac{1}{2} \tau | T \, 2\tau \rangle^2 \langle \alpha_1 \alpha_2 T | v | \alpha_3 \alpha_4 T \rangle_A =$$

$$\langle \alpha_1 \alpha_2 T = 1 | v | \alpha_3 \alpha_4 T = 1 \rangle_A \quad \text{for } \tau = \pm 1/2 ,$$

the $|T_z| = 1$ potential is

$$\Delta_{\tau \tau}(\alpha) = \sum_{\beta > 0} \langle \alpha \bar{\alpha} \, T = 1 | v | \beta \bar{\beta} \, T = 1 \rangle_A \langle a_{\bar{\beta} \tau} a_{\beta \tau} \rangle . \tag{4.48}$$

Since $\langle a_{\bar{\beta}\tau} a_{\beta\tau} \rangle$ is real

$$\Delta_{pp}(\alpha) \quad \text{and} \quad \Delta_{nn}(\alpha) \quad \text{are Real.} \tag{4.49}$$

The $T_z = 0$ potential may be reduced to T = 0 and T = 1 components. Consider the matrix element

$$\langle \alpha_1 \tau, \alpha_2 -\tau | v | \alpha_3 \tau', \alpha_4 -\tau' \rangle_A =$$

$$\sum_T \langle \tfrac{1}{2}\tau \tfrac{1}{2} -\tau | T 0 \rangle \langle \tfrac{1}{2}\tau' \tfrac{1}{2} -\tau' | T 0 \rangle \langle \alpha_1 \alpha_2 T | v | \alpha_3 \alpha_4 T \rangle_A .$$

The product of the Clebsch-Gordon coefficients is evaluated in the table below.

	$T=0$	$T=1$
$\tau' = \tau$	$1/2$	$1/2$
$\tau' = -\tau$	$-1/2$	$1/2$

Then the $T_z = 0$ potential may be written as

$$\Delta_{\tau-\tau}(\alpha) =$$

$$1/2 \sum_{\beta>0} \langle \alpha\bar{\alpha}\, T=1 | v | \beta\bar{\beta}\, T=1 \rangle_A \{ \langle a_{\bar{\beta}-\tau} a_{\beta\tau} \rangle + \langle a_{\bar{\beta}\tau} a_{\beta-\tau} \rangle \} \tag{4.50}$$

$$+ 1/2 \sum_{\beta>0} \langle \alpha\bar{\alpha}\, T=0 | v | \beta\bar{\beta}\, T=0 \rangle_A \{ \langle a_{\bar{\beta}-\tau} a_{\beta\tau} \rangle - \langle a_{\bar{\beta}\tau} a_{\beta-\tau} \rangle \}.$$

Since

$$\langle a_{\bar{\beta}-\tau} a_{\beta\tau} \rangle = \langle a_{\bar{\beta}\tau} a_{\beta-\tau} \rangle^*,$$

$$\Delta_{\tau-\tau}(\alpha) = \sum_{\beta>0} \langle \alpha\bar{\alpha}\, T=1 | v | \beta\bar{\beta}\, T=1 \rangle_A \, \mathrm{Re} \langle a_{\bar{\beta}-\tau} a_{\beta\tau} \rangle$$

$$+ i \sum_{\beta>0} \langle \alpha\bar{\alpha}\, T=0 | v | \beta\bar{\beta}\, T=0 \rangle_A \, \mathrm{Im} \langle a_{\bar{\beta}-\tau} a_{\beta\tau} \rangle . \tag{4.51}$$

The pair potential has the remarkable feature that its real part describes T = 1 pairing while the imaginary part describes T = 0 pairing. Let

$$\Delta^{T=1}_{\tau-\tau}(\alpha) = \sum_{\beta>0}{}' \langle \alpha\bar{\alpha}\, T=1 | v | \beta\bar{\beta}\, T=1 \rangle_A \, \mathrm{Re} \langle a_{\bar{\beta}-\tau}\, a_{\beta\tau} \rangle \tag{4.52}$$

$$\Delta^{T=0}_{\tau-\tau}(\alpha) = \sum_{\beta>0}{}' \langle \alpha\bar{\alpha}\, T=0 | v | \beta\bar{\beta}\, T=0 \rangle_A \, \mathrm{Im} \langle a_{\bar{\beta}-\tau}\, a_{\beta\tau} \rangle \tag{4.53}$$

then

$$\Delta_{\tau-\tau}(\alpha) = \Delta^{T=1}_{\tau-\tau}(\alpha) + i\, \Delta^{T=0}_{\tau-\tau}(\alpha) . \tag{4.54}$$

Furthermore, since

$$\mathrm{Re} \langle a_{\bar{\beta}-\tau}\, a_{\beta\tau} \rangle = \mathrm{Re} \langle a_{\bar{\beta}\tau}\, a_{\beta-\tau} \rangle$$
$$\mathrm{Im} \langle a_{\bar{\beta}-\tau}\, a_{\beta\tau} \rangle = -\mathrm{Im} \langle a_{\bar{\beta}\tau}\, a_{\beta-\tau} \rangle$$

we have

$$\Delta^{T=1}_{\tau-\tau}(\alpha) = \Delta^{T=1}_{-\tau\tau}(\alpha) \tag{4.55}$$

$$\Delta^{T=0}_{\tau-\tau}(\alpha) = -\Delta^{T=0}_{-\tau\tau}(\alpha) \tag{4.56}$$

so that

$$\Delta_{\tau-\tau}(\alpha) = \Delta^{*}_{-\tau\tau}(\alpha) . \tag{4.57}$$

Therefore the matrix

$$\Delta(\alpha) = \begin{bmatrix} \Delta_{pp}(\alpha) & \Delta_{pn}(\alpha) \\ \Delta_{np}(\alpha) & \Delta_{nn}(\alpha) \end{bmatrix} \tag{4.58}$$

is self-adjoint.

$$\Delta^{+}(\alpha) = \Delta(\alpha) \tag{4.59}$$

The adjoint operation refers only to the isospin co-ordinates, i.e.

$$\Delta^{\dagger}_{\tau_1\tau_2}(\alpha) = \Delta^{*}_{\alpha\tau_2,\bar{\alpha}\tau_1} \neq \Delta^{*}_{\bar{\alpha}\tau_2,\alpha\tau_1} .$$

Since the pair potential is anti-symmetric

$$\Delta_{\alpha\tau_1,\bar{\alpha}\tau_2} = -\Delta_{\bar{\alpha}\tau_2,\alpha\tau_1} \tag{4.60}$$

the time reversal symmetry is

$$\Delta(\bar{\alpha}) = -\Delta^*(\alpha) \tag{4.61}$$

where $\Delta_{\tau_1\tau_2}(\bar{\alpha}) = \Delta_{\bar{\alpha}\tau_1,\alpha\tau_2}$.

The explicit expressions for the pair potentials are

$$\Delta_{pp}(\alpha) = \sum_{\beta>0} \langle \alpha\bar{\alpha}\, T=1 | v | \beta\bar{\beta}\, T=1 \rangle_A \langle a_{\bar{\beta}p}\, a_{\beta p} \rangle \tag{4.62}$$

$$\Delta_{nn}(\alpha) = \sum_{\beta>0} \langle \alpha\bar{\alpha}\, T=1 | v | \beta\bar{\beta}\, T=1 \rangle_A \langle a_{\bar{\beta}n}\, a_{\beta n} \rangle \tag{4.63}$$

$$\Delta_{pn}^{T=1}(\alpha) = \sum_{\beta>0} \langle \alpha\bar{\alpha}\, T=1 | v | \beta\bar{\beta}\, T=1 \rangle_A \, Re \langle a_{\bar{\beta}n}\, a_{\beta p} \rangle \tag{4.64}$$

$$\Delta_{pn}^{T=0}(\alpha) = \sum_{\beta>0} \langle \alpha\bar{\alpha}\, T=0 | v | \beta\bar{\beta}\, T=0 \rangle_A \, Im \langle a_{\bar{\beta}n}\, a_{\beta p} \rangle \tag{4.65}$$

where

$$\Delta_{pn}(\alpha) = \Delta_{pn}^{T=1}(\alpha) + i\,\Delta_{pn}^{T=0}(\alpha) \tag{4.66}$$

and

$$\Delta_{np}(\alpha) = \Delta_{pn}^*(\alpha). \tag{4.67}$$

The derivation of these expressions depends only upon the phase choice (4.7)

$$U_{\bar{\alpha}} = U_\alpha^* \qquad V_{\bar{\alpha}} = -V_\alpha^*$$

and the unitarity conditions (4.9). No other information or assumption was required.

Let us now consider what would have resulted from the conventional phase choice.

$$U_{\bar{\alpha}} = U_\alpha \qquad V_{\bar{\alpha}} = -V_\alpha$$

The quasiparticle transformation (4.4) becomes

$$\begin{bmatrix} B_\alpha^\dagger \\ B_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} U_\alpha & -V_\alpha \\ V_\alpha^* & U_\alpha^* \end{bmatrix} \begin{bmatrix} A_\alpha^\dagger \\ A_{\bar{\alpha}} \end{bmatrix}.$$

The inverse transformation (4.5) would be

$$\begin{bmatrix} A^{+}_{\alpha} \\ A_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} \tilde{U}^{*}_{\alpha} & \tilde{V}_{\alpha} \\ -\tilde{V}^{*}_{\alpha} & \tilde{U}_{\alpha} \end{bmatrix} \begin{bmatrix} B^{+}_{\alpha} \\ B_{\bar{\alpha}} \end{bmatrix} .$$

The unitarity condition (4.6d) is

$$U^{+}_{\alpha} V_{\alpha} - (V^{+}_{\alpha} U_{\alpha})^{*} = 0$$

or

$$\sum_{\tau} (U_{\alpha\tau\tau_1} V^{*}_{\alpha\tau\tau_2} - V^{*}_{\alpha\tau\tau_1} U_{\alpha\tau\tau_2}) = 0$$

instead of (4.9d). The pairing tensor would be

$$\langle a_{\bar{\alpha}\tau_1} a_{\alpha\tau_2} \rangle = \sum_{\tau} U_{\alpha\tau\tau_1} V^{*}_{\alpha\tau\tau_2}$$

so that $\langle a_{\bar{\alpha}p} a_{\alpha n} \rangle = \langle a_{\bar{\alpha}n} a_{\alpha p} \rangle$.

The $T_z = 0$ pair potential (4.50) reduces to

$$\Delta_{\tau-\tau}(\alpha) = \sum_{\beta>0} \langle \alpha\bar{\alpha}\, T=1 | V | \beta\bar{\beta}\, T=1 \rangle_A \langle a_{\bar{\beta}-\tau} a_{\beta\tau} \rangle .$$

Consequently, with the conventional phase choice, the unitarity conditions alone forbid the possibility of $T = 0$ pairing. This is true even if the pair parameters are complex.

The Hamiltonian is now completely determined. The ground state energy is given by (3.38a)

$$\begin{aligned} H_0' &= E_0 - \lambda_p Z - \lambda_n (A - Z) \\ &= \sum_{\alpha>0,\tau_1\tau_2} (T - \lambda_p P_p - \lambda_n P_n + \tfrac{1}{2}\Gamma)_{\alpha\tau_1,\alpha\tau_2} \langle a^{+}_{\alpha\tau_1} a_{\alpha\tau_2} \rangle \\ &\quad + \sum_{\alpha>0,\tau_1\tau_2} \Delta_{\alpha\tau_1,\bar{\alpha}\tau_2} \langle a^{+}_{\alpha\tau_1} a^{+}_{\bar{\alpha}\tau_2} \rangle \end{aligned} \tag{4.68}$$

or by (3.38b)

$$H_0' = E_0 - \lambda_p Z - \lambda_n (A-Z)$$

$$= \sum_{\substack{\alpha>0,\tau}} \langle \alpha\tau | T - \lambda_p P_p - \lambda_n P_n | \alpha\tau \rangle \langle a^\dagger_{\alpha\tau} a_{\alpha\tau} \rangle$$
$$+ \frac{1}{2} \sum_{\substack{\alpha\beta>0\\ \tau_1\tau_2\tau_3\tau_4}} \langle \alpha\tau_1, \beta\tau_2 | v | \alpha\tau_3, \beta\tau_4 \rangle_A \langle a^\dagger_{\alpha\tau_1} a_{\alpha\tau_3} \rangle \langle a^\dagger_{\beta\tau_2} a_{\beta\tau_4} \rangle \tag{4.69}$$
$$+ \sum_{\substack{\alpha\beta>0\\ \tau_1\tau_2\tau_3\tau_4}} \langle \alpha\tau_1, \bar{\alpha}\tau_2 | v | \beta\tau_3, \bar{\beta}\tau_4 \rangle_A \langle a^\dagger_{\alpha\tau_1} a^\dagger_{\bar{\alpha}\tau_2} \rangle \langle a_{\bar{\beta}\tau_4} a_{\beta\tau_3} \rangle$$

where P_τ is a projection operator.

$$P_\tau = |\tau\rangle\langle\tau| \tag{4.70}$$

H_2' is given by (3.39)

$$H_2' = \sum_{\alpha_1\alpha_2>0,\tau_1\tau_2} \hat{\mathcal{H}}_{\alpha_1\tau_1,\alpha_2\tau_2} N[a^\dagger_{\alpha_1\tau_1} a_{\alpha_2\tau_2}]$$
$$+ \sum_{\alpha_1\alpha_2>0,\tau_1\tau_2} \Delta_{\alpha_1\tau_1,\bar{\alpha}_2\tau_2} N[a^\dagger_{\alpha_1\tau_1} a^\dagger_{\bar{\alpha}_2\tau_2}] \tag{4.71}$$
$$+ \sum_{\alpha_1\alpha_2>0,\tau_1\tau_2} \Delta^*_{\alpha_1\tau_1,\bar{\alpha}_2\tau_2} N[a_{\bar{\alpha}_2\tau_2} a_{\alpha_1\tau_1}]$$

where
$$\hat{\mathcal{H}} = \mathcal{H} - \lambda_p P_p - \lambda_n P_n \,. \tag{4.72}$$

Note that

$$\hat{\mathcal{H}}_{pp}(\alpha) = \mathcal{H}_{pp}(\alpha) - \lambda_p \tag{4.73a}$$

$$\hat{\mathcal{H}}_{nn}(\alpha) = \mathcal{H}_{nn}(\alpha) - \lambda_n \tag{4.73b}$$

$$\hat{\mathcal{H}}_{pn}(\alpha) = \mathcal{H}_{pn}(\alpha) \tag{4.73c}$$

$$\hat{\mathcal{H}}_{np}(\alpha) = \mathcal{H}_{np}(\alpha) \,. \tag{4.73d}$$

4. Equation of Motion

The pairing parameters may be determined by the equation of motion method. It is assumed that

$$\overline{|\langle \alpha_1 \bar{\alpha}_2 T | N | \beta \bar{\beta} T \rangle_A|} \ll \overline{|\langle \alpha_1 \bar{\alpha}_1 T | N | \beta \bar{\beta} T \rangle_A|} \quad (\alpha_1 \neq \alpha_2) \tag{4.74a}$$

so that

$$|\Delta_{\alpha_1 \tau_1, \bar{\alpha}_2 \tau_2}| \ll |\Delta_{\alpha_1 \tau_1, \bar{\alpha}_1 \tau_2}|. \quad (\alpha_1 \neq \alpha_2) \tag{4.74b}$$

Elements of Δ connecting different spatial orbitals are neglected. It is also assumed that

$$|\mathcal{H}_{\alpha_1 \tau_1, \alpha_2 \tau_2}| \ll |\mathcal{H}_{\alpha_1 \tau_1, \alpha_1 \tau_2}|. \quad (\alpha_1 \neq \alpha_2) \tag{4.75}$$

Then H_2' is simplified.

$$H_2' = \sum_{\alpha > 0, \tau_1 \tau_2} \hat{\mathcal{H}}_{\tau_1 \tau_2}(\alpha) \, N[a^\dagger_{\alpha \tau_1} a_{\alpha \tau_2}] + \sum_{\alpha > 0, \tau_1 \tau_2} \{ \Delta_{\tau_1 \tau_2}(\alpha) N[a^\dagger_{\alpha \tau_1} a^\dagger_{\bar{\alpha} \tau_2}] + \Delta^*_{\tau_1 \tau_2}(\alpha) N[a_{\bar{\alpha} \tau_2} a_{\alpha \tau_1}] \} \tag{4.76}$$

H' has the form of an independent quasiparticle Hamiltonian if H_4' may be neglected and if

$$H_2' = \sum_{\alpha \tau} E_{\alpha \tau} b^\dagger_{\alpha \tau} b_{\alpha \tau}. \tag{4.77}$$

It is therefore required that

$$[H_2', b^\dagger_{\alpha \tau}]_- = E_{\alpha \tau} b^\dagger_{\alpha \tau} \tag{4.78a}$$

or

$$[H_2', b^\dagger_{\alpha \tau}]_- = E_{\alpha \tau} \sum_{\tau} (U_{\alpha \tau \tau} a^\dagger_{\alpha \tau} - N_{\alpha \tau \tau} a_{\bar{\alpha} \tau}). \tag{4.78b}$$

The commutator may also be evaluated with (4.76).

$$[H_2', b^{\dagger}_{\alpha\tau}]_- = \sum_{\tau_1\tau_2} \{ \hat{\mathcal{H}}_{\tau_1\tau_2}(\alpha) U_{\alpha\tau\tau_2} - \Delta_{\tau_1\tau_2}(\alpha) V_{\alpha\tau\tau_2} \} a^{\dagger}_{\alpha\tau_1}$$
$$+ \sum_{\tau_1\tau_2} \{ \Delta^{\dagger}_{\tau_1\tau_2}(\alpha) U_{\alpha\tau\tau_2} + \tilde{\hat{\mathcal{H}}}_{\tau_1\tau_2}(\bar{\alpha}) V_{\alpha\tau\tau_2} \} a_{\bar{\alpha}\tau_1} . \tag{4.79}$$

The time reversal symmetry $\mathcal{H}(\bar{\alpha}) = \mathcal{H}^*(\alpha)$ and the Hermiticity of $\mathcal{H}$ result in $\tilde{\mathcal{H}}(\bar{\alpha}) = \mathcal{H}(\alpha)$. Also $\Delta(\alpha)$ is self-adjoint. Therefore

$$[H_2', b^{\dagger}_{\alpha\tau}]_- = \sum_{\tau_1\tau_2} \{ \hat{\mathcal{H}}_{\tau_1\tau_2}(\alpha) U_{\alpha\tau\tau_2} - \Delta_{\tau_1\tau_2}(\alpha) V_{\alpha\tau\tau_2} \} a^{\dagger}_{\alpha\tau_1} \tag{4.80}$$
$$+ \sum_{\tau_1\tau_2} \{ \Delta_{\tau_1\tau_2}(\alpha) U_{\alpha\tau\tau_2} + \hat{\mathcal{H}}_{\tau_1\tau_2}(\alpha) V_{\alpha\tau\tau_2} \} a_{\bar{\alpha}\tau_1} .$$

Compare (4.78b) and (4.80) and equate coefficients of $a^{\dagger}_{\alpha\tau}$ and $a_{\bar{\alpha}\tau}$.

$$\sum_{\tau_2} \{ \hat{\mathcal{H}}_{\tau_1\tau_2}(\alpha) U_{\alpha\tau\tau_2} - \Delta_{\tau_1\tau_2}(\alpha) V_{\alpha\tau\tau_2} \} = E_{\alpha\tau} U_{\alpha\tau\tau_1} \tag{4.81a}$$

$$\sum_{\tau_2} \{ \Delta_{\tau_1\tau_2}(\alpha) U_{\alpha\tau\tau_2} + \hat{\mathcal{H}}_{\tau_1\tau_2}(\alpha) V_{\alpha\tau\tau_2} \} = -E_{\alpha\tau} V_{\alpha\tau\tau_1} . \tag{4.81b}$$

In matrix form (4.81) is

$$\begin{bmatrix} \hat{\mathcal{H}}_{pp}(\alpha) & \hat{\mathcal{H}}_{pn}(\alpha) & \Delta_{pp}(\alpha) & \Delta_{pn}(\alpha) \\ \hat{\mathcal{H}}_{np}(\alpha) & \hat{\mathcal{H}}_{nn}(\alpha) & \Delta_{np}(\alpha) & \Delta_{nn}(\alpha) \\ \Delta_{pp}(\alpha) & \Delta_{pn}(\alpha) & -\hat{\mathcal{H}}_{pp}(\alpha) & -\hat{\mathcal{H}}_{pn}(\alpha) \\ \Delta_{np}(\alpha) & \Delta_{nn}(\alpha) & -\hat{\mathcal{H}}_{np}(\alpha) & -\hat{\mathcal{H}}_{nn}(\alpha) \end{bmatrix} \begin{bmatrix} U_{\alpha\tau 1} \\ U_{\alpha\tau 2} \\ -V_{\alpha\tau 1} \\ -V_{\alpha\tau 2} \end{bmatrix} = E_{\alpha\tau} \begin{bmatrix} U_{\alpha\tau 1} \\ U_{\alpha\tau 2} \\ -V_{\alpha\tau 1} \\ -V_{\alpha\tau 2} \end{bmatrix} \tag{4.82}$$

or more compactly

$$\begin{bmatrix} \hat{\mathcal{H}}(\alpha) & \Delta(\alpha) \\ \Delta(\alpha) & -\hat{\mathcal{H}}(\alpha) \end{bmatrix} \begin{bmatrix} U_\tau(\alpha) \\ -V_\tau(\alpha) \end{bmatrix} = E_\tau(\alpha) \begin{bmatrix} U_\tau(\alpha) \\ -V_\tau(\alpha) \end{bmatrix} \tag{4.83}$$

where $$E_\tau(\alpha) = E_{\alpha\tau} \tag{4.84}$$

$$U_\tau(\alpha) = \begin{bmatrix} U_{\alpha\tau 1} \\ U_{\alpha\tau 2} \end{bmatrix} \qquad V_\tau(\alpha) = \begin{bmatrix} V_{\alpha\tau 1} \\ V_{\alpha\tau 2} \end{bmatrix}. \tag{4.85}$$

The result is a four dimensional eigenvalue equation. The eigenvalues are $\pm E_{\alpha 1}, \pm E_{\alpha 2}$. The eigenvectors corresponding to the positive eigenvalues provide the pairing parameters. The normalization condition is

$$|U_{\alpha\tau 1}|^2 + |U_{\alpha\tau 2}|^2 + |V_{\alpha\tau 1}|^2 + |V_{\alpha\tau 2}|^2 = 1. \tag{4.86}$$

5. Gap Equations for N = Z Nuclei

For N = Z nuclei the eigenvalue problem is considerably simplified. We are able to obtain a generalized set of gap equations. Since both T = 0 and T = 1 pairing are included, the wave function violates isospin conservation. This is analogous to the mixing of different J orbitals in HF instrinsic wave functions, thereby violating angular momentum conservation. Both violations are performed in the same spirit. If the binding energy may be increased by forsaking a symmetry of H, then the intrinsic state shall be permitted to forgo that symmetry. States of good symmetry are later obtained by appopriate projections upon the intrinsic state. Just as the J deformed HF state still satisfies $\langle \underline{J} \rangle = 0$, so do we require our T deformed state to satisfy

$$\langle \underline{T} \rangle = 0 \tag{4.87}$$

where $$\underline{T} = T_x \underline{i} + T_y \underline{j} + T_z \underline{k} \tag{4.88}$$

All components of $\underline{T}$ are to have vanishing ground state expectation values.

$$\langle T_x \rangle = \langle T_y \rangle = \langle T_z \rangle = 0 \tag{4.89}$$

This constraint will simplify our eigenvalue equations. Since $\underline{T} = \frac{1}{2}\underline{\tau}$, the isospin operator has the second quantized form

$$\underline{T} = \tfrac{1}{2} \sum_{\alpha \tau_1 \tau_2} \langle \underline{\tau} \rangle_{\tau_1 \tau_2} \, a^{+}_{\alpha \tau_1} a_{\alpha \tau_2} \tag{4.90}$$

where $$\underline{\tau} = \tau_x \underline{i} + \tau_y \underline{j} + \tau_z \underline{k} \tag{4.91}$$

and τ_n are represented by the Pauli spin matrices.

$$\tau_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \tau_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \tau_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4.92}$$

The expectation values $\langle \tau_n \rangle_{\tau_1 \tau_2} = \langle \tau_1 | \tau_n | \tau_2 \rangle$ are easily evaluated, the bra and ket being represented by Pauli spinors.

$$|p\rangle \sim \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |n\rangle \sim \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\langle p| \sim (1 \;\; 0) \qquad \langle n| \sim (0 \;\; 1) \tag{4.93}$$

The values of $\langle \tau_n \rangle_{\tau_1 \tau_2}$ are in the tables below.

$\langle \tau_x \rangle_{\tau_1 \tau_2}$

$\tau_1 \backslash \tau_2$	p	n
p	0	1
n	1	0

$\langle \tau_y \rangle_{\tau_1 \tau_2}$

$\tau_1 \backslash \tau_2$	p	n
p	0	$-i$
n	i	0

$\langle \tau_z \rangle_{\tau_1 \tau_2}$

$\tau_1 \backslash \tau_2$	p	n
p	1	0
n	0	-1

(4.94)

The isospin projection conservation requirement is

$$\langle T_z \rangle = \tfrac{1}{2} \sum_{\alpha} \{ \langle a^{+}_{\alpha p} a_{\alpha p} \rangle - \langle a^{+}_{\alpha n} a_{\alpha n} \rangle \} = 0 . \qquad (4.95)$$

It is therefore required that

$$\langle a^{+}_{\alpha p} a_{\alpha p} \rangle = \langle a^{+}_{\alpha n} a_{\alpha n} \rangle . \qquad (4.96)$$

Consequently

$$\mathcal{H}_{pp}(\alpha) = \mathcal{H}_{nn}(\alpha) . \qquad (4.97)$$

The other components of the constraint are

$$\langle T_x \rangle = \tfrac{1}{2} \sum_{\alpha} \{ \langle a^{+}_{\alpha p} a_{\alpha n} \rangle + \langle a^{+}_{\alpha n} a_{\alpha p} \rangle \} = 0 \qquad (4.98)$$

$$\langle T_y \rangle = -\tfrac{i}{2} \sum_{\alpha} \{ \langle a^{+}_{\alpha p} a_{\alpha n} \rangle - \langle a^{+}_{\alpha n} a_{\alpha p} \rangle \} = 0 . \qquad (4.99)$$

Since each bracket must vanish

$$\langle a^{+}_{\alpha p} a_{\alpha n} \rangle = \langle a^{+}_{\alpha n} a_{\alpha p} \rangle = 0 \qquad (4.100)$$

and

$$\mathcal{H}_{pn}(\alpha) = \mathcal{H}_{np}(\alpha) = 0 . \qquad (4.101)$$

Constraints (4.96, 4.100) are satisfied by

$$V_{\alpha} = \begin{bmatrix} v_{\alpha 11} & v_{\alpha 12} \\ v^{*}_{\alpha 12} & -v^{*}_{\alpha 11} \end{bmatrix} . \qquad (4.102)$$

That is $$\mathcal{N}_{\alpha 22} = -\mathcal{N}_{\alpha 11}^{*} \tag{4.103a}$$

$$\mathcal{N}_{\alpha 21} = \mathcal{N}_{\alpha 12}^{*} . \tag{4.103b}$$

Then the matrix V_α has the property

$$V_\alpha V_\alpha^{\dagger} = |\mathrm{Det}\, V_\alpha|\, I = \{ |\mathcal{N}_{\alpha 11}|^2 + |\mathcal{N}_{\alpha 12}|^2 \}\, I \tag{4.104}$$

where $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

Neutron - proton symmetry ensures that

$$|\Delta_{pp}(\alpha)| = |\Delta_{nn}(\alpha)| .$$

It has been demonstrated that $\Delta_{\tau\tau}(\alpha)$ is real. Therefore

$$\Delta_{pp}(\alpha) = \pm\, \Delta_{nn}(\alpha).$$

The relative phase is as yet undetermined. For reasons which will later become apparent, we choose

$$\Delta_{pp}(\alpha) = -\Delta_{nn}(\alpha) . \tag{4.105}$$

The matrix $\Delta(\alpha)$ then has the property

$$\Delta(\alpha)\Delta^{\dagger}(\alpha) = |\mathrm{Det}\, \Delta(\alpha)|\, I = \{ \Delta_{pp}^2(\alpha) + |\Delta_{pn}(\alpha)|^2 \}\, I . \tag{4.106}$$

The eigenvalue equation (4.83)

$$\begin{bmatrix} \hat{\mathcal{H}} & \Delta \\ \Delta & -\hat{\mathcal{H}} \end{bmatrix} \begin{bmatrix} \mathcal{U}_\tau \\ -\mathcal{N}_\tau \end{bmatrix} = E_\tau \begin{bmatrix} \mathcal{U}_\tau \\ -\mathcal{N}_\tau \end{bmatrix}$$

is simplified since

$$\hat{\mathcal{H}} = \begin{bmatrix} \hat{\mathcal{H}}_{pp} & 0 \\ 0 & \hat{\mathcal{H}}_{pp} \end{bmatrix} \qquad \Delta = \begin{bmatrix} \Delta_{pp} & \Delta_{pn} \\ \Delta_{pn}^{*} & -\Delta_{pp} \end{bmatrix} .$$

(The α dependence is implicit.) To determine the eigenvalue E_t multiply (4.83) by $\begin{bmatrix} \hat{\mathcal{H}} & \Delta \\ \Delta & -\hat{\mathcal{H}} \end{bmatrix}$.

$$\begin{bmatrix} \hat{\mathcal{H}}^2 + \Delta^2 & [\hat{\mathcal{H}}, \Delta]_- \\ -[\hat{\mathcal{H}}, \Delta]_- & \hat{\mathcal{H}}^2 + \Delta^2 \end{bmatrix} \begin{bmatrix} \mathcal{U}_\tau \\ -\mathcal{V}_\tau \end{bmatrix} = E_\tau^2 \begin{bmatrix} \mathcal{U}_\tau \\ -\mathcal{V}_\tau \end{bmatrix}$$

$\hat{\mathcal{H}}$ and Δ commute

$$[\hat{\mathcal{H}}, \Delta]_- = 0$$

and the two dimensional matrix $\hat{\mathcal{H}}^2 + \Delta^2$ is diagonal.

$$\hat{\mathcal{H}}^2 + \Delta^2 = \{ \hat{\mathcal{H}}_{pp}^2 + \Delta_{pp}^2 + |\Delta_{pn}|^2 \} I$$

The 4 x 4 matrix is therefore diagonal, so that the eigenvalues are

$$E_1^2(\alpha) = E_2^2(\alpha) = \hat{\mathcal{H}}_{pp}^2(\alpha) + \Delta_{pp}^2(\alpha) + |\Delta_{pn}(\alpha)|^2 . \tag{4.107}$$

The positive square roots correspond to the desired eigenvectors. The two quasiparticles $b_{\alpha 1}^{+}$ and $b_{\alpha 2}^{+}$ are degenerate in energy. Let

$$\hat{\epsilon}(\alpha) = \hat{\mathcal{H}}_{pp}(\alpha) = \hat{\mathcal{H}}_{nn}(\alpha) . \tag{4.108}$$

The second equality assumes

$$\lambda_p = \lambda_n . \tag{4.109}$$

The set of linear equations

$$\begin{bmatrix} (\hat{\epsilon}-E) & 0 & \Delta_{pp} & \Delta_{pn} \\ 0 & (\hat{\epsilon}-E) & \Delta_{pn}^* & -\Delta_{pp} \\ \Delta_{pp} & \Delta_{pn} & -(\hat{\epsilon}+E) & 0 \\ \Delta_{pn}^* & -\Delta_{pp} & 0 & -(\hat{\epsilon}+E) \end{bmatrix} \begin{bmatrix} U_{\tau 1} \\ U_{\tau 2} \\ -V_{\tau 1} \\ -V_{\tau 2} \end{bmatrix} = 0$$

can not be solved by the usual method since all cofactors of the energy matrix vanish. Instead the eigenvectors may be found by inspection.

$$\begin{bmatrix} U_{11} \\ U_{12} \\ -V_{11} \\ -V_{12} \end{bmatrix} = K \begin{bmatrix} \hat{\epsilon}+E \\ 0 \\ \Delta_{pp} \\ \Delta_{pn}^* \end{bmatrix} \qquad \begin{bmatrix} U_{21} \\ U_{22} \\ -V_{21} \\ -V_{22} \end{bmatrix} = K \begin{bmatrix} 0 \\ \hat{\epsilon}+E \\ \Delta_{pn} \\ -\Delta_{pp} \end{bmatrix} \tag{4.110}$$

K is a constant of normalization. The two vectors are orthogonal. Notice that

$$\begin{aligned} U_{11} &= U_{22} && \text{Real} \\ U_{12} &= U_{21} = 0 && \\ V_{11} &= -V_{22} && \text{Real} \\ V_{12} &= V_{21}^* . && \text{Complex} \end{aligned} \tag{4.111}$$

The expressions for the density matrix and the pairing tensor are considerably simplified. Let

$$V_\alpha^2 = V_{\alpha 11}^2 + |V_{\alpha 12}|^2 . \tag{4.112}$$

$$\langle a^+_{\alpha p} a_{\alpha p} \rangle = \langle a^+_{\alpha n} a_{\alpha n} \rangle = V_\alpha^2 \tag{4.113}$$

$$\langle a^{\dagger}_{\alpha p}\, a_{\alpha n}\rangle = \langle a^{\dagger}_{\alpha n}\, a_{\alpha p}\rangle = 0 \tag{4.114}$$

$$\langle a_{\bar{\alpha} p}\, a_{\alpha p}\rangle = -\langle a_{\bar{\alpha} n}\, a_{\alpha n}\rangle = u_{\alpha 11}\, v_{\alpha 11} \tag{4.115}$$

$$\langle a_{\bar{\alpha} p}\, a_{\alpha n}\rangle = \langle a_{\bar{\alpha} n}\, a_{\alpha p}\rangle^{*} = u_{\alpha 11}\, v_{\alpha 12} \tag{4.116}$$

All of our phase conventions are self-consistent. That is, if the set (4.111) is assumed in constructing the potentials, then the eigenvectors of the energy matrix will reproduce (4.111). Therefore no artificial constraints have been imposed. If the trial wave function contains the symmetries in (4.111), then they will propagate through to the final self-consistent wave function.

Had we chosen $\Delta_{pp}(\alpha) = +\Delta_{nn}(\alpha)$, we would find that the isospin degeneracy is lost $(E_1(\alpha) \neq E_2(\alpha))$ and that the density matrix is not diagonal in isospin co-ordinates $(\rho_{pn}(\alpha) \neq 0)$. Since the constraint $\langle \underline{T} \rangle = 0$ requires that $\rho_{pn}(\alpha) = 0$, the choice $\Delta_{pp}(\alpha) = \Delta_{nn}(\alpha)$ is unacceptable.

To recapitulate, the quasiparticle transformation

$$\begin{bmatrix} b^{\dagger}_{\alpha 1} \\ b^{\dagger}_{\alpha 2} \\ b_{\bar{\alpha} 1} \\ b_{\bar{\alpha} 2} \end{bmatrix} = \begin{bmatrix} u_{\alpha 11} & 0 & -v_{\alpha 11} & -v_{\alpha 12} \\ 0 & u_{\alpha 11} & -v^{*}_{\alpha 12} & v_{\alpha 11} \\ v_{\alpha 11} & v_{\alpha 12} & u_{\alpha 11} & 0 \\ v^{*}_{\alpha 12} & -v_{\alpha 11} & 0 & u_{\alpha 11} \end{bmatrix} \begin{bmatrix} a^{\dagger}_{\alpha p} \\ a^{\dagger}_{\alpha n} \\ a_{\bar{\alpha} p} \\ a_{\bar{\alpha} n} \end{bmatrix} \tag{4.117}$$

is obtained from (4.4) with the aid of the unitarity conditions and by choosing

$$U_{\bar{\alpha}} = U^{*}_{\alpha} \qquad V_{\bar{\alpha}} = -V^{*}_{\alpha}$$

$$\langle \underline{T} \rangle = 0 .$$

The following matrices are all self-adjoint in isospin co-ordinates.

$$U_\alpha = \begin{bmatrix} u_{\alpha 11} & 0 \\ 0 & u_{\alpha 11} \end{bmatrix} \qquad V_\alpha = \begin{bmatrix} v_{\alpha 11} & v_{\alpha 12} \\ v_{\alpha 12}^* & -v_{\alpha 11} \end{bmatrix}$$

$$\rho(\alpha) = \begin{bmatrix} \rho_{pp}(\alpha) & 0 \\ 0 & \rho_{pp}(\alpha) \end{bmatrix} \qquad \tau(\alpha) = \begin{bmatrix} \tau_{pp}(\alpha) & \tau_{pn}(\alpha) \\ \tau_{pn}^*(\alpha) & -\tau_{pp}(\alpha) \end{bmatrix}$$

$$\mathcal{H}(\alpha) = \begin{bmatrix} \mathcal{H}_{pp}(\alpha) & 0 \\ 0 & \mathcal{H}_{pp}(\alpha) \end{bmatrix} \qquad \Delta(\alpha) = \begin{bmatrix} \Delta_{pp}(\alpha) & \Delta_{pn}(\alpha) \\ \Delta_{pn}^*(\alpha) & -\Delta_{pp}(\alpha) \end{bmatrix} \tag{4.118}$$

The normalized wave function is

$$u_{\alpha 11}^2 = \tfrac{1}{2}\left(1 + \hat{\epsilon}(\alpha)/E(\alpha)\right)$$

$$u_{\alpha 12}^2 = 0$$

$$v_{\alpha 11}^2 = \tfrac{1}{2}\left(1 - \hat{\epsilon}(\alpha)/E(\alpha)\right)\left(\Delta_{pp}(\alpha)/\Delta(\alpha)\right)^2$$

$$(\mathrm{Re}\, v_{\alpha 12})^2 = \tfrac{1}{2}\left(1 - \hat{\epsilon}(\alpha)/E(\alpha)\right)\left(\Delta_{np}^{T=1}(\alpha)/\Delta(\alpha)\right)^2$$

$$(\mathrm{Im}\, v_{\alpha 12})^2 = \tfrac{1}{2}\left(1 - \hat{\epsilon}(\alpha)/E(\alpha)\right)\left(\Delta_{np}^{T=0}(\alpha)/\Delta(\alpha)\right)^2$$

$$v_\alpha^2 = \tfrac{1}{2}\left(1 - \hat{\epsilon}(\alpha)/E(\alpha)\right) \tag{4.119}$$

with corresponding expressions for the second eigenvector. The quasiparticle energy is

$$E(\alpha) = \sqrt{\hat{\epsilon}^2(\alpha) + \Delta^2(\alpha)} \quad . \tag{4.120}$$

For (4.119, 4.120) $\Delta^2(\alpha)$ is regarded as a one, rather than two, dimensional matrix.

$$\Delta^2(\alpha) = \Delta_{pp}^2(\alpha) + \{\Delta_{np}^{T=1}(\alpha)\}^2 + \{\Delta_{np}^{T=0}(\alpha)\}^2 \tag{4.121}$$

The final expressions for the potentials are

$$\epsilon(\alpha) = \langle\alpha|T|\alpha\rangle + \sum_{\beta>0}{}' \{\langle\alpha p, \beta p|v|\alpha p, \beta p\rangle_A + \langle\alpha p, \beta n|v|\alpha p, \beta n\rangle_A\} v_\beta^2 \tag{4.122}$$

$$\Delta_{pp}(\alpha) = -\Delta_{nn}(\alpha) = \sum_{\beta>0}{}' \langle\alpha\bar{\alpha}\, T=1|v|\beta\bar{\beta}\, T=1\rangle_A\, u_{\beta 11} v_{\beta 11} \tag{4.123}$$

$$\Delta_{np}^{T=1}(\alpha) = \Delta_{pn}^{T=1}(\alpha) = \sum_{\beta>0}{}' \langle\alpha\bar{\alpha}\, T=1|v|\beta\bar{\beta}\, T=1\rangle_A\, u_{\beta 11}\, \mathrm{Re}\, v_{\beta 12}$$

$$\Delta_{np}^{T=0}(\alpha) = -\Delta_{pn}^{T=0}(\alpha) = \sum_{\beta>0}{}' \langle\alpha\bar{\alpha}\, T=0|v|\beta\bar{\beta}\, T=0\rangle_A\, u_{\beta 11}\, \mathrm{Im}\, v_{\beta 12}$$

where

$$\Delta_{np}(\alpha) = \Delta_{np}^{T=1}(\alpha) + i\,\Delta_{np}^{T=0}(\alpha) \tag{4.124}$$

and

$$\Delta_{pn}(\alpha) = \Delta_{np}^{*}(\alpha). \tag{4.125}$$

The number conservation constraint is

$$Z = A - Z = 2\sum_{\alpha>0}{}' v_\alpha^2 . \tag{4.126}$$

There are three sets of gap equations. The different modes of pairing have been separated, so that the physical interpretation of the wave function is enhanced. The potentials are self-consistently determined. An initial guess is made for the pairing parameters. The potentials may then be

calculated, and a new set of pair parameters (consistent with number conservation) is computed. The procedure is continued until convergence is achieved. The existence or absence of a particular pairing mode represents a self-consistent symmetry. If the occupation probabilities corresponding to one mode $\{\mathcal{N}_{\alpha 11}^2, (Re\,\mathcal{N}_{\alpha 12})^2, (Im\,\mathcal{N}_{\alpha 12})^2\}$ are non-zero (zero), then the pair potentials corresponding to that mode $\{\Delta_{pp}(\alpha), \Delta_{np}^{T=1}(\alpha), \Delta_{np}^{T=0}(\alpha)\}$ are non-zero (zero), and vice-versa. If the trial wave function excludes a particular mode of pairing, then so will the final self-consistent wave function.

The pairing parameters may be eliminated from the gap equations. From(4.110), we find

$$
\begin{aligned}
U_{\alpha 11}\mathcal{N}_{\alpha 11} &= -\Delta_{pp}(\alpha)/2E(\alpha) \\
U_{\alpha 11}\,Re\,\mathcal{N}_{\alpha 12} &= -\Delta_{np}^{T=1}(\alpha)/2E(\alpha) \\
U_{\alpha 11}\,Im\,\mathcal{N}_{\alpha 12} &= -\Delta_{np}^{T=0}(\alpha)/2E(\alpha).
\end{aligned}
\tag{4.127}
$$

Substitute these expressions into (4.123).

$$
\begin{aligned}
\Delta_{pp}(\alpha) &= -\tfrac{1}{2}\sum_{\beta>0}{}' \langle\alpha\bar{\alpha}\,T=1|\mathcal{N}|\beta\bar{\beta}\,T=1\rangle_A\,\Delta_{pp}(\beta)/E(\beta) \\
\Delta_{np}^{T=1}(\alpha) &= -\tfrac{1}{2}\sum_{\beta>0}{}' \langle\alpha\bar{\alpha}\,T=1|\mathcal{N}|\beta\bar{\beta}\,T=1\rangle_A\,\Delta_{np}^{T=1}(\beta)/E(\beta) \\
\Delta_{np}^{T=0}(\alpha) &= -\tfrac{1}{2}\sum_{\beta>0}{}' \langle\alpha\bar{\alpha}\,T=0|\mathcal{N}|\beta\bar{\beta}\,T=0\rangle_A\,\Delta_{np}^{T=0}(\beta)/E(\beta)
\end{aligned}
\tag{4.128}
$$

The pp and np (T = 1) gap equations are formally identical. Consequently if the trial wave-function is such that $\Delta_{pp}(\alpha)/\Delta_{np}^{T=1}(\alpha) = r$, then the final wave-function will

have the same property. Choosing Δ_{pp} and $\Delta_{np}^{T=1}$ in any ratio such that $(\Delta^{T=1})^2 = (\Delta_{pp})^2 + (\Delta_{np}^{T=1})^2$ is constant leaves the quasiparticle energies, the density matrix, the HF single particle energies, and the binding energy invariant. For N = Z nuclei, therefore, generalized T = 1 pairing is not really a generalization.

Other works have approximated the pairing matrix elements by a constant.

$$\overline{\langle \alpha\bar{\alpha}\, T=1 | v | \beta\bar{\beta}\, T=1 \rangle_A} = -G_1$$

$$\overline{\langle \alpha\bar{\alpha}\, T=0 | v | \beta\bar{\beta}\, T=0 \rangle_A} = -G_0$$

The gap equations are then considerably simplified.

$$\Delta_{pp}(\alpha) = G_1 \sum_{\beta>0} \Delta_{pp}(\beta)/2E(\beta)$$

$$\Delta_{np}^{T=1}(\alpha) = G_1 \sum_{\beta>0} \Delta_{np}^{T=1}(\beta)/2E(\beta)$$

$$\Delta_{np}^{T=0}(\alpha) = G_0 \sum_{\beta>0} \Delta_{np}^{T=0}(\beta)/2E(\beta)$$

If $G_0 \neq G_1$, it is energetically favorable to disperse the particles entirely into the pairing mode with the larger G. The pair potential for the mode with the smaller G is identically zero. If $G_0 = G_1$, the pair potentials may be chosen in arbitrary ratios without affecting E, ρ, ϵ, or E_0.

The expressions for the ground state energy (4.68, 4.69) may be simplified. Since $\Gamma_{pp}(\alpha) = \Gamma_{nn}(\alpha)$ and $\langle a^+_{\alpha p} a_{\alpha p} \rangle = \langle a^+_{\alpha n} a_{\alpha n} \rangle$

$$\sum_{\tau} \Gamma_{\alpha\tau,\alpha\tau} \langle a^{+}_{\alpha\tau} a_{\alpha\tau} \rangle = 2\Gamma_{pp}(\alpha) \langle a^{+}_{\alpha p} a_{\alpha p} \rangle .$$

Similarly $\Delta_{pp}(\alpha) = -\Delta_{nn}(\alpha)$ and $\langle a^{+}_{\alpha p} a^{+}_{\bar{\alpha} p} \rangle = -\langle a^{+}_{\alpha n} a^{+}_{\bar{\alpha} n} \rangle$ so that

$$\sum_{\tau} \Delta_{\alpha\tau,\bar{\alpha}\tau} \langle a^{+}_{\alpha\tau} a^{+}_{\bar{\alpha}\tau} \rangle = 2\Delta_{pp}(\alpha) \langle a^{+}_{\alpha p} a^{+}_{\bar{\alpha} p} \rangle .$$

Finally $\Delta_{pn}(\alpha) = \Delta^{*}_{np}(\alpha)$ and $\langle a^{+}_{\alpha p} a^{+}_{\bar{\alpha} n} \rangle = \langle a^{+}_{\alpha n} a^{+}_{\bar{\alpha} p} \rangle^{*}$ and

$$\sum_{\tau} \Delta_{\alpha\tau,\bar{\alpha}-\tau} \langle a^{+}_{\alpha\tau} a^{+}_{\bar{\alpha}-\tau} \rangle = 2\,\mathrm{Re}\{\Delta_{np}(\alpha) \langle a^{+}_{\alpha n} a^{+}_{\bar{\alpha} p} \rangle\} =$$

$$2\{\Delta^{T=1}_{np}(\alpha)\,\mathrm{Re}\langle a^{+}_{\alpha n} a^{+}_{\bar{\alpha} p} \rangle - \Delta^{T=0}_{np}(\alpha)\,\mathrm{Im}\langle a^{+}_{\alpha n} a^{+}_{\bar{\alpha} p} \rangle\} .$$

Collecting terms we have

$$H_0' = E_0 - \lambda A = 2\Big\{\sum_{\alpha>0} \big(T_{pp}(\alpha) - \lambda + \tfrac{1}{2}\Gamma_{pp}(\alpha)\big) v_\alpha^2 + \tag{4.129}$$

$$\sum_{\alpha>0} \big(\Delta_{pp}(\alpha) u_{\alpha 11} v_{\alpha 11} + \Delta^{T=1}_{np}(\alpha) u_{\alpha 11}\,\mathrm{Re}\, v_{\alpha 12} + \Delta^{T=0}_{np}(\alpha) u_{\alpha 11}\,\mathrm{Im}\, v_{\alpha 12}\big)\Big\}$$

or

$$H_0' = E_0 - \lambda A = 2\Big\{\sum_{\alpha>0} \langle \alpha | T - \lambda | \alpha \rangle v_\alpha^2 +$$

$$\sum_{\alpha\beta>0} \big(\langle \alpha p, \beta p | v | \alpha p, \beta p \rangle_A + \langle \alpha p, \beta n | v | \alpha p, \beta n \rangle_A\big) v_\alpha^2 v_\beta^2 +$$

$$\sum_{\alpha\beta>0} \langle \alpha\bar{\alpha}\, T=1 | v | \beta\bar{\beta}\, T=1 \rangle_A\, u_{\alpha 11} v_{\alpha 11} u_{\beta 11} v_{\beta 11} +$$

$$\sum_{\alpha\beta>0} \langle \alpha\bar{\alpha}\, T=1 | v | \beta\bar{\beta}\, T=1 \rangle_A\, u_{\alpha 11}\,\mathrm{Re}\, v_{\alpha 12}\, u_{\beta 11}\,\mathrm{Re}\, v_{\beta 12} + \tag{4.130}$$

$$\sum_{\alpha\beta>0} \langle \alpha\bar{\alpha}\, T=0 | v | \beta\bar{\beta}\, T=0 \rangle_A\, u_{\alpha 11}\,\mathrm{Im}\, v_{\alpha 12}\, u_{\beta 11}\,\mathrm{Im}\, v_{\beta 12}\Big\}$$

where

$$\lambda = \lambda_p = \lambda_n . \tag{4.131}$$

The energy corresponding to the various modes of pairing is readily identifiable.

6. Canonical Representation

The representation for which

$$\rho_{\alpha\beta} = \rho_{\alpha\alpha}\,\delta_{\alpha\beta} \tag{4.132a}$$

and

$$\tau_{\alpha\beta} = \tau_{\alpha\bar{\alpha}}\,\delta_{\bar{\alpha}\beta} \tag{4.132b}$$

is termed the canonical representation. Our generalized pairing formalism results in a diagonal density matrix, but the pairing tensor is a two dimensional matrix in isospin co-ordinates.

$\rho_{\alpha_1\tau_1,\alpha_2\tau_2}$

$\alpha_1\tau_1 \backslash \alpha_2\tau_2$	αp	αn	$\bar{\alpha} p$	$\bar{\alpha} n$
αp	$\rho_{pp}(\alpha)$	0	0	0
αn	0	$\rho_{pp}(\alpha)$	0	0
$\bar{\alpha} p$	0	0	$\rho_{pp}(\alpha)$	0
$\bar{\alpha} n$	0	0	0	$\rho_{pp}(\alpha)$

$\tau_{\alpha_1\tau_1,\alpha_2\tau_2}$

$\alpha_1\tau_1 \backslash \alpha_2\tau_2$	αp	αn	$\bar{\alpha} p$	$\bar{\alpha} n$
αp	0	0	$\tau_{pp}(\alpha)$	$\tau_{pn}(\alpha)$
αn	0	0	$\tau_{pn}^*(\alpha)$	$-\tau_{pp}(\alpha)$
$\bar{\alpha} p$	$-\tau_{pp}(\alpha)$	$-\tau_{pn}^*(\alpha)$	0	0
$\bar{\alpha} n$	$-\tau_{pn}(\alpha)$	$\tau_{pp}(\alpha)$	0	0

where

$$\rho_{pp}(\alpha) = N_{\alpha 11}^2 + |N_{\alpha 12}|^2 \qquad \tau_{pp}(\alpha) = U_{\alpha 11} N_{\alpha 11}$$

$$\tau_{pn}(\alpha) = U_{\alpha 11} N_{\alpha 12}^*$$

The canonical representation is obtained by finding a basis in which the matrix

$$\tau(\alpha) = \begin{bmatrix} \tau_{pp}(\alpha) & \tau_{pn}(\alpha) \\ \tau_{pn}^*(\alpha) & -\tau_{pp}(\alpha) \end{bmatrix}$$

is diagonal. The eigenvalue equation is

$$\tau(\alpha)\,\underline{C}(\alpha) = \tau_c(\alpha)\,\underline{C}(\alpha) \tag{4.133a}$$

or $$\begin{bmatrix} t_{pp}(\alpha) & t_{pn}(\alpha) \\ t_{pn}^{*}(\alpha) & -t_{pp}(\alpha) \end{bmatrix} \begin{bmatrix} C_{\alpha 1} \\ C_{\alpha 2} \end{bmatrix} = t_c(\alpha) \begin{bmatrix} C_{\alpha 1} \\ C_{\alpha 2} \end{bmatrix}. \tag{4.133b}$$

The eigenvalues are given by

$$\begin{vmatrix} (t_{pp}(\alpha) - t_c(\alpha)) & t_{pn}(\alpha) \\ t_{pn}^{*}(\alpha) & -(t_{pp}(\alpha) + t_c(\alpha)) \end{vmatrix} = 0 \tag{4.134}$$

so that $$t_c^2(\alpha) = t_{pp}^2(\alpha) + |t_{pn}(\alpha)|^2 . \tag{4.135}$$

Define $$\begin{aligned} u_\alpha &= u_{\alpha 11} \\ v_\alpha &= [v_{\alpha 11}^2 + |v_{\alpha 12}|^2]^{1/2} \end{aligned} \tag{4.136}$$

then $$t_c^2(\alpha) = (u_\alpha v_\alpha)^2 . \tag{4.137}$$

The eigenvectors are

$$\begin{bmatrix} a_{\alpha 1}^{\dagger} \\ a_{\alpha 2}^{\dagger} \end{bmatrix} = \begin{bmatrix} C_{\alpha 1} & C_{\alpha 2} \\ C_{\alpha 2}^{*} & -C_{\alpha 1} \end{bmatrix} \begin{bmatrix} a_{\alpha p}^{\dagger} \\ a_{\alpha n}^{\dagger} \end{bmatrix} \tag{4.138}$$

where $$\begin{bmatrix} C_{\alpha 1} \\ C_{\alpha 2} \end{bmatrix} = K \begin{bmatrix} t_{pp}(\alpha) + t_c(\alpha) \\ t_{pn}^{*}(\alpha) \end{bmatrix}. \tag{4.139}$$

The normalized vector is

$$\begin{aligned} C_{\alpha 1} &= [\tfrac{1}{2}(1 + v_{\alpha 11}/v_\alpha)]^{1/2} \\ C_{\alpha 2} &= [\tfrac{1}{2}(1 - v_{\alpha 11}/v_\alpha)]^{1/2} e^{-i\theta} \end{aligned} \tag{4.140}$$

where $\theta = \mathrm{Tan}^{-1}$ (Im $v_{\alpha 12}$ / Re $v_{\alpha 12}$).

Let $$t_c(\alpha) = u_\alpha v_\alpha \tag{4.141}$$

then $|\alpha 1\rangle$ and $|\alpha 2\rangle$ correspond respectively to the eigenvalues $+t_c(\alpha)$ and $-t_c(\alpha)$. The eigenvalue

equation for the time reversed space is

$$\mathcal{T}(\bar{\alpha})\,\underline{C}(\bar{\alpha}) = \mathcal{T}_c(\bar{\alpha})\,\underline{C}(\bar{\alpha}) \,. \tag{4.142}$$

Since $t(\bar{\alpha}) = -t^*(\alpha)$, the solution is

$$\underline{C}(\bar{\alpha}) = \underline{C}^*(\alpha) \tag{4.143}$$

$$\mathcal{T}_c(\bar{\alpha}) = -\mathcal{T}_c(\alpha) \tag{4.144}$$

or

$$\begin{bmatrix} a^{\dagger}_{\bar{\alpha}1} \\ a^{\dagger}_{\bar{\alpha}2} \end{bmatrix} = \begin{bmatrix} C_{\alpha 1} & C^*_{\alpha 2} \\ C_{\alpha 2} & -C_{\alpha 1} \end{bmatrix} \begin{bmatrix} a^{\dagger}_{\bar{\alpha}p} \\ a^{\dagger}_{\bar{\alpha}n} \end{bmatrix} \tag{4.145}$$

where $|\bar{\alpha}1\rangle$ and $|\bar{\alpha}2\rangle$ correspond respectively to the eigenvalues $-t_c(\alpha)$ and $+t_c(\alpha)$. In this new single particle basis $t(\alpha)$ is real and has the form

$$\mathcal{T}(\alpha) = \begin{bmatrix} \mathcal{T}_c(\alpha) & 0 \\ 0 & -\mathcal{T}_c(\alpha) \end{bmatrix} \tag{4.146}$$

$$\mathcal{T}(\bar{\alpha}) = -\mathcal{T}(\alpha) \,. \tag{4.147}$$

Since $t_{ij}(\alpha) = t_{\alpha i,\, \bar{\alpha} j}$ (see 4.28) the components of the rotated matrix $t(\alpha)$ have the meaning

$$\mathcal{T}_c(\alpha) = \begin{cases} \mathcal{T}_{11}(\alpha) = \mathcal{T}_{\alpha 1, \bar{\alpha} 1} \,. \\ -\mathcal{T}_{22}(\alpha) = -\mathcal{T}_{\alpha 2, \bar{\alpha} 2} \end{cases}$$

Also $t_{ij}(\bar{\alpha}) = t_{\bar{\alpha} i,\, \alpha j}$ (see 4.32 ff) so that

$$\mathcal{T}_c(\alpha) = \begin{cases} -\mathcal{T}_{11}(\bar{\alpha}) = -\mathcal{T}_{\bar{\alpha}1, \alpha 1} \,. \\ \mathcal{T}_{22}(\bar{\alpha}) = \mathcal{T}_{\bar{\alpha}2, \alpha 2} \end{cases}$$

Consequently the pairing tensor has the canonical form.

$$\mathcal{T}_{\alpha_1 c_1, \alpha_2 c_2}$$

$\alpha_1 c_1 \backslash \alpha_2 c_2$	$\alpha 1$	$\bar{\alpha} 1$	$\alpha 2$	$\bar{\alpha} 2$
$\alpha 1$	0	$\mathcal{T}_c(\alpha)$	0	0
$\bar{\alpha} 1$	$-\mathcal{T}_c(\alpha)$	0	0	0
$\alpha 2$	0	0	0	$-\mathcal{T}_c(\alpha)$
$\bar{\alpha} 2$	0	0	$\mathcal{T}_c(\alpha)$	0

(4.148)

Since $\rho(\alpha)$ is diagonal and doubly degenerate the density matrix remains diagonal in the rotated basis with the same representation.

$$\rho(\alpha) = \begin{bmatrix} \mathcal{N}_\alpha^2 & 0 \\ 0 & \mathcal{N}_\alpha^2 \end{bmatrix}. \tag{4.149}$$

Therefore the new basis does indeed furnish the canonical representation. Consider the various limiting cases.

a) $|T_z| = 1$ pairing $(\mathcal{N}_{\alpha 12} = 0)$ (4.150)

$C_{\alpha 1} = 1$

$C_{\alpha 2} = 0$

b) $|T_z| = 0$ pairing $(\mathcal{N}_{\alpha 11} = 0)$ (4.151)

$C_{\alpha 1} = \sqrt{1/2}$

$C_{\alpha 2} = \sqrt{1/2}\, e^{-i\theta}$

c) $T = 1$ pairing $(\mathcal{N}_{\alpha 11} = \mathcal{N}_{\alpha 12} = \text{Real})$ (4.152)

$C_{\alpha 1} = \left[\frac{1}{2}\left(1 + \sqrt{1/2}\right)\right]^{1/2}$

$C_{\alpha 2} = \left[\frac{1}{2}\left(1 - \sqrt{1/2}\right)\right]^{1/2}$

d) $T = 0$ pairing $(\mathcal{N}_{\alpha 11} = \text{Re}\, \mathcal{N}_{\alpha 12} = 0)$ (4.153)

$C_{\alpha 1} = \sqrt{1/2}$

$C_{\alpha 2} = -\sqrt{1/2}\, i$

The density matrix and pairing tensor may be reproduced by a new set of quasiparticle operators.

$$
\begin{aligned}
b^{+}_{\alpha 1} &= u_\alpha a^{+}_{\alpha 1} - v_\alpha a_{\bar{\alpha} 1} \\
b^{+}_{\alpha 2} &= u_\alpha a^{+}_{\alpha 2} + v_\alpha a_{\bar{\alpha} 2} \\
b^{+}_{\bar{\alpha} 1} &= u_\alpha a^{+}_{\bar{\alpha} 1} + v_\alpha a_{\alpha 1} \\
b^{+}_{\bar{\alpha} 2} &= u_\alpha a^{+}_{\bar{\alpha} 2} - v_\alpha a_{\alpha 2}
\end{aligned}
\tag{4.154}
$$

Therefore in the canonical representation the ground state wave function

$$
|\Phi_0\rangle = \prod_{\alpha>0} b_{\alpha 2}\, b_{\bar{\alpha} 2}\, b_{\alpha 1}\, b_{\bar{\alpha} 1}\, |0\rangle \tag{4.155}
$$

assumes the familiar BCS form.

$$
|\Phi_0\rangle = \prod_{\alpha>0} (u_\alpha - v_\alpha a^{+}_{\alpha 2} a^{+}_{\bar{\alpha} 2})(u_\alpha + v_\alpha a^{+}_{\alpha 1} a^{+}_{\bar{\alpha} 1})|0\rangle \tag{4.156}
$$

Even if T = 0 and T = 1 pairing co-exist, so that the original pair parameters are complex numbers, the ground state wave function may be expressed in terms of a special quasiparticle transformation with real pairing parameters. The single particle basis, however, may contain complex coefficients.

With the aid of (4.138, 4.145), $|\Phi_0\rangle$ may be expressed in terms of proton and neutron states. Noting that

$$
\begin{aligned}
C_{\alpha 1}^2 - C_{\alpha 2}^2 &= v_{\alpha 11} / v_\alpha \\
2 C_{\alpha 1} C_{\alpha 2} &= v_{\alpha 12} / v_\alpha
\end{aligned}
$$

and using $a^{+}_{k} a^{+}_{k} |0\rangle = 0$, we find

$$|\Phi_0\rangle = \prod_{\alpha>0} \{ u_{\alpha 11} (u_{\alpha 11} + v_{\alpha 11} a^{+}_{\alpha p} a^{+}_{\bar{\alpha} p} - v_{\alpha 11} a^{+}_{\alpha n} a^{+}_{\bar{\alpha} n} + v^{*}_{\alpha 12} a^{+}_{\alpha p} a^{+}_{\bar{\alpha} n} + v_{\alpha 12} a^{+}_{\alpha n} a^{+}_{\bar{\alpha} p}) + (v^{2}_{\alpha 11} + |v_{\alpha 12}|^{2}) a^{+}_{\alpha p} a^{+}_{\alpha n} a^{+}_{\bar{\alpha} p} a^{+}_{\bar{\alpha} n} \} |0\rangle . \quad (4.157)$$

($|\Phi_0\rangle$ is normalized.) Note that the wave function contains all pairs of particles for which we wish to permit correlations. In addition there is an α - particle term. This should not, however, be regarded as a genuine 4 particle correlation. The coefficient of this term is not an independent parameter. Even if there is no neutron - proton pairing ($v_{\alpha 12} = 0$) the α - particle term remains. That is, the conventional $|T_z| = 1$ pairing theory contains the same component in its wave function. Finally our conclusion that our wave function may be expressed in the usual BCS form demonstrates that the " 4 particle correlations" are fictitious.[8]

In conclusion we recall that elements of $\mathcal{H}$ and Δ connecting different spatial orbitals have been neglected (4.74, 4.75). This is the same approximation encountered in the familiar BCS theory (3.51, 3.52). The discussion following (3.52) applies here as well. Since we have expressed the generalized wave function in the BCS form, section 3.6 concerning the Hartree - Bogoliubov equations is directly applicable. Therein the reader will find a formalism for which approximations (4.74, 4.75) are not

required, as well as some reflections concerning the choice of the "best" single particle basis.

7. Generalized Pairing in the 2s-1d Shell

The generalized pairing equations were solved for the N = Z even-even nuclei in the 2s-1d shell. For experimental data on these nuclei the reader is referred to II.7. All HF solutions reported in Table 2.15 were tried as single particle bases. The solutions to the pairing equations are listed in Table 4.1. The energy gap for elementary excitations, $E(\alpha) + E(\beta)$, is calculated with α and β being the two levels adjacent to the Fermi energy. If there is no re-ordering of levels, in the limit of weak pairing $E(\alpha) + E(\beta)$ then equals the HF gap. The moments of inertia and multipole moments are given by (3.119, 3.120).

Ne^{20}

For all forces the lowest prolate state has a large HF gap, thereby excluding pairing correlations.

The asymmetric state permits pairing (T = 0) only for the Yale force.

The other higher lying states do not have physical relevance, although some numerical oddities may be of interest. Since the single particle energies $\epsilon(\alpha)$ are dispersion dependent, an inversion of the HF level ordering may occur (oblate, Rosenfeld 2, see Table 4.1). Since the pair potential is different for each orbital,

it may happen that the smallest quasiparticle energy does not correspond to either of the orbitals adjacent to the Fermi energy (asymmetric, Yale, see Table 4.1).

The result for Ne^{20}, therefore, is that the physically relevant HF wave function is stable against both T = 0 and T = 1 pairing admixtures.

Mg^{24}

The asymmetric HF state does not admit pairing correlations for any force.

The prolate HF state with $\Omega = \frac{1}{2}$, 3/2 occupied orbitals favors T = 0 pairing for all forces. The solutions to the pairing equations are in Tables 4.2- 4.6. The HF wave functions displayed small HF gaps, whereas the corresponding two quasiparticle energies are substantially larger (Rosenfeld 1, 3.06 and 5.42 Mev; Rosenfeld 2, 1.48 and 5.73 Mev; Yale, 0.46 and 4.99 Mev; NDKB 1, 1.64 and 5.15 Mev; NDKB 2, 2.11 and 5.08 Mev). Although the deformation parameters are not significantly altered, the inertial parameter is considerably larger (0.05 to 0.26 Mev for Yale) and is force independent (0.25 to 0.29 Mev). Since the cranking formula is expected to overestimate $\hbar^2/2\mathcal{J}$, we are in reasonable agreement with experiment. The binding energy of the prolate state is now comparable to that of the asymmetric state (-132.333 vs. -133.144 Mev for Yale). The energy difference between these two states

is negligible compared to neglected corrections to the binding energy. T = 0 pairing correlations have therefore eliminated all of the deficiencies of this prolate HF wave function. The results of this calculation have been reported [6], the one difference being that the published calculation did not use occupation dependent single particle energies.

All oblate states contain T = 0 pairing. However, these are not physically relevant since Mg^{24} is prolate in the intrinsic frame. Most remarkable, nevertheless, are the two oblate solutions for the Yale force. The pairing energies are -11.012 and -13.866 Mev. The inertial parameters are considerably increased (0.01 to 0.47 Mev and 0.10 to 0.58 Mev). So is the energy for elementary excitations (0.10 to 5.54 Mev and 0.92 to 6.05 Mev). Although HF predicts these oblate states to be 3.3 and 4.7 Mev above the prolate state, the paired oblate states are only 1.4 and 1.5 Mev above the paired prolate state.

Si^{28}

The lowest oblate state is stable against pairing admixtures for all forces. Since the intrinsic state is oblate, and the lowest HF oblate state fails to explain the energy spectrum, we may reconsider the higher lying oblate states. Most of them show reasonable energy gaps induced by T = 0 pairing.

The low lying prolate state displays pairing ($T = 0$) only for the NDKB 1 force.

The spherical states contain both $T = 0$ and $T = 1$ correlations. The small deformations arise because pairs of nucleons can not be in a $T = 0$, $J = 0$ state. The $T = 0$ pairing force has the effect that $v^2_{jm} \neq v^2_{jm'}$, $\epsilon_{jm} \neq \epsilon_{jm'}$ ($m \neq m'$). Therefore a fully self-consistent calculation in which pairing and HF degrees of freedom are allowed to vary simultaneously can not result in a $T = 0$ paired spherical state. It may be of interest, nevertheless, to present one of these combined $T = 0$ and $T = 1$ pairing solutions (Table 4.7). Note that for some orbitals $T = 0$ pairing is more dominant than $T = 1$ pairing, while for other orbitals the reverse is true. Yet both modes contribute in all orbitals. Also notice that $v_{\alpha 11} = \mathrm{Re}\, v_{\alpha 12}$ and $\Delta_{pp}(\alpha) = \Delta^{T=1}_{np}(\alpha)$.

S^{32}

The asymmetric state does not admit pairing correlations.

The two oblate states with $Q_{40} < 0$ (Rosenfeld) contain $T = 0$ pairing admixtures.

The oblate state with $Q_{40} > 0$ shows strong $T = 0$ pairing with the NDKB force. In the HF approximation, this state is well above the prolate state (6.0 Mev, NDKB 1; 7.2 Mev, NDKB 2), whereas the paired wave functions lie nearer to one another (2.6 Mev, NDKB 1; 4.2 Mev,

NDKB 2). For the Rosenfeld force, however, this oblate state does not admit pairing.

The prolate state is stabilized by T = 0 pairing for all forces.

If the HF asymmetric wave function can not explain the S^{32} spectrum, then several oblate and prolate states, stabilized by T = 0 pairing, may now be considered as candidates.

Ar^{36}

Neither the oblate nor the asymmetric state contains pairing correlations. Since these states have a small inertial parameter they do not correspond to the physically relevant intrinsic state.

T = 0 pairing correlations alter the properties of the prolate state. For all forces the inertial parameter is considerably increased (0.20 to 0.85 Mev, Rosenfeld 1; 0.22 to 0.69 Mev, Rosenfeld 2; 0.14 to 0.49 Mev, Yale; 0.06 to 0.77 Mev, NDKB 1; 0.11 to 0.56 Mev, NDKB 2). Since $\hbar^2/2\mathcal{J}$ is so large, the excitation energy of the rotational states might be greater than that of the vibrational states. The prolate state with T = 0 pair correlations may therefore explain the vibrational character of the Ar^{36} spectrum.

The binding energy of the spherical state is substantially increased by T = 0 pairing, so that the prolate and spherical states have nearly the same energy.

Even if T = 0 correlations are rejected for a spherical state, recall that $|T_z| = 1$ correlations lower the spherical state by 5 Mev for the Rosenfeld 2 and Yale forces (see Table 3.10). For the NDKB force the spherical and prolate HF states are only an Mev or less apart. The conclusion remains that the spherical and prolate states are nearly degenerate. Perhaps they are admixed in the physically relevant intrinsic wave function.

We conclude that T = 0 pairing correlations are significant in the 2s - 1d shell. In particular, axial symmetry is restored to Mg^{24} and S^{32}, and an explanation is provided for the vibrational nature of Ar^{36}.

Table 4.1: Generalized Pairing in 2s - 1d Shell (BCS)

Nucleus	Force	Shape	Mode	E_{PAIR}	E_{TOTAL}	Q_{20}	Q_{40}	A_x	$E_\alpha + E_\beta$	
Ne^{20}	Rosenfeld 1	Oblate	T = 0	-5.032	-40.857	-4.7	14.0	0.95	4.34	
		Prolate 2	T = 0	-5.500	-41.297	3.1	-47.5	0.37	4.91	
	Rosenfeld 2	Oblate	T = 0	-6.737	-30.898	-5.3	19.4	0.75	3.84	a
		Prolate 2								b
	Yale	Asymmetric	T = 0	-4.963	-97.210	3.7 (4.5)	-45.0 (43.4) (6.0)	0.52 (0.24) (0.52)	4.61	c
		Spherical	T = 1	-6.490	-95.518	0	0	∞	3.45	d

For the asymmetric wave function (Q_{22}), (Q_{42}, Q_{44}) and (A_y, A_z) are given in parentheses under Q_{20}, Q_{40}, and A_x.

Table 4.1 (continued)

Nucleus	Force	Shape	Mode	E_{PAIR}	E_{TOTAL}	Q_{20}	Q_{40}	A_x	$E_\alpha + E_\beta$	
Mg^{24}	Rosenfeld 1	Prolate 1	T = 0	-3.985	-95.027	15.1	-0.9	0.25	5.42	
		Oblate 1	T = 0	-5.545	-93.480	-12.5	51.9	0.30	5.59	
		Oblate 2	T = 0	-3.511	-92.037	-1.8	104.1	0.17	4.20	
		Oblate 3	T = 0	-5.513	-91.696	-9.2	28.2	0.46	4.57	
	Rosenfeld 2	Oblate 1	T = 0	-5.083	-76.855	-12.9	38.4	0.38	5.39	
		Prolate 2	T = 0	-6.024	-77.392	15.7	-9.4	0.29	5.73	
		Oblate 2	T = 0	-7.478	-74.168	-11.6	52.9	0.30	6.07	e
	Yale	Prolate	T = 0	-6.308	-132.333	19.1	-6.4	0.26	4.99	f
		Oblate 1	T = 0	-11.012	-130.904	-14.5	43.7	0.47	5.54	g
		Oblate 2	T = 0	-13.866	-130.791	-13.0	40.2	0.58	6.05	h
	NDKB 1	Prolate	T = 0	-6.226	-110.133	16.1	10.0	0.27	5.15	
		Oblate	T = 0	-6.404	-107.585	-11.8	30.4	0.39	4.25	
	NDKB 2	Prolate	T = 0	-4.763	-115.883	22.9	1.1	0.26	5.08	
		Oblate	T = 0	-7.485	-111.540	-16.7	38.0	0.41	4.74	

Table 4.1 (continued)

Nucleus	Force	Shape	Mode	E_{PAIR}	E_{TOTAL}	Q_{20}	Q_{40}	A_x	$E_\alpha + E_\beta$
Si^{28}	Rosenfeld 1	Oblate 2	T = 0	-1.904	-150.019	-0.5	-94.3	0.26	6.08
		Oblate 3	T = 0	-3.661	-147.091	0.2	105.5	0.17	4.05
	Rosenfeld 2	Oblate 2	T = 0	-4.870	-122.752	0.2	114.0	0.18	4.85
		Oblate 3							
		Spherical	T=0+T=1	-5.011	-114.900	0.1	0.5	31	4.99
	NDKB 1	Prolate	T = 0	-5.431	-139.625	17.0	-58.4	0.26	3.38
		Oblate 2	T = 0	-11.426	-138.327	- 0.03	-87.4	0.35	6.14
		Spherical	T=0+T=1	-2.982	-134.395	0.4	- 1.0	9.9	2.77
	NDKB 2	Oblate 2	T = 0	-7.904	-139.361	-0.3	-123.0	0.26	5.82
		Spherical	T = 0	-2.581	-135.621	0.3	-1.0	8.2	2.87

Table 4.1 (continued)

Nucleus	Force	Shape	Mode	E_{PAIR}	E_{TOTAL}	Q_{20}	Q_{40}	A_x	$E_\alpha + E_\beta$	
S^{32}	Rosenfeld 1	Oblate 1	T = 0	-1.009	-212.882	-1.5	-94.5	0.26	5.78	
		Oblate 3	T = 0	-6.148	-209.457	-7.5	-61.7	0.39	5.94	
	Rosenfeld 2	Oblate 2	T = 0	-5.481	-178.331	-1.4	-108.0	0.22	6.14	
		Prolate	T = 0	-5.743	-175.347	9.7	- 40.9	0.33	3.89	k
		Spherical	T=0+T=1	-3.818	-173.943	0.1	0.7	28	4.56	l
		Oblate 3	T = 0	-7.498	-175.353	-9.5	-64.8	0.35	4.70	m
	Yale	Prolate	T = 0	-4.753	-223.764	15.5	-68.5	0.24	4.23	n
	NDKB 1	Prolate	T = 0	-2.717	-178.880	13.3	-43.8	0.26	4.41	o
		Oblate	T = 0	-7.392	-176.238	-8.3	73.2	0.29	4.38	p
		Spherical	T = 0	-2.975	-173.784	0.3	-0.2	32	2.16	q
	NDKB 2	Prolate	T = 0	-2.164	-182.091	17.9	-61.6	0.28	5.38	
		Oblate	T = 0	-7.862	-177.852	-10.1	101.0	0.29	4.58	
		Spherical	T = 0	-3.545	-174.096	0.4	-0.2	27	2.28	r

Table 4.1 (continued)

Nucleus	Force	Shape	Mode	E_{PAIR}	E_{TOTAL}	Q_{20}	Q_{40}	A_x	$E_\alpha + E_\beta$	
Ar^{36}	Rosenfeld 1	Prolate	T = 0	-3.108	-277.243	4.0	-8.5	0.85	3.13	
		Spherical	T = 0	-3.562	-277.314	0.4	-0.4	23	2.97	s
	Rosenfeld 2	Prolate	T = 0	-3.732	-236.036	4.8	-11.8	0.69	3.68	
		Spherical	T = 0	-4.003	-235.783	0.8	-0.8	7.9	3.20	s
	Yale	Prolate	T = 0	-3.392	-287.096	6.1	-24.8	0.49	2.93	t
		Spherical	T = 0+T=1	-3.931	-286.457	-0.1	- 0.02	285	2.09	u
	NDKB 1	Prolate	T = 0	-2.663	-223.562	4.1	-12.6	0.77	2.26	
		Spherical	T = 0	-2.023	-223.343	0.1	-0.1	12	1.80	u
	NDKB 2	Prolate	T = 0	-3.556	-224.540	7.1	- 19.2	0.56	2.99	
		Spherical								v

All energies are in Mev. Q_{LM} has units of fm^L.

a. Levels 2 and 3 exchange position.

b. $v_4^2 = 1$.

c. $E_3 < E_1, E_2$. In parentheses are (Q_{22}), (Q_{42}, Q_{44}), (A_y, A_z).

d. 300+ iterations.

e. Levels 2 and 3 exchange, 4 and 5 exchange.

f. HF gap increases to 2 Mev.

g. Levels 1 and 2 exchange position.

h. Levels 2 and 3 exchange position.

i. $v_1^2 = v_2^2 = v_5^2 = 1$.

j. All sd levels contribute equally to E_{PAIR}.

k. E_{PAIR} twice as large as when $\Gamma \neq \Gamma(v^2)$.

l. 298 iterations.

m. Level order is 2,1,5,3,4,6. $E_\alpha + E_\beta = E_3 + E_4$.

n. Levels 5 and 6 exchange. $E_\alpha + E_\beta = E_4 + E_6$.

o. $v_4^2 > v_3^2$.

p. Levels 4 and 5 exchange.

q. $1d_{3/2}$ below $2s_{1/2}$.

r. $1d_{3/2}$ 200 kev below $2s_{1/2}$, equally occupied.

s. No pairing for $\Gamma \neq \Gamma(v^2)$. $2s_{1/2}$ lowered by 9 Mev.
$E_\alpha + E_\beta = E_4 + E_5$.

t. 284 iterations.

u. $2s_{1/2}$ below $1d_{3/2}$. $E_\alpha + E_\beta = E_4 + E_5$.

v. At pairing cutoff.

(All level numberings are with respect to level ordering within sd shell.)

Table 4.2: Prolate Mg^{24} (Prolate 1, Rosenfeld 1)

$\epsilon(\alpha)$	-19.500	-15.045	-11.738	-10.184	-6.343	-4.011
$(Im\, N_{\alpha 12})^2$	(-)0.993	(+)0.798	(+)0.189	(-)0.013	(-)0.002	(-) 0.005
$\Delta_{np}^{T=0}(\alpha)$	0.987	-1.930	-2.363	0.793	0.618	1.357
$E(\alpha)$	5.970	2.403	3.016	3.519	7.295	9.697

Table 4.3: Prolate Mg^{24} (Prolate 2, Rosenfeld 2)

$\epsilon(\alpha)$	-17.940	-12.284	-10.303	-7.024	-5.318	-2.625
$(Im\, N_{\alpha 12})^2$	(-)0.988	(+)0.665	(+)0.321	(-)0.015	(-)0.005	(-)0.008
$\Delta_{np}^{T=0}(\alpha)$	1.492	-2.551	-2.832	1.087	0.831	1.538
$E(\alpha)$	6.716	2.703	3.034	4.501	6.130	8.900

Table 4.4 Prolate Mg^{24} (Yale)

$\epsilon(\alpha)$	-14.646	-10.103	-8.171	-5.536	-4.273	-1.611
$(Im\, N_{\alpha 12})^2$	(-)0.968	(+)0.693	(+)0.306	(-)0.024	(-)0.009	(-)0.007
$\Delta_{np}^{T=0}(\alpha)$	2.087	-2.317	-2.288	1.166	0.956	1.225
$E(\alpha)$	5.895	2.512	2.482	3.782	4.954	7.622

For prolate Mg^{24}: $N_{\alpha 11} = Re\, N_{\alpha 12} = \Delta_{pp}(\alpha) = \Delta_{np}^{T=1}(\alpha) = 0$.
The sign of $Im\, N_{\alpha 12}$ is given in parentheses before $(Im\, N_{\alpha 12})^2$.
$U_{\alpha 11} > 0$.

Table 4.5: Prolate Mg^{24} (NDKB 1)

$\epsilon(\alpha)$	-11.373	-7.740	-4.822	-4.286	-0.685	1.638
$(Im\, \mathcal{N}_{\alpha 12})^2$	(-)0.975	(+)0.746	(+)0.185	(-)0.079	(-)0.011	(-)0.014
$\Delta_{np}^{T=0}(\alpha)$	1.589	-2.061	-2.160	1.465	1.236	1.998
$E(\alpha)$	5.051	2.366	2.784	2.720	6.021	8.455

Table 4.6: Prolate Mg^{24} (NDKB 2)

$\epsilon(\alpha)$	-13.477	-8.417	-5.186	-2.756	0.739	3.654
$(Im\, \mathcal{N}_{\alpha 12})^2$	(-)0.990	(+)0.810	(+)0.173	(-)0.022	(-)0.004	(-)0.005
$\Delta_{np}^{T=0}(\alpha)$	1.346	-1.930	-1.984	1.258	1.013	1.558
$E(\alpha)$	6.716	2.457	2.620	4.327	7.702	10.665

For prolate Mg^{24}: $\mathcal{N}_{\alpha 11} = Re\, \mathcal{N}_{\alpha 12} = \Delta_{pp}(\alpha) = \Delta_{np}^{T=1}(\alpha) = 0$.
The sign of $Im\, \mathcal{N}_{\alpha 12}$ is given in parentheses before $(Im\, \mathcal{N}_{\alpha 12})^2$.
$U_{\alpha 11} > 0$.

Table 4.7: Spherical Si^{28} (Rosenfeld 2)

Jm	5/2 -3/2	5/2 1/2	5/2 5/2	3/2 1/2	3/2 -3/2	1/2 1/2
$\epsilon(\alpha)$	- 14.914	- 14.928	- 14.926	- 10.911	-10.835	- 9.630
$N_{\alpha 11}^2$	0.251	0.402	0.167	0.025	0.018	0.007
$(Re\, N_{\alpha 12})^2$	0.251	0.402	0.167	0.025	0.018	0.007
$(Im\, N_{\alpha 12})^2$	(-) 0.410	(+) 0.133	(+) 0.557	(-) 0.035	(+)0.093	(+)0.035
N_α^2	0.912	0.936	0.890	0.085	0.129	0.048
$\Delta_{pp}(\alpha)$	- 0.715	- 0.728	- 0.689	- 0.736	-0.707	- 0.575
$\Delta_{np}^{T=1}(\alpha)$	- 0.715	- 0.728	- 0.689	- 0.736	-0.707	- 0.575
$\Delta_{np}^{T=0}(\alpha)$	0.915	- 0.420	- 1.259	0.870	-1.617	- 1.335
$E(\alpha)$	2.402	2.280	2.547	2.438	2.834	3.658

The sign of $Im\, N_{\alpha 12}$ is given in parentheses before $(Im\, N_{\alpha 12})^2$. $N_{\alpha 11}, Re\, N_{\alpha 12}, U_{\alpha 11} > 0$.

References to Chapter 4

1. A.M. Lane, Nuclear Theory. New York: W.A. Benjamin, 1964. Section I.5.1 has a good review of previous attempts to formulate an isospin generalized pairing theory.

2. A. Goswami, Nucl. Phys. 60, 228 (1964).

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5. The Pauli principle does not prevent the pairing of neutrons and protons in identical spatial orbitals. However, we restrict ourselves, as is conventional, to the pairing of particles in time-reversed orbitals.

6. A.L. Goodman, G.L. Struble, and A. Goswami, Phys. Letters 26B, 260 (1968).

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8. The wave function may also be expressed as

$$|\Phi_0\rangle = \prod_{\alpha>0} (u_{\alpha 11} + v_{\alpha 11}\, a^{+}_{\alpha p}\, a^{+}_{\bar{\alpha} p} + v^{*}_{\alpha 12}\, a^{+}_{\alpha p}\, a^{+}_{\bar{\alpha} n})$$
$$\times (u_{\alpha 11} - v_{\alpha 11}\, a^{+}_{\alpha n}\, a^{+}_{\bar{\alpha} n} + v_{\alpha 12}\, a^{+}_{\alpha n}\, a^{+}_{\bar{\alpha} p})\,|0\rangle .$$

V. THE GENERAL QUASIPARTICLE TRANSFORMATION

1. Introduction

A satisfactory theory of self-consistent fields should allow the Hartree-Fock (HF) and pairing degrees of freedom to interact with one another. There are two methods by which this may be accomplished.

The pairing theory has been described by the special quasiparticle transformation. Unless special care is taken in the choice of the single particle orbitals $|\alpha\rangle$, the formulation is equivalent to neglecting elements of the HF and pair potentials which connect different spatial orbitals. It is assumed that

$$\overline{|\langle\alpha\beta T|v|\alpha'\beta T\rangle_A|} \ll \overline{|\langle\alpha\beta T|v|\alpha\beta T\rangle_A|}$$

$$\overline{|\langle\alpha\bar{\alpha}' T|v|\beta\bar{\beta} T\rangle_A|} \ll \overline{|\langle\alpha\bar{\alpha} T|v|\beta\bar{\beta} T\rangle_A|}$$

where $\alpha \neq \alpha'$. For reasonable forces there is no a priori reason to expect that these assumptions are justified. However if the single particle basis is judiciously selected, these approximations need not be made. The appropriate formalism consists of coupled Hartree-Bogoliubov (HB) and BCS equations. It may be derived by eliminating the terms in the Hamiltonian which create or annihilate two quasiparticles. A further rotation in quasiparticle space is required to diagonalize the terms

containing one quasiparticle creation operator and one quasiparticle annihilation operator. The HB equations have the disadvantage that the HB Hamiltonian is a functional of the orbital $|\alpha\rangle$. Hence they can not be solved in the usual way.

The general quasiparticle transformation provides an alternative, but equivalent description.[1,2] Instead of restricting the transformation to a linear combination of a^+_α and $a_{\bar{\alpha}}$

$$b^+_\alpha = u_\alpha a^+_\alpha - v_\alpha a_{\bar{\alpha}} \qquad \text{(special)}$$

we permit each quasiparticle to be a linear combination of all particle creation and annihilation operators.

$$b^+_i = \sum_j (U_{ij} a^+_j + V_{ij} a_j) \qquad \text{(general)}$$

Although the simplicity of the special transformation appears to be discarded, thereby rendering the interpretation of the wave function more difficult, we shall see that the general transformation may be described in terms of the special, so that in fact, no ease of interpretation is lost. The resulting Hartree-Fock-Bogoliubov (HFB) equations are a natural generalization of the HF equations. The HFB equations are easier to solve than the HB equations. Also no additional rotation in quasiparticle space is required. The general transformation provides the more elegant of the two formulations of the pairing theory.

2. Quasiparticle Transformation

The general Bogoliubov quasiparticle is given by the most general linear transformation

$$b_i^\dagger = \sum_j (U_{ij} a_j^\dagger + V_{ij} a_j) \tag{5.1a}$$

$$b_i = \sum_j (U_{ij}^* a_j + V_{ij}^* a_j^\dagger) \tag{5.1b}$$

or

$$\begin{bmatrix} \underline{b}^\dagger \\ \underline{b} \end{bmatrix} = \begin{bmatrix} U & V \\ V^* & U^* \end{bmatrix} \begin{bmatrix} \underline{a}^\dagger \\ \underline{a} \end{bmatrix} \tag{5.2}$$

where $\underline{a}$ and $\underline{b}$ are N dimensional vectors and U and V are N x N dimensional matrices. Since the transformation is required to be unitary, the inverse transformation is

$$\begin{bmatrix} \underline{a}^\dagger \\ \underline{a} \end{bmatrix} = \begin{bmatrix} \tilde{U}^* & \tilde{V} \\ \tilde{V}^* & \tilde{U} \end{bmatrix} \begin{bmatrix} \underline{b}^\dagger \\ \underline{b} \end{bmatrix} \tag{5.3}$$

or

$$a_j^\dagger = \sum_i (U_{ij}^* b_i^\dagger + V_{ij} b_i) \tag{5.4a}$$

$$a_j = \sum_i (U_{ij} b_i + V_{ij}^* b_i^\dagger). \tag{5.4b}$$

The unitarity conditions are($XX^\dagger = I$)

$$UU^\dagger + VV^\dagger = I \tag{5.5a}$$

$$U\tilde{V} + V\tilde{U} = 0 \tag{5.5b}$$

and ($X^\dagger X = I$)

$$U^\dagger U + (V^\dagger V)^* = I \tag{5.5c}$$

$$U^\dagger V + (V^\dagger U)^* = 0. \tag{5.5d}$$

That is

$$\sum_j (U_{ij} U^*_{kj} + V_{ij} V^*_{kj}) = \delta_{ik} \tag{5.6a}$$

$$\sum_j (U_{ij} V_{kj} + V_{ij} U_{kj}) = 0 \tag{5.6b}$$

$$\sum_j (U^*_{ji} U_{jk} + V_{ji} V^*_{jk}) = \delta_{ik} \tag{5.6c}$$

$$\sum_j (U^*_{ji} V_{jk} + V_{ji} U^*_{jk}) = 0 \ . \tag{5.6d}$$

These relations may also be obtained by requiring the particle and quasiparticle operators to satisfy the Fermion commutation rules. Substituting (5.1) into

$$[b^\dagger_i, b_k]_+ = \delta_{ik} \tag{5.7a}$$

$$[b^\dagger_i, b^\dagger_k]_+ = [b_i, b_k]_+ = 0 \tag{5.7b}$$

results in (5.6a,b). Substituting (5.4) into

$$[a^\dagger_i, a_k]_+ = \delta_{ik} \tag{5.8a}$$

$$[a^\dagger_i, a^\dagger_k]_+ = [a_i, a_k]_+ = 0 \tag{5.8b}$$

results in (5.6c,d).

The reference state $|\Phi_0\rangle$ is defined as a quasiparticle vacuum. Therefore

$$b_i \, |\Phi_0\rangle = 0 \ . \qquad (\text{all } i) \tag{5.9}$$

Since $[b_i, b_i]_+$ vanishes, $b_i b_i = 0$. Therefore a solution to (5.9) is

$$|\Phi_0\rangle = C \prod_i b_i |0\rangle \tag{5.10}$$

where C is a constant of normalization.

3. The Hamiltonian

The Hamiltonian is

$$H' = H - \lambda N \tag{5.11}$$

$$= \sum_{ij} \langle i | T - \lambda | j \rangle a^\dagger_i a_j + \frac{1}{4} \sum_{ijkl} \langle ij | v | kl \rangle_A a^\dagger_i a^\dagger_j a_l a_k \tag{5.12a}$$

where

$$N = \sum_i a^\dagger_i a_i \tag{5.12b}$$

$$\lambda = \lambda_p P_p + \lambda_n P_n \tag{5.12c}$$

$$P_\tau = | \tau \rangle \langle \tau | .$$

λ_p and λ_n are Lagrange multipliers to be chosen so that the average numbers of protons and neutrons in the wave function equal the experimental values.

$$\langle N_p \rangle = Z \qquad \langle N_n \rangle = A - Z \tag{5.13a}$$

where

$$N_\tau = \sum_k a^\dagger_{k\tau} a_{k\tau} \tag{5.13b}$$

and

$$N_p + N_n = N \tag{5.13c}$$

We have used Wick's theorem (I.3) to express H' as

$$H' = H_0' + H_2' + H_4' \tag{5.14}$$

where

$$H_0' = \sum_{ij} (T - \lambda + \tfrac{1}{2}\Gamma)_{ij} \rho_{ji} + \tfrac{1}{2} \sum_{ij} \Delta_{ij} \kappa^\dagger_{ji} \tag{5.15}$$

$$H_2' = \sum_{ij} (\mathcal{H} - \lambda)_{ij} N[a^\dagger_i a_j] + \tfrac{1}{2} \sum_{ij} \Delta_{ij} N[a^\dagger_i a^\dagger_j] \tag{5.16}$$

$$+ \tfrac{1}{2} \sum_{ij} \Delta^\dagger_{ij} N[a_i a_j] \tag{5.17}$$

$$H_4' = \frac{1}{4} \sum_{ijkl} \langle ij | v | kl \rangle_A N[a^\dagger_i a^\dagger_j a_l a_k] .$$

ρ is the density matrix.

$$\rho_{ji} = \langle a^{\dagger}_i a_j \rangle \tag{5.18}$$

$$\rho^{\dagger} = \rho \tag{5.19}$$

t is the pairing tensor.

$$t_{ji} = \langle a_i a_j \rangle \tag{5.20}$$

$$t^{*}_{ji} = \langle a^{\dagger}_j a^{\dagger}_i \rangle \tag{5.21}$$

$$\tilde{t} = -t \tag{5.22}$$

Γ is the HF potential.

$$\Gamma_{ij} = \sum_{kl} \langle ik | v | jl \rangle_A \rho_{lk} \tag{5.23}$$

$$\Gamma^{\dagger} = \Gamma \tag{5.24}$$

$\mathcal{H}$ is the HF Hamiltonian.

$$\mathcal{H}_{ij} = T_{ij} + \Gamma_{ij} \tag{5.25}$$

$$\mathcal{H}^{\dagger} = \mathcal{H} \tag{5.26}$$

Δ is the pair potential.

$$\Delta_{ij} = \frac{1}{2} \sum_{kl} \langle ij | v | kl \rangle_A t_{kl} \tag{5.27}$$

$$\Delta^{*}_{ij} = \frac{1}{2} \sum_{kl} \langle kl | v | ij \rangle_A t^{*}_{kl} \tag{5.28}$$

$$\tilde{\Delta} = -\Delta \tag{5.29}$$

The expectation values and normal orderings are with respect to a reference state, which is chosen to be the quasiparticle vacuum. It follows that

$$\langle b^\dagger_k b^\dagger_\ell \rangle = \langle b_k b_\ell \rangle = \langle b^\dagger_k b_\ell \rangle = 0 \tag{5.30}$$

$$\langle b_k b^\dagger_\ell \rangle = \delta_{k\ell} \tag{5.31}$$

where the last equality uses (5.7a).

The density matrix may be evaluated in terms of U and V. Use the inverse transformation (5.4)

$$\langle a^\dagger_i a_j \rangle = \langle \sum_k (U^*_{ki} b^\dagger_k + V_{ki} b_k) \sum_\ell (U_{\ell j} b_\ell + V^*_{\ell j} b^\dagger_\ell) \rangle$$

and (5.30 - 5.31).

$$\rho_{ji} = \sum_k V_{ki} V^*_{kj} \tag{5.32a}$$

or

$$\rho = V^\dagger V \, . \tag{5.32b}$$

Similarly the pairing tensor is

$$\langle a_i a_j \rangle = \langle \sum_k (U_{ki} b_k + V^*_{ki} b^\dagger_k) \sum_\ell (U_{\ell j} b_\ell + V^*_{\ell j} b^\dagger_\ell) \rangle$$

so that

$$t_{ji} = \sum_k U_{ki} V^*_{kj} \tag{5.33a}$$

or

$$t = V^\dagger U \, . \tag{5.33b}$$

4. Hartree - Fock - Bogoliubov Equations

The Hamiltonian will acquire the desired form of an independent quasiparticle Hamiltonian if H_4' (the quasi-particle interactions) may be neglected and if

$$H_2' = \sum_k E_k b_k^+ b_k . \tag{5.34}$$

The problem therefore is to choose U and V so that (5.34) is satisfied. The commutator $[H_2', b_k^+]_-$ may be evaluated with (5.34)

$$[H_2', b_k^+]_- = E_k b_k^+ \tag{5.35}$$

or

$$[H_2', b_k^+]_- = E_k \sum_i (U_{ki} a_i^+ + V_{ki} a_i). \tag{5.36}$$

Alternatively, (5.16) may be used.

$$\begin{aligned}[H_2', b_k^+]_- = &\sum_{ij} \{(\mathcal{H}-\lambda)_{ij} U_{kj} + \Delta_{ij} V_{kj}\} a_i^+ \\ &+ \sum_{ij} \{\Delta_{ij}^+ U_{kj} + (\lambda - \tilde{\mathcal{H}})_{ij} V_{kj}\} a_i\end{aligned} \tag{5.37}$$

Equate the coefficients of a_i^+ and a_i in (5.36) and (5.37).

$$\sum_j \{(\mathcal{H}-\lambda)_{ij} U_{kj} + \Delta_{ij} V_{kj}\} = E_k U_{ki} \tag{5.38a}$$

$$\sum_j \{\Delta_{ij}^+ U_{kj} + (\lambda - \tilde{\mathcal{H}})_{ij} V_{kj}\} = E_k V_{ki} \tag{5.38b}$$

Let

$$\underline{U}_k = \begin{bmatrix} U_{k1} \\ U_{k2} \\ \vdots \\ U_{kN} \end{bmatrix} \qquad \underline{V}_k = \begin{bmatrix} V_{k1} \\ V_{k2} \\ \vdots \\ V_{kN} \end{bmatrix} \tag{5.39}$$

then (5.38) is

$$(\mathcal{H}-\lambda)\,\underline{U}_K + \Delta\,\underline{V}_K = E_K\,\underline{U}_K \tag{5.40a}$$

$$\Delta^{\dagger}\,\underline{U}_K + (\lambda-\tilde{\mathcal{H}})\,\underline{V}_K = E_K\,\underline{V}_K\,. \tag{5.40b}$$

Equations (5.40) form an eigenvalue equation.

$$\begin{bmatrix} (\mathcal{H}-\lambda) & \Delta \\ \Delta^{\dagger} & (\lambda-\tilde{\mathcal{H}}) \end{bmatrix} \begin{bmatrix} \underline{U}_K \\ \underline{V}_K \end{bmatrix} = E_K \begin{bmatrix} \underline{U}_K \\ \underline{V}_K \end{bmatrix} \tag{5.41}$$

Let

$$\mathcal{K} = \begin{bmatrix} (\mathcal{H}-\lambda) & \Delta \\ \Delta^{\dagger} & (\lambda-\tilde{\mathcal{H}}) \end{bmatrix} \tag{5.42}$$

and

$$\underline{X}_K = \begin{bmatrix} \underline{U}_K \\ \underline{V}_K \end{bmatrix} \tag{5.43}$$

then (5.41) is more compactly represented by

$$\mathcal{K}\,\underline{X}_K = E_K\,\underline{X}_K\,. \tag{5.44}$$

$\mathcal{K}$ is self adjoint. Therefore its eigenvalues are real.

$$\mathcal{K}^{\dagger} = \mathcal{K} \qquad\qquad E_K = \mathrm{Real} \tag{5.45}$$

Equations (5.44) are called the HFB equations. The eigenvectors provide the quasiparticle coefficients U and V for which (5.34) is satisfied. The eigenvalues E_K are the corresponding quasiparticle energies.

The HFB equations are a natural generalization of the HF equations (2.17). The eigenvalue problem is of the same nature, except that the generalized potential $\mathcal{K}$ has twice the dimension of the HF potential. The HF and

pair potentials are treated simultaneously and on an equal basis. HF and pair degrees of freedom interact with one another during each iteration of the calculation.

The potentials $\mathcal{H}, \Delta$ are determined by the wave function ρ, t and vice-versa. Therefore the potentials are self-consistent. An initial guess is made for ρ, t. Then $\mathcal{H}, \Delta$ are calculated (5.23, 5.25, 5.27). The HFB equations (5.44) are solved, providing the coefficients U, V from which a new ρ, t may be calculated (5.32, 5.33). λ_p, λ_n are adjusted so that the number conservation constraints (5.13) are satisfied. The procedure is repeated until ρ, t are the same on successive iterations.

In the limit of zero pairing (Δ = 0), the HFB equations are equivalent to the HF equations.

Consider the 2N x 2N dimensional matrix A.

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{5.46}$$

The product AKA is $\begin{bmatrix} (\lambda - \tilde{\mathcal{H}}) & \Delta^{+} \\ \Delta & (\mathcal{H} - \lambda) \end{bmatrix}$.

Since $\mathcal{H}$ is Hermitian and Δ is antisymmetric

$$AKA = -K^{*} . \tag{5.47}$$

Complex conjugate (5.44).

$$K^{*} \underline{X}_k^{*} = E_k \underline{X}_k^{*}$$

Substitute (5.47).

$$-AKA \underline{X}_k^{*} = E_k \underline{X}_k^{*}$$

Since

$$A^2 = 1 \tag{5.48}$$

multiplying through by A gives

$$\mathcal{K} A \underline{X}_K^* = -E_K A \underline{X}_K^* . \tag{5.49}$$

Therefore if $\underline{X}_K$ is an eigenvector of $\mathcal{K}$ associated with the eigenvalue E_K, it follows that $A\underline{X}_K^*$ is an eigenvector of $\mathcal{K}$ corresponding to the eigenvalue $-E_K$. Since H_2' is Hermitian, the adjoint of (5.35) is

$$[H_2', b_K]_- = -E_K b_K . \tag{5.50}$$

Therefore it is clear why the eigenvectors and eigenvalues come in pairs: $\underline{X}_K$, E_K and $A\underline{X}_K^*$, $-E_K$. If b_K^+ is given by $\underline{X}_K = \begin{bmatrix} \underline{U}_K \\ \underline{V}_K \end{bmatrix}$, then b_K is given by $A\underline{X}_K^* = \begin{bmatrix} \underline{V}_K^* \\ \underline{U}_K \end{bmatrix}$

(see(5.1)). In constructing ρ and t (5.32,5.33), the summations are over eigenvectors with positive energy.

It is desirable to know whether the HFB equations may be derived from a variational principle. One might hope to succeed with the principle

$$\frac{\partial \mathcal{L}}{\partial U_{rs}} = \frac{\partial \mathcal{L}}{\partial V_{rs}} = 0$$

where (5.51)

$$\mathcal{L} = H_0' - \sum_K \mathcal{E}_K \left\{ \sum_j (U_{Kj}^* U_{Kj} + V_{Kj}^* V_{Kj}) - 1 \right\}$$

and

$$H_0' = \sum_{ijm} (T-\lambda)_{ij} \, V_{mi} V_{mj}^* + \frac{1}{2} \sum_{ijklmn} \mathcal{N}_{ijkl} \, V_{mi} V_{mk}^* \, V_{nj} V_{nl}^* + \frac{1}{4} \sum_{ijklmn} \mathcal{N}_{ijkl} \, U_{mj}^* V_{mi} \, U_{nl} V_{nk}^* \, . \tag{5.52}$$

Unfortunately the resulting energy matrix is

$$\begin{bmatrix} \mathcal{H} & \frac{1}{2}\Delta \\ \frac{1}{2}\Delta^+ & 0 \end{bmatrix}$$

which is not $\mathcal{K}$. The lack of symmetry in this energy matrix arises because H_0 is not symmetrical in U and V. Furthermore U and V are not independent parameters, but are coupled to each other through the unitarity conditions. The correct variational principle is

$$\frac{\delta \mathcal{L}}{\delta V_{rs}} = \frac{\partial \mathcal{L}}{\partial V_{rs}} + \frac{\partial \mathcal{L}}{\partial U_{rs}} \frac{\partial U_{rs}}{\partial V_{rs}} = 0 \, . \tag{5.53}$$

However $\partial U_{rs} / \partial V_{rs}$ is not readily obtainable.

A more elegant approach is to proceed with the aid of the generalized density matrix. In the discussion which follows we use the notation,

$$1 \leq i, j, k, l, p \leq N$$
$$1 \leq m, n, r, s, q \leq 2N$$
$$\bar{i} = i + N, \text{ etc.}$$

Let $\quad \underline{A}^+ = \begin{bmatrix} \underline{a}^+ \\ \underline{a} \end{bmatrix} \qquad \underline{A} = \begin{bmatrix} \underline{a} \\ \underline{a}^+ \end{bmatrix} . \qquad (5.54)$

Then the generalized particle density matrix is

$$R_{mn} = \langle A_n^\dagger A_m \rangle . \tag{5.55}$$

It may be verified that

$$R = \begin{bmatrix} \rho & t \\ t^\dagger & 1-\tilde{\rho} \end{bmatrix} . \tag{5.56}$$

For example $R_{ij} = \langle A_j^\dagger A_i \rangle = \langle a_j a_i^\dagger \rangle = \langle \delta_{ij} - a_i^\dagger a_j \rangle = (1-\tilde{\rho})_{ij}$. Alternatively one may define

$$\underline{B}^\dagger = \begin{bmatrix} \underline{b}^\dagger \\ \underline{b} \end{bmatrix} \qquad \underline{B} = \begin{bmatrix} \underline{b} \\ \underline{b}^\dagger \end{bmatrix} . \tag{5.57}$$

The generalized quasiparticle density matrix is

$$G_{mn} = \langle B_n^\dagger B_m \rangle . \tag{5.58}$$

Noting (5.30 -5.31)

$$G = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} . \tag{5.59}$$

Let $$X = \begin{bmatrix} U & V \\ V^* & U^* \end{bmatrix} . \tag{5.60}$$

Then the quasiparticle transformation (5.2) is

$$\underline{B}^\dagger = X \underline{A}^\dagger \qquad B_m^\dagger = \sum_n X_{mn} A_n^\dagger \tag{5.61}$$

and the inverse transformation is

$$\underline{A}^\dagger = X^\dagger \underline{B}^\dagger \qquad A_n^\dagger = \sum_m X_{mn}^* B_m^\dagger . \tag{5.62}$$

Then R is easily evaluated.

$$\langle A_n^+ A_m \rangle = \sum_{rs} X_{sn}^* X_{rm} \langle B_s^+ B_r \rangle$$

Substitute G,

$$R_{mn} = \sum_{k} X_{kn}^* X_{km} \tag{5.63}$$

R is symmetrical in U and V.

$$R = \begin{bmatrix} V^+V & V^+U \\ U^+V & U^+U \end{bmatrix} \tag{5.64}$$

This form of R is equivalent to (5.56). For example, $U^+U = 1 - (V^+V)^* = 1 - \rho^* = 1 - \tilde{\rho}$. The program is to express H_o' in terms of R and then vary H_o' with respect to X. H_o' (5.15) may be written as

$$H_o' = Tr\left[(T - \lambda + \tfrac{1}{2}\Gamma)\rho + \tfrac{1}{2}\Delta\mathcal{L}^+\right]. \tag{5.65}$$

Define $\hat{T} = \begin{bmatrix} T & 0 \\ 0 & -\tilde{T} \end{bmatrix}$ $\hat{\lambda} = \begin{bmatrix} \lambda & 0 \\ 0 & -\lambda \end{bmatrix}$. (5.66)

Since H_o' is real; $T, \mathcal{H}, \rho$ are Hermitian; $\Delta, \mathcal{L}$ are antisymmetric; it may be shown that

$$H_o' = \tfrac{1}{4} Tr\left[(\hat{T} - \hat{\lambda} + \mathcal{K})R + 2(T - \lambda) + \Gamma\right].$$

$\mathcal{K}$ may be expressed in terms of R with the aid of a generalized potential $\hat{\Gamma}$

$$\hat{\Gamma}_{mn} = \sum_{rs} \hat{v}_{mrns} R_{sr} \tag{5.67}$$

where $\hat{v}$ remains to be defined. Choose

$$\hat{v}_{ijkl} = \tfrac{1}{2} v_{ijkl} \qquad \hat{v}_{\bar{i}\bar{j}\bar{k}\bar{l}} = \tfrac{1}{2} v_{klij}$$

$$\hat{v}_{i\bar{j}k\bar{l}} = -\tfrac{1}{2} v_{ilkj} \qquad \hat{v}_{\bar{i}j\bar{k}l} = -\tfrac{1}{2} v_{kjil} \tag{5.68}$$

$$\hat{v}_{i\bar{j}\bar{k}l} = -\tfrac{1}{2} v_{ikjl} \qquad \hat{v}_{\bar{i}jk\bar{l}} = -\tfrac{1}{2} v_{jlik}$$

all other components of $\hat{v}$ being zero.[3] Then

$$\hat{\Gamma} = \begin{bmatrix} (\Gamma - \tfrac{1}{2} V) & \Delta \\ \Delta^{\dagger} & -(\tilde{\Gamma} - \tfrac{1}{2} \tilde{V}) \end{bmatrix} \tag{5.69}$$

where $$V_{ij} = \sum_k v_{ikjk} \, . \tag{5.70}$$

Let $$\hat{V} = \begin{bmatrix} V & 0 \\ 0 & -\tilde{V} \end{bmatrix} \tag{5.71}$$

and $$\hat{\mathcal{J}} = \hat{T} - \hat{\lambda} + \tfrac{1}{2} \hat{V} \tag{5.72}$$

then $$\mathcal{K} = \hat{\mathcal{J}} + \hat{\Gamma} \, . \tag{5.73}$$

Substitute into H_o'.

$$H_o' = \tfrac{1}{4} \mathrm{Tr} \left[(2\hat{\mathcal{J}} + \hat{\Gamma} - \tfrac{1}{2}\hat{V}) R + 2(T-\lambda) + \Gamma \right]$$

Fortunately $\mathrm{Tr}[-\tfrac{1}{2}\hat{V} R + \Gamma] = \mathrm{Tr}[\tfrac{1}{2} V]$,

so that all dependence on ρ, Σ is eliminated.

$$H_o' = \tfrac{1}{2} \mathrm{Tr} \left[(\hat{\mathcal{J}} + \tfrac{1}{2}\hat{\Gamma}) R + \tfrac{1}{4} V + (T-\lambda) \right] \tag{5.74a}$$

or $$H_o' = \tfrac{1}{2} \sum_{mn} \hat{\mathcal{J}}_{mn} R_{nm} + \tfrac{1}{4} \sum_{mnrs} \hat{v}_{mnrs} R_{sn} R_{rm}$$

$$+ \tfrac{1}{8} \sum_{kl} v_{klkl} + \tfrac{1}{2} \sum_k (T-\lambda)_{kk} \tag{5.74b}$$

This expression is similar in form to that obtained in HF theory.

$$H_0 = \sum_{ij} T_{ij} \rho_{ji} + \frac{1}{2} \sum_{ijkl} v_{ijkl} \rho_{lj} \rho_{ki}$$

The variational principle is

$$\frac{\partial \mathcal{L}}{\partial X^*_{\bar{p}q}} = 0 \tag{5.75}$$

where $$\mathcal{L} = H_0' - \sum_m \varepsilon_m \left(\sum_n X^*_{mn} X_{mn} - 1 \right) \tag{5.76}$$

and

$$H_0' = \frac{1}{2} \sum_{kmn} \hat{T}_{mn} X^*_{\bar{k}m} X_{\bar{k}n} + \frac{1}{4} \sum_{klmnrs} \hat{v}_{mnrs} X^*_{\bar{k}n} X_{\bar{k}s} X^*_{\bar{l}m} X_{\bar{l}r}$$
$$+ \frac{1}{8} \sum_{kl} v_{klkl} + \frac{1}{2} \sum_k (T - \lambda)_{kk} . \tag{5.77}$$

Performing the variation we find

$$\sum_n \mathcal{K}_{qn} X_{\bar{p}n} = E_{\bar{p}} X_{\bar{p}q} \tag{5.78a}$$

or $$\mathcal{K} \underline{X}_{\bar{p}} = E_{\bar{p}} \underline{X}_{\bar{p}} \tag{5.78b}$$

where $$E_{\bar{p}} = 2 \varepsilon_{\bar{p}} . \tag{5.79}$$

By the argument following (5.46) we find

$$\mathcal{K} \underline{X}_p = E_p \underline{X}_p \tag{5.80}$$

where $$E_p = - E_{\bar{p}} . \tag{5.81}$$

The HFB theory has been derived by a variational principle applied directly to the quasiparticle co-ordinates.

The generalized density matrix R has other interesting properties. (5.63) may be written as

$$R_{mn} = \sum_{rs} X^*_{sn} G_{rs} X_{rm}$$

so that $$R = (X^*)^\dagger G (X^*) \; . \tag{5.82}$$

Since R is obtained from G by a unitary transformation, it has the same eigenvalues as G, that is, N eigenvalues equal to 0 and N equal to 1. It follows that

$$R^2 = R \tag{5.83}$$

and $$Tr\, R = N \; . \tag{5.84}$$

Inspection of (5.56) shows that (5.84) is automatically satisfied. (5.83) implies

$$\rho - \rho^2 = \tau \tau^\dagger \tag{5.85}$$

$$\rho \tau = \tau \tilde{\rho} \; . \tag{5.86}$$

For zero pairing (5.85) reduces to the HF relation $\rho^2 = \rho$.

If ρ and τ are given, one may ask whether it is possible to determine the co-ordinates of the quasiparticle transformation. The adjoint of (5.9) is

$$\langle \Phi_0 | b_k^\dagger = 0 \; . \tag{5.87}$$

Consequently

$$\langle b_k^\dagger a_j \rangle = \langle b_k^\dagger a_j^\dagger \rangle = 0 \; .$$

Substituting (5.1a)

$$\sum_i \left(U_{ki} \langle a_i^\dagger a_j \rangle + V_{ki} \langle a_i a_j \rangle \right) = 0$$

$$\sum_i \left(U_{ki} \langle a_i^\dagger a_j^\dagger \rangle + V_{ki} \langle a_i a_j^\dagger \rangle \right) = 0$$

we find

$$\sum_i (\rho_{ji} U_{ki} + \tau_{ji} V_{ki}) = 0$$
$$\sum_i (\tau^\dagger_{ji} U_{ki} + (1-\tilde{\rho})_{ji} V_{ki}) = 0 .$$

The matrix equation is

$$R \underline{X}_k = 0 . \tag{5.88}$$

$\underline{X}_k$ is an eigenvector of the generalized density matrix R corresponding to eigenvalue 0 as well as being an eigenvector of the generalized energy matrix $\mathcal{K}$ corresponding to the eigenvalue E_k. To determine the eigenvectors of R corresponding to eigenvalues of 1, consider the relation (see 5.48, 5.82)

$$ARA = A(X^*)^\dagger AAGAA(X^*)A .$$

It may be verified that

$$AX^*A = X \qquad A(X^*)^\dagger A = X^\dagger \qquad AGA = 1-G .$$

Consequently $\qquad ARA = X^\dagger(1-G)X .$

Since $X^+X = 1$

$$ARA = 1 - R^* . \tag{5.89}$$

Complex conjugate (5.88).

$$R^* \underline{X}_k^* = 0$$

Substitute (5.89).

$$ARA \underline{X}_k^* = \underline{X}_k^*$$

Since $A^2 = 1$

$$R A \underline{X}_K^* = A \underline{X}_K^* . \tag{5.90}$$

$A\underline{X}_k^*$ are the eigenvectors of R corresponding to eigenvalues of 1. Recall that $A\underline{X}_k^*$ are also the eigenvectors of $\mathcal{K}$ associated with the eigenvalues $-E_k$.

It might appear that the quasiparticle co-ordinates are determined by the eigenvectors of R. However because of the high degeneracy (of order N), the eigenvectors of R are not uniquely determined. If the quasiparticle co-ordinates are $\underline{X}_k$ then any set of linear combinations of $\underline{X}_k$ are also eigenvectors of R with eigenvalue 0. We conclude that defining the reference state (that is, giving R) defines the quasiparticle co-ordinates up to an arbitrary unitary transformation. This result follows directly from the definition of the reference state.

$$b_K | \Phi_0 \rangle = 0$$

If

$$b'_K = \sum_\ell \mathcal{U}_{K\ell} b_\ell$$

where $\mathcal{U}$ is an arbitrary unitary transformation, then

$$b'_K | \Phi_0 \rangle = 0 .$$

This is reminiscent of our conclusion in III.6 that a rotation in particle space followed by a special quasiparticle transformation are sufficient to define the BCS wave function (that is, determine ρ and τ), whereas a further unitary transformation of quasiparticle co-ordinates

is required to make H_2' diagonal in quasiparticle co-ordinates.

The analogous situation in HF theory is given by the relation

$$\rho^2 = \rho$$

so that ρ has eigenvalues of 0 or 1. The eigenvalue equation is

$$\rho \underline{D}_\alpha = e_\alpha \underline{D}_\alpha \qquad e_\alpha = 0 \text{ or } 1 .$$

The eigenvalues of 1 correspond to hole states, and the eigenvalues of 0 correspond to "particle" states.

$$b_\alpha = \begin{cases} a_\alpha & e_\alpha = 0 \\ a^\dagger_\alpha & e_\alpha = 1 \end{cases}$$

The reference state is defined by

$$b_\alpha |\Phi_0\rangle = 0 .$$

Any unitary transformation of hole states (occupied orbitals) leaves the wave function (ρ) invariant.

The derivation of the HFB equations by the equation of motion method is more transparent with the generalized co-ordinates. H_2' (5.16) may be written as

$$H_2' = \frac{1}{2} \sum_{mn} K_{mn} N[A^\dagger_m A_n] . \qquad (5.91)$$

Substitute the inverse transformation (5.62).

$$H_2' = \frac{1}{2} \sum_{mnrs} K_{mn} X^*_{rm} X_{sn} N[B^\dagger_r B_s]$$

or

$$H_2' = \frac{1}{2} \sum_{rs} [(X^*) K (X^*)^\dagger]_{rs} N[B^\dagger_r B_s] \qquad (5.92)$$

H_2' acquires the desired form if X is chosen so that $(X^*)\ \mathcal{K}\ (X^*)^+$ is diagonal. It is therefore required that

$$(X^*)\mathcal{K}(X^*)^+ = E \tag{5.93}$$

where E is diagonal. The components of this equation are

$$\mathcal{K}\,\underline{X}_r = E_r\,\underline{X}_r$$

which is the HFB equation. Then

$$H_2' = \frac{1}{2}\sum_r E_r\, N[B^+_r B_r].$$

Since $E_{\bar{k}} = -E_k$

and $-N[b_k b^+_k] = N[b^+_k b_k] = b^+_k b_k$

we arrive at

$$H_2' = \sum_k E_k b^+_k b_k .$$

5. Symmetries of the HFB Solutions

If S is a symmetry of the Hamiltonian H, then

$$[H, S]_- = 0 , \tag{5.94}$$

We have partitioned H as

$$H = H_0 + H_2 + H_4 .$$

It may not be true that

$$[H_2, S]_- = 0 \tag{5.95a}$$

or equivalently

$$[\mathcal{K}, S]_- = 0 . \tag{5.95b}$$

If S commutes with H (5.94) and leaves the reference state invariant

$$S|\Phi_0\rangle = |\Phi_0\rangle \tag{5.96a}$$

or

$$[R, S]_- = 0 \tag{5.96b}$$

then S commutes with $\mathcal{K}$ (5.95), and S is termed a "self-consistent symmetry." If a self-consistent symmetry is introduced into R, then $\mathcal{K}$ will reflect that symmetry, and therefore so will R of the following iteration. Consequently if the trial generalized density matrix contains a self-consistent symmetry, it will propagate through to the final self-consistent R.

Harmonic oscillator (HO) wave functions are chosen as the basis states.

$$|K\rangle = |N\ell JM\tau\rangle \tag{5.97}$$

Parity is a self-consistent symmetry. Restrict the quasiparticle transformation so that all components have the same parity. Since

$$P\begin{Bmatrix} a_k^\dagger \\ a_k \end{Bmatrix} P^{-1} = \pm \begin{Bmatrix} a_k^\dagger \\ a_k \end{Bmatrix} \tag{5.98a}$$

it follows that

$$P b_j P^{-1} = \pm b_j . \tag{5.98b}$$

The ground state wave function is

$$|\Phi_0\rangle = \prod_j b_j |0\rangle .$$

Since $\quad P|0\rangle = |0\rangle \qquad$ (5.98c)

we have

$$P|\Phi_0\rangle = \prod_j P b_j P^{-1}|0\rangle = \pm \prod_j b_j |0\rangle$$

so that $|\Phi_0\rangle$ is parity invariant.

$$P|\Phi_0\rangle = \pm |\Phi_0\rangle \tag{5.99}$$

Therefore parity is a self-consistent symmetry. The density matrix and pairing tensor will connect only states of the same parity.

$$\rho = \begin{bmatrix} \rho_{++} & 0 \\ 0 & \rho_{--} \end{bmatrix} \qquad \kappa = \begin{bmatrix} \kappa_{++} & 0 \\ 0 & \kappa_{--} \end{bmatrix} \tag{5.100a}$$

Since the two nucleon interaction conserves the parity of

the two particle state, $\mathcal{H}$ and Δ have the same structure.

$$\mathcal{H} = \begin{bmatrix} \mathcal{H}_{++} & 0 \\ 0 & \mathcal{H}_{--} \end{bmatrix} \qquad \Delta = \begin{bmatrix} \Delta_{++} & 0 \\ 0 & \Delta_{--} \end{bmatrix} \tag{5.100b}$$

The energy matrix has the form

$$\mathcal{K} = \begin{bmatrix} \mathcal{H}_{++} - \lambda & 0 & \Delta_{++} & 0 \\ 0 & \mathcal{H}_{--} - \lambda & 0 & \Delta_{--} \\ \Delta^{\dagger}_{++} & 0 & \lambda - \tilde{\mathcal{H}}_{++} & 0 \\ 0 & \Delta^{\dagger}_{--} & 0 & \lambda - \tilde{\mathcal{H}}_{--} \end{bmatrix}. \tag{5.100c}$$

The eigenvalue equations for positive and negative parity states are therefore de-coupled. Consequently the new set of eigenvectors is also parity invariant, thereby confirming the self-consistent nature of the parity symmetry.

We shall consider in some detail the time-reversal symmetry. $\mathcal{J}$ operating on a HO state gives

$$\mathcal{J}\,|N\ell J m \tau\rangle \equiv |\overline{N\ell J m \tau}\rangle = (-1)^{J-m+\ell}\,|N\ell J - m\,\tau\rangle . \tag{5.101}$$

(We choose $\langle \underline{r} | \ell m_\ell \rangle = Y_{\ell m_\ell}$. For the choice $\langle r | \ell m_\ell \rangle = i^\ell Y_{\ell m_\ell}$, $\mathcal{J}\,|Jm\rangle = (-1)^{J-m}\,|J-m\rangle$.)

Divide the basis states into two sets: the first containing states with $m - \frac{1}{2}$ = even integer, the second containing states with $m - \frac{1}{2}$ = odd integer. Denote the sets respectively by $\{|K\rangle\}$ and $\{|\bar{K}\rangle\}$. More specifically $\{|K\rangle\}$ is composed of states with

$$m = \cdots -7/2, -3/2, 1/2, 5/2, \cdots \qquad |K\rangle \tag{5.102a}$$

and $\{|\bar{k}\rangle\}$ is composed of the states

$$\{|\bar{k}\rangle\} = \mathcal{J}\{|k\rangle\} \tag{5.102b}$$

so that

$$m = \cdots -5/2, -1/2, 3/2, 7/2, \cdots \qquad |\bar{k}\rangle . \tag{5.102c}$$

In the following discussion we use the notation

$$\begin{aligned} &1 \leq i, j, k, \ell \leq N/2 \\ &1 \leq m, n, r, s \leq N \\ &\bar{k} = k + N/2, \text{ etc.} \end{aligned} \tag{5.102d}$$

and $\quad |\bar{k}\rangle = \mathcal{J}\,|k\rangle .$

To restrict the pairing to pairs of states, one of which is composed of $\{|k\rangle\}$ the other having components in $\{|\bar{k}\rangle\}$, the appropriate choice for the trial quasi-particle transformation is

$$U = \begin{bmatrix} u & 0 \\ 0 & \bar{u} \end{bmatrix} \qquad V = \begin{bmatrix} 0 & v \\ \bar{v} & 0 \end{bmatrix} \tag{5.103}$$

where

$$\begin{aligned} u_{jk} &= U_{jk} & v_{jk} &= V_{j\bar{k}} \\ \bar{u}_{jk} &= U_{\bar{j}\bar{k}} & \bar{v}_{jk} &= V_{\bar{j}k} . \end{aligned} \tag{5.104}$$

Then X has the form

$$\begin{bmatrix} u & 0 & 0 & v \\ 0 & \bar{u} & \bar{v} & 0 \\ 0 & v^* & u^* & 0 \\ \bar{v}^* & 0 & 0 & \bar{u}^* \end{bmatrix} \tag{5.105}$$

therefore separating into two subspaces:

$$b_J^\dagger = \sum_K (u_{JK}\, a_K^\dagger + v_{JK}\, a_{\bar{K}}) \tag{5.106a}$$

$$b_{\bar{J}} = \sum_K (\bar{u}_{JK}^*\, a_{\bar{K}} + \bar{v}_{JK}^*\, a_K^\dagger) \tag{5.106b}$$

and

$$b_{\bar{J}}^\dagger = \sum_K (\bar{u}_{JK}\, a_{\bar{K}}^\dagger + \bar{v}_{JK}\, a_K) \tag{5.106c}$$

$$b_J = \sum_K (u_{JK}^*\, a_K + v_{JK}^*\, a_{\bar{K}}^\dagger)\,. \tag{5.106d}$$

The density matrix (5.32) and the pairing tensor (5.33) are also partitioned.

$$\rho = \begin{bmatrix} \rho & 0 \\ 0 & \bar{\rho} \end{bmatrix} = \begin{bmatrix} \bar{v}^\dagger \bar{v} & 0 \\ 0 & v^\dagger v \end{bmatrix} \tag{5.107}$$

$$\tau = \begin{bmatrix} 0 & \tau \\ \bar{\tau} & 0 \end{bmatrix} = \begin{bmatrix} 0 & \bar{v}^\dagger \bar{u} \\ v^\dagger u & 0 \end{bmatrix} \tag{5.108}$$

where

$$\begin{aligned} \rho_{ij} &= \rho_{ij} & \tau_{ij} &= \tau_{i\bar{j}} \\ \bar{\rho}_{ij} &= \rho_{\bar{i}\bar{j}} & \bar{\tau}_{ij} &= \tau_{\bar{i}j}\,. \end{aligned} \tag{5.109}$$

Since the two nucleon interaction conserves angular momentum projection ($m_i + m_j = m_k + m_l$ for v_{ijkl}), the HF Hamiltonian and the pair potential follow the partitioning of ρ and τ.

$$\mathcal{H} = \begin{bmatrix} \mathcal{H} & 0 \\ 0 & \bar{\mathcal{H}} \end{bmatrix} \qquad \Delta = \begin{bmatrix} 0 & \Delta \\ \bar{\Delta} & 0 \end{bmatrix} \tag{5.110}$$

where $\quad H_{ij} = \mathcal{H}_{ij} \qquad \Delta_{ij} = \Delta_{i\bar{j}} \qquad (5.111)$

$$\bar{H}_{ij} = \mathcal{H}_{\bar{i}\bar{j}} \qquad \bar{\Delta}_{ij} = \Delta_{\bar{i}j} .$$

The elements of the HF Hamiltonian (5.23,5.25) are

$$H_{ij} = T_{ij} + \sum_{k\ell} \{ \langle ik|v|j\ell\rangle_A \rho_{\ell k} + \langle i\bar{k}|v|j\bar{\ell}\rangle_A \bar{\rho}_{\ell k} \} \qquad (5.112)$$

$$\bar{H}_{ij} = T_{ij} + \sum_{k\ell} \{ \langle ik|v|j\ell\rangle_A \bar{\rho}_{\ell k} + \langle i\bar{k}|v|j\bar{\ell}\rangle_A \rho_{\ell k} \}$$

where we have used $T_{\bar{i}\bar{j}} = T_{ij}$ and $\langle \bar{i}\bar{j}|v|\bar{k}\bar{\ell}\rangle_A = \langle ij|v|k\ell\rangle_A$. The expression for the pair potential (5.27) simplifies.

$$\Delta_{mn} = \tfrac{1}{2} \sum_{k\ell} \langle mn|v|k\bar{\ell}\rangle_A \tau_{k\bar{\ell}} + \tfrac{1}{2} \sum_{k\ell} \langle mn|v|\bar{k}\ell\rangle_A \tau_{\bar{k}\ell}$$

Since τ is anti-symmetric and $\langle mn|v|\bar{k}\ell\rangle_A = -\langle mn|v|\ell\bar{k}\rangle_A$, the second sum equals the first sum.

$$\Delta_{mn} = \sum_{k\ell} \langle mn|v|k\bar{\ell}\rangle_A \tau_{k\bar{\ell}} \qquad (5.113)$$

The non-vanishing components of Δ are $\Delta_{i\bar{j}}$ and $\Delta_{\bar{i}j}$.

$$\Delta_{ij} = \sum_{k\ell} \langle i\bar{j}|v|k\bar{\ell}\rangle_A \tau_{k\ell}$$

$$\bar{\Delta}_{ij} = \sum_{k\ell} \langle i\bar{j}|v|k\bar{\ell}\rangle_A \bar{\tau}_{k\ell} \qquad (5.114)$$

The $\mathcal{K}$ matrix (5.42) has the form

$$\begin{bmatrix} H-\lambda & 0 & 0 & \Delta \\ 0 & \bar{H}-\lambda & \bar{\Delta} & 0 \\ 0 & \bar{\Delta}^{+} & \lambda-\tilde{H} & 0 \\ \Delta^{+} & 0 & 0 & \lambda-\tilde{\bar{H}} \end{bmatrix} \qquad (5.115)$$

so that the HFB equations (5.41) decouple into two sets.

$$\begin{bmatrix} H-\lambda & \Delta \\ \Delta^{+} & \lambda-\tilde{\tilde{H}} \end{bmatrix} \begin{bmatrix} \underline{u}_k \\ \underline{v}_k \end{bmatrix} = E_k \begin{bmatrix} \underline{u}_k \\ \underline{v}_k \end{bmatrix}$$

$$\begin{bmatrix} \bar{H}-\lambda & \bar{\Delta} \\ \bar{\Delta}^{+} & \lambda-\tilde{H} \end{bmatrix} \begin{bmatrix} \bar{\underline{u}}_k \\ \bar{\underline{v}}_k \end{bmatrix} = E_{\bar{k}} \begin{bmatrix} \bar{\underline{u}}_k \\ \bar{\underline{v}}_k \end{bmatrix} \qquad (5.116)$$

Consequently the new set of quasiparticle co-ordinates has the form of (5.103). Therefore, choosing the quasiparticle transformation to be a linear combination of the set $\{a^{+}_{k}\}$ and the set $\{a_{\bar{k}}\}$ is a self-consistent representation which will propagate through at each iteration. Note that the argument so far does not require time-reversal symmetry, nor does it require the mass number A to be even. We have derived simplified expressions for H_o' and H_2' which are valid whenever $\Gamma_{ij} = \Gamma_{\bar{i}\bar{j}} = \Delta_{ij} = \Delta_{\bar{i}\bar{j}} = 0$ (see equations 3.35 - 3.40).

We now restrict our attention to systems with time-reversal degeneracy. This is achieved by relating $\bar{u}$ to u and $\bar{v}$ to v . The usual convention is

$$\bar{u} = u \qquad \bar{v} = -v.$$

Instead we determine the phases by

$$b^{+}_{\bar{j}} = \mathcal{T} b^{+}_{j} \mathcal{T}^{-1}. \qquad (5.117a)$$

Since

$$\mathcal{T} \begin{Bmatrix} a^{+}_{k} \\ a_{k} \end{Bmatrix} \mathcal{T}^{-1} = + \begin{Bmatrix} a^{+}_{\bar{k}} \\ a_{\bar{k}} \end{Bmatrix} \qquad (5.117b)$$

$$\mathcal{T} \begin{Bmatrix} a^{+}_{\bar{k}} \\ a_{\bar{k}} \end{Bmatrix} \mathcal{T}^{-1} = - \begin{Bmatrix} a^{+}_{k} \\ a_{k} \end{Bmatrix}$$

and since $\mathcal{T}$ is anti-linear, we find

$$\mathcal{T} b_J^+ \mathcal{T}^{-1} = \sum_K (u_{JK}^* a_{\bar{K}}^+ - v_{JK}^* a_K) . \tag{5.117c}$$

Compare to (5.106c). The phases are

$$\bar{u}_{JK} = u_{JK}^* \qquad \bar{v}_{JK} = - v_{JK}^* . \tag{5.117d}$$

It then follows that

$$\mathcal{T} \begin{Bmatrix} b_J^+ \\ b_J \end{Bmatrix} \mathcal{T}^{-1} = + \begin{Bmatrix} b_{\bar{J}}^+ \\ b_{\bar{J}} \end{Bmatrix} \tag{5.117e}$$

$$\mathcal{T} \begin{Bmatrix} b_{\bar{J}}^+ \\ b_{\bar{J}} \end{Bmatrix} \mathcal{T}^{-1} = - \begin{Bmatrix} b_J^+ \\ b_J \end{Bmatrix} .$$

Therefore

$$\mathcal{T} b_J b_{\bar{J}} \mathcal{T}^{-1} = (\mathcal{T} b_J \mathcal{T}^{-1})(\mathcal{T} b_{\bar{J}} \mathcal{T}^{-1}) = - b_{\bar{J}} b_J = b_J b_{\bar{J}} . \tag{5.117f}$$

The ground state wave function is

$$|\Phi_0\rangle = \prod_{J>0} b_J b_{\bar{J}} |0\rangle . \tag{5.117g}$$

Since $\qquad \mathcal{T}|0\rangle = |0\rangle \qquad$ (5.117h)

we have

$$\mathcal{T}|\Phi_0\rangle = \prod_{J>0} \mathcal{T} b_J b_{\bar{J}} \mathcal{T}^{-1} |0\rangle = \prod_{J>0} b_J b_{\bar{J}} |0\rangle$$

so that $|\Phi_0\rangle$ is invariant under time-reversal.

$$\mathcal{T}|\Phi_0\rangle = |\Phi_0\rangle \tag{5.117i}$$

Therefore time-reversal is a self-consistent symmetry.

The quasiparticle transformations(5.106) become

$$b_J^\dagger = \sum_K{}' \left(u_{JK}\, a_K^\dagger + v_{JK}\, a_{\bar{K}} \right) \tag{5.118a}$$

$$b_{\bar{J}} = \sum_K{}' \left(u_{JK}\, a_{\bar{K}} - v_{JK}\, a_K^\dagger \right) \tag{5.118b}$$

and

$$b_{\bar{J}}^\dagger = \sum_K{}' \left(u_{JK}^*\, a_{\bar{K}}^\dagger - v_{JK}^*\, a_K \right) \tag{5.118c}$$

$$b_J = \sum_K{}' \left(u_{JK}^*\, a_K + v_{JK}^*\, a_{\bar{K}}^\dagger \right). \tag{5.118d}$$

The unitarity conditions (5.5) are

$$u u^\dagger + v v^\dagger = I \tag{5.119a}$$

$$u v^\dagger - v u^\dagger = 0 \tag{5.119b}$$

$$u^\dagger u + v^\dagger v = I \tag{5.119c}$$

$$u^\dagger v - v^\dagger u = 0 . \tag{5.119d}$$

The density matrix (5.107) is

$$\rho = (v^\dagger v)^* \quad \text{or} \quad \rho_{JL} = \sum_K{}' v_{KL}^*\, v_{KJ} \tag{5.120}$$

with the time-reversal symmetry

$$\bar{\rho} = \rho^* . \tag{5.121}$$

Clearly ρ is self-adjoint.

$$\rho^\dagger = \rho \tag{5.122}$$

The pairing tensor (5.108) is

$$\tau = -(v^\dagger u)^* \quad \text{or} \quad \tau_{JL} = -\sum_K{}' u_{KL}^*\, v_{KJ} \tag{5.123}$$

with the time-reversal symmetry

$$\bar{\tau} = -\tau^* . \tag{5.124}$$

Also, since τ is antisymmetric (see 5.109)

$$\bar{\tau} = -\tilde{\tau} . \tag{5.125}$$

Combining the last two relations, we find that the reduced pairing tensor τ is Hermitian.

$$\tau^{\dagger} = \tau \tag{5.126}$$

The unitarity condition (5.119d) also provides (5.126). The constraints (5.85, 5.86) reduce to

$$\rho - \rho^2 = \tau^2 \tag{5.127}$$

$$[\rho, \tau]_- = 0 . \tag{5.128}$$

The HF Hamiltonian (5.112) is

$$\mathcal{H}_{ij} = T_{ij} + \sum_{k\ell} \{ \langle ik|v|j\ell\rangle_A \rho_{\ell k} + \langle i\bar{k}|v|j\bar{\ell}\rangle_A \rho^*_{\ell k} \} \tag{5.129}$$

with the time-reversal symmetry

$$\bar{\mathcal{H}} = \mathcal{H}^* . \tag{5.130}$$

Since $\mathcal{H}$ is Hermitian

$$\mathcal{H}^{\dagger} = \mathcal{H} . \tag{5.131}$$

The pair potential is given in (5.114). The time-reversal symmetry is

$$\bar{\Delta} = -\Delta^* , \tag{5.132}$$

Since Δ is anti-symmetric (see 5.111)

$$\bar{\Delta} = -\tilde{\Delta} . \tag{5.133}$$

The last two relations combine to show that the reduced pair potential is self-adjoint.

$$\Delta^{\dagger} = \Delta \tag{5.134}$$

The HFB equations (5.116) become

$$\begin{bmatrix} \mathcal{H}-\lambda & \Delta \\ \Delta & \lambda-\mathcal{H} \end{bmatrix} \begin{bmatrix} \underline{u}_k \\ \underline{v}_k \end{bmatrix} = E_k \begin{bmatrix} \underline{u}_k \\ \underline{v}_k \end{bmatrix}. \tag{5.135}$$

The equations are reduced in dimension by a factor of two. Note that the form of this energy matrix is somewhat different than that of the complete $\mathcal{K}$ matrix (5.42). The second set of equations in (5.116) are

$$\begin{bmatrix} \mathcal{H}^*-\lambda & -\Delta^* \\ -\Delta^* & \lambda-\mathcal{H}^* \end{bmatrix} \begin{bmatrix} \underline{\bar{u}}_k \\ \underline{\bar{v}}_k \end{bmatrix} = E_{\bar{k}} \begin{bmatrix} \underline{\bar{u}}_k \\ \underline{\bar{v}}_k \end{bmatrix}.$$

Rewriting

$$\begin{bmatrix} \mathcal{H}^*-\lambda & \Delta^* \\ \Delta^* & \lambda-\mathcal{H}^* \end{bmatrix} \begin{bmatrix} \underline{\bar{u}}_k \\ -\underline{\bar{v}}_k \end{bmatrix} = E_{\bar{k}} \begin{bmatrix} \underline{\bar{u}}_k \\ -\underline{\bar{v}}_k \end{bmatrix}$$

and complex conjugating

$$\begin{bmatrix} \mathcal{H}-\lambda & \Delta \\ \Delta & \lambda-\mathcal{H} \end{bmatrix} \begin{bmatrix} \underline{\bar{u}}_k^* \\ -\underline{\bar{v}}_k^* \end{bmatrix} = E_{\bar{k}} \begin{bmatrix} \underline{\bar{u}}_k^* \\ -\underline{\bar{v}}_k^* \end{bmatrix}$$

and comparing to (5.135) we find

$$\bar{u} = u^* \qquad \bar{v} = -v^*$$

so that our phase choice is self-consistent. Also

$$E_{\bar{k}} = E_k$$

so that the quasiparticles possess time-reversal degeneracy.

Since the rotation operator $R_y(\pi)$ is

$$R_y(\pi) = K P \mathcal{J} \tag{5.136a}$$

where $K =$ complex conjugation (5.136b)

it follows that

$$R_y(\pi)\,|\Phi_0\rangle = K\,|\Phi_0\rangle. \tag{5.136c}$$

Consider the rotation operator $R_Z(\theta)$.

$$R_z(\theta)\,|Jm\rangle = e^{-im\theta}\,|Jm\rangle \tag{5.137a}$$

The particle operators transform as

$$R_z(\theta)\begin{Bmatrix} a^{\dagger}_{Jm} \\ a_{\overline{Jm}} \end{Bmatrix} R_z^{-1}(\theta) = e^{-im\theta}\begin{Bmatrix} a^{\dagger}_{Jm} \\ a_{\overline{Jm}} \end{Bmatrix} \tag{5.137b}$$

$$R_z(\theta)\begin{Bmatrix} a^{\dagger}_{\overline{Jm}} \\ a_{Jm} \end{Bmatrix} R_z^{-1}(\theta) = e^{+im\theta}\begin{Bmatrix} a^{\dagger}_{\overline{Jm}} \\ a_{Jm} \end{Bmatrix}.$$

Since the states $\{|K\rangle\}$ have $(m-\frac{1}{2})$ = even integer and the states $\{|\bar{K}\rangle\}$ have $(m-\frac{1}{2})$ = odd integer, they transform under $R_Z(\pi)$ as

$$R_z(\pi)\begin{Bmatrix} a^{\dagger}_{K} \\ a_{\bar{K}} \end{Bmatrix} R_z^{-1}(\pi) = -i\begin{Bmatrix} a^{\dagger}_{K} \\ a_{\bar{K}} \end{Bmatrix}$$

$$R_z(\pi)\begin{Bmatrix} a^{\dagger}_{\bar{K}} \\ a_{K} \end{Bmatrix} R_z^{-1}(\pi) = +i\begin{Bmatrix} a^{\dagger}_{\bar{K}} \\ a_{K} \end{Bmatrix}. \tag{5.137c}$$

The quasiparticle operators (5.118) therefore transform as

$$R_z(\pi)\begin{Bmatrix} b^{\dagger}_{J} \\ b_{\bar{J}} \end{Bmatrix} R_z^{-1}(\pi) = -i\begin{Bmatrix} b^{\dagger}_{J} \\ b_{\bar{J}} \end{Bmatrix}$$

$$R_z(\pi)\begin{Bmatrix} b^{\dagger}_{\bar{J}} \\ b_{J} \end{Bmatrix} R_z^{-1}(\pi) = +i\begin{Bmatrix} b^{\dagger}_{\bar{J}} \\ b_{J} \end{Bmatrix}. \tag{5.137d}$$

Consequently

$$R_z(\pi)\, b_j\, b_{\bar{j}}\, R_z^{-1}(\pi) = \tag{5.137e}$$
$$\{R_z(\pi)\, b_j\, R_z^{-1}(\pi)\}\{R_z(\pi)\, b_{\bar{j}}\, R_z^{-1}(\pi)\} = b_j\, b_{\bar{j}} \,.$$

The refererence state wave function is (5.117g).

Since $$R_z(\theta)\,|0\rangle = |0\rangle \tag{5.137f}$$

we have

$$R_z(\pi)\,|\Phi_0\rangle = \prod_{j>0} R_z(\pi)\, b_j\, b_{\bar{j}}\, R_z^{-1}(\pi)|0\rangle = \prod_{j>0} b_j\, b_{\bar{j}}\,|0\rangle$$

so that $|\Phi_0\rangle$ is invariant under $R_z(\pi)$.

$$R_z(\pi)\,|\Phi_0\rangle = |\Phi_0\rangle \tag{5.138}$$

Therefore rotation by π about the Z axis is a self-consistent symmetry.

Axial symmetry is introduced by restricting the quasiparticle transformation (5.118) to states $|k\rangle$ with the same value of m. The quasiparticle operators then transform as

$$R_z(\theta)\begin{Bmatrix} b^{+}_{j} \\ b_{\bar{j}} \end{Bmatrix} R_z^{-1}(\theta) = e^{-im\theta}\begin{Bmatrix} b^{+}_{j} \\ b_{\bar{j}} \end{Bmatrix} \tag{5.139a}$$

$$R_z(\theta)\begin{Bmatrix} b^{+}_{\bar{j}} \\ b_{j} \end{Bmatrix} R_z^{-1}(\theta) = e^{+im\theta}\begin{Bmatrix} b^{+}_{\bar{j}} \\ b_{j} \end{Bmatrix}.$$

Therefore

$$R_z(\theta)\, b_j\, b_{\bar{j}}\, R_z^{-1}(\theta) = \tag{5.139b}$$
$$\{R_z(\theta)\, b_j\, R_z^{-1}(\theta)\}\{R_z(\theta)\, b_{\bar{j}}\, R_z^{-1}(\theta)\} = b_j\, b_{\bar{j}} \,.$$

The ground state transforms as

$$R_z(\theta)\,|\Phi_0\rangle = \prod_{J>0} R_z(\theta)\, b_J\, b_{\bar{J}}\, R_z^{-1}(\theta)\,|0\rangle = \prod_{J>0} b_J\, b_{\bar{J}}\,|0\rangle$$

so that $|\Phi_0\rangle$ is invariant under $R_z(\theta)$.

$$R_z(\theta)\,|\Phi_0\rangle = |\Phi_0\rangle \qquad (\text{for all } \theta) \tag{5.139c}$$

Therefore axial symmetry is a self-consistent symmetry. The components of R and $\mathcal{K}$ have the structure

$$\rho_{ij} = \tau_{ij} = \mathcal{H}_{ij} = \Delta_{ij} = 0 \qquad \text{unless } m_i = m_j \tag{5.140}$$

The $\mathcal{K}$ matrix therefore separates into blocks like (5.135) for each m.

Spherical symmetry is introduced by restricting the quasiparticle transformation (5.118) to states $|K\rangle$ with the same value of ljm, with degeneracy in m for each lj (that is, $u_{Nljm\tau}$ and $v_{Nljm\tau}$ are independent of m). Then ρ and τ will not connect states with differing lj. Only radial and isospin mixing are permitted.

The isospin symmetries are of special importance to us. The isospin quantum number will now be explicitly denoted, with the notation

$$(M_{\tau_1\tau_2})_{ij} = M_{i\tau_1, j\tau_2} \tag{5.141}$$

where $M_{\tau_1\tau_2}$ is a sub-matrix of M. The quasiparticle co-ordinates are

$$\mathcal{U} = \begin{bmatrix} \mathcal{U}_{pp} & \mathcal{U}_{pn} \\ \mathcal{U}_{np} & \mathcal{U}_{nn} \end{bmatrix} \qquad \mathcal{V} = \begin{bmatrix} \mathcal{V}_{pp} & \mathcal{V}_{pn} \\ \mathcal{V}_{np} & \mathcal{V}_{nn} \end{bmatrix} . \tag{5.142}$$

The unitarity conditions (5.119) are

$$\sum_{\tau} (\mathcal{U}_{\tau_1\tau} \mathcal{U}^{\dagger}_{\tau_2\tau} + \mathcal{V}_{\tau_1\tau} \mathcal{V}^{\dagger}_{\tau_2\tau}) = \delta_{\tau_1\tau_2} \tag{5.143a}$$

$$\sum_{\tau} (\mathcal{U}_{\tau_1\tau} \mathcal{V}^{\dagger}_{\tau_2\tau} - \mathcal{V}_{\tau_1\tau} \mathcal{U}^{\dagger}_{\tau_2\tau}) = 0 \tag{5.143b}$$

$$\sum_{\tau} (\mathcal{U}^{\dagger}_{\tau\tau_1} \mathcal{U}_{\tau\tau_2} + \mathcal{V}^{\dagger}_{\tau\tau_1} \mathcal{V}_{\tau\tau_2}) = \delta_{\tau_1\tau_2} \tag{5.143c}$$

$$\sum_{\tau} (\mathcal{U}^{\dagger}_{\tau\tau_1} \mathcal{V}_{\tau\tau_2} - \mathcal{V}^{\dagger}_{\tau\tau_1} \mathcal{U}_{\tau\tau_2}) = 0 . \tag{5.143d}$$

The reduced density matrix and pairing tensor are

$$\rho = \begin{bmatrix} \rho_{pp} & \rho_{pn} \\ \rho_{np} & \rho_{nn} \end{bmatrix} \qquad \tau = \begin{bmatrix} \tau_{pp} & \tau_{pn} \\ \tau_{np} & \tau_{nn} \end{bmatrix} . \tag{5.144}$$

Since ρ and τ are self-adjoint

$$\begin{aligned} \rho^{\dagger}_{pp} &= \rho_{pp} & \tau^{\dagger}_{pp} &= \tau_{pp} \\ \rho^{\dagger}_{pn} &= \rho_{np} & \tau^{\dagger}_{pn} &= \tau_{np} \\ \rho^{\dagger}_{nn} &= \rho_{nn} & \tau^{\dagger}_{nn} &= \tau_{nn} . \end{aligned} \tag{5.145}$$

The density matrix is evaluated with (5.120).

$$\rho_{\tau_1\tau_2} = \sum_{\tau} (\mathcal{V}^{\dagger}_{\tau\tau_1} \mathcal{V}_{\tau\tau_2})^* \tag{5.146}$$

The various components are

$$\begin{aligned} \rho_{pp} &= (\mathcal{V}^{\dagger}_{pp} \mathcal{V}_{pp} + \mathcal{V}^{\dagger}_{np} \mathcal{V}_{np})^* \\ \rho_{pn} &= (\mathcal{V}^{\dagger}_{pp} \mathcal{V}_{pn} + \mathcal{V}^{\dagger}_{np} \mathcal{V}_{nn})^* \\ \rho_{np} &= (\mathcal{V}^{\dagger}_{pn} \mathcal{V}_{pp} + \mathcal{V}^{\dagger}_{nn} \mathcal{V}_{np})^* \\ \rho_{nn} &= (\mathcal{V}^{\dagger}_{pn} \mathcal{V}_{pn} + \mathcal{V}^{\dagger}_{nn} \mathcal{V}_{nn})^* . \end{aligned} \tag{5.147}$$

Similarly the pairing tensor is given by (5.123)

$$\tau_{\tau_1\tau_2} = -\sum_{\tau}{}' \left(V^{\dagger}_{\tau\tau_1} U_{\tau\tau_2} \right)^* \tag{5.148}$$

so that

$$\begin{aligned}
\tau_{pp} &= -\left(V^{\dagger}_{pp} U_{pp} + V^{\dagger}_{np} U_{np} \right)^* \\
\tau_{pn} &= -\left(V^{\dagger}_{pp} U_{pn} + V^{\dagger}_{np} U_{nn} \right)^* \\
\tau_{np} &= -\left(V^{\dagger}_{pn} U_{pp} + V^{\dagger}_{nn} U_{np} \right)^* \\
\tau_{nn} &= -\left(V^{\dagger}_{pn} U_{pn} + V^{\dagger}_{nn} U_{nn} \right)^* .
\end{aligned} \tag{5.149}$$

The reduced HF Hamiltonian and pair potential are

$$\mathcal{H} = \begin{bmatrix} \mathcal{H}_{pp} & \mathcal{H}_{pn} \\ \mathcal{H}_{np} & \mathcal{H}_{nn} \end{bmatrix} \qquad \Delta = \begin{bmatrix} \Delta_{pp} & \Delta_{pn} \\ \Delta_{np} & \Delta_{nn} \end{bmatrix} . \tag{5.150}$$

Since $\mathcal{H}$ and Δ are self-adjoint

$$\begin{aligned}
\mathcal{H}^{\dagger}_{pp} &= \mathcal{H}_{pp} & \Delta^{\dagger}_{pp} &= \Delta_{pp} \\
\mathcal{H}^{\dagger}_{pn} &= \mathcal{H}_{np} & \Delta^{\dagger}_{pn} &= \Delta_{np} \\
\mathcal{H}^{\dagger}_{nn} &= \mathcal{H}_{nn} & \Delta^{\dagger}_{nn} &= \Delta_{nn} .
\end{aligned} \tag{5.151}$$

The HF Hamiltonian (5.129) has matrix elements

$$\begin{aligned}
(\mathcal{H}_{\tau_1\tau_2})_{ij} = T_{i\tau_1, j\tau_2} + \sum_{\substack{k\ell \\ \tau_3\tau_4}}{}' \Big\{ & \langle i\tau_1, k\tau_3 | v | j\tau_2, \ell\tau_4 \rangle_A \left(\rho_{\tau_4\tau_3} \right)_{\ell k} \\
& + \langle i\tau_1, \bar{k}\tau_3 | v | j\tau_2, \bar{\ell}\tau_4 \rangle_A \left(\rho_{\tau_4\tau_3} \right)^*_{\ell k} \Big\} .
\end{aligned} \tag{5.152}$$

Matrix elements of v are non-zero only if $\tau_1 + \tau_2 = \tau_3 + \tau_4$.

Therefore the diagonal-isospin elements of $\mathcal{H}$ are

$$(\mathcal{H}_{\tau\tau})_{ij} = T_{ij} + \sum_{k\ell\tau'} \{ \langle i\tau, k\tau' | v | j\tau, \ell\tau' \rangle_A (\rho_{\tau'\tau'})_{\ell k} + \langle i\tau, \bar{k}\tau' | v | j\tau, \bar{\ell}\tau' \rangle_A (\rho_{\tau'\tau'})^*_{\ell k} \} \tag{5.153}$$

and the off-diagonal -isospin elements are

$$(\mathcal{H}_{\tau-\tau})_{ij} = \sum_{k\ell} \{ \langle i\tau, k-\tau | v | j-\tau, \ell\tau \rangle_A (\rho_{\tau-\tau})_{\ell k} + \langle i\tau, \bar{k}-\tau | v | j-\tau, \bar{\ell}\tau \rangle_A (\rho_{\tau-\tau})^*_{\ell k} \} . \tag{5.154}$$

The pair potential (5.114) has elements

$$(\Delta_{\tau_1\tau_2})_{ij} = \sum_{\substack{k\ell \\ \tau_3\tau_4}} \langle i\tau_1, \bar{j}\tau_2 | v | k\tau_3, \bar{\ell}\tau_4 \rangle_A (\tau_{\tau_3\tau_4})_{k\ell} . \tag{5.155}$$

The $|T_Z| = 1$ pair potential is $\Delta_{\tau\tau}$. Only protons (neutrons) may contribute to the proton (neutron) pair potential.

$$(\Delta_{\tau\tau})_{ij} = \sum_{k\ell} \langle i\tau, \bar{j}\tau | v | k\tau, \bar{\ell}\tau \rangle_A (\tau_{\tau\tau})_{k\ell} \tag{5.156}$$

Since $\langle i\tau, j\tau | v | k\tau, \ell\tau \rangle_A =$

$$\sum_{T} \langle \tfrac{1}{2}\tau\, \tfrac{1}{2}\tau | T\, 2\tau \rangle^2 \langle i j T | v | k \ell T \rangle_A =$$

$$\langle i j\, T=1 | v | k \ell\, T=1 \rangle_A \quad \text{for } \tau = \pm 1/2$$

the $|T_Z| = 1$ potential is

$$(\Delta_{\tau\tau})_{ij} = \sum_{k\ell} \langle i \bar{j}\, T=1 | v | k \bar{\ell}\, T=1 \rangle_A (\tau_{\tau\tau})_{k\ell} . \tag{5.157}$$

The $T_Z = 0$ pair potential is $\Delta_{\tau-\tau}$.

$$(\Delta_{\tau-\tau})_{ij} = \sum_{k\ell\tau'} \langle i\tau, \bar{j}-\tau | v | k\tau', \bar{\ell}-\tau' \rangle_A (\tau_{\tau'-\tau'})_{k\ell} \tag{5.158}$$

It may be separated into T = 0 and T = 1 components. Consider the matrix element

$$\langle i\tau, j-\tau | v | k\tau', l-\tau' \rangle_A =$$

$$\sum_T \langle \tfrac{1}{2}\tau\, \tfrac{1}{2}-\tau | T0 \rangle \langle \tfrac{1}{2}\tau'\, \tfrac{1}{2}-\tau' | T0 \rangle \langle ijT | v | klT \rangle_A .$$

The product of the Clebsch-Gordon coefficients is evaluated in the table below.

	$T=0$	$T=1$
$\tau'=\tau$	$1/2$	$1/2$
$\tau'=-\tau$	$-1/2$	$1/2$

Therefore the $T_Z = 0$ potential is

$$(\Delta_{\tau-\tau})_{ij} = \frac{1}{2}\sum_{kl} \langle i\bar{j}\, T=1 | v | k\bar{l}\, T=1 \rangle_A (\tau_{\tau-\tau} + \tau_{-\tau\tau})_{kl}$$
$$+ \frac{1}{2}\sum_{kl} \langle i\bar{j}\, T=0 | v | k\bar{l}\, T=0 \rangle_A (\tau_{\tau-\tau} - \tau_{-\tau\tau})_{kl} . \tag{5.159}$$

Since $\tau_{-\tau\tau} = \tau^{+}_{\tau-\tau}$

$$(\Delta_{\tau-\tau})_{ij} = \frac{1}{2}\sum_{kl} \langle i\bar{j}\, T=1 | v | k\bar{l}\, T=1 \rangle_A (\tau_{\tau-\tau} + \tau^{+}_{\tau-\tau})_{kl} \tag{5.160}$$
$$+ \frac{1}{2}\sum_{kl} \langle i\bar{j}\, T=0 | v | k\bar{l}\, T=0 \rangle_A (\tau_{\tau-\tau} - \tau^{+}_{\tau-\tau})_{kl} .$$

The T = 1 and T = 0 components of the $T_Z = 0$ pair potential are

$$(\Delta^{T=1}_{\tau-\tau})_{ij} = \frac{1}{2}\sum_{kl} \langle i\bar{j}\, T=1 | v | k\bar{l}\, T=1 \rangle_A (\tau_{\tau-\tau} + \tau^{+}_{\tau-\tau})_{kl} \tag{5.161}$$

$$(\Delta^{T=0}_{\tau-\tau})_{ij} = -\frac{1}{2} i \sum_{kl} \langle i\bar{j}\, T=0 | v | k\bar{l}\, T=0 \rangle_A (\tau_{\tau-\tau} - \tau^{+}_{\tau-\tau})_{kl} \tag{5.162}$$

so that

$$\Delta_{\tau-\tau} = \Delta^{T=1}_{\tau-\tau} + i\,\Delta^{T=0}_{\tau-\tau} \quad . \tag{5.163}$$

Since $\left\{ \begin{array}{l} (\tau_{\tau-\tau} + \tau^{+}_{\tau-\tau}) \\ -i\,(\tau_{\tau-\tau} - \tau^{+}_{\tau-\tau}) \end{array} \right\}$ are Hermitian

and $\langle i\,\bar{j}\,T|N|k\,\bar{l}\,T\rangle_A = \langle j\,\bar{i}\,T|N|l\,\bar{k}\,T\rangle_A$,

the T = 1 and T = 0 potentials are Hermitian.

$$(\Delta^{T=1}_{\tau-\tau})^{+} = \Delta^{T=1}_{\tau-\tau} \tag{5.164}$$

$$(\Delta^{T=0}_{\tau-\tau})^{+} = \Delta^{T=0}_{\tau-\tau} \tag{5.165}$$

From (5.159) we note that

$$\Delta^{T=1}_{\tau-\tau} = \Delta^{T=1}_{-\tau\tau} \tag{5.166}$$

$$\Delta^{T=0}_{\tau-\tau} = -\Delta^{T=0}_{-\tau\tau} \tag{5.167}$$

which verifies that

$$\Delta^{+}_{\tau-\tau} = \Delta_{-\tau\tau} \quad . \tag{5.168}$$

$i\,\Delta^{T=0}_{\tau-\tau}$ is anti-Hermitian. If the quasiparticle transformation is restricted to real parameters, it follows that

$$(\Delta^{T=0}_{\tau-\tau})_{KK} = 0 \quad . \tag{5.169}$$

The unitarity conditions would cause the diagonal elements of the T = 0 pair potential to vanish. This is certainly

unsatisfactory, since the diagonal elements are usually considered to be the most important ones. In the BCS theory only the diagonal elements of Δ are included, in which case there will be no T = 0 pairing. (The phases may be altered so that T = 1 pairing vanishes instead of T = 0 pairing.) We conclude that for generalized pairing to exist, the unitarity conditions alone require that the quasiparticle transformation be complex.

The same reasoning accounts for choosing

$$\bar{u} = u^* \qquad \bar{v} = -v^*$$

rather than

$$\bar{u} = u \qquad \bar{v} = -v .$$

Had we selected the latter phase, unitarity condition (5.5d) would reduce to

$$u^\dagger v - (v^\dagger u)^* = 0 .$$

The reduced pairing tensor (5.108) becomes

$$\tau = -v^\dagger u$$

so that τ is symmetric.

$$\tilde{\tau} = \tau$$

Therefore

$$\tilde{\tau}_{pn} = \tau_{np} .$$

The $T_Z = 0$ potentials would be (see 5.159)

$$(\Delta^{T=1}_{\tau-\tau})_{ij} = \frac{1}{2} \sum_{kl} \langle i\bar{j}\, T=1 | v | k\bar{l}\, T=1 \rangle_A \, (\tau_{\tau-\tau} + \tilde{\tau}_{\tau-\tau})_{kl}$$

$$(\Delta^{T=0}_{\tau-\tau})_{ij} = -\frac{1}{2} i \sum_{kl} \langle i\bar{j}\, T=0 | v | k\bar{l}\, T=0 \rangle_A \, (\tau_{\tau-\tau} - \tilde{\tau}_{\tau-\tau})_{kl} .$$

Since $(\tau_{\tau-\tau} - \tilde{\tau}_{\tau-\tau})_{K\ell}$ is antisymmetric

$$\tilde{\Delta}^{T=0}_{\tau-\tau} = -\Delta^{T=0}_{\tau-\tau}$$

so that

$$(\Delta^{T=0}_{\tau-\tau})_{KK} = 0$$

even if the quasiparticle co-ordinates are complex. For the reasons given above, this phase choice is therefore unacceptable for generalized pairing.

The wave function is rotationally invariant if

$$e^{i\underline{J}\cdot\underline{\theta}} \, |\Phi_0\rangle = |\Phi_0\rangle .$$

Then $|\Phi_0\rangle$ will be an eigenstate of $\underline{J}$ with J = 0. Similarly the wave function is rotationally invariant in isospin space if

$$e^{i\underline{T}\cdot\underline{\theta}} \, |\Phi_0\rangle = |\Phi_0\rangle .$$

Then $|\Phi_0\rangle$ will be an eigenstate of $\underline{T}$ with T = 0. If T = 1 pairing is present the several T = 1 vectors (one from each pair) can couple to different resultants, so that $|\Phi_0\rangle$ will probably be a linear combination of states with various T values. States of good T may be obtained by isospin projection. In general, therefore, $|\Phi_0\rangle$ is not rotationally invariant in isospin space. For T = 0 pairing, however, the resultant isospin vector is ensured to be T = 0, so that $|\Phi_0\rangle$ is invariant under $e^{i\underline{T}\cdot\underline{\theta}}$.

6. Generalized Pairing in N = Z Even - Even Nuclei

For N = Z even - even nuclei the time-reversal and isospin symmetries may be used to simplify the form of the HFB equations. Guided by our experience with the generalized gap equations (Chapter IV.) we choose the following symmetries and shall demonstrate that they may be self-consistent.

$$\rho = \begin{bmatrix} \rho_{pp} & 0 \\ 0 & \rho_{pp} \end{bmatrix} \qquad \tau = \begin{bmatrix} \tau_{pp} & \tau_{pn} \\ \tau_{pn}^{*} & -\tau_{pp} \end{bmatrix} \tag{5.170a}$$

$$\rho_{pp}, \tau_{pp} \text{ are Real.} \tag{5.170b}$$

Let $$\tau_{pn} = \tau_{pn}^{R} + i\,\tau_{pn}^{I} . \tag{5.171}$$

The unitarity conditions (5.127, 5.128) require that

$$\rho_{pp}, \tau_{pp}, \tau_{pn}^{R}, \tau_{pn}^{I} \tag{5.172}$$

a) are symmetric

b) commute with one another

and that

$$\rho_{pp} - \rho_{pp}^{2} = \tau_{pp}^{2} + (\tau_{pn}^{R})^{2} + (\tau_{pn}^{I})^{2} . \tag{5.173}$$

The HF Hamiltonian (5.152 - 5.154) and the pair potential (5.155 - 5.168) have the representation

$$\mathcal{H} = \begin{bmatrix} \mathcal{H}_{pp} & 0 \\ 0 & \mathcal{H}_{pp} \end{bmatrix} \qquad \Delta = \begin{bmatrix} \Delta_{pp} & \Delta_{pn} \\ \Delta_{pn}^{*} & -\Delta_{pp} \end{bmatrix} \tag{5.174}$$

where

$$\Delta_{pn} = \Delta_{pn}^{T=1} + i\,\Delta_{pn}^{T=0} \tag{5.175}$$

and

$$\mathcal{H}_{pp},\ \Delta_{pp},\ \Delta_{pn}^{T=1},\ \Delta_{pn}^{T=0} \quad \text{are} \tag{5.176}$$

a) real

b) symmetric.

Δ_{pn} is also symmetric. The components of $\mathcal{H}$ and Δ are

$$(\mathcal{H}_{pp})_{ij} = T_{ij} + \sum_{k\ell T} \{ \langle i p, k \tau | v | j p, \ell \tau \rangle_A + \langle i p, \bar{k} \tau | v | j p, \bar{\ell} \tau \rangle_A \} (\rho_{pp})_{k\ell} \tag{5.177}$$

$$(\Delta_{pp})_{ij} = \sum_{k\ell} \langle i \bar{j}\, T=1 | v | k \bar{\ell}\, T=1 \rangle_A \, (\tau_{pp})_{k\ell} \tag{5.178}$$

$$(\Delta_{pn}^{T=1})_{ij} = \sum_{k\ell} \langle i \bar{j}\, T=1 | v | k \bar{\ell}\, T=1 \rangle_A \, (\tau_{pn}^{R})_{k\ell} \tag{5.179}$$

$$(\Delta_{pn}^{T=0})_{ij} = \sum_{k\ell} \langle i \bar{j}\, T=0 | v | k \bar{\ell}\, T=0 \rangle_A \, (\tau_{pn}^{I})_{k\ell} \,. \tag{5.180}$$

The reduced HFB equations (5.135) have the form

$$\begin{bmatrix} \mathcal{H}_{pp}-\lambda & 0 & \Delta_{pp} & \Delta_{pn} \\ 0 & \mathcal{H}_{pp}-\lambda & \Delta_{pn}^{*} & -\Delta_{pp} \\ \Delta_{pp} & \Delta_{pn} & \lambda-\mathcal{H}_{pp} & 0 \\ \Delta_{pn}^{*} & -\Delta_{pp} & 0 & \lambda-\mathcal{H}_{pp} \end{bmatrix} \begin{bmatrix} (\underline{u}_{\tau p})_k \\ (\underline{u}_{\tau n})_k \\ (\underline{v}_{\tau p})_k \\ (\underline{v}_{\tau n})_k \end{bmatrix} = E_{\tau k} \begin{bmatrix} (\underline{u}_{\tau p})_k \\ (\underline{u}_{\tau n})_k \\ (\underline{v}_{\tau p})_k \\ (\underline{v}_{\tau n})_k \end{bmatrix} \tag{5.181}$$

where

$$(\underline{u}_{\tau_1 \tau_2})_k = \begin{bmatrix} (u_{\tau_1 \tau_2})_{k1} \\ (u_{\tau_1 \tau_2})_{k2} \\ \vdots \\ (u_{\tau_1 \tau_2})_{k\frac{N}{2}} \end{bmatrix} . \tag{5.182}$$

If

$$\begin{bmatrix} \mathcal{U}_{pp} \\ \mathcal{U}_{pn} \\ \mathcal{V}_{pp} \\ \mathcal{V}_{pn} \end{bmatrix} = \begin{bmatrix} \text{Real} \\ 0 \\ \text{Real} \\ \text{Complex} \end{bmatrix} \tag{5.183}$$

are a set of eigenvectors with eigenvalues E_1, then

$$\begin{bmatrix} \mathcal{U}_{np} \\ \mathcal{U}_{nn} \\ \mathcal{V}_{np} \\ \mathcal{V}_{nn} \end{bmatrix} = \begin{bmatrix} \mathcal{U}_{pn} \\ \mathcal{U}_{pp} \\ \mathcal{V}_{pn} \\ -\mathcal{V}_{pp} \end{bmatrix} \tag{5.184a}$$

are a set of eigenvectors with eigenvalues

$$E_2 = E_1 \, . \tag{5.184b}$$

This may be seen by writing out the components of the eigenvalue equation $\mathcal{K}\tilde{\mathcal{X}} = \tilde{\mathcal{X}}E$, where $\mathcal{K}$ is given in (5.181), $\mathcal{U}$ and $\mathcal{V}$ are given by (5.142), and E is

$$\begin{bmatrix} E_1 & 0 & 0 & 0 \\ 0 & E_2 & 0 & 0 \\ 0 & 0 & -E_1 & 0 \\ 0 & 0 & 0 & -E_2 \end{bmatrix} .$$

The unitarity conditions (5.143c) may then be applied to show that the new ρ and τ have the form (5.170).

The symmetries (5.170) have been introduced to ensure that

$$\langle \underline{T} \rangle = 0 \, . \tag{5.185a}$$

This constraint is satisfied if

$$\begin{aligned} \mathrm{Tr}\,\rho_{pn} &= \mathrm{Tr}\,\rho_{np} = 0 \\ \mathrm{Tr}\,\rho_{pp} &= \mathrm{Tr}\,\rho_{nn} \quad . \end{aligned} \tag{5.185b}$$

The implications of (5.185a) and the derivation of (5.185b) are given in IV.5.

7. Canonical Representation

For a system with time-reversal symmetry the unitarity conditions are (5.122, 5.126-5.128).

$$\rho^{+} = \rho \qquad\qquad [\rho, \tau]_{-} = 0$$

$$\tau^{+} = \tau \qquad\qquad \tau^{2} = \rho(1-\rho)$$

Since ρ and τ are Hermitian and commute they may be diagonalized by the same unitary transformation .

$$\begin{aligned} \rho &\rightarrow u^{+}\rho u \\ \tau &\rightarrow u^{+}\tau u \end{aligned} \tag{5.186}$$

In the rotated single particle basis ρ and τ are diagonal and real. Since

$$\rho = \begin{bmatrix} \rho & 0 \\ 0 & \rho^{*} \end{bmatrix} \qquad t = \begin{bmatrix} 0 & \tau \\ -\tau^{*} & 0 \end{bmatrix} \tag{5.187}$$

the density matrix and pairing tensor in the rotated basis have the form

$$\rho = \left[\begin{array}{cc|cc|c} \rho_{\alpha\alpha} & 0 & & 0 & \\ 0 & \rho_{\alpha\alpha} & & & \\ \hline & 0 & \rho_{\beta\beta} & 0 & \\ & & 0 & \rho_{\beta\beta} & \\ \hline & & & & \ddots \end{array}\right] \tag{5.188}$$

$$t = \left[\begin{array}{cc|cc|c} 0 & \tau_{\alpha\bar{\alpha}} & & 0 & \\ -\tau_{\alpha\bar{\alpha}} & 0 & & & \\ \hline & 0 & 0 & \tau_{\beta\bar{\beta}} & \\ & & -\tau_{\beta\bar{\beta}} & 0 & \\ \hline & & & & \ddots \end{array}\right]. \tag{5.189}$$

The time-reversal symmetries are

$$\rho_{\bar{\alpha}\bar{\alpha}} = \rho_{\alpha\alpha} \tag{5.190a}$$

$$\tau_{\bar{\alpha}\alpha} = -\tau_{\alpha\bar{\alpha}} \ . \tag{5.190b}$$

From the last unitarity condition we have

$$|\tau_{\alpha\bar{\alpha}}| = \sqrt{\rho_{\alpha\alpha}(1-\rho_{\alpha\alpha})} \ . \tag{5.191}$$

ρ is real and diagonal. τ is real and has non-vanishing elements only between time-reversed states. This representation of ρ and τ is termed the canonical representation, and the single particle states $|\alpha\rangle$, $|\beta\rangle$ ... are termed the canonical single particle basis.

The canonical representation was first determined by Bloch and Messiah.[4] They did not assume time-reversal symmetry, in which case $\tau_{\alpha\bar{\alpha}}$ may be complex. Since they work with τ (which is antisymmetric and does not transform in the usual way) rather than τ (which is Hermitian and transforms in the usual way) their proof is considerably more complicated than ours.

That ρ and τ transform in the same manner also follows from their definitions.

$$\rho_{jk} = \langle a^{+}_{k} a_{j} \rangle \qquad \tau_{jk} = \langle a_{\bar{k}} a_{j} \rangle$$

If a^{+}_{i} transforms as

$$a^{+}_{\alpha} = \sum_{k} D^{\alpha}_{k} a^{+}_{k}$$

then a_i transforms as

$$a_\alpha = \sum_k D_k^{\alpha *} a_k$$

and $a^+_i a_j$ transforms as

$$a^+_\alpha a_\beta = \sum_{k\ell} D_k^\alpha a^+_k a_\ell D_\ell^{\beta *} . \tag{5.192a}$$

Since $\bar{\rho} = \rho^*$

$$D_{\bar{k}}^{\bar{\alpha}} = D_k^{\alpha *}$$

so that $a_{\bar{i}}$ transforms as

$$a_{\bar{\alpha}} = \sum_k D_k^\alpha a_{\bar{k}}$$

and $a_{\bar{i}} a_j$ transforms as

$$a_{\bar{\alpha}} a_\beta = \sum_{k\ell} D_k^\alpha a_{\bar{k}} a_\ell D_\ell^{\beta *} . \tag{5.192b}$$

Similarly from the definitions of $\mathcal{H}$ and Δ (5.112, 5.114), it follows that the HF Hamiltonian and the pair potential transform in the same manner as ρ and τ .

$$\mathcal{H}_{\alpha\beta} = \sum_{k\ell} D_k^\alpha \mathcal{H}_{k\ell} D_\ell^{\beta *} \tag{5.192c}$$

$$\Delta_{\alpha\beta} = \sum_{k\ell} D_k^\alpha \Delta_{k\ell} D_\ell^{\beta *} \tag{5.192d}$$

The generalized density matrix R (5.56) separates into blocks.

$$R(\alpha) = \begin{bmatrix} \rho_{\alpha\alpha} & 0 & 0 & \tau_{\alpha\bar{\alpha}} \\ 0 & \rho_{\alpha\alpha} & -\tau_{\alpha\bar{\alpha}} & 0 \\ 0 & -\tau_{\alpha\bar{\alpha}} & 1-\rho_{\alpha\alpha} & 0 \\ \tau_{\alpha\bar{\alpha}} & 0 & 0 & 1-\rho_{\alpha\alpha} \end{bmatrix} \tag{5.193}$$

The quasiparticle co-ordinates are eigenvectors of R with eigenvalues of 0 (5.88).

$$\begin{bmatrix} \rho_{\alpha\alpha} & \tau_{\alpha\bar{\alpha}} \\ \tau_{\alpha\bar{\alpha}} & 1-\rho_{\alpha\alpha} \end{bmatrix} \begin{bmatrix} u_\alpha \\ -v_\alpha \end{bmatrix} = 0 \qquad \begin{bmatrix} \rho_{\alpha\alpha} & -\tau_{\alpha\bar{\alpha}} \\ -\tau_{\alpha\bar{\alpha}} & 1-\rho_{\alpha\alpha} \end{bmatrix} \begin{bmatrix} u_{\bar{\alpha}} \\ -v_{\bar{\alpha}} \end{bmatrix} = 0 \tag{5.194}$$

where (5.195)

$$u_\alpha = u_{\alpha\alpha} \qquad u_{\bar{\alpha}} = \bar{u}_{\alpha\alpha}$$
$$v_\alpha = -v_{\alpha\alpha} \qquad v_{\bar{\alpha}} = -\bar{v}_{\alpha\alpha}$$

The co-ordinates may be chosen real with the phase

$$u_{\bar{\alpha}} = u_\alpha = \text{Real} \tag{5.196}$$
$$v_{\bar{\alpha}} = -v_\alpha = \text{Real}.$$

The quasiparticle transformations are

$$b^+_\alpha = u_\alpha a^+_\alpha - v_\alpha a_{\bar{\alpha}} \tag{5.197}$$

$$b^+_{\bar{\alpha}} = u_\alpha a^+_{\bar{\alpha}} + v_\alpha a_\alpha .$$

This is simply the special quasiparticle transformation. We may conclude that the ground state wave function (ρ, τ) may always be given by the special transformation in the canonical basis. $|\Phi_0\rangle$ may always be given in the form

$$|\Phi_0\rangle = \prod_{\alpha>0} (u_\alpha + v_\alpha a^+_\alpha a^+_{\bar{\alpha}}) |0\rangle . \tag{5.198}$$

The density matrix and pairing tensor are

$$\rho_{\alpha\alpha} = v_\alpha^2 \qquad \tau_{\alpha\bar{\alpha}} = u_\alpha v_\alpha . \tag{5.199}$$

We have shown that the wave function is invariant under an arbitrary unitary transformation of quasi-particle co-ordinates. (See discussion following 3.95 and 5.90.) Therefore the most general set of quasi-particle co-ordinates is given by the product of three transfomations:

$$B_{gen} = U_2 B_{sp} U_1 \tag{5.200}$$

where

U_1: Rotation in particle space

$$a^+_\alpha = \sum_K D^\alpha_K a^+_K \tag{5.201}$$

B_{sp}: Special Bogoliubov quasiparticle transformation

$$b^+_\alpha = u_\alpha a^+_\alpha - v_\alpha a_{\bar{\alpha}} \tag{5.202}$$

U_2: Rotation in quasiparticle space

$$b^+_\nu = \sum_\alpha R^\nu_\alpha b^+_\alpha \tag{5.203}$$

If U_2 is neglected the HFB equations with time-reversal symmetry reduce to the HB-BCS equations. We restrict ourselves to real co-ordinates. Then

$$D^{\bar{\beta}}_{\bar{K}} = D^\beta_K \tag{5.204}$$

and

$$U_{\beta K} = u_\beta D^\beta_K \qquad V_{\beta K} = -v_\beta D^\beta_K . \tag{5.205}$$

The components of (5.135) are

$$\sum_{K_2} (H'_{K_1K_2} u_\beta - \Delta_{K_1K_2} v_\beta) D^\beta_{K_2} = E_\beta u_\beta D^\beta_{K_1} \tag{5.206a}$$

$$\sum_{K_2} (H'_{K_1K_2} v_\beta + \Delta_{K_1K_2} u_\beta) D^\beta_{K_2} = -E_\beta v_\beta D^\beta_{K_1} \tag{5.206b}$$

where $H' = H - \lambda$. (5.207)

Multiply (5.206a) by $v_\alpha D^\alpha_{K_1}$ and sum on K_1.

$$H'_{\alpha\beta} u_\beta v_\alpha - \Delta_{\alpha\beta} v_\alpha v_\beta = E_\beta u_\beta v_\alpha \delta_{\alpha\beta}$$

Multiply (5.206b) by $u_\alpha D^\alpha_{K_1}$ and sum on K_1.

$$H'_{\alpha\beta} u_\alpha v_\beta + \Delta_{\alpha\beta} u_\alpha u_\beta = -E_\beta u_\alpha v_\beta \delta_{\alpha\beta}$$

Add the last two equations.

$$H'_{\alpha\beta} (u_\alpha v_\beta + u_\beta v_\alpha) + \Delta_{\alpha\beta} (u_\alpha u_\beta - v_\alpha v_\beta) = 0 \tag{5.208}$$

We have shown that these equations correspond to the elimination of $H'_{02} + H'_{20}$. The diagonal elements ($\alpha = \beta$) give the BCS equations, while the off-diagonal elements ($\alpha \neq \beta$) may be rearranged to give the HB equations. (See equation 3.82 ff.) The HB equations may be obtained more directly by multiplying (5.206b) by $\mathcal{N}_\beta D^\alpha_{K_1}$ and summing on K_1.

$$\mathcal{H}'_{\alpha\beta}\mathcal{N}_\beta^2 + \Delta_{\alpha\beta}\mathcal{U}_\beta\mathcal{N}_\beta = -E_\beta\mathcal{N}_\beta^2\delta_{\alpha\beta}$$

Exchange the indices α and β, recalling that $\mathcal{H}$ and Δ are symmetric.

$$\mathcal{H}'_{\alpha\beta}\mathcal{N}_\alpha^2 + \Delta_{\alpha\beta}\mathcal{U}_\alpha\mathcal{N}_\alpha = -E_\alpha\mathcal{N}_\alpha^2\delta_{\alpha\beta}$$

By subtracting, we arrive at the HB equations.

$$\mathcal{H}'_{\alpha\beta}(\mathcal{N}_\alpha^2 - \mathcal{N}_\beta^2) + \Delta_{\alpha\beta}(\mathcal{U}_\alpha\mathcal{N}_\alpha - \mathcal{U}_\beta\mathcal{N}_\beta) = 0 \qquad (5.209)$$

The relationship between the HFB and HB-BCS formalisms is now transparent. Both provide the ground state wave-function which has the simple BCS form. Both minimize the energy of the ground state and eliminate $H'_{02} + H'_{20}$. However, HB-BCS does not provide the third transformation, U_2, which diagonalizes H'_{11}.

If and only if Δ is diagonal in the canonical basis then U_2 will be unity and the HB equations reduce to the pair-modified HF equations. For a non-trivial force there is no reason to expect that Δ will be diagonal. We have found no cases of physical interest for which these simplifications are justified.

Our generalized isospin-pairing wave function has the form (5.170). The basis which diagonalizes ρ is doubly degenerate in isospin.

$$D = \begin{bmatrix} \mathcal{D} & 0 \\ 0 & \mathcal{D} \end{bmatrix} \tag{5.210a}$$

where $$\mathcal{D}^{\alpha}_{\kappa} = D^{\alpha p}_{\kappa p} = D^{\alpha n}_{\kappa n} \, . \tag{5.210b}$$

Since ρ_{pp} is real and symmetric

$$\mathcal{D} \text{ is real and orthogonal} \, . \tag{5.210c}$$

The density matrix is

$$\rho^{(\alpha)} = \begin{bmatrix} \rho_{pp}(\alpha) & 0 \\ 0 & \rho_{pp}(\alpha) \end{bmatrix} . \tag{5.211a}$$

Any rotation in isospin co-ordinates leaves $\rho(\alpha)$ invariant. Therefore the basis $\{|\alpha\rangle\}$ must reduce τ to two-dimensional matrices in isospin space. (We assume $\rho_{pp}(\alpha) \neq \rho_{pp}(\beta)$ for $\alpha \neq \beta$.)

$$\tau(\alpha) = \begin{bmatrix} \tau_{pp}(\alpha) & \tau_{pn}(\alpha) \\ \tau^{*}_{pn}(\alpha) & -\tau_{pp}(\alpha) \end{bmatrix} \tag{5.211b}$$

ρ and τ have therefore been reduced to the form encountered in the isospin generalization of the special transformations (4.118). The canonical representation is obtained by diagonalizing $\tau(\alpha)$. (See IV.6.), and is therefore a linear combination of $|\alpha p\rangle$ and $|\alpha n\rangle$.

$$|\alpha_c\rangle = C_p^\alpha |\alpha p\rangle + C_n^\alpha |\alpha n\rangle \tag{5.212}$$

where $|\alpha\rangle = \sum_K D_K^\alpha |K\rangle$.

This diagonalization has not been performed, since the interpretation of the wave function is enhanced with the form (5.210-5.211). Nevertheless, knowing that the canonical representation (5.212) does exist, the argument for our choice of phases may be strengthened. Since $\bar{\tau} = -\tau^*$

$$|\bar{\alpha}_c\rangle = C_p^{\alpha *} |\bar{\alpha} p\rangle + C_n^{\alpha *} |\bar{\alpha} n\rangle \tag{5.213}$$

where $|\bar{\alpha}\rangle = \sum_K D_K^\alpha |\bar{K}\rangle$.

Because $\{|\alpha_c\rangle\}$ form a complete orthonormal set, Δ may be expressed as

$$(\Delta_{T_1 T_2})_{K\ell} = \sum_{\alpha_c > 0} \langle K T_1, \bar{\ell} T_2 | v | \alpha_c \bar{\alpha}_c \rangle_A \, t_{\alpha_c \bar{\alpha}_c} \tag{5.214}$$

where $t_{\alpha_c \bar{\alpha}_c}$ is real. Substitute (5.212, 5.213) and couple the isospin co-ordinates to T. The pn pair potential becomes

$$\begin{aligned}(\Delta_{pn})_{K\ell} = {} & \tfrac{1}{2} \sum_{\alpha_c > 0} \langle K \bar{\ell}\, T=1 | v | \alpha \bar{\alpha}\, T=1 \rangle_A \left(C_p^\alpha C_n^{\alpha *} + C_p^{\alpha *} C_n^\alpha \right) t_{\alpha_c \bar{\alpha}_c} \\ & + \tfrac{1}{2} \sum_{\alpha_c > 0} \langle K \bar{\ell}\, T=0 | v | \alpha \bar{\alpha}\, T=0 \rangle_A \left(C_p^\alpha C_n^{\alpha *} - C_p^{\alpha *} C_n^\alpha \right) t_{\alpha_c \bar{\alpha}_c} .\end{aligned} \tag{5.215}$$

If the quasiparticle tranformation is restricted to real co-ordinates, C_p^α and C_n^α are real, so that all elements of the T = 0 pair potential vanish. Similarly, if the co-ordinates are complex, but the phase choice $\bar{u} = u$, $\bar{v} = -v$ is retained, then $\bar{\tau} = -\tau$ (see 5,108), and

$$|\bar{\alpha}_c\rangle = C_p^\alpha |\bar{\alpha} p\rangle + C_n^\alpha |\bar{\alpha} n\rangle .$$

Consequently

$$(\Delta_{pn})_{k\ell} = \sum_{\alpha_c > 0} \langle k\bar{\ell}\, T=1 | v | \alpha\bar{\alpha}\, T=1\rangle_A\, C_p^\alpha C_n^\alpha\, \tau_{\alpha_c \bar{\alpha}_c}$$

and all elements of the T = 0 potential vanish. Implicit in these proofs is the fact that D_k^α is independent of isospin.

If ρ and τ are given by (5.211) then the eigenvectors of R are given by (4.117)

$$\begin{bmatrix} b^+_{\alpha 1} \\ b^+_{\alpha 2} \\ b_{\bar{\alpha} 1} \\ b_{\bar{\alpha} 2} \end{bmatrix} = \begin{bmatrix} u_{\alpha 11} & 0 & -v_{\alpha 11} & -v_{\alpha 12} \\ 0 & u_{\alpha 11} & -v^*_{\alpha 12} & v_{\alpha 11} \\ v_{\alpha 11} & v_{\alpha 12} & u_{\alpha 11} & 0 \\ v^*_{\alpha 12} & -v_{\alpha 11} & 0 & u_{\alpha 11} \end{bmatrix} \begin{bmatrix} a^+_{\alpha p} \\ a^+_{\alpha n} \\ a_{\bar{\alpha} p} \\ a_{\bar{\alpha} n} \end{bmatrix} \tag{5.216}$$

plus the time-reversed set.

$$u_{\alpha 11},\ v_{\alpha 11} = \text{Real} \tag{5.217}$$

The density matrix and pairing tensor are (see 4.112 - 4.116, 5.147)

$$\rho_{pp}(\alpha) = v_\alpha^2 \equiv v_{\alpha 11}^2 + |v_{\alpha 12}|^2 \tag{5.218}$$

$$\tau_{pp}(\alpha) = u_{\alpha 11} v_{\alpha 11} \tag{5.219}$$

$$\tau_{pn}(\alpha) = u_{\alpha 11} v^*_{\alpha 12} . \tag{5.220}$$

$\tau^2(\alpha)$ is diagonal.

$$\tau^2(\alpha) = (u_\alpha v_\alpha)^2 I \tag{5.221}$$

where $u_\alpha \equiv u_{\alpha 11}$. (5.222)

u_α is given by

$$|u_\alpha| = \sqrt{\tau^2(\alpha)/\rho(\alpha)} \tag{5.223a}$$

or by

$$|u_\alpha| = \sqrt{1-\rho_{pp}(\alpha)} \quad . \tag{5.223b}$$

We choose $u_\alpha > 0$. (5.224)

Then $v_{\alpha 11}$ and $v_{\alpha 12}$ are determined by (5.219, 5.220).

The third transformation, U_2 , is determined as follows. First express the general tranformation in terms of the canonical basis.

$$b^+_\nu = \sum_\alpha{}' \left(u_{\nu\alpha} a^+_\alpha + v_{\nu\alpha} a_{\bar\alpha} \right) \tag{5.225}$$

Inverting (5.201) and substituting into (5.118) we find

$$b^+_\nu = \sum_{\alpha k}{}' \left(u_{\nu k} D^{\alpha *}_k a^+_\alpha + v_{\nu k} D^{\alpha *}_k a_{\bar\alpha} \right).$$

Comparing the last two equations we obtain

$$u_{\nu\alpha} = \sum_k{}' u_{\nu k} D^{\alpha *}_k \qquad v_{\nu\alpha} = \sum_k{}' v_{\nu k} D^{\alpha *}_k \, . \tag{5.226}$$

Combining (5.202, 5.203), we have a third expression for b^+_ν in terms of the canonical basis.

$$b^+_\nu = \sum_\alpha{}' \left(R^\nu_\alpha u_\alpha a^+_\alpha - R^\nu_\alpha v_\alpha a_{\bar\alpha} \right)$$

Comparing with (5.225), the matrix R may be evaluated.

$$R^\nu_\alpha = u_{\nu\alpha} / u_\alpha \tag{5.227}$$

For generalized isospin pairing R has a simple structure. By comparing (5.216) and (5.183, 5.184) it may be seen that the quasiparticles are divided into two groups according to

$$b^{+}_{\nu 1} = \sum_{\alpha 1} R^{\nu 1}_{\alpha 1} \, b^{+}_{\alpha 1} \qquad (5.228)$$

$$b^{+}_{\nu 2} = \sum_{\alpha 2} R^{\nu 2}_{\alpha 2} \, b^{+}_{\alpha 2} \, .$$

That is $R^{\nu 1}_{\alpha 2} = R^{\nu 2}_{\alpha 1} = 0 .$ (5.229)

Furthermore the two sets transform by the same rotation, so that R has the form

$$R = \begin{bmatrix} \mathcal{R} & 0 \\ 0 & \mathcal{R} \end{bmatrix} \qquad (5.230)$$

where $\mathcal{R}^{\nu}_{\alpha} = R^{\nu 1}_{\alpha 1} = R^{\nu 2}_{\alpha 2} \, .$ (5.231)

Comparing (5.183) and (5.216) $\mathcal{R}$ may be evaluated.

$$\mathcal{R}^{\nu}_{\alpha} = (\mathcal{U}_{pp})_{\nu\alpha} / u_{\alpha} \qquad (5.232)$$

Since R is unitary and $\mathcal{U}_{pp}$ and u_{α} are real

$\mathcal{R}$ is real and orthogonal . (5.233)

To recapitulate, for generalized isospin pairing the general transformation may be expressed as the product of three transformations.

1. Rotation in particle space

$$\begin{bmatrix} \underline{a}^{\dagger}_{\alpha p} \\ \underline{a}^{\dagger}_{\alpha n} \\ \underline{a}_{\bar{\alpha} p} \\ \underline{a}_{\bar{\alpha} n} \end{bmatrix} = \begin{bmatrix} \mathcal{D} & 0 & 0 & 0 \\ 0 & \mathcal{D} & 0 & 0 \\ 0 & 0 & \mathcal{D} & 0 \\ 0 & 0 & 0 & \mathcal{D} \end{bmatrix} \begin{bmatrix} \underline{a}^{\dagger}_{\kappa p} \\ \underline{a}^{\dagger}_{\kappa n} \\ \underline{a}_{\bar{\kappa} p} \\ \underline{a}_{\bar{\kappa} n} \end{bmatrix} \tag{5.234}$$

where $\mathcal{D}$ is real and orthogonal

2. A "generalized" special quasiparticle transformation

$$\begin{bmatrix} \underline{b}^{\dagger}_{\beta 1} \\ \underline{b}^{\dagger}_{\beta 2} \\ \underline{b}_{\bar{\beta} 1} \\ \underline{b}_{\bar{\beta} 2} \end{bmatrix} = \begin{bmatrix} \mathcal{U}_{11} & 0 & -\mathcal{V}_{11} & -\mathcal{V}_{12} \\ 0 & \mathcal{U}_{11} & -\mathcal{V}_{12}^{*} & \mathcal{V}_{11} \\ \mathcal{V}_{11} & \mathcal{V}_{12} & \mathcal{U}_{11} & 0 \\ \mathcal{V}_{12}^{*} & -\mathcal{V}_{11} & 0 & \mathcal{U}_{11} \end{bmatrix} \begin{bmatrix} \underline{a}^{\dagger}_{\alpha p} \\ \underline{a}^{\dagger}_{\alpha n} \\ \underline{a}_{\bar{\alpha} p} \\ \underline{a}_{\bar{\alpha} n} \end{bmatrix} \tag{5.235}$$

where $\mathcal{U}_{11}, \mathcal{V}_{11}, \mathcal{V}_{12}$ are diagonal

$$\begin{aligned} (\mathcal{U}_{11})_{\beta\alpha} &= U_{\alpha 11}\, \delta_{\alpha\beta} \\ (\mathcal{V}_{11})_{\beta\alpha} &= \mathcal{V}_{\alpha 11}\, \delta_{\alpha\beta} \\ (\mathcal{V}_{12})_{\beta\alpha} &= \mathcal{V}_{\alpha 12}\, \delta_{\alpha\beta} \end{aligned} \tag{5.236}$$

and $U_{\alpha 11}, \mathcal{V}_{\alpha 11} = \text{Real}$

3. A rotation in quasiparticle space

$$\begin{bmatrix} \underline{b}^{\dagger}_{\nu 1} \\ \underline{b}^{\dagger}_{\nu 2} \\ \underline{b}_{\bar{\nu} 1} \\ \underline{b}_{\bar{\nu} 2} \end{bmatrix} = \begin{bmatrix} \mathcal{R} & 0 & 0 & 0 \\ 0 & \mathcal{R} & 0 & 0 \\ 0 & 0 & \mathcal{R} & 0 \\ 0 & 0 & 0 & \mathcal{R} \end{bmatrix} \begin{bmatrix} \underline{b}^{\dagger}_{\beta 1} \\ \underline{b}^{\dagger}_{\beta 2} \\ \underline{b}_{\bar{\beta} 1} \\ \underline{b}_{\bar{\beta} 2} \end{bmatrix} \tag{5.237}$$

where $\mathcal{R}$ is real and orthogonal.

The general transformation is therefore determined by

$$\mathcal{R}, \mathcal{U}_{11}, \mathcal{V}_{11}, \mathcal{V}_{12}, \mathcal{D}.$$

8. HFB in the 2s - 1d Shell

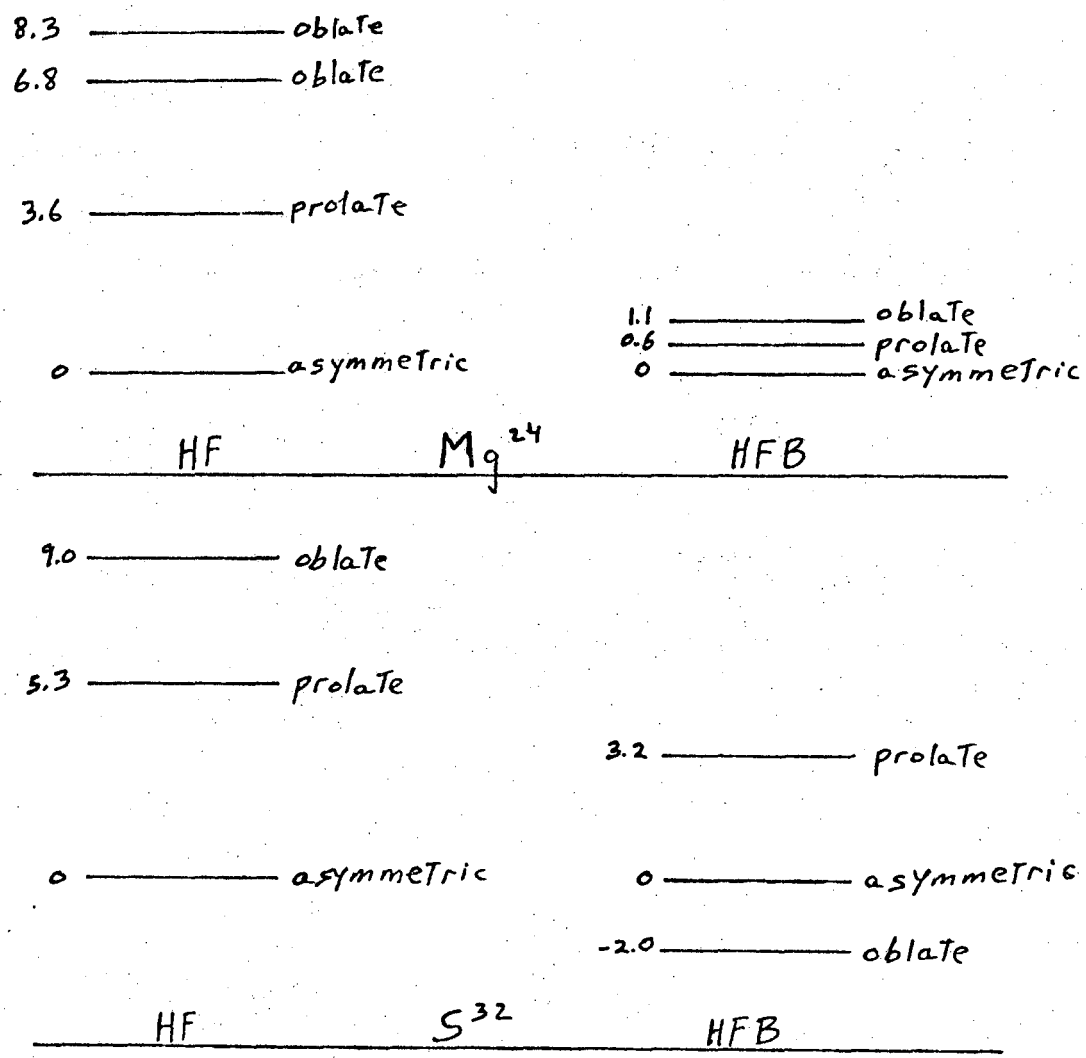
The HFB equations with generalized isospin pairing have been solved for the N = Z even-even nuclei in the 2s - 1d shell. The nucleon - nucleon interactions used are the Rosenfeld force (sd), the Yale-Shakin t matrix (s-p-sd), and the Nestor-Davies-Krieger-Baranger (NDKB) force (s-p-sd and s-p-sd-pf). These interactions are described in II.6. The wave - functions (ρ, t) obtained from the generalized gap equations (4.123) have been used as HFB trial wave-functions. The non-trivial solutions to the HFB equations are listed in Table 5.1. The energy for elementary excitations, $E_1 + E_2$, is the sum of the two smallest distinct quasiparticle energies. In the limit of small pairing, this energy equals the HF gap. The multipole moments Q_{LM} and the deformation parameter β are given by (2.74) and (2.76). The solutions to the HF equations (Table 2.15) are also trivial solutions to the HFB equations.

A consistent feature of the generalized pairing solutions is the mutual exclusion of T = 0 and T = 1 pairing. All HFB wave-functions encountered here display only T = 0 pairing correlations.

Most remarkable is the uniformity of the quasi-particle gap. Although the HF bases employed as trial wave-functions have HF gaps ranging from 0.1 to 5.3 Mev,

the corresponding two quasiparticle excitation energies range from 4.7 to 6.0 Mev. There are very few exceptions. All HF solutions with small excitation energies have been stabilized by T = 0 pairing.

Equally remarkable is the magnitude of the pairing energy. Physically relevant solutions display pairing energies of 5 to 17 Mev. With such large contributions to the binding energy, the HF relative ordering of intrinsic states is often drastically altered. Most notable are Mg^{24} and S^{32}. The results for the Yale force are depicted below.[5] (Energies are in Mev.)



Very often BCS wave - functions based on different HF intrinsic states converge to the same HFB limit. The HFB equations therefore alleviate a major difficulty of the HF theory: having too many intrinsic states from which to choose the physically relevant one. Also discrepancies between the different forces in HF theory concerning the relative ordering of prolate and oblate states are eliminated in HFB.

The NDKB calculations were performed with and without the pf shell to test the effects of core polarization. Inclusion of the pf shell generally increases the deformation β by 40 - 50%[9] and results in a substantial increase in pairing energy (Table 5.22) and in the quasi-particle gap (Table 5.24).

Although the inertial parameter $\hbar^2/2\mathcal{J}$ appears to be much increased by T = 0 pairing (see IV.7), the multipole moments are not significantly altered.

Most encouraging is our finding that physically relevant results are reproduced by all forces used.

Having obtained the exact solutions to the HFB equations we may now evaluate the justifiability of various approximations.

The BCS approximation is to neglect off-diagonal elements of $\mathcal{H}$ and Δ. Equivalently, it is assumed that the HF basis is very similar to the HFB canonical basis and that the third transformation, U_2, is near

unity. If these assumptions are valid then HF-BCS and HFB result in the same ground state wave function and quasiparticle excitations. Our calculations show that these approximations are not justified in the 2s - 1d shell. We have found no case of physical interest for which U_2 is near unity. The canonical basis is sometimes similar to the HF basis, but often they bear no resemblance. Even in the canonical basis the pair potential usually has large off-diagonal elements.

The HFB formalism consistently results in stronger pairing correlations than does HF -BCS. This is reflected in the increase of the pairing energy (often by a factor of 2 or 3), and in the dispersion of the occupation probabilities v_α^2 . (See Table 5.21.) That this should occur appears reasonable. The HF basis is chosen only to maximize E_{HF}, with no regard for E_{PAIR}. The HFB canonical basis is chosen to maximize the sum $E_{HF} + E_{PAIR}$. The excitation energy $E_1 + E_2$ usually changes very little between HF -BCS and HFB; although in a few significnat cases where BCS gives a small gap, HFB considerably increases the gap. (See Table 5.23.)

The HB - BCS formalism will give the same ground state wave function as HFB. However, since U_2 is not near unity, the quasiparticle wave functions and energies would be gravely in error (unless, of course, the quasiparticle energy matrix resulting from HB-BCS is diagonalized).

An approximation which has enjoyed some popularity is to neglect the pair potential in the HB equations. This is justified if off - diagonal elements of Δ in the canonical basis are negligible. The HB equations then reduce to the HF equations, where the HF potential accounts for the dispersion of the occupation probability. One then iterates between the HF and the BCS equations until self-consistency is achieved in both HF and pair degrees of freedom. It has been thought that this procedure would be an improvement upon the BCS calculation with the original HF basis. We have made a thorough study of this approximation, using all HF solutions reported in Table 2.15 as starting points. The conclusion is that approximate HB-BCS is most remarkable for its consistency -- it is always a worse approximation to HFB than the simpler method (HF-BCS) upon which it is intended to improve. More precisely-- it has never been advantageous to iterate between the HF and the BCS equations. The specific failures of the method are as follows:

1. It usually results in a small decrease in pairing correlations (compared to BCS), whereas HFB almost always considerably increases pairing correlations.
2. It sometimes decreases the total binding energy from E_{BCS}, whereas HFB always increases binding energy. This should not be surprising, since the approximate HB equations can not be derived from a variational principle.

3. The single particle basis obtained is always very similar to the original HF basis. HFB often produces large changes in the single particle (canonical) basis. Furthermore, the changes induced by iterating between HF and BCS are usually in the wrong direction -- away from rather than toward the HFB canonical basis.

Some possible rebuttals are:

1. In some cases Δ may be diagonal in the canonical basis, so that approximate HB-BCS will be reliable.

This is true. In fact, for this case HF-BCS, approximate HB-BCS, and HFB will all give very similar results. Nevertheless, approximate HB-BCS will still differ from HFB more than does HF-BCS.

2. Because this approximation gives wave functions drastically different from HFB does not render its results meaningless. The wave functions might simply correspond to different "wells," i.e. different HFB solutions.

This position is not defensible since the pair potential in the HF or approximate - HB basis is generally not diagonal. If the wave function approximated a HFB solution, Δ would be diagonal. The example of prolate Ar^{36} is presented in Table 5.20. The BCS pair potential in the HF basis is presented. (The approximate - HB result is nearly identical.) Note that in the $\Omega, \pi = 1/2, +$ subspace $|\Delta_{2,3}| = 2.3\ |\Delta_{2,2}|$.

We hope these comments will be heeded, so that future students will not be misled into imagining that something is to be gained by iterating between the HF and the BCS equations. Most likely only disadvantage will result - and- most telling perhaps- one can never know whether the approximation is justifiable unless one calculates off-diagonal elements of the pair potential - but then one might as well do HFB and obtain the exact result.

We may now proceed to discuss the HFB solutions for the various nuclei. For experimental details and angular momentum projection calculations concerning these nuclei the reader is referred to I.7.

Ne^{20}

The state with maximum binding is axially symmetric and prolate. The solution is a trivial one (no pairing) and corresponds to the HF solution given in Table 2.4. The properties of this state do not depend upon the choice of force. Angular momentum projection on this intrinsic state adequately explains the low-lying Ne^{20} energy spectrum.

Although the prolate HF state obtained with the Yale force has a gap large enough to prevent pairing, the spherical HF state does admit T = 0 pairing. The T = 0 pair force then deforms the underlying HF field, so that the final density distribution is prolate. The binding energy of this paired prolate state is slightly greater than that of the trivial prolate state. Their canonical single particle bases are very similar.

There are several other higher-lying trivial (Table 2.15) and non-trivial (Table 5.1) solutions of assorted shapes, but these are not thought to have any physical significance.

Mg^{24}

HF theory predicts only one stable solution: the asymmetric one. This state fails to agree with experiment. a) The predicted spacing between the K = 0 and K = 2 bands is 1.18 Mev, whereas the experimental value is 2.86 Mev.

b) Angular momentum projection fails to reproduce the approximate I (I + 1) spectra for the K = 0 and K = 2 bands.

c) Experimental data on stripping spectroscopic factors and the γ -branching ratio of Mg^{25} can not be explained in terms of the asymmetric state.

It is clear that the HF prediction must be rejected.

The other HF intrinsic states have the following defects.

a) The binding energy is several Mev above the asymmetric state.

b) The inertial parameter $\hbar^2/2\mathcal{J}$ is too small.

c) The gap for elementary excitations is very small (0.5 Mev for Yale prolate) so that these higher lying states are not stable against particle-hole admixtures. Introducing pairing correlations should eliminate these deficiencies.

The HFB equations have three almost degenerate solutions with the Yale-Shakin t matrix elements.

a) The trivial (Δ = 0) asymmetric state with $\langle H \rangle$ = -133.144 Mev.

b) An axially symmetric prolate T = 0 paired state with $\langle H \rangle$ = -132.527 Mev, E_{PAIR} = -7.802 Mev.

c) An axially symmetric oblate T = 0 paired state with $\langle H \rangle$ = -132.049 Mev, E_{PAIR} = -17.205 Mev.

The corresponding HF states are separated in energy by 8.3 Mev. Also, introducing pairing into each of the two distinct oblate HF states leads to the same HFB solution. The energy for elementary excitations is increased from 0.46 Mev to 4.81 Mev (prolate) and 0.10, 0.92 Mev to 6.05 Mev (oblate).

Since the measured quadrupole moment of the first 2^+ state is negative, the intrinsic state must be prolate. Futhermore, the stripping spectroscopic data favors a prolate intrinsic state.

The axially symmetric prolate $T = 0$ paired state is therefore chosen as the physically relevant intrinsic state. The predicted energy of the lowest $K = 2^+$ two quasiparticle state, 4.81 Mev, is in reasonable agreement with the experimental value of 4.23 Mev, since residual quasiparticle interactions may be expected to lower the energy of this state.

The NDKB force yields prolate and oblate paired states which are almost identical to the Yale solutions. Addition of the pf shell increases the pairing energy and quasiparticle gap somewhat, but the structure of the prolate state is essentially unchanged. The HF energy is increased by $\sim$ 5 Mev, and the deformation β is increased by $\sim$ 50%, as is expected from HF calculations. Again the oblate and prolate states are nearly degenerate.

The Rosenfeld force also yields nearly degenerate asymmetric, paired prolate, and paired oblate states.

All three distinct oblate HF states lead to the same HFB limit. The structure of the prolate state is very similar to that obtained with the other forces.

Since the T = 0 paired axially symmetric prolate state has been stabilized and lowered in energy, and has a structure which is invariant under change of forces, we suggest that T = 0 pairing correlations restore axial symmetry to Mg^{24}.

The wave function and pair potential for the prolate state are presented in Table 5.2 - 5.6, 5.11 - 5.15. Neither $\mathcal{R}$ nor Δ may be approximated by diagonal matrices. Nevertheless, the canonical basis is very similar to the HF basis (Tables 2.5 - 2.9).

Si^{28}

HF theory predicts orthogonal prolate and oblate states with similar binding energy. Angular momentum projection from these two states fails to reproduce the energy spectrum. Experimentally there is only one low-lying K = 0 band. Since the matrix element of the Hamiltonian connecting these two states (or rather, the J projected states) has been shown to be small, the two HF bands could not be separated by mixing.

The rotational spectrum corresponding to the ground, K = 0 band deviates considerably from the I (I + 1) spectrum characteristic of axially symmetric shapes.

However, the $I \neq 0$ members of the band do satisfy the $I(I+1)$ rule. Only the ground state $I = 0^+$ seems to be depressed from its predicted position. This depression may be understood as a result of mixing with a coexisting spherical state at 4.98 Mev.

The coexistence picture assumes the existence of a spherical and one deformed low-lying intrinsic state. HF predicts two low-lying deformed states and a spherical state some 15 Mev higher.

The energy of the spherical state is not lowered very much by $|T_z| = 1$ pairing (Table 3.8). Also the Rosenfeld and Yale forces fail to give any low-lying non-trivial solutions to the HFB equations. This is because the first oblate and prolate HF states possess large single particle gaps.

With the NDKB force, however, a find a $T = 0$ paired axially symmetric prolate state almost degenerate with the prolate and oblate HF states. Moreover this paired state is not orthogonal to either of the HF states. For all forces the oblate state has $\Omega\pi = 5/2+, 1/2+, 3/2+$ occupied orbitals; and the trivial prolate state has $\Omega\pi = 1/2+, 3/2+, 1/2+$ occupied orbitals, with 5/2+ being the first unoccupied orbital. In the paired prolate state the 5/2+ orbital becomes partially occupied. Consequently, the overlap of this state with the oblate state becomes significant.

With realistic forces the prolate HF state has a small energy gap, so that the only physically relevant states are the trivial oblate and the paired prolate states. However, experiments indicate that the intrinsic state is oblate, so that the prolate paired state may also be disregarded. We have already noted that angular momementum projection on the oblate state fails to predict the experimental energy spectrum.

We must conclude that a satisfactory self-consistent field description of Si^{28} has not yet been achieved.

S^{32}

The experimental spectrum is not characteristic of a rotator. However, if the ground 0^+ state is lowered to its observed position by interacting with the first excited 0^+ state at 3.78 Mev, then the unperturbed ground state band exhibits an $I(I + 1)$ dependence.

HF theory predicts an asymmetric shape for S^{32}. It has recently been demonstrated that 2p-2h admixtures to this state result in a spherical ground state.[6] The asymmetric HF state is therefore not reliable. There is a considerable overlap between 2p-2h and pairing admixtures.

HF also predicts low-lying oblate and prolate states with small energy gaps and large moments of inertia. The relative ordering of these two states is force dependent,

and they are separated by 4 to 7 Mev. Since these HF states are unstable against particle-hole admixtures , and lie several Mev above the asymmetric state, they are not suitable intrinsic ground states.

The HFB equations have three close-lying solutions: trivial asymmetric and T = 0 paired axially symmetric prolate and oblate. For all forces the oblate state lies lower than the prolate state. For the Rosenfeld and NDKB forces the two states are nearly degenerate. For the Yale force the oblate state is tremendously lowered in energy by T = 0 pairing. Although the trivial oblate state lies 9 Mev above the asymmetric state, the paired oblate state is 2 Mev below the asymmetric state. The HFB binding energies for the Yale force are ;

a) T = 0 paired axially symmetric oblate, $\langle H \rangle$ = -229.658 Mev, E_{PAIR} = -13.233 Mev.

b) trivial asymmetric, $\langle H \rangle$ =-227.737 Mev.

c) T = 0 paired axially symmetric prolate, $\langle H \rangle$ =-224.531 Mev, E_{PAIR} = -9.208 Mev.

Although the asymmetric solution can be disregarded, no choice can be made at present between the prolate and oblate T = 0 paired states. A determination of the quadrupole moment of the 2.23 Mev 2^+ state of S^{32} can lead to a choice between these two solutions.

The wave functions and pair potentials for the paired states are presented in Tables 5.7-8, 5.16-17.

For the paired oblate state all forces result in $\mathcal{R}$ and Δ with large off-diagonal elements. The canonical basis is very different from the HF basis (Table 2.11) for the Yale and NDKB forces, but for the Rosenfeld force the two bases are very similar. Addition of the pf shell does not alter $|\Phi_0\rangle$ or $\mathcal{R}$. The Yale and NDKB forces provide similar wave functions, but these differ from the Rosenfeld wave functions.

For the paired prolate state as well, all forces yield large off-diagonal elements in $\mathcal{R}$ and Δ. Also the canonical basis is very different from the HF basis. Including the pf shell does not change the ground state wave function $|\Phi_0\rangle$, but the quasiparticle transformation $\mathcal{R}$ is altered. The various forces give states with similar properties, but the wave function is somewhat force dependent.

The spherical intrinsic state usually contains $|T_Z| = 1$ pairing correlations (Table 3.9) and is 3½ to 8½ Mev above the ground state, depending upon the choice of force.

Since the T = 0 paired axially symmetric states are stabilized and lowered in energy, and have properties which are relatively independent of the choice of force, we suggest that T = 0 pairing correlations restore axial symmetry to S^{32}.

Ar^{36}

The low-lying spectrum is characteristic of a vibrator. However, HF gives a well deformed oblate ground state with a small inertial parameter. This, of course, predicts a low-lying rotational spectrum, in obvious disagreement with experiment.

The HF equations also have a prolate solution some 5 Mev above the oblate state. It has a small energy gap and is therefore unstable. Also the moment of inertia is large.

Introduction of T = 0 pairing correlations lowers the energy of the prolate state so that it is nearly degenerate with the trivial oblate state. The excitation energy is considerably increased, thereby stabilizing the wave function. Pairing is known to increase the inertial parameter $\hbar^2/2\mathcal{J}$. With the isospin generalized gap equations (Chapter IV) we found that $\hbar^2/2\mathcal{J}$ for prolate Ar^{36} was increased from the HF value of 0.06 - 0.22 Mev to the T = 0 paired value of 0.49 -0.85 Mev. Since the HFB quasiparticle gap is even larger than the BCS gap (see Table 5.23), it is reasonable to expect an unusually large inertial parameter from the HFB prolate paired state. This suggests that the rotational states should appear at energies comparable with or above the two quasiparticle states. The resulting spectrum

may then tend to look vibrational.

For the Yale force the paired state lies below the trivial oblate state. Futhermore, the pairing correlations are so strong as to drastically alter the underlying single particle (canonical) basis, so that the resulting self-consistent shape is oblate. This serves as a dramatic confirmation of the necessity of allowing the HF and pair degrees of freedom to interact with one another.

For all forces the canonical basis bears no resemblance to the corresponding prolate HF basis. The transformation $\mathcal{R}$ is exceedingly non-diagonal. The T = 0 pair potential has substantial off-diagonal elements. The wave function is very force dependent, although it is not altered very much by including the pf shell. Some examples of wave functions and pair potentials are presented in Tables 5.9-10, 5.18-19.

The spherical intrinsic state is substantially lowered by $|T_z| = 1$ pairing correlations (see III.7). If the barrier between the paired spherical state and the paired deformed state is small, they may be admixed in the physically relevant intrinsic wave function.

We conclude that T = 0 pairing correlations are significant in the 2s-1d shell. They rectify most of the failures of the HF theory in explaining the properties of N = Z even-even nuclei in this shell. Axial symmetry is restored to Mg^{24} and S^{32}, and an explanation is provided for the vibrational nature of Ar^{36}. [7, 8]

Tables for Chapter V

Table 5.1. Non-trivial solutions to the HFB equations.
The shape of the trial wave function is given in parentheses.
O = Oblate, P = Prolate, S = Spherical. The properties of the trial wave function are given in Tables 2.15, 4.1. All energies are in units of Mev. Q_{LM} has units of fm^L.

Tables 5.2 - 5.10. HFB wave functions.
The general quasiparticle transformation is expressed as the product of three transformations. See equations 5.234-5.237. For each subspace the following quantities are given (read tables from left to right):

1. Ω ,π
2. $\underline{E}_\nu$, the column vector of quasiparticle energies (Mev).
3. $\mathcal{R}^\nu_\alpha$, a square matrix.
4. $(\mathrm{Im}\ \underline{v}_{\alpha 12})^2$, a column vector. In parentheses is given the sign of Im $v_{\alpha 12}$. Since there is no T = 1 pairing, $v_{\alpha 11}$ = Re $v_{\alpha 12}$ = 0. $u_{\alpha 11}$ is real and positive; it is given by $u_{\alpha 11} = \left[1 - (\mathrm{Im}\ v_{\alpha 12})^2 \right]^{1/2}$.
5. $\mathcal{D}^\alpha_k$, a square matrix.

The Fermi energy, λ, is also given (Mev).

Tables 5.11 - 5.19. HFB T = 0 pair potentials, $\Delta^{T=0}_{pn}$, in canonical basis $|\alpha\rangle$. $\Delta_{pp} = \Delta^{T=1}_{pn} = 0$. Energies are in Mev.

Table 5.20. BCS T = 0 pair potential, $\Delta_{pn}^{T=1}$, in HF basis. Energies are in Mev.

Table 5.21. Relative magnitudes of pairing energy resulting from BCS and HFB.

Table 5.22. Effect of pf shell on pairing energy. NDKB 2 (s-p-sd-pf), NDKB 1 (s-p-sd).

Table 5.23. Relative magnitudes of quasiparticle gap, $E_1 + E_2$, resulting from BCS and HFB.

Table 5.24. Effect of pf shell on quasiparticle gap, $E_1 + E_2$. NDKB 2 (s-p-sd-pf), NDKB 1 (s-p-sd).

Table 5.1: Generalized Pairing in 2s-1d Shell (HFB)

Nucleus	Force	Shape	Mode	E_{PAIR}	E_{TOTAL}	Q_{20}	Q_{40}	β	$E_1 + E_2$	
Ne^{20}	Rosenfeld 1	Oblate (0)	T = 0	-7.625	-41.697	-5.9	25.9		5.02	
		Prolate (P2)	T = 0	-6.587	-41.444	2.7	- 53.5		4.86	
	Rosenfeld 2	Oblate (0)								a
	Yale	Prolate (S)	T = 0	-2.324	-101.505	15.4	80.0	0.255	5.74	b

(continued)

Table 5.1 (continued)

Nucleus	Force	Shape	Mode	E_{PAIR}	E_{TOTAL}	Q_{20}	Q_{40}	β	$E_1 + E_2$
Mg^{24}	Rosenfeld 1	Prolate (P1)	T = 0	-4.576	-95.170	15.6	-0.5		5.51
		Oblate (O1,O2,O3)	T = 0	-6.857	-93.865	-12.4	58.1		5.99
	Rosenfeld 2	Prolate (P2)	T = 0	-6.438	-77.526	15.6	-14.9		5.74
		Oblate (O1, O2)	T = 0	-6.551	-77.238	-13.0	40.8		5.80
	Yale	Prolate (P)	T = 0	-7.802	-132.527	19.0	-12.1	0.244	4.81
		Oblate (O1, O2)	T = 0	-17.205	-132.049	-12.1	31.4	-0.155	6.05
	NDKB 1	Prolate (P)	T = 0	-8.121	-110.388	15.9	13.4	0.218	5.01
		Oblate (O)	T = 0	- 11.802	-109.301	-12.5	47.5	-0.171	4.72
	NDKB 2	Prolate (P)	T = 0	-9.637	-116.651	22.5	6.0	0.314	5.90
		Oblate (O)	T = 0	-15.887	-114.131	-16.6	52.8	-0.232	5.83

(continued)

Table 5.1 (continued)

Nucleus	Force	Shape	Mode	E_{PAIR}	E_{TOTAL}	Q_{20}	Q_{40}	β	$E_1 + E_2$
Si^{28}	Rosenfeld 1	Oblate (02)	T = 0	-2.207	-150.041	-0.5	-96.5		6.13
		Prolate (03)	T = 0	-6.050	-147.808	0.14	110.5		4.91
	Rosenfeld 2	Prolate (02)	T = 0	-7.234	-123.420	0.13	116.0		5.43
		Spherical (S)							
	NDKB 1	Prolate (P,S)	T = 0	-9.933	-140.610	15.1	- 20.9	0.169	4.09
		Prolate (02)	T = 0	-14.375	-138.733	3.1	-84.0	0.035	4.74
	NDKB 2	Prolate (02,S)	T = 0	-8.359	-146.853	24.9	-72.0	0.282	4.71

(continued)

Table 5.1 (continued)

Nucleus	Force	Shape	Mode	E_{PAIR}	E_{TOTAL}	Q_{20}	Q_{40}	β	$E_1 + E_2$
S^{32}	Rosenfeld 1	Oblate (01, 03)	T = 0	-1.385	-212.901	-1.5	-95.8		5.89
	Rosenfeld 2	Oblate (02,03)	T = 0	-5.835	-178.385	-1.3	-110.0		6.16
		Prolate (P)	T = 0	-7.276	-178.179	6.5	-94.5		6.23 b
		Prolate (S)	T = 0	-12.724	-176.173	3.4	37.9		4.97
	Yale	Oblate (NDKB1-0)	T = 0	-13.233	-229.658	-17.0	2.5	-0.151	6.17
		Prolate (P)	T = 0	-9.208	-224.531	13.6	- 66.3	0.121	4.68
	NDKB 1	Oblate (0)	T = 0	-6.988	-179.696	-15.5	5.9	-0.147	3.68
		Prolate (P,S)	T = 0	-6.031	-179.266	12.8	-38.2	0.121	4.69
	NDKB 2	Oblate (0)	T = 0	-9.977	-183.910	-20.4	0.9	-0.194	4.54
		Prolate (P,S)	T = 0	-10.953	-183.153	16.8	-52.6	0.160	6.47

(continued)

Table 5.1 (continued)

Nucleus	Force	Shape	Mode	E_{PAIR}	E_{TOTAL}	Q_{20}	Q_{40}	β	$E_1 + E_2$
Ar^{36}	Rosenfeld 1	Prolate (P,S)	T = 0	-5.079	-277.826	3.9	-21.5		3.75
	Rosenfeld 2	Prolate (P,S)	T = 0	-7.722	-237.234	4.9	-26.3		4.69
	Yale	Oblate (P,S)	T = 0	-9.523	-291.765	-11.3	-37.0	-0.086	5.24
	NDKB 1	Prolate (P,S)	T = 0	-5.904	-224.664	6.0	-17.7	0.049	2.82
	NDKB 2	Prolate (P)	T = 0	-11.260	-226.519	7.5	-19.9	0.061	4.05

a. E_{PAIR} peaks at -9.30 Mev, then wave function falls to spherical HF solution.

b. 100+ iterations.

c. E_{PAIR} peaks at -13.9 Mev, then wave function falls to prolate HF solution.

Table 5.2 : Prolate Mg^{24} (Prolate 1, Rosenfeld 1)

					$1d_{5/2}$
5/2, +	1.	3.566	1.000	(+).017	1.000

					$1d_{5/2}$	$1d_{3/2}$
-3/2, +	1.	2.598	.035	.999	(+).006	.231	-.973
	2.	9.740	.999	-.035	(-).779	.973	.231

						$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
1/2, +	1.	2.911	.163	.977	.138	(+).003	.304	.784	-.542
	2.	6.433	-.047	-.132	.990	(-).203	.501	.352	.791
	3.	7.354	.986	-.167	.024	(+).991	.810	-.512	-.286

$\lambda = -13.535$

Table 5.3 : Prolate Mg^{24} (Prolate 2, Rosenfeld 2)

					$1d_{5/2}$				
5/2, +	1.	4.612	1.000	(+).017	1.000				
						$1d_{5/2}$	$1d_{3/2}$		
-3/2, +	1.	2.841	.039	.999	(+).008	.278	-.961		
	2.	9.005	.999	-.039	(-).658	.961	.278		
							$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
1/2, +	1.	2.903	.212	.973	.092	(+).007	.405	.681	-.610
	2.	6.333	.969	-.197	-.147	(-).325	.625	.280	.729
	3.	6.788	.125	-.120	.985	(+).985	.667	-.676	-.312

$\lambda = -11.425$

Table 5.4 : Prolate Mg^{24} (Yale)

					$1d_{5/2}$
5/2, +	1.	3.777	1.000	(+).034	1.000

						$1d_{5/2}$	$1d_{3/2}$
-3/2, +	1.	2.651	.167	.986	(+).008	.347	-.938
	2.	7.982	.986	-.167	(-).684	.938	.347

								$1s_{1/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
1/2, +	1.	2.158	.247	.923	-.296	.015	(+).014	.143	-.409	-.747	.504
	2.	5.058	.926	-.134	.351	-.036	(-).317	.024	-.617	-.175	-.767
	3.	6.503	.285	-.361	-.888	.021	(+).953	.067	.672	-.622	-.396
	4.	49.655	.024	-.011	.036	.999	(+)1.000	.987	.029	.155	-.027

					$1p_{3/2}$
-3/2, -	1.	19.334	1.000	(-).997	1.000

						$1p_{3/2}$	$1p_{1/2}$
1/2, -	1.	16.958	.990	.139	(-).996	.570	.821
	2.	26.094	-.139	.990	(+).998	.821	-.570

$\lambda = -9.150$

Table 5.5 : Prolate Mg^{24} (NDKB 1)

					$1d_{5/2}$
5/2, +	1.	2.807	1.000	(+).109	1.000

					$1d_{5/2}$	$1d_{3/2}$
-3/2, +	1.	2.494	.151	.989	(+).018	.285	-.959
	2.	8.710	.989	-.151	(-).717	.959	.285

								$1s_{1/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
1/2, +	1.	2.516	.242	.892	-.381	.016	(+).018	.092	-.316	-.842	.428
	2.	5.354	.564	.190	.803	-.034	(-).187	.005	-.501	-.235	-.833
	3.	6.570	.789	-.409	-.458	-.004	(+).962	.004	.805	-.479	-.349
	4.	54.353	.018	-.009	.032	.999	(+)1.000	.996	.028	.081	-.034

					$1p_{3/2}$
-3/2, +	1.	22.403	1.000	(-).997	1.000

					$1p_{3/2}$	$1p_{1/2}$
1/2, -	1.	19.370	.990	.141	(-).994	.526	.851
	2.	28.126	-.141	.990	(+).998	.851	-.526

$\lambda = -6.582$

Table 5.6 : Prolate Mg^{24} (NDKB 2)

					$1d_{5/2}$
5/2, +	1.	4.363	1.000	(+).053	1.000

						$1d_{5/2}$	$1d_{3/2}$
-3/2, +	1.	3.016	.104	.995	(+).011	.308	-.951
	2.	10.839	.995	-.104	(-).743	.951	.308

								$1s_{1/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
1/2, +	1.	2.885	.191	.941	-.280	.017	(+).013	.118	-.352	-.811	.452
	2.	7.020	.479	.160	.861	-.053	(-).205	.003	-.526	-.228	-.820
	3.	8.011	.856	-.299	-.421	.003	(+).974	.013	.774	-.528	-.349
	4.	55.786	.020	-.007	.052	.998	(+)1.000	.993	.033	.104	-.047

					$1f_{7/2}$
-7/2, -	1.	22.513	1.000	(-).001	1.000

						$1f_{7/2}$	$1f_{5/2}$
5/2, -	1.	19.081	.210	.978	(-).001	.399	.917
	2.	29.594	.978	-.210	(+).002	.917	-.399

(cont.)

Table 5.6 : (continued)

								$1p_{3/2}$	$1f_{7/2}$	$2p_{3/2}$	$1f_{5/2}$
-3/2, -	1.	16.163	-.161	-.419	.890	.077	(-).000	.091	-.243	-.951	-.166
	2.	21.816	.921	-.284	.010	.267	(+).002	.003	.598	-.013	-.801
	3.	22.053	-.276	-.005	-.134	.952	(-).003	.074	-.760	.301	-.572
	4.	26.124	.224	.862	.435	.131	(-).995	.993	.077	.064	.060

1/2, -	1.	14.365	-.166	-.165	.570	.785	.070	.016
	2.	18.528	.070	.267	.063	-.061	.953	.085
	3.	19.722	.223	.861	.361	-.008	-.277	-.050
	4.	22.811	.632	.068	-.542	.542	.014	-.093
	5.	24.733	.720	-.386	.484	-.283	-.006	.138
	6.	30.659	-.033	.084	-.115	.083	-.095	.981

	$1p_{3/2}$	$1p_{1/2}$	$1f_{7/2}$	$2p_{3/2}$	$1f_{5/2}$	$2p_{1/2}$
(-).000	.050	.058	-.169	-.623	-.255	-.716
(+).001	.042	-.028	-.349	-.682	.272	.580
(-).003	.047	.076	-.634	.225	-.703	.214
(+).004	.077	-.063	-.661	.308	.595	-.323
(-).992	.521	.845	.061	.030	.091	.032
(+).998	.846	-.521	.085	.012	-.069	.011

$\lambda = -6.871$

Table 5.7 : Prolate S^{32} (NDKB 2)

					$1d_{5/2}$
5/2, +	1.	3.501	1.000	(-).822	1.000

						$1d_{5/2}$	$1d_{3/2}$
-3/2, +	1.	3.854	.974	.228	(-).125	.293	-.956
	2.	8.193	-.228	.974	(+).976	.956	.293

								$1s_{1/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
1/2, +	1.	2.969	.443	.818	.367	.003	(-).153	.063	-.345	-.817	.459
	2.	3.901	.892	-.362	-.271	-.014	(+).923	.019	-.609	-.176	-.773
	3.	9.957	.089	-.447	.890	-.022	(-).985	.042	-.711	.549	.437
	4.	62.893	.014	-.017	.015	1.000	(-)1.000	.997	.064	.032	-.032

					$1f_{7/2}$
-7/2, -	1.	18.768	1.000	(+).002	1.000

						$1f_{7/2}$	$1f_{5/2}$
5/2, -	1.	15.120	.313	.950	(+).001	.451	.892
	2.	25.962	.950	-.313	(-).004	.892	-.451

Table 5.7 (continued)

								$1p_{3/2}$	$1f_{7/2}$	$2p_{3/2}$	$1f_{5/2}$
-3/2, -	1.	13.404	-.227	.528	.818	-.003	(+).001	.048	-.080	-.995	-.029
	2.	20.531	.966	.224	.123	-.040	(-).002	.001	-.591	.024	.806
	3.	23.078	.113	-.813	.556	-.129	(+).005	.081	-.800	.085	-.589
	4.	30.544	.053	-.095	.080	.991	(+).998	.996	.069	.041	.049

1/2, -	1.	12.749	-.172	.179	.631	.735	-.010	-.008
	2.	18.927	.357	-.895	.252	.084	-.008	-.007
	3.	21.624	.631	.158	-.518	.554	.027	-.039
	4.	23.253	.658	.371	.505	-.373	-.187	.023
	5.	27.525	.109	.059	.114	-.072	.970	.159
	6.	35.056	-.007	-.017	-.043	.049	-.151	.986

	$1p_{3/2}$	$1p_{1/2}$	$1f_{7/2}$	$2p_{3/2}$	$1f_{5/2}$	$2p_{1/2}$
(+).001	.025	.027	-.071	-.662	-.025	-.745
(-).001	.009	-.001	.096	.739	-.045	-.665
(+).003	.046	.056	-.662	.068	-.742	.031
(-).004	.047	-.021	-.737	.100	.666	-.040
(+).997	.522	.849	.055	.015	.050	.027
(-).999	.850	-.524	.044	-.007	-.026	.012

$\lambda = -9.878$

Table 5.8 : Oblate S^{32} (NDKB 2)

					$1d_{5/2}$
5/2, +	1.	9.778	1.000	(-).990	1.000

					$1d_{5/2}$	$1d_{3/2}$
-3/2, +	1.	2.074	.938	.347	(+).542	.670	.743
	2.	7.136	.347	-.938	(-).974	.743	-.670

								$1s_{1/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
1/2, +	1.	2.471	.209	.954	-.211	.037	(-).024	.083	.428	-.567	-.699
	2.	6.554	.124	.191	.963	-.146	(+).479	.025	.608	-.390	.691
	3.	7.254	.970	-.230	-.081	-.010	(-).988	.137	-.668	-.709	.182
	4.	63.609	.020	-.010	.150	.989	(-).999	.987	.041	.155	.016

					$1f_{7/2}$
-7/2, -	1.	11.492	1.000	(+).002	1.000

					$1f_{7/2}$	$1f_{5/2}$
5/2, -	1.	14.297	.768	.640	(+).001	.593	.806
	2.	21.680	-.640	.768	(-).002	.806	-.593

Table 5.8 : (continued)

								$1p_{3/2}$	$1f_{7/2}$	$2p_{3/2}$	$1f_{5/2}$
-3/2, -	1.	15.396	.901	.061	.430	.002	(+).001	.038	.548	.811	.202
	2.	19.149	-.384	.572	.724	.021	(+).002	.062	.543	-.531	.648
	3.	24.912	.199	.814	-.533	-.116	(-).002	.008	.633	-.246	-.734
	4.	34.668	.029	.083	-.078	.993	(+).998	.997	-.060	.004	-.042

1/2, -	1.	16.057	.799	.268	-.521	.127	.056	.014
	2.	20.942	-.457	.476	-.274	.686	.133	.012
	3.	23.021	.367	.231	.762	.427	-.187	-.122
	4.	24.756	.107	-.158	.207	.078	.946	.137
	5.	26.839	-.078	.787	.166	-.559	.131	.132
	6.	32.846	.035	-.065	.055	.108	-.177	.974

	$1p_{3/2}$	$1p_{1/2}$	$1f_{7/2}$	$2p_{3/2}$	$1f_{5/2}$	$2p_{1/2}$
(+).001	.029	.022	.479	.554	.258	.629
(-).001	.087	-.065	.623	-.347	-.684	.111
(-).001	.010	-.005	-.324	-.599	.128	.721
(+).002	.040	.044	.520	-.461	.665	-.267
(-).996	.746	-.657	-.068	.040	.070	-.024
(+).997	.658	.749	-.053	.012	-.043	-.010

$\lambda = -9.865$

Table 5.9 : Prolate Ar^{36} (Rosenfeld 2)

					$1d_{5/2}$
5/2, +	1.	4.676	1.000	(-).876	1.000

					$1d_{5/2}$	$1d_{3/2}$
-3/2, +	1.	2.506	.994	.111	(-).391	.221	-.975
	2.	6.594	-.111	.994	(+).986	.975	.221

						$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
1/2, +	1.	2.177	.835	.528	.154	(-).773	.486	-.769	.416
	2.	5.784	.542	-.743	-.392	(+).982	.786	.592	.176
	3.	7.386	.092	-.411	.907	(-).991	.382	-.241	-.892

$\lambda = -15.847$

Table 5.10 : Prolate Ar^{36} (NDKB 2)

					$1d_{5/2}$
5/2, +	1.	7.006	1.000	(-).950	1.000

					$1d_{5/2}$	$1d_{3/2}$
-3/2, +	1.	1.973	.982	.190	(-).450	.238	-.971
	2.	9.123	-.190	.982	(+).981	.971	.238

								$1s_{1/2}$	$1d_{5/2}$	$2s_{1/2}$	$1d_{3/2}$
1/2, +	1.	2.077	.622	.697	.356	.004	(-).675	.052	-.308	-.825	.471
	2.	3.623	.768	-.452	-.454	-.016	(+).944	.034	-.628	-.193	-.753
	3.	9.989	.155	-.555	.817	-.032	(-).979	.021	-.713	.530	.459
	4.	66.395	.015	-.028	.017	.999	(-)1.000	.998	.053	.039	-.008

					$1f_{7/2}$
-7/2, -	1.	15.685	1.000	(+).004	1.000

					$1f_{7/2}$	$1f_{5/2}$
5/2, -	1.	14.058	.372	.928	(+).001	.425	.905
	2.	24.488	.928	-.372	(-).005	.905	-.425

(cont.)

Table 5.10 (continued)

								$1p_{3/2}$	$1f_{7/2}$	$2p_{3/2}$	$1f_{5/2}$
-3/2, -	1.	13.260	-.167	.561	.811	-.004	(+).001	.018	.026	-.999	.004
	2.	19.662	.985	.101	.133	-.030	(-).002	.002	-.584	-.011	.812
	3.	23.247	.004	-.817	.565	-.112	(+).005	.038	-.811	-.023	-.583
	4.	33.925	.030	-.087	.072	.993	(+).998	.999	.031	.019	.020

1/2, -	1.	12.950	-.117	.127	.657	.734	-.003	-.005
	2.	19.013	.550	-.817	.123	.119	-.011	-.005
	3.	22.711	.546	.359	-.551	.517	.026	-.040
	4.	23.372	.617	.430	.492	-.417	-.140	.017
	5.	29.891	.079	.042	.075	-.056	.946	.297
	6.	35.804	-.011	-.009	-.051	.051	-.291	.954

	$1p_{3/2}$	$1p_{1/2}$	$1f_{7/2}$	$2p_{3/2}$	$1f_{5/2}$	$2p_{1/2}$
(+).000	.009	.004	.005	-.650	.040	-.759
(-).001	.004	-.005	-.002	.760	.033	-.649
(+).003	.021	.021	-.670	-.003	-.741	-.040
(-).004	.024	-.007	-.742	-.003	.669	.033
(+).998	.494	.869	.023	.007	.018	.006
(-).999	.869	-.495	.024	-.001	-.011	.008

$\lambda = -11.988$

Table 5.11 : T = 0 Pair Potential ($\Delta_{pn}^{T=0}$) in Canonical Basis

Prolate Mg^{24} (Prolate 1, Rosenfeld 1)

5/2, +	.922		
-3/2, +	1.483	.210	
	.210	-2.162	
1/2, +	.806	.285	-.057
	.285	-2.494	-.406
	-.057	-.406	1.188

Table 5.12: T = 0 Pair Potential ($\Delta_{pn}^{T=0}$) in Canonical Basis

Prolate Mg^{24} (Prolate 2, Rosenfeld 2)

5/2, +	1.198		
-3/2, +	1.616	.183	
	.183	-2.704	
1/2, +	1.001	.357	-.011
	.357	-2.896	-.269
	-.011	-.269	1.635

Table 5.13 : T = 0 Pair Potential ($\Delta^{T=0}_{pn}$) in Canonical Basis

Prolate Mg^{24} (Yale)

5/2, +	1.372			
-3/2, +	1.428	.678		
	.678	-2.604		
1/2, +	1.189	.378	-.116	1.058
	.378	-2.589	.845	-.458
	-.116	.845	2.547	.367
	1.058	-.458	.367	1.656
-3/2, -	-2.178			
1/2, -	-2.264	-.022		
	- .022	2.537		

Table 5.14 : T = 0 Pair Potential ($\Delta_{pn}^{T=0}$) in Canonical Basis

Prolate Mg^{24} (NDKB 1)

5/2, +	1.750			
-3/2, +	2.276	.713		
	.713	-2.375		
1/2, +	1.601	.311	-.149	.879
	.311	-2.576	.943	-.431
	-.149	.943	1.997	.339
	.879	-.431	.339	2.154
3/2, -	-2.598			
1/2, -	-3.052	-.041		
	- .041	2.497		

Table 5.15 : T = 0 Pair Potential ($\Delta_{pn}^{T=0}$) in Canonical Basis

Prolate Mg^{24} (NDKB 2)

5/2, +	1.954			
-3/2, +	2.281	.649		
	.649	-2.710		
1/2, +	1.746	.348	-.087	.940
	.348	-2.784	.965	-.359
	-.087	.965	2.228	.466
	.940	-.359	.466	2.431
-7/2, -	-1.013			
5/2, -	-1.376	-.040		
	-.040	1.652		

(cont.)

Table 5.15 : (Continued)

-3/2, -	-.751	.010	-.091	-.134
	.010	1.906	-.063	-.662
	-.091	-.063	-2.052	.173
	-.134	-.662	.173	-2.965

1/2, -	-.863	-.011	-.088	.031	-.022	-.035
	-.011	1.064	.018	.127	.313	.605
	-.088	.018	-2.140	-.035	.202	-.797
	.031	.127	-.035	2.191	.274	.482
	-.022	.313	.202	.274	-3.282	-.050
	-.035	.605	-.797	.482	-.050	2.647

Table 5.16 : T = 0 Pair Potential ($\Delta^{T=0}_{pn}$) in Canonical Basis
Prolate S^{32} (NDKB 2)

5/2, +	-2.681			
-3/2, +	-2.695	-.836		
	-.836	2.460		
1/2, +	-2.721	-.460	-.327	-.730
	-.460	2.403	.426	.244
	-.327	.426	-2.091	-.106
	-.730	.244	-.106	-2.537
-7/2, -	1.648			
5/2, -	1.857	.083		
	.083	-2.039		

(cont.)

Table 5.16 (continued)

-3/2, -

.904	-.015	.138	.484
-.015	-1.981	-.083	-.663
.138	-.083	2.254	.631
.484	-.663	.631	2.898

1/2, -

.937	-.019	.107	-.025	.433	-.025
-.019	-1.315	-.001	.119	.252	.158
.107	-.001	2.163	.022	.646	.396
-.025	.119	.022	-2.175	-.328	-.624
.433	.252	.646	-.328	2.976	.021
-.025	.158	.396	-.624	.021	-2.425

Table 5.17 : T = 0 Pair Potential ($\Delta_{pn}^{T=0}$) in Canonical Basis

Oblate S^{32} (NDKB 2)

5/2, +	-1.937			
-3/2, +	2.675	.907		
	.907	-2.066		
1/2, +	-2.177	-.560	-.297	-1.095
	- .560	2.876	-.481	.490
	-.297	-.481	-1.676	-1.184
	-1.095	.490	-1.184	-3.735
-7/2, -	.919			
5/2, -	1.220	.035		
	.035	-1.673		

(cont.)

Table 5.17 (continued)

-3/2, -	.768	.050	.046	.311
	.050	1.947	.008	.736
	.046	.008	-1.827	-.850
	.311	.736	-.850	3.376

1/2, -	.830	.004	-.019	.010	.106	.256
	.004	-1.263	-.092	-.040	-.012	-.304
	-.019	-.092	-1.278	.006	-.605	.716
	.010	-.040	.006	1.896	.575	.737
	.106	-.012	-.605	.575	-3.218	-.015
	.256	-.304	.716	.737	-.015	3.520

Table 5.18 : T = 0 Pair Potential ($\Delta_{pn}^{T=0}$) in Canonical Basis

Prolate Ar^{36} (Rosenfeld 2)

5/2, +	-3.079		
-3/2, +	-2.495	-.316	
	-.316	1.523	
1/2, +	-2.748	-.585	.184
	-.585	1.340	0.035
	.184	.035	-1.317

Table 5.19 : T = 0 Pair Potential ($\Delta_{pn}^{T=0}$) in Canonical Basis

Prolate Ar^{36} (NDKB 2)

5/2, +	-3.065			
-3/2, +	-2.220	-.859		
	-.859	2.408		
1/2, +	-2.991	-.448	-.327	-.530
	-.448	2.240	.308	.360
	-.327	.308	-2.196	-.149
	-.530	.360	-.149	-2.441
-7/2, -	2.068			
5/2, -	1.520	.132		
	.132	-2.151		

(cont.)

Table 5.19 (continued)

-3/2, -	.923	-.012	.085	.416
	-.012	-1.809	-.116	-.881
	.085	-.116	2.324	.809
	.416	-.881	.809	2.976

1/2, -	.763	-.034	.056	-.018	.540	-.044
	-.034	-1.393	-.006	.069	.247	.024
	.056	-.006	2.127	.039	.688	.436
	-.018	.069	.039	-2.274	-.505	-.557
	.540	.247	.688	-.505	2.529	.011
	-.044	.024	.436	-.557	.011	- 2.482

Table 5.20 : BCS T = 0 Pair Potential ($\Delta_{pn}^{T=0}$) in HF Basis

Prolate Ar^{36} (Rosenfeld 2)

5/2, +	-2.105		
-3/2, +	-0.181	-.078	
	-.078	-1.780	
1/2, +	.071	.263	.299
	.263	-.399	.915
	.299	.915	-1.221

Table 5.21

$$\frac{E_{PAIR}\ (HFB) - E_{PAIR}\ (BCS)}{E_{PAIR}\ (BCS)}$$

	Prolate Mg^{24}	Prolate S^{32}	Oblate S^{32}	Prolate Ar^{36}
Rosenfeld 1	0.15	-	0.38	0.63
Rosenfeld 2	0.07	0.27	0.06	1.07
Yale	0.24	0.94	-	1.81 *
NDKB 1	0.30	1.22	-0.05	1.18
NDKB 2	1.02	4.06	0.27	2.16

* HFB solution is Oblate

Table 5.22

$$\frac{E_{PAIR}\ (\text{NDKB } 2) - E_{PAIR}\ (\text{NDKB } 1)}{E_{PAIR}\ (\text{NDKB } 1)}$$

Prolate Mg^{24}	0.19
Oblate Mg^{24}	0.35
Prolate Si^{28}	-0.16
Prolate S^{32}	0.52
Oblate S^{32}	0.43
Prolate Ar^{36}	0.90

Table 5.23

$$\frac{(E_1 + E_2)_{HFB} - (E_1 + E_2)_{BCS}}{(E_1 + E_2)_{BCS}}$$

	Prolate Mg^{24}	Prolate S^{32}	Oblate S^{32}	Prolate Ar^{36}
Rosenfeld 1	0.02	-	0.02	0.20
Rosenfeld 2	0.00	0.60	0.00	0.27
Yale	-0.04	0.11	-	0.79 *
NDKB 1	-0.03	0.06	-0.16	0.25
NDKB 2	0.16	0.20	-0.01	0.36

* HFB solution is Oblate

Table 5.24

$$\frac{(E_1 + E_2)_{NDKB\ 2} - (E_1 + E_2)_{NDKB\ 1}}{(E_1 + E_2)_{NDKB\ 1}}$$

Prolate Mg^{24}	0.18
Oblate Mg^{24}	0.24
Prolate Si^{28}	0.15
Prolate S^{32}	0.38
Oblate S^{32}	0.23
Prolate Ar^{36}	0.44

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SUMMARY

The Schroedinger equation with nucleon-nucleon interactions provides a starting point for a many - body description of nuclear properties. Application of the partition method results in an effective interaction operating in a model space. If the model space is suitably chosen, the same effective interaction may be used in both the pair potential and the HF potential. The self-consistent field formalisms are then to be interpreted as approximations to exact diagonalization of the effective Hamiltonian in the model space. (Ch.I)

HF theory is the first order approximation to exact diagonalization. It is an independent particle description and provides a one body self-consistent potential. With the exception of Ne^{20}, HF theory fails to explain the ground state properties of the N = Z even - even nuclei in the 2s-1d shell. (Ch.II)

Components of the effective interaction unaccounted for by the HF potential give rise to correlations between pairs of nucleons in time-reversed degenerate orbitals. With these pairing correlations is associated a self-consistent pair potential. The approximately independent modes of excitation are no longer particles, but quasi-particles. They may be described by the special Bogoliubov quasiparticle transformation. Unless special care is

taken in choosing the single particle basis states, use of the special transformation assumes that the pair potential only connects time-reversed orbitals. For a non-trivial force, this assumption is not justifiable. It is demonstrated that p-p and n-n pairing correlations are not significant in N = Z even-even nuclei in the 2s-1d shell. (Ch III)

The pairing theory is generalized to include p-p, n-n, n-p (T = 1), and n-p (T = 0), pairing. All modes are treated on an equal basis. The quasiparticle co-ordinates must be complex. A generalized set of gap equations are derived for N = Z nuclei. Solution of the gap equations indicates that T = 0 pairing correlations play a very important role, altering the properties of several of the nuclei considered. However the generalized gap equations still assume that the pair potential is diagonal in spatial co-ordinates. Their utility, therefore, is twofold. a) The isospin generalized special transformation demonstrates how to introduce appropriate symmetries into the HF and pair potentials so as to permit both T = 0 and T = 1 pairing. b) The solutions to the generalized gap equations are natural starting points for HFB calculations. (Ch. IV)

The general quasiparticle transformation permits the HF and pair degrees of freedom to interact with one another. The pair potential is not assumed to be diagonal.

Requiring the quasiparticles to be approximately non-interacting results in the HFB equations, which provide the quasiparticle co-ordinates and energies. The HFB equations are also derived by a variational principle: minimization of the binding energy with respect to arbitrary variations in quasiparticle co-ordinates. This proof requires the assistance of the generalized density matrix. The self-consistent symmetries of the HFB solutions are discussed in some detail. It is demonstrated that complex quasiparticle co-ordinates are required for generalized isospin pairing. (Ch.V.1-7.)

Unitarity conditions and the assumption of time-reversal symmetry quite trivially provide the canonical form of the density matrix and the pairing tensor. The general quasiparticle transformation is then described as the product of three transformations: (1) an isospin-conserving rotation in particle space, (2) an isospin-generalized special quasiparticle transformation, (3) a rotation in quasiparticle space. This representation facilitates an evaluation of the various approximations to HFB. We find that the BCS approximation of neglecting off-diagonal elements of the pair potential is not justified. Furthermore, attempting to permit the HF and pair degrees of freedom to interact with one another by iterating between the HF and BCS equations is an even worse approximation. The HFB canonical single particle basis

often bears no resemblance to the "corresponding" HF single particle basis. The third transformation may not be approximated by the unit transformation, nor is the pair potential diagonal in the canonical basis. (Ch. III.6, IV.6, V.7-8)

The HFB equations with generalized isospin pairing have been solved for the N = Z even-even nuclei in the 2s-1d shell. A variety of model spaces and interactions, both realistic and phenomenological, all reproduce the following conclusions: T = 0 pairing correlations dominate over T = 1 pairing correlations. They play a very significant role, drastically altering the properties of many intrinsic states. Most of the failures of the HF theory in explaining the properties of these nuclei are rectified. T = 0 pairing restores axial symmetry to the equilibrium shapes of Mg^{24} and S^{32} and provides an explanation for the vibrational nature of Ar^{36}. (Ch.V.8)

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