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(Ph. D. Thesis)

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CONTENTS

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 inter-
actions 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 t-matrix. Pairing correlations alter the t-matrix in a fairly obvious fashion. A more perplexing problem is whether the t-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.

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

One then observes that if the interaction $\mathcal{N}_{12}$ has a hard core, the matrix elements diverge, rendering the HF equations meaningless. Brueckner theory is then invoked to justify the replacement of $\mathcal{N}$ 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 $\mathcal{N}_{ij}$. The Hamiltonian is
separated into two parts.

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

where Ho contains only single particle operators

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

and H_1 contains the residual interactions unaccounted for
by U .

$$H_1 = V - U = \sum_{i<j=1}^{A} N_{ij} - \sum_{i=1}^{A} U_i \qquad (1.5)$$

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_o satisfy

$$\langle T_i + U_i \rangle |\phi(i)\rangle = \epsilon_\phi |\phi(i)\rangle . \qquad (1.6)$$

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

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

$$H_o |\Phi_i\rangle = E_i |\Phi_i\rangle \qquad (1.7b)$$

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

$$E_i = \sum_{\phi \ occupied} \epsilon_\phi \qquad (1.8)$$

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

The set $\{|\Phi_c\rangle\}$ 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 $\langle\Phi_c|$.

$$\sum_j \langle\Phi_c|H_o + H_i|\Phi_j\rangle a_j = \sum_j \langle\Phi_c|E|\Phi_j\rangle a_j \tag{1.10}$$

or

$$\sum_j \{E_c \delta_{cj} + \langle\Phi_c|H_i|\Phi_j\rangle\} a_j = E a_c \tag{1.11}$$

We have simply rewritten the Schroedinger equation as

$$[H_o + H_i] \underline{a} = E \underline{a}. \tag{1.12}$$

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 $\langle\Phi_c|H_i|\Phi_j\rangle$ may be expressed in terms of the two body matrix elements

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

The nucleon-nucleon interaction $\mathcal{N}_{12}$, 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).
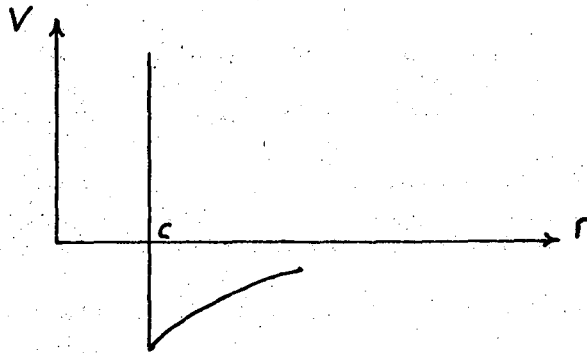
Figure (1.1)

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 $\mathcal{N}_{ij}$ 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_i 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

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

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

$$\langle \Phi_i | H_1^{eff}(E) | \Phi_j \rangle = \langle \Phi_i | H_1 | \Phi_j \rangle +$$

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

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

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

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

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

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.

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

One of the eigenvalues of

$$H^{eff}(E) = H_o + H_1^{eff}(E) \qquad (1.29)$$

is the exact ground state energy of the system of inter-
acting 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 $i\epsilon d$, $j\epsilon d$, (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.

$$\langle \Psi_d | \Psi_d \rangle = 1$$

$$(1.30)$$

Then

$$\langle \Psi | \Psi_d \rangle = 1. \qquad (1.31)$$

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

$$H_1^{eff}(E) = H_1 \sum_{m=0}^{\infty} (GH_1)^m \qquad (1.32)$$

Define the effective interaction V^{eff} by

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

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

$$V^{eff}(E) = H_1^{eff}(E) + U .$$ (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.

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

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

$$H_0 |N\ell jm\tau\rangle = \epsilon_{N\ell j} |N\ell jm\tau\rangle \qquad (1.36)$$

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

$$\epsilon_\nu > \epsilon_A . \qquad (1.37)$$

Choose the model space to consist of all A dimensional

Slater determinants where the single particle orbitals

are HO states with $\epsilon_i \leq \epsilon_\nu$.

The HO spectrum is presented in Figure (1.2).
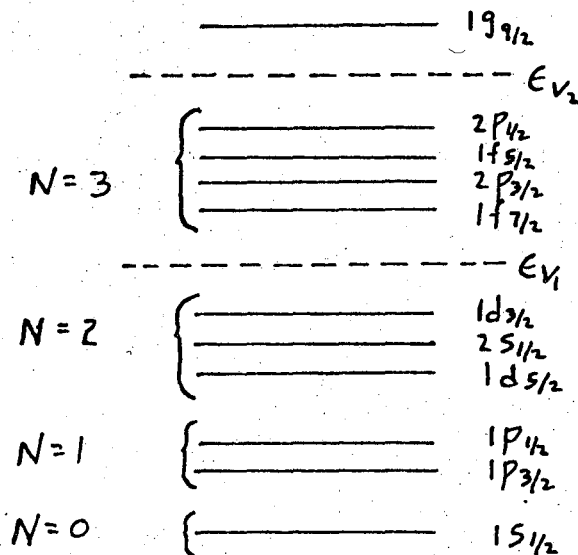
Figure(1.2)

For nuclei filling the 2s-1d shell the dashed lines in
Figure (1.2) are two reasonable choices for ϵ_ν . Suppose
we choose $\epsilon_\nu = \epsilon_{\nu_1}$. The number of proton states with
$\epsilon_c \lessgtr \epsilon_\nu$ 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
$\epsilon_\nu = \epsilon_{\nu_2}$, 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
$H_1 = V - U$.

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

The terms outside the bracket contain at least one U

factor. If they are neglected

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

Combining (1.33),(1.39)

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

or

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

$$Q = Q_{2p}$$ (approximation) (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 $\epsilon_m, \epsilon_n > \epsilon_v$, the remaining particles having $\epsilon_i \leq \epsilon_v$. 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

$$\langle \phi_i(1) \; \phi_j(2) | \mathcal{N}_{12} | \phi_K(1) \; \phi_\ell(2) \rangle$$

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

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

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

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

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
$v_{ijk...}^{eff}$.

K (E) has the matrix representation

$$\langle ij|K(E)|kl\rangle = \langle ij|v|kl\rangle +$$

$$\sum_i' \frac{\langle ij|v|mn\rangle\langle mn|K(E)|kl\rangle}{E-H_o} \qquad (1.46)$$
$$\epsilon_m, \epsilon_n > \epsilon_v$$

Actually this representation of K is deceptive. The
energy denominator $1/(E - H_o)$ 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.

$$\frac{1}{E-H_o} = \frac{1}{E-\epsilon_i + \epsilon_k + \epsilon_l - \epsilon_m - \epsilon_n}$$

where E_1 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_1 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 $|\Phi_o\rangle$.

$$H_o \, | \, \Phi_o \rangle = E_o \, | \, \Phi_o \rangle \tag{1.47}$$

The model space eigenvalue equation (1.28) is simply

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

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

Inserting (1.32)

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

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

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

$\mathcal{N}_{ij}$ is $\quad\quad \langle \Phi_0 | V^{eff}(E) | \Phi_0 \rangle$

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

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

$$U = U_{HF}$$

$$(T + U_{HF})_i |\phi(i)\rangle = \mathcal{E}_\phi |\phi(i)\rangle$$

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

$$E_{HF} = \sum_{i=1}^{A} \mathcal{E}_i$$

(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.
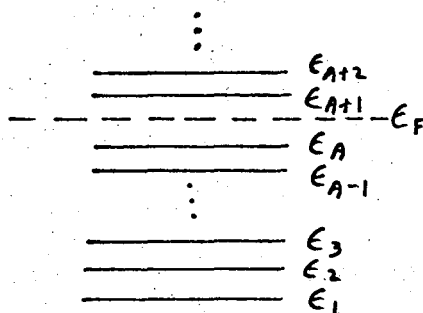
Figure (1.3)

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

$$Q_{2p} = \sum_{\mathcal{E}_m, \mathcal{E}_n > \mathcal{E}_F} |mn\rangle\langle mn| \quad\quad (1.53)$$

(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

$$\langle ij | K(E) | k\ell \rangle = \langle ij | \mathcal{N} | k\ell \rangle +$$

$$\sum_{\epsilon_m, \epsilon_n > \epsilon_f} \frac{\langle ij | \mathcal{N} | mn \rangle \langle mn | K(E) | k\ell \rangle}{E - E_{HF} + \epsilon_K + \epsilon_\ell - \epsilon_m - \epsilon_n} \cdot \quad (1.54)$$

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

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

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

$$\langle ij | K | k\ell \rangle = \langle ij | \mathcal{N} | k\ell \rangle +$$

$$\sum_{\epsilon_m, \epsilon_n > \epsilon_F} \frac{\langle ij | \mathcal{N} | mn \rangle \langle mn | K | k\ell \rangle}{\epsilon_K + \epsilon_\ell - \epsilon_m - \epsilon_n} \qquad (1.56)$$

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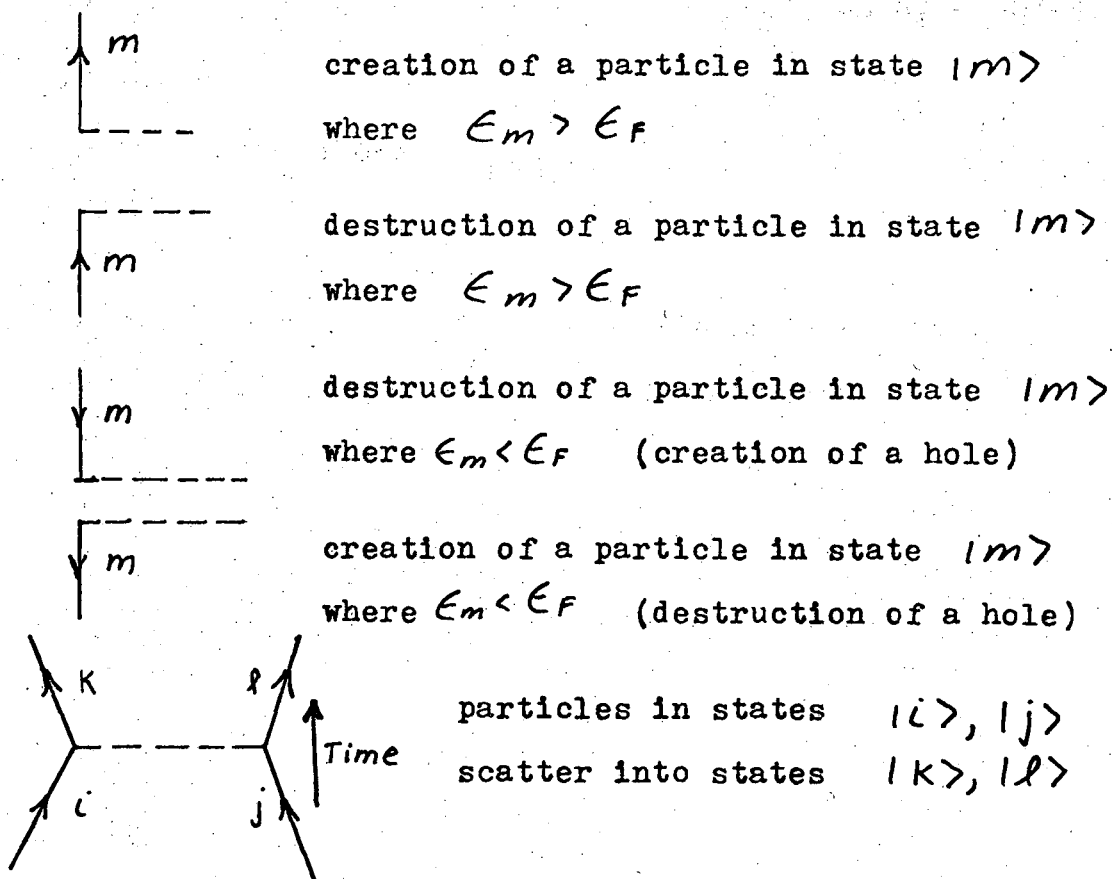
Consider the process whereby particles in occupied states $|i\rangle, |j\rangle$ forward scatter, remaining in $|i\rangle, |j\rangle$.

The energy contribution is $\langle i'j' | \mathcal{N} | i'j \rangle$. Summing over distinct pairs

$$\text{(diagram)} = \frac{1}{2} \sum_{\epsilon_i, \epsilon_j < \epsilon_F} \langle i'j' | \mathcal{N} | i'j \rangle. \tag{1.57}$$

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

$$E_0 - H_0 = \text{(sum of hole energies)} - \text{(sum of particle energies)}.$$

$$\text{(diagram)} = \frac{1}{2} \sum_{\substack{\epsilon_i, \epsilon_j < \epsilon_F \\ \epsilon_K, \epsilon_\ell > \epsilon_F}} \frac{\langle i'j' | \mathcal{N} | K\ell \rangle \langle K\ell | \mathcal{N} | i'j \rangle}{\epsilon_i + \epsilon_j - \epsilon_K - \epsilon_\ell} \tag{1.58}$$

The third order process is

$$\text{(diagram)} = \frac{1}{2} \sum_{\substack{\epsilon_i, \epsilon_j < \epsilon_F \\ \epsilon_K, \epsilon_\ell, \epsilon_m, \epsilon_n > \epsilon_F}} \frac{\langle i'j' | \mathcal{N} | mn \rangle \langle mn | \mathcal{N} | K\ell \rangle \langle K\ell | \mathcal{N} | i'j \rangle}{(\epsilon_i + \epsilon_j - \epsilon_m - \epsilon_n)(\epsilon_i + \epsilon_j - \epsilon_K - \epsilon_\ell)}, \tag{1.59}$$

and so on.

Returning to our expression for the reaction matrix (1.56), let $i = k$, $j = 1$, and iterate.
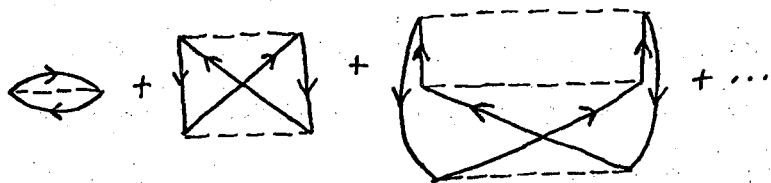
$$\langle ij | K | ij \rangle = \langle ij | N | ij \rangle + \sum_{\epsilon_k, \epsilon_\ell > \epsilon_F} \frac{\langle ij | N | k\ell \rangle \langle k\ell | N | ij \rangle}{\epsilon_i + \epsilon_j - \epsilon_k - \epsilon_\ell}$$

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

It is therefore clear that

$$(1.61)$$

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

Similarly the exchange terms may be evaluated.

$$(1.62)$$

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

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

$$\frac{1}{2} \sum_{\epsilon_i, \epsilon_j < \epsilon_F} \left\{ \langle ij | K | ij \rangle - \langle ij | K | ji \rangle \right\} \cdot \qquad (1.63)$$

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

$$\langle i \bar{i} | \mathcal{N} | j \bar{j} \rangle = \lambda \, \mathcal{N}_i \, \mathcal{N}_j \tag{1.64}$$

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

$$\langle i \bar{i} | K | j \bar{j} \rangle = \lambda \, \mathcal{N}_i \mathcal{N}_j +$$

$$\sum_{\epsilon_m > \epsilon_F} \frac{\lambda \, \mathcal{N}_i \mathcal{N}_m \, \langle m \bar{m} | K | j \bar{j} \rangle}{2 \, (\epsilon_j - \epsilon_m)} \tag{1.65}$$

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

$$\langle i\,\bar{i}\,|K|\,j\,\bar{j}\rangle = \lambda\,N_i\,K_j \qquad (1.66)$$

where

$$K_j = N_j + \sum_{\epsilon_m > \epsilon_F} \frac{\lambda\,N_m^2\,K_j}{2(\epsilon_j - \epsilon_m)} . \qquad (1.67)$$

Solving for K_j

$$K_j = \frac{N_j}{1 + \dfrac{\lambda}{2}\displaystyle\sum_{\epsilon_m > \epsilon_F}\dfrac{N_m^2}{(\epsilon_m - \epsilon_j)}} . \qquad (1.68)$$

Substituting into (1.66)

$$\langle i\,\bar{i}\,|K|\,j\,\bar{j}\rangle = \frac{N_i\,N_j}{\dfrac{1}{\lambda} + \dfrac{1}{2}\displaystyle\sum_{\epsilon_m > \epsilon_F}\dfrac{N_m^2}{(\epsilon_m - \epsilon_j)}} . \qquad (1.69)$$

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_ν . The effective force may be approximated by the reaction matrix (1.46). The intermediate states have HO energies $\epsilon_m, \epsilon_n > \epsilon_\nu$. 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 $|\Phi_o\rangle$. If $|\Phi_o\rangle$ 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

$$Q = \sum_{i \neq o}' |\Phi_i\rangle\langle\Phi_i| = 1 - |\Phi_o\rangle\langle\Phi_o|. \tag{1.70}$$

If $|\Phi_o\rangle$ 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

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

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

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

$$H = E_0 + H_{q \cdot p} + H_{q \cdot p - int}$$

(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

$$H = \sum_{ij} \langle i|T|j\rangle a_i^\dagger a_j + \frac{1}{4} \sum_{ijk\ell} \langle ij|N|k\ell\rangle_A a_i^\dagger a_j^\dagger a_\ell a_k \quad (1.74)$$

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

$$\langle ij|N|k\ell\rangle_A = \langle ij|N|k\ell\rangle - \langle ij|N|\ell k\rangle. \quad (1.75)$$

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

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

where

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

A system with particles in states $|K_1\rangle$, $|K_2\rangle$, $\cdots$ $|K_A\rangle$ 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

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

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

$$b_k^+ = a_k^+ \qquad \text{creates a "particle"}$$

$$b_k = a_k \qquad \text{annihilates a "particle"}$$

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

$$b_k^+ = a_k \qquad \text{creates a hole}$$

$$b_k = a_k^+ \qquad \text{annihilates a hole}$$
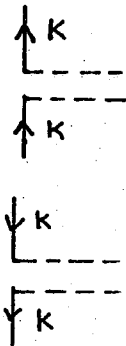
The normal product of a number of creation operators b_k^+ and annihilation operators b_k is defined as the product of these operators rearranged so that the

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

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

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

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

$$\langle \Phi_0 | N\left[ABC\cdots\right] | \Phi_0 \rangle = 0 \qquad (1.80)$$

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

$$\overline{AB} \equiv \langle AB \rangle = \langle \Phi_0 | AB | \Phi_0 \rangle . \qquad (1.81)$$

In particular

$$\langle b_i^\dagger b_j \rangle = \langle b_i^\dagger b_j^\dagger \rangle = \langle b_i b_j \rangle = 0 \qquad (1.82)$$

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

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

$$N[\overline{ABCD}] = -\overline{AC}\, N[BD]$$
$$N[\overline{AB\,CDEF}] = -\overline{AC}\,\overline{BD}\, N[EF].$$

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

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

$$ABCD = N[ABCD] + \overline{AB}\, N[CD] - \overline{AC}\, N[BD]$$
$$+ \overline{AD}\, N[BC] + \overline{BC}\, N[AD] - \overline{BD}\, N[AC]$$
$$+ \overline{CD}\, N[AB] + \overline{AB}\,\overline{CD} - \overline{AC}\,\overline{BD} + \overline{AD}\,\overline{BC}.$$

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.

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

$$\frac{1}{2} \sum_{ijk\ell} <ij|N|k\ell>_A <a^\dagger_i a_k><a^\dagger_j a_\ell> +$$

$$\frac{1}{4} \sum_{ijk\ell} <ij|N|k\ell>_A <a^\dagger_i a_j><a_\ell a_k> \tag{1.84}$$

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

$$\sum_{ijk\ell} <ij|N|k\ell>_A <a^\dagger_j a_\ell> N[a^\dagger_i a_k] +$$

$$\frac{1}{4} \sum_{ijk\ell} <ij|N|k\ell>_A <a^\dagger_i a^\dagger_j> N[a_\ell a_k] +$$

$$\frac{1}{4} \sum_{ijk\ell} <ij|N|k\ell>_A <a_\ell a_k> N[a^\dagger_i a^\dagger_j] \tag{1.85}$$

$$H_4 = \frac{1}{4} \sum_{ijk\ell} <ij|N|k\ell>_A N[a^\dagger_i a^\dagger_j a_\ell a_k] \tag{1.86}$$

It has been assumed that

$$<ij|N|k\ell>_A = <k\ell|N|ij>_A = <ji|N|\ell k>_A .$$

Define a density matrix ρ .

$$\rho_{ji} = <a^\dagger_i a_j> \tag{1.87a}$$

ρ is clearly Hermitian.

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

Define a pairing tensor $\mathcal{L}$.

$$\mathcal{L}_{ji} = \langle a_i a_j \rangle \tag{1.88a}$$

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

Recalling the anti-commutation relation (1.76) it is apparent that $\mathcal{L}$ is anti-symmetric.

$$\tilde{\mathcal{L}} = -\mathcal{L} \tag{1.88c}$$

Define a HF potential Γ .

$$\Gamma_{ij} = \sum_{k\ell} \langle ik | N | j\ell \rangle_A \, \rho_{\ell k} \tag{1.89a}$$

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 .

$$\Delta_{ij} = \tfrac{1}{2} \sum_{k\ell} \langle ij | N | k\ell \rangle_A \, \mathcal{L}_{k\ell} \tag{1.91a}$$

$$\Delta^*_{ij} = \tfrac{1}{2} \sum_{k\ell} \langle k\ell | N | ij \rangle_A \, \mathcal{L}^*_{k\ell} \tag{1.91b}$$

Since $\langle ij|N|k\ell\rangle_A = -\langle ji|N|k\ell\rangle_A$, Δ is anti-symmetric.

$$\tilde{\Delta} = -\Delta \qquad (1.91c)$$

H_0 and H_2 may be more simply expressed.

$$H_0 = \sum_{ij} \{T_{ij} + \tfrac{1}{2}\Gamma_{ij}\}\rho_{ji} + \tfrac{1}{2}\sum_{ij}\Delta_{ij}\zeta_{ij}^* \qquad (1.92)$$

$$H_2 = \sum_{ij}\mathcal{H}_{ij}N[a_i^\dagger a_j] + \tfrac{1}{2}\sum_{ij}\Delta_{ij}N[a_i^\dagger a_j^\dagger]$$
$$+ \tfrac{1}{2}\sum_{ij}\Delta_{ij}^\dagger N[a_i a_j] \qquad (1.93)$$

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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    This review article is a good introduction, with references to original papers.

2. B.H. Brandow, "Linked-Cluster Expansions for the Nuclear Many-Body Problem," Rev. Mod. Phys. 39, 771 (1967).
    The reader is referred to Brandow's discussion of superfluidity.

3. C. Bloch, Lectures on Nuclear Many-Body Problem, Tata Institute, Bombay, 1962.
    The reader is referred to section XXIII.

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.
    The reader is also referred to Brandow's review article.

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 $|\overline{\Phi}_0\rangle$.

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

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

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

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

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

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

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

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)

$$E_0 = \sum_{\substack{\alpha \, occ. \\ ij}} D^{\alpha}_i D^{\alpha}_j \langle i | T | j \rangle + \frac{1}{2} \sum_{\substack{\alpha\beta \, occ. \\ ijk\ell}} D^{\alpha}_i D^{\beta}_j D^{\alpha}_k D^{\beta}_\ell \langle ij | v | k\ell \rangle_A \, . \tag{2.12}$$

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

$$\langle a^\dagger_i a_j \rangle = \sum_{\alpha\beta} D^\alpha_i \; D^\beta_j \; \langle a^\dagger_\alpha a_\beta \rangle$$

Noting (2.5) we obtain

$$\rho_{ji} = \langle a^\dagger_i a_j \rangle = \sum_{\alpha \; occ.} D^\alpha_i \; D^\alpha_j \; . \tag{2.13}$$

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.

$$\sum_j \left\{ \langle i | T | j \rangle + \sum_{\beta \; occ.} \langle i\beta | N | j\beta \rangle_A \right\} D^\alpha_j = \epsilon_\alpha D^\alpha_i \tag{2.16}$$

or $\quad \sum_j \mathcal{H}_{ij} D^\alpha_j = \epsilon_\alpha D^\alpha_i \; . \tag{2.17a}$

The HF equations present an eigenvalue problem.

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

or $\quad \mathcal{H} |\alpha\rangle = \epsilon_\alpha |\alpha\rangle \; . \tag{2.17c}$

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 .

$$\epsilon_\alpha = \langle \alpha | T | \alpha \rangle + \sum_{\beta \, occ.} \langle \alpha \beta | \mathcal{N} | \alpha \beta \rangle_A \qquad (2.18)$$

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 $|\Phi_o\rangle$ 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

$$H = H_0 + H_2 + H_4 .$$

If there is a basis in which H_2 has the form

$$H_2 = \sum_{\alpha} \epsilon_{\alpha} \, N \, [\, a_{\alpha}^{\dagger} \, a_{\alpha} \,] \qquad (2.19)$$

then

$$H = E_0 + \sum_{\alpha} \epsilon_{\alpha} \, N \, [\, a_{\alpha}^{\dagger} \, a_{\alpha} \,] + H_4 .$$

The H F ground state has one particle in each of the A lowest energy states.
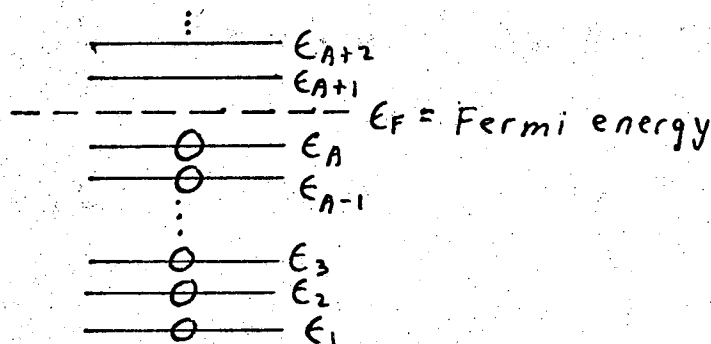
Figure (2.1)

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

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

$$\qquad (2.20)$$

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

and

$$H = E_o + \sum_{\substack{\epsilon_\alpha > \epsilon_F}}' \epsilon_\alpha \, a^\dagger_\alpha \, a_\alpha - \sum_{\substack{\epsilon_\alpha < \epsilon_F}}' \epsilon_\alpha \, a_\alpha \, a^\dagger_\alpha$$

$$\hspace{8cm} (2.21)$$

$$+ \tfrac{1}{4} \sum_{\alpha_1 \alpha_2 \alpha_3 \alpha_4}' \langle \alpha_1 \alpha_2 | \wr \vee | \alpha_3 \alpha_4 \rangle^N_A [a^\dagger_{\alpha_1} \, a^\dagger_{\alpha_2} \, a_{\alpha_4} \, a_{\alpha_3}].$$

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

$$H \approx E_o + \sum_{\substack{\epsilon_\alpha > \epsilon_F}}' \epsilon_\alpha \, a^\dagger_\alpha \, a_\alpha - \sum_{\substack{\epsilon_\alpha < \epsilon_F}}' \epsilon_\alpha \, a_\alpha \, a^\dagger_\alpha$$

$$\hspace{8cm} (2.22)$$

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

$$[H_2, a^\dagger_\alpha]_- = \epsilon_\alpha \, a^\dagger_\alpha$$

$$\hspace{8cm} (2.23)$$

or

$$[H_2, a^\dagger_\alpha]_- = \epsilon_\alpha \sum_i' D^\alpha_i \, a^\dagger_i .$$

$$\hspace{8cm} (2.24)$$

The commutator may also be evaluated using (2.9).

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

$$\hspace{8cm} (2.25)$$

Equating coefficients of a_1^+ 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 $\mathcal{N}_{ij}$ 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

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

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 $\mathcal{H}$.

$$\mathcal{H}_{ij} = \langle i|T|j\rangle + \sum_{k\ell}^{A} \langle ik|\mathcal{N}|j\ell\rangle_A \, \rho_{\ell k}$$

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.

$$|\alpha\rangle = \sum_K D_K^\alpha \, |\, N\ell J m T \rangle_K \qquad (2.29)$$

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

$$|\alpha\rangle = \sum_K D_K^\alpha \, |\, N\ell J m T_\alpha \rangle_K \qquad (2.30)$$

Then

$$T_z \{\, |\alpha\rangle \,\}_{occ.} = \{\, |\alpha\rangle \,\}_{occ.} \qquad (2.31a)$$

or

$$T_z \, |\, \Phi_0 \rangle = |\, \Phi_0 \rangle \qquad (2.31b)$$

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

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

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

$$\mathcal{H} = \begin{bmatrix} \mathcal{H}_{pp} & o \\ o & \mathcal{H}_{nn} \end{bmatrix} \qquad (2.32b)$$

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

$$P \, |\Phi_0\rangle = |\Phi_b\rangle \qquad (2.33)$$

and ρ and $\mathcal{H}$ have the form

$$\rho = \begin{bmatrix} \rho_{++} & o \\ o & \rho_{--} \end{bmatrix} \qquad \mathcal{H} = \begin{bmatrix} \mathcal{H}_{++} & o \\ o & \mathcal{H}_{--} \end{bmatrix}. \qquad (2.34)$$

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

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

(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

$$|\bar{\alpha}\rangle = \sum_K D_K^{\bar{\alpha}} |\overline{N\ell Jm T_\alpha}\rangle_K = \sum_K D_K^{\alpha} (-1)^{J-m+\ell} |N\ell J-m T_\alpha\rangle_K . \quad (2.36)$$

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

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

we have

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

so that

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

and time - reversal is a self - consistent symmetry.

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

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

and

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

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 $\{|Jm\rangle\}$, with

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

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

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

$$(2.42b)$$

This choice diagonalizes the inertia tensor.[2]

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

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

so that

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

Noting the restriction (2.42)

$$R_z(\pi)|\alpha\rangle = -i\,|\alpha\rangle \qquad\qquad (2.45a)$$

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

Therefore

$$R_z(\pi)|\Phi_0\rangle = |\Phi_0\rangle \qquad\qquad (2.46)$$

and

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

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.

$$\rho = \begin{bmatrix} \overset{\substack{m-\frac{1}{2}\\even}}{\rho} & \overset{\substack{m-\frac{1}{2}\\odd}}{0} \\ 0 & \bar{\rho} \end{bmatrix} \begin{matrix} m-\frac{1}{2}\\even\\[6pt] m-\frac{1}{2}\\odd \end{matrix} \qquad\qquad (2.48)$$

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.

$$\mathcal{H} = \begin{array}{cc} \overset{\substack{m-\frac{1}{2}\\ even}}{} & \overset{\substack{m-\frac{1}{2}\\ odd}}{} \\ \begin{bmatrix} \mathcal{H} & 0 \\ 0 & \bar{\mathcal{H}} \end{bmatrix} & \begin{array}{c} \substack{m-\frac{1}{2}\\ even} \\ \substack{m-\frac{1}{2}\\ odd} \end{array} \end{array} \qquad (2.49)$$

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

$$(2.51)$$

$$R_z(\theta) | \Phi_o \rangle = | \Phi_o \rangle \quad \text{for all } \theta .$$

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 $|m\rangle$.

$$|\alpha\rangle = \sum_K D_K^\alpha \, |N \ell J m_\alpha T_\alpha\rangle_K \qquad (2.52)$$

Then

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

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.

$$|\alpha\rangle = \sum_K D_K^\alpha \, |N \ell_\alpha J_\alpha m_\alpha T_\alpha\rangle \qquad (2.54)$$

$\underline{J}\{|\alpha\rangle\}$ 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

$$| \Phi_o \rangle = | \Phi_v \rangle | \Phi_c \rangle \qquad (2.55)$$

Let $|K\rangle$ represent a HO state $(|K\rangle = |N\ell Jm\tau\rangle)$. Then the
core component of $| \Phi_o \rangle$ is

$$| \Phi_c \rangle = a^\dagger_{K_1} a^\dagger_{K_2} \cdots a^\dagger_{K_{A_c}} |0\rangle \qquad (2.56)$$

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.

$$E_c = \sum_{k \in core}' \langle k|T|k \rangle + \tfrac{1}{2} \sum_{k_1 k_2 \in core}' \langle k_1 k_2 | \mathcal{N} | k_1 k_2 \rangle_A \qquad (2.57)$$

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

$$E_c = \sum_{(N\ell J) \in core}' 2(2J+1) \langle (N\ell J)m | T | (N\ell J)m \rangle +$$

$$\tfrac{1}{2} \sum_{\substack{JT \\ (N\ell J)_1 (N\ell J)_2 \in core}}' (2J+1)(2T+1) \langle (N\ell J)_1 (N\ell J)_2 JT | \mathcal{N} | (N\ell J)_1 (N\ell J)_2 JT \rangle_A$$

$$\qquad (2.58)$$

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).

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

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

$$\frac{1}{2(2J+1)} \sum_{\substack{JT \\ (N'\ell'J') \in core}} (2J+1)(2T+1) \langle (N\ell J)(N'\ell'J') JT \mid \mathscr{N} \mid (N\ell J)(N'\ell'J') JT \rangle_A \cdot$$

$$\tag{2.62}$$

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

$$H = E_c + \sum_{K \in valence} e_K a_K^\dagger a_K - \sum_{K \in core} e_K a_K a_K^\dagger$$

$$+ \tfrac{1}{4} \sum_{K_1 K_2 K_3 K_4} \langle K_1 K_2 \mid \mathscr{N} \mid K_3 K_4 \rangle_A N[a_{K_1}^\dagger a_{K_2}^\dagger a_{K_4} a_{K_3}] \cdot$$

$$\tag{2.63}$$

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 splitting 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 $\mid \mathscr{F}_c \rangle$ (2.56) as the reference state. If the wave function $\mid \mathscr{F}_0 \rangle$ is then restricted to the form (2.55), there can be no holes, and the Hamiltonian is simplified.

$$H = E_c + \sum_{K \in valence}' e_K\, a^\dagger_K\, a_K$$
$$+ \tfrac{1}{4} \sum_{K_1 K_2 K_3 K_4}' \langle K_1 K_2 | w | K_3 K_4 \rangle_A\, a^\dagger_{K_1}\, a^\dagger_{K_2}\, a_{K_4}\, a_{K_3} \qquad (2.64)$$

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

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

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

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

with

$$|\alpha\rangle = \sum_{K \in valence}' D^\alpha_K\, |K\rangle . \qquad (2.67)$$

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.

$$E_V = \sum_{\alpha=1}^{A_V} \langle \alpha | t | \alpha \rangle + \tfrac{1}{2} \sum_{\alpha,\beta=1}^{A_V} \langle \alpha\beta | v | \alpha\beta \rangle_A \qquad (2.68)$$

with

$$\langle jm\tau | t | j'm'\tau' \rangle = e_j \, \delta_{jj'} \, \delta_{mm'} \, \delta_{\tau\tau'} . \qquad (2.69)$$

The HF Hamiltonian is

$$\mathcal{H}_{ij} = \langle i | t | j \rangle + \sum_{\alpha=1}^{A_V} \langle i\alpha | v | j\alpha \rangle_A . \qquad (2.70)$$

The eigenvalue equation

$$\mathcal{H} \underline{D}^\alpha = \epsilon_\alpha \, \underline{D}^\alpha \qquad (2.71)$$

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

$$Q_{LM} = \sum_{ij} \langle i | Q_{LM} | j \rangle \, a_i^\dagger a_j \tag{2.73}$$

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 $M \leqslant L$. The units are fm^L.

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

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

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

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

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

$$R_I = (E_I - E_0)/(E_2 - E_0) \; .$$

(2.81)

For a good rotator

$$R_4 = 3\tfrac{1}{3} \quad \text{and} \quad R_6 = 7.$$

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.

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

(2.82)

In particular

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

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.

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

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

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

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

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

where $| i \rangle, | j \rangle$ are HO orbitals. A realistic force contains a $\underline{L} \cdot \underline{S}$ 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 $\underline{L} \cdot \underline{S}$ 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 inter-
action: 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.

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

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

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

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

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 $b = 1.70 fm$. 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 inter-
pretation 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}.

$(1p_{3/2})$ ————— 6.16 ————— $3/2-$

$(1d_{3/2})$ ————— 5.08 ————— $3/2+$

$(2s_{1/2})$ ————— 0.871 ————— $1/2+$

$(1d_{5/2})$ ————— 0 ————— $5/2+$ $(1p_{1/2})$ ————— 0 ————— $1/2-$

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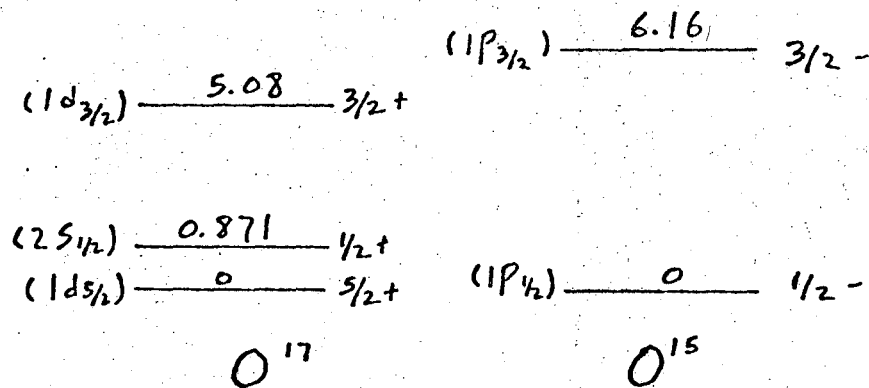
Figure 2.2: The lowest positive parity levels in O^{17} and the lowest negative parity levels in O^{15}.

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

$$\text{Ne}^{20}$$

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.

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

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 0^{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_o 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 $\Omega = \frac{1}{2}, \frac{3}{2}$ 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 Λ should therefore be determined from the $2^+ - 4^+$ spacing.

$$R_2 = 2.59$$

$$A_{2-0} = 0.299 \text{ Mev}$$

$$A_{4-2} = 0.202 \text{ Mev}$$

$$A_{exp.} = 0.202 \text{ Mev}$$

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.

$$R_2 = 2.00$$
$$A_{2-0} = 0.374 \text{ Mev}$$
$$A_{4-2} = 0.161 \text{ Mev}$$
$$A_{exp} = 0.161 \text{ Mev}$$

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.

6+	————————	8.71
	• • •	
4-	————————	7.03
0+	————————	6.72
1-	————————	5.785
3-	————————	5.623
2-	————————	4.97
4+	————————	4.25
2+	————————	1.63
0+	————————	0
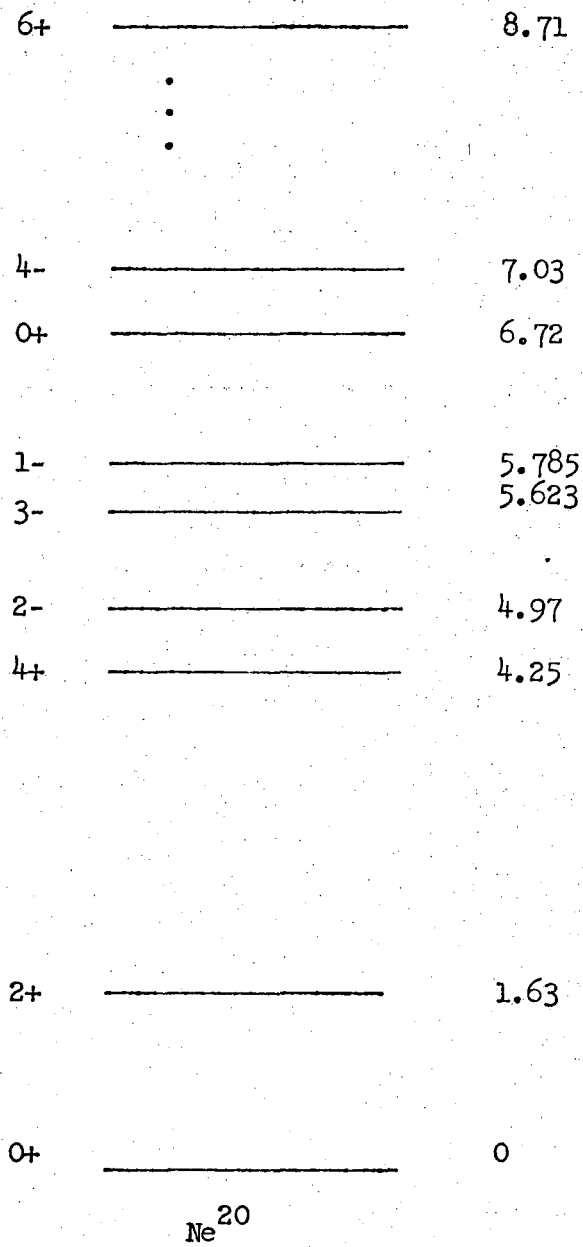
Ne^{20}

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

(2)+ ——————————— 7.35

0+ ——————————— 6.44
4+ ——————————— 6.00

3+ ——————————— 5.22

2+ ——————————— 4.23
4+ ——————————— 4.1225

2+ ——————————— 1.36853

0+ ——————————— 0
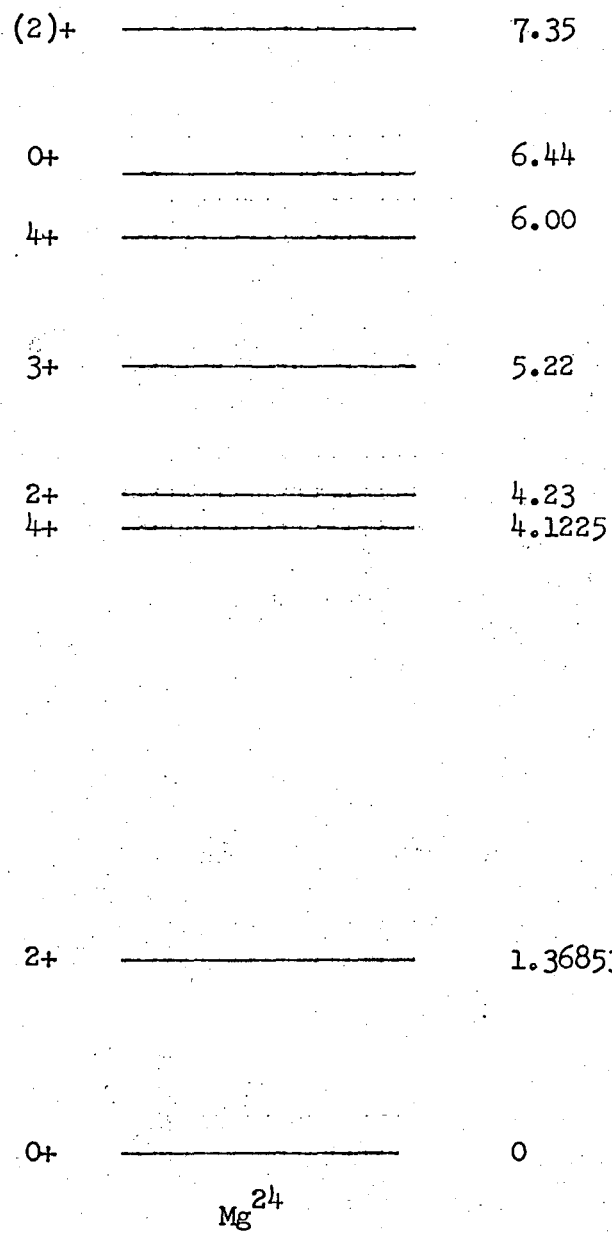
Mg^{24}

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

4+	————————	6.887
3-	————————	6.878
0+	————————	6.69
3+	————————	6.27
0+	————————	4.97
4+	————————	4.61
2+	————————	1.7787
0+	————————	0

$$Si^{28}$$
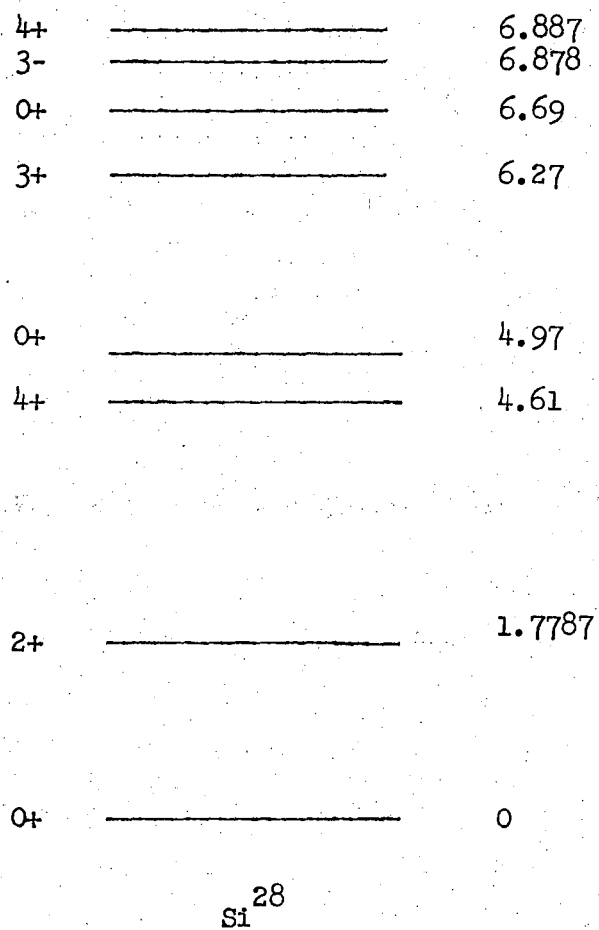
Fig. 2.5 Si^{28} energy level diagram (Ref. 19)
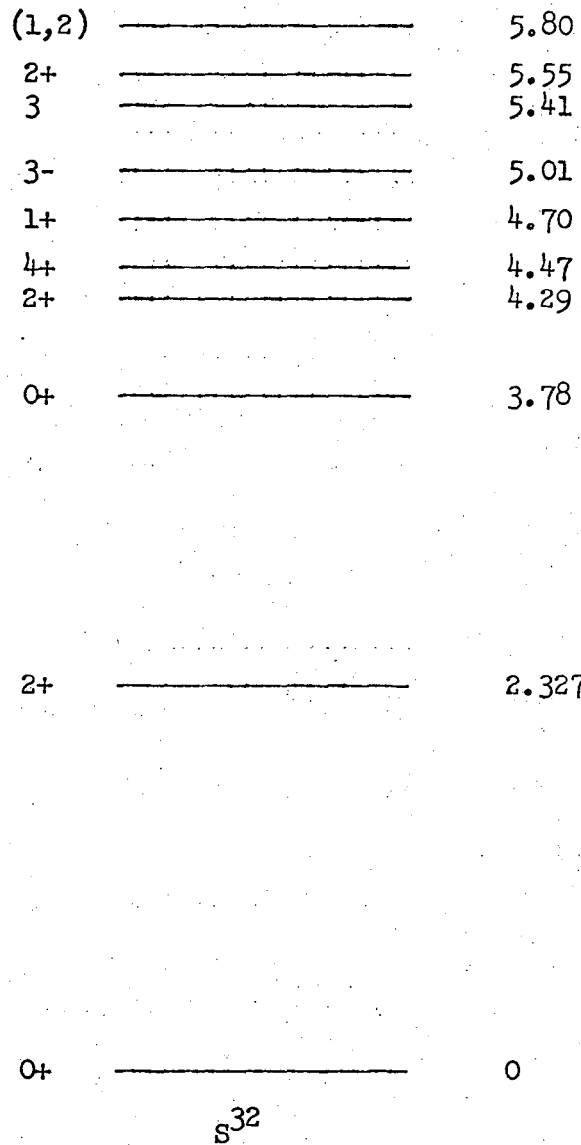
Fig. 2.6   S^{32} energy level diagram (Ref. 19,20)

(0+)	————————	5.19
5-	————————	5.17
2-(3-)	————————	4.98
(2+)	————————	4.96
2(+)	————————	4.440
4+	————————	4.41
(0+)	————————	4.33
3-	————————	4.178
2+	————————	1.970
0+	————————	0
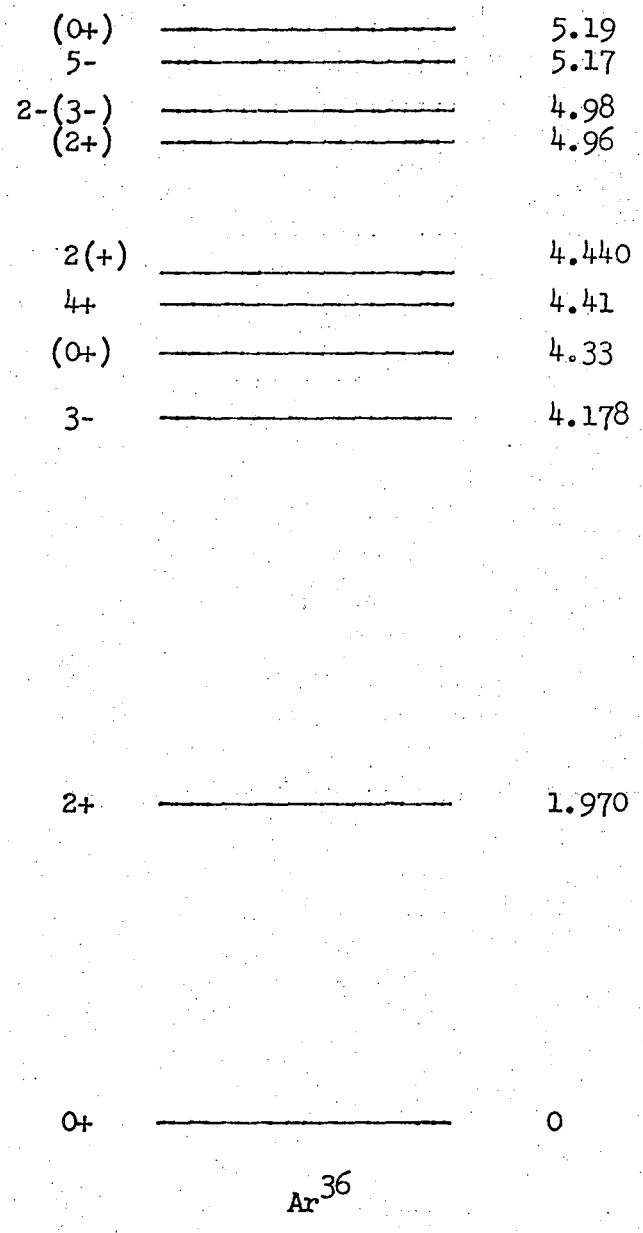
Ar^{36}

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	Λ_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	Λ_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	Λ_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.

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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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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 energeti-
cally 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

$$\langle \alpha(1) \ \beta(2) \ | \ \nu \ | \ \alpha(1) \ \beta(2) \ \rangle_A .$$

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

$$\langle \alpha(1) \; \bar{\alpha}(2) \mid \mathcal{N} \mid \beta(1) \; \bar{\beta}(2) \rangle_A \; .$$

The sharp Fermi surface of the HF theory is replaced by a diffuse Fermi surface (in particle space).
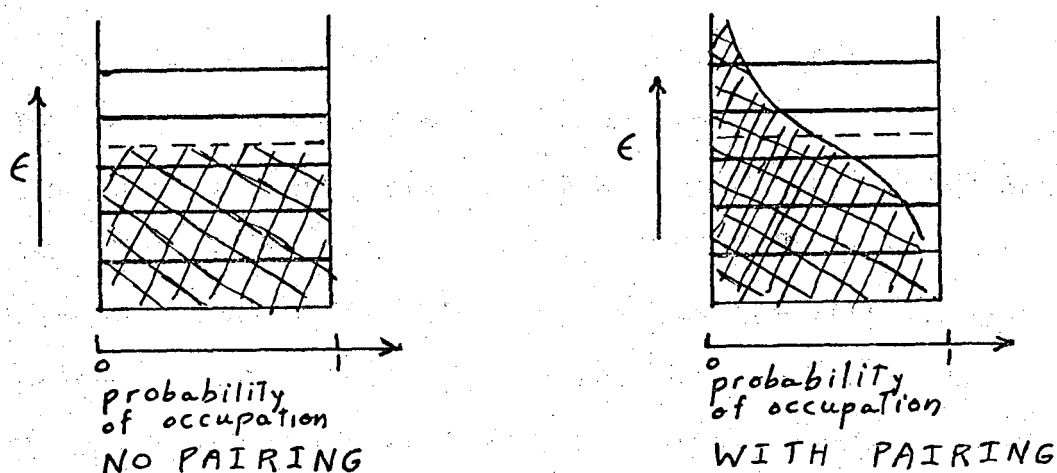
Figure (3.1)

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"

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

(3.1a)

or holes.

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

(3.1b)

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

$$b^{\dagger}_{\alpha} = U_{\alpha} a^{\dagger}_{\alpha} - N_{\alpha} a_{\bar{\alpha}}$$

(3.2a)

$$b_{\alpha} = U^*_{\alpha} a_{\alpha} - N^*_{\alpha} a^{\dagger}_{\bar{\alpha}}$$

(3.2b)

$$b^{\dagger}_{\bar{\alpha}} = U_{\bar{\alpha}} a^{\dagger}_{\bar{\alpha}} - N_{\bar{\alpha}} a_{\alpha}$$

(3.2c)

$$b_{\bar{\alpha}} = U^*_{\bar{\alpha}} a_{\bar{\alpha}} - N^*_{\bar{\alpha}} a^{\dagger}_{\alpha}$$

(3.2d)

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

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

$$[b^{\dagger}_{\alpha}, b^{\dagger}_{\beta}]_{+} = [b_{\alpha}, b_{\beta}]_{+} = 0 \qquad (3.3a)$$

$$[b^{\dagger}_{\alpha}, b_{\beta}]_{+} = \delta_{\alpha\beta} \qquad (3.3b)$$

In particular

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

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

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

$$|U_{\alpha}|^{2} + |N_{\alpha}|^{2} = 1 \qquad (3.4a)$$

$$U_{\alpha} N_{\bar{\alpha}} + U_{\bar{\alpha}} N_{\alpha} = 0 \qquad (3.4b)$$

It is therefore required that

$$|U_{\alpha}| = |U_{\bar{\alpha}}| \qquad (3.5a)$$

$$|N_{\alpha}| = |N_{\bar{\alpha}}| \qquad (3.5b)$$

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

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

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

Rewriting (3.2)

$$b^{\dagger}_{\alpha} = U_{\alpha} a^{\dagger}_{\alpha} - N_{\alpha} a_{\bar{\alpha}} \tag{3.7a}$$

$$b_{\alpha} = U_{\alpha} a_{\alpha} - N_{\alpha} a^{\dagger}_{\bar{\alpha}} \tag{3.7b}$$

$$b^{\dagger}_{\bar{\alpha}} = U_{\alpha} a^{\dagger}_{\bar{\alpha}} + N_{\alpha} a_{\alpha} \tag{3.7c}$$

$$b_{\bar{\alpha}} = U_{\alpha} a_{\bar{\alpha}} + N_{\alpha} a^{\dagger}_{\alpha} . \tag{3.7d}$$

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

$$\begin{bmatrix} b^{\dagger}_{\alpha} \\ b_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} U_{\alpha} & -N_{\alpha} \\ -N^{*}_{\bar{\alpha}} & U^{*}_{\bar{\alpha}} \end{bmatrix} \begin{bmatrix} a^{\dagger}_{\alpha} \\ a_{\bar{\alpha}} \end{bmatrix} \tag{3.8}$$

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

$$\begin{bmatrix} b^{\dagger}_{\alpha} \\ b_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} U_{\alpha} & -N_{\alpha} \\ N_{\alpha} & U_{\alpha} \end{bmatrix} \begin{bmatrix} a^{\dagger}_{\alpha} \\ a_{\bar{\alpha}} \end{bmatrix} . \tag{3.9}$$

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

$$|\Phi_0\rangle = \prod_{\alpha > 0} (U_\alpha + \mathcal{N}_\alpha \, a^\dagger_\alpha \, a^\dagger_{\bar{\alpha}}) |0\rangle \, . \qquad (3.14)$$

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

$$N = \sum_\alpha a^\dagger_\alpha \, a_\alpha \qquad (3.15)$$

We require that the average number of particles in the ground state equals the true particle number N_0.

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

The Hamiltonian H is replaced by $H - \lambda N$

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

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 $T - \lambda$.

4. The Hamiltonian

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

$$\rho_{\alpha\beta} = \langle a^\dagger_\beta a_\alpha \rangle$$

$$= \langle \Phi_0 | (u_\beta b^\dagger_\beta + N_\beta b_{\bar\beta})(u_\alpha b_\alpha + N_\alpha b^\dagger_{\bar\alpha}) | \Phi_0 \rangle \qquad (3.18)$$

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

$$\rho_{\alpha\beta} = N_\beta N_\alpha \langle \Phi_0 | b_{\bar\beta} b^\dagger_{\bar\alpha} | \Phi_0 \rangle .$$

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

$$\rho_{\alpha\beta} = N_\alpha^2 \delta_{\alpha\beta} . \qquad (3.19)$$

The occupation probability is N_α^2 .

The number conservation constraint (3.17) is simply

$$Tr \rho = N_0 \qquad (3.20)$$

or $$2 \sum_{\alpha > 0} N_\alpha^2 = N_0 . \qquad (3.21)$$

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

$$t_{\alpha\beta} = \langle a_\beta a_\alpha \rangle \qquad (3.22)$$

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

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

$$t_{\alpha\bar{\beta}} = \langle a_{\bar{\beta}} a_{\alpha} \rangle = U_\alpha N_\alpha \delta_{\alpha\beta} \tag{3.23b}$$

$$t_{\bar{\alpha}\beta} = \langle a_{\beta} a_{\bar{\alpha}} \rangle = -U_\alpha N_\alpha \delta_{\alpha\beta} \tag{3.23c}$$

The adjoint of the pairing tensor (1.88b)

$$t^*_{\alpha\beta} = \langle a^\dagger_\alpha a^\dagger_\beta \rangle \tag{3.24}$$

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

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

$$t^*_{\alpha\bar{\beta}} = \langle a^\dagger_\alpha a^\dagger_{\bar{\beta}} \rangle = U_\alpha N_\alpha \delta_{\alpha\beta} \tag{3.25b}$$

$$t^*_{\bar{\alpha}\beta} = \langle a^\dagger_{\bar{\alpha}} a_\beta \rangle = -U_\alpha N_\alpha \delta_{\alpha\beta} \ . \tag{3.25c}$$

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

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

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 $\langle \alpha_1 \beta | N | \alpha_2 \beta \rangle_A = \langle \alpha_2 \beta | N | \alpha_1 \beta \rangle_A$.

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)

$$\Delta_{ij} = \tfrac{1}{2} \sum_{k\ell} \langle ij | N | k\ell \rangle_A \, t_{k\ell}$$

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

$$\Delta_{ij} = \tfrac{1}{2} \sum_{k\ell > 0}' \langle ij | N | k\bar{\ell} \rangle_A \, t_{k\bar{\ell}} + \tfrac{1}{2} \sum_{k\ell > 0}' \langle ij | N | \bar{k}\ell \rangle_A \, t_{\bar{k}\ell}$$

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

$$\Delta_{ij} = \sum_{k\ell > 0}' \langle ij | N | k\bar{\ell} \rangle_A \, t_{k\bar{\ell}} .$$

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

$$\Delta_{i\bar{j}} = \sum_{k l > 0} \langle i\bar{j} | \mathcal{N} | k\bar{l} \rangle_A \, L_{k\bar{l}} \qquad (3.30)$$

This result is not restricted to the special transformation.
The pair potential for the special transformation is

$$\Delta_{\alpha_1 \bar{\alpha}_2} = \sum_{\beta > 0} \langle \alpha_1 \bar{\alpha}_2 | \mathcal{N} | \beta\bar{\beta} \rangle_A \, U_\beta N_\beta \, . \qquad (3.31)$$

Although Δ is antisymmetric, so that

$$\Delta_{\alpha_1 \bar{\alpha}_2} = - \Delta_{\bar{\alpha}_2 \alpha_1} \qquad (3.32)$$

it is not true that $\Delta_{\alpha_1 \bar{\alpha}_2} = - \Delta_{\alpha_2 \bar{\alpha}_1}$. Since

$$\langle \alpha_1 \bar{\alpha}_2 | \mathcal{N} | \beta\bar{\beta} \rangle_A = \langle \bar{\alpha}_1 \alpha_2 | \mathcal{N} | \bar{\beta}\beta \rangle_A = \langle \alpha_2 \bar{\alpha}_1 | \mathcal{N} | \beta\bar{\beta} \rangle_A \, ,$$

the correct symmetry relation is

$$\Delta_{\alpha_1 \bar{\alpha}_2} = \Delta_{\alpha_2 \bar{\alpha}_1} \, . \qquad (3.33)$$

The Hamiltonian

$$H' = H_0' + H_2' + H_4' \qquad (3.34)$$

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_0' 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 $i,j < 0$.

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

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

$$E_{pair} = \sum_{ij > 0} \Delta_{i\bar{j}} t_{i\bar{j}}^* . \tag{3.36}$$

Similarly

$$\frac{1}{2} \sum_{ij} \Delta_{ij} N[a^{\dagger}_i a^{\dagger}_j] = \sum_{ij > 0} \Delta_{i\bar{j}} N[a^{\dagger}_i a^{\dagger}_{\bar{j}}] . \tag{3.37}$$

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

$$H_0' = E_0 - \lambda N_0 = \sum_{ij} (T - \lambda + \tfrac{1}{2}\Gamma)_{ij} \rho_{ji} + \sum_{ij > 0} \Delta_{i\bar{j}} t_{i\bar{j}}^* \tag{3.38a}$$

or

$$H_0' = E_0 - \lambda N_0 = \sum_{ij}' \langle i|T-\lambda|j \rangle \rho_{ji} +$$

$$\frac{1}{2} \sum_{ijkl} \langle ij|N|kl \rangle_A \rho_{ki} \rho_{lj} +$$

$$\sum_{ijkl>0} \langle i\bar{j}|N|k\bar{l} \rangle_A \mathcal{L}_{ij}^* \mathcal{L}_{k\bar{l}} \qquad (3.38b)$$

$$H_2' = \sum_{ij}' (H-\lambda)_{ij} N[a_i^\dagger a_j] + \sum_{ij>0} \Delta_{ij} N[a_i^\dagger a_j^\dagger]$$

$$+ \sum_{ij>0}' \Delta_{ij}^* N[a_{\bar{j}} a_i] \qquad (3.39)$$

$$H_4' = \frac{1}{4} \sum_{ijkl} \langle ij|N|kl \rangle_A N[a_i^\dagger a_j^\dagger a_l a_k] \cdot \qquad (3.40)$$

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

$$H_0' = E_0 - \lambda N_0 = \sum_{\alpha \geq 0}' (T-\lambda+\tfrac{1}{2}\Gamma)_{\alpha\alpha} N_\alpha^2 +$$

$$\sum_{\alpha>0} \Delta_{\alpha\bar{\alpha}} U_\alpha N_\alpha \qquad (3.41a)$$

or

$$H_0' = E_0 - \lambda N_0 = \sum_{\alpha \geq 0}' \langle \alpha|T-\lambda|\alpha \rangle N_\alpha^2 +$$

$$\frac{1}{2} \sum_{\alpha\beta \geq 0}' \langle \alpha\beta|N|\alpha\beta \rangle_A N_\alpha^2 N_\beta^2 +$$

$$\sum_{\alpha\beta>0} \langle \alpha\bar{\alpha}|N|\beta\bar{\beta} \rangle_A U_\alpha N_\alpha U_\beta N_\beta \qquad (3.41b)$$

$$H_2' = \sum_{\alpha\beta > 0}{}' (\mathcal{H} - \lambda)_{\alpha\beta} \; N [\, a^{\dagger}_{\alpha} \, a_{\beta} \,] +$$

$$\sum_{\alpha\beta > 0}{}' \Delta_{\alpha\bar{\beta}} \; (\, N[\, a^{\dagger}_{\alpha} \, a^{\dagger}_{\bar{\beta}} \,] + N [\, a_{\bar{\beta}} \, a_{\alpha} \,]) \, .$$

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

$$U_\alpha^2 + N_\alpha^2 = 1$$

restricts the variation of V_α . The variational principle is

$$\frac{\delta H_0'}{\delta N_\alpha} = \frac{\partial H_0'}{\partial N_\alpha} + \frac{\partial H_0'}{\partial U_\alpha} \frac{\partial U_\alpha}{\partial N_\alpha} = 0 \qquad (3.42a)$$

or $$\frac{\delta H_0'}{\delta N_\alpha} = \frac{\partial H_0'}{\partial N_\alpha} - \frac{N_\alpha}{U_\alpha} \frac{\partial H_0'}{\partial U_\alpha} = 0 \qquad (3.42b)$$

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

$$(H_{\alpha\alpha} - \lambda) U_\alpha N_\alpha + \tfrac{1}{2} \Delta_{\alpha\bar\alpha} (U_\alpha^2 - N_\alpha^2) = 0 \qquad (3.43a)$$

or $$(\mathcal{E}_\alpha - \lambda) U_\alpha N_\alpha + \tfrac{1}{2} \Delta_\alpha (U_\alpha^2 - N_\alpha^2) = 0 \qquad (3.43b)$$

where $\mathcal{E}_\alpha$ denotes $H_{\alpha\alpha}$ and Δ_α is $\Delta_{\alpha\bar\alpha}$.

$$\mathcal{E}_\alpha = \langle \alpha | T | \alpha \rangle + \sum_{\beta>0}' \langle \alpha\beta | N | \alpha\beta \rangle_A N_\beta^2 \qquad (3.44)$$

$$\Delta_\alpha = \sum_{\beta>0}' \langle \alpha\bar\alpha | N | \beta\bar\beta \rangle_A U_\beta N_\beta \qquad (3.45)$$

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

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

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

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, N_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, N_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 L have opposite signs. $U_\alpha V_\alpha$ is therefore given by

$$U_\alpha N_\alpha = -\frac{1}{2} \frac{\Delta_\alpha}{\sqrt{(\epsilon_\alpha - \lambda)^2 + \Delta_\alpha^2}} . \qquad (3.47)$$

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

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

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

$$|\overline{\langle \alpha \bar{\alpha}' | \mathcal{N} | \beta \bar{\beta} \rangle_A}| << |\overline{\langle \alpha \bar{\alpha} | \mathcal{N} | \beta \bar{\beta} \rangle_A}|. \quad (3.51a)$$
$$(\alpha' \neq \alpha)$$

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

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

$$\mid \mathcal{H}_{\alpha\alpha'} \mid \ll \mid \mathcal{H}_{\alpha\alpha} \mid . \qquad (\alpha \neq \alpha') \qquad (3.52)$$

This assumption is satisfied, of course, if $\mathcal{H}$ is diagonal in the $\mid \alpha \rangle$ basis. That is, $\mid \alpha \rangle$ 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

$$H_2' = \sum_{\alpha \gtrless 0} (\epsilon_\alpha - \lambda) N [a_\alpha^\dagger a_\alpha] +$$
$$\sum_{\alpha > 0} \Delta_\alpha (N[a_\alpha^\dagger a_{\bar\alpha}^\dagger] + N[a_{\bar\alpha} a_\alpha]) . \qquad (3.53)$$

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

$$[H_2', b_\alpha^\dagger]_- = E_\alpha b_\alpha^\dagger . \qquad (3.54)$$

Substituting (3.7a) into (3.54)

$$[H_2', b_\alpha^\dagger]_- = E_\alpha (U_\alpha a_\alpha^\dagger - \mathcal{N}_\alpha a_{\bar\alpha}) . \qquad (3.55)$$

The commutator may also be evaluated with (3.53).

$$[H_2', b_\alpha^\dagger]_- = \{(\epsilon_\alpha - \lambda) U_\alpha - \Delta_\alpha \mathcal{N}_\alpha\} a_\alpha^\dagger +$$
$$\{\Delta_\alpha U_\alpha + (\epsilon_{\bar\alpha} - \lambda) \mathcal{N}_\alpha\} a_{\bar\alpha} \quad (\alpha > 0) \quad (3.56)$$

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

$$(\epsilon_\alpha - \lambda) U_\alpha - \Delta_\alpha \mathcal{N}_\alpha = E_\alpha U_\alpha \qquad (3.57a)$$

$$\Delta_\alpha U_\alpha + (\epsilon_{\bar\alpha} - \lambda) \mathcal{N}_\alpha = -E_\alpha \mathcal{N}_\alpha \qquad (3.57b)$$

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

$$\begin{bmatrix} (\epsilon_\alpha - \lambda) & \Delta_\alpha \\ \Delta_\alpha & -(\epsilon_\alpha - \lambda) \end{bmatrix} \begin{bmatrix} U_\alpha \\ -\mathcal{N}_\alpha \end{bmatrix} = E_\alpha \begin{bmatrix} U_\alpha \\ -\mathcal{N}_\alpha \end{bmatrix} \qquad (3.58)$$

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

$$(\epsilon_\alpha - \lambda) U_\alpha \mathcal{N}_\alpha + \tfrac{1}{2} \Delta_\alpha (U_\alpha^2 - \mathcal{N}_\alpha^2) = 0 \quad .$$

The quasiparticle energy E_α is determined by

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

Solving for E_α

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

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

$$\mathcal{E}_{ex} = \mathcal{E}_{\alpha_1} - \mathcal{E}_{\alpha_2} \cdot \quad (\mathcal{E}_{\alpha_1} > \mathcal{E}_F > \mathcal{E}_{\alpha_2}) \qquad (3.61)$$

$\mathcal{E}_{ex}$ 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

$$\mathcal{E}_{ex} = E_{\alpha_1} + E_{\alpha_2}$$
$$= \sqrt{(\mathcal{E}_{\alpha_1} - \lambda)^2 + \Delta_{\alpha_1}^2} + \sqrt{(\mathcal{E}_{\alpha_2} - \lambda)^2 + \Delta_{\alpha_2}^2} \cdot \qquad (3.62)$$

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

$$\mathcal{E}_{ex}^{min} = |\Delta_{\alpha_1}| + |\Delta_{\alpha_2}|. \qquad (3.63)$$

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

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

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

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

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

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

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

Substituting (3.65 - 3.67) into (3.41b)

$$H_o' = E_o - \lambda N_o = \sum_{\substack{\alpha > 0 \\ k_1 k_2}} D^{\alpha}_{k_1} D^{\alpha}_{k_2} \mathcal{N}_\alpha^2 \langle k_1 | T - \lambda | k_2 \rangle +$$

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

$$\sum_{\substack{\alpha_1 \alpha_2 > 0 \\ k_1 k_2 k_3 k_4}} D^{\alpha_1}_{k_1} D^{\alpha_1}_{k_2} D^{\alpha_2}_{k_3} D^{\alpha_2}_{k_4} U_{\alpha_1} \mathcal{N}_{\alpha_1} U_{\alpha_2} \mathcal{N}_{\alpha_2} \langle k_1 \bar{k}_2 | \mathcal{N} | k_3 \bar{k}_4 \rangle_A \ .$$

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

Inserting (3.19)

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

Similarly

$$t_{k_2 \bar{k}_1} = \langle a_{\bar{k}_1} a_{k_2} \rangle = \sum_{\alpha} D^{\alpha}_{k_1} D^{\alpha}_{k_2} U_\alpha \mathcal{N}_\alpha \ . \tag{3.71}$$

(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.

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

Substituting (3.68) into (3.72) leads to

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

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

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

so that

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

The HB equations present an eigenvalue problem.

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

or

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

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

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

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)

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

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

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

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

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

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,

$$N[b_\alpha^\dagger b_\beta^\dagger] = b_\alpha^\dagger b_\beta^\dagger \qquad (3.78a)$$

$$N[b_\alpha b_\beta] = b_\alpha b_\beta \qquad (3.78b)$$

$$N[b_\alpha^\dagger b_\beta] = b_\alpha^\dagger b_\beta \qquad (3.78c)$$

$$N[b_\alpha b_\beta^\dagger] = -b_\beta^\dagger b_\alpha. \qquad (3.78d)$$

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

$$H_2' = H_{11}' + H_{20}' + H_{02}' \qquad (3.79)$$

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

$$H_{11}' = \sum_{\alpha\beta>0} \left\{ (\mathcal{H}-\lambda)_{\alpha\beta} (U_\alpha U_\beta - \mathcal{N}_\alpha \mathcal{N}_\beta) \right.$$
$$\left. - \Delta_{\alpha\bar\beta} (U_\alpha \mathcal{N}_\beta + \mathcal{N}_\alpha U_\beta) \right\} (b_\alpha^\dagger b_\beta + b_{\bar\alpha}^\dagger b_{\bar\beta}) \qquad (3.80)$$

$$H_{20}' + H_{02}' = \sum_{\alpha\beta>0} \left\{ (\mathcal{H}-\lambda)_{\alpha\beta} (U_\alpha \mathcal{N}_\beta + \mathcal{N}_\alpha U_\beta) \right.$$
$$\left. + \Delta_{\alpha\bar\beta} (U_\alpha U_\beta - \mathcal{N}_\alpha \mathcal{N}_\beta) \right\} (b_\alpha^\dagger b_{\bar\beta}^\dagger + b_{\bar\alpha} b_\beta). \qquad (3.81)$$

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

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

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

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

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

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

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}.

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

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)

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

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

$$E_{\alpha\beta} = -\Delta_{\alpha\bar{\beta}} / (U_\alpha N_\beta + N_\alpha U_\beta) \qquad (3.88)$$

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

$$b_\nu^\dagger = \sum_\alpha R_\alpha^\nu b_\alpha^\dagger \qquad (3.89)$$

is chosen to diagonalize the energy matrix $E_{\alpha\beta}$.

$$\sum_\beta E_{\alpha\beta} R_\beta^\nu = \tilde{E}_\nu R_\alpha^\nu \qquad (3.90a)$$

or $$E\underline{R}^\nu = \tilde{E}_\nu \underline{R}^\nu . \qquad (3.90b)$$

Then $$H_2' = \sum_\nu \tilde{E}_\nu b_\nu^\dagger b_\nu . \qquad (3.91)$$

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

$$a_\alpha^\dagger = \sum_k D_k^\alpha a_k^\dagger \qquad (3.92)$$

B_{sp}: Special Bogoliubov quasiparticle transformation

$$b_\alpha^\dagger = U_\alpha a_\alpha^\dagger - N_\alpha a_{\bar\alpha}$$

(3.93)

U_2: Rotation in quasiparticle space

$$b_\nu^\dagger = \sum_\alpha R_\alpha^\nu b_\alpha^\dagger$$

(3.94)

The final Bogoliubov quasiparticle co-ordinates are given by the product of these transformations.

$$B = U_2 B_{sp} \cdot U_1$$

(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

$$\rho_{\alpha\beta} = \langle a_\beta^\dagger a_\alpha \rangle = N_\alpha^2 \delta_{\alpha\beta}$$

and the pairing tensor is

$$t_{\alpha\bar\beta} = \langle a_{\bar\beta} a_\alpha \rangle = U_\alpha N_\alpha \delta_{\alpha\beta} .$$

Substitute (3.93) into (3.94).

$$b_\nu^\dagger = \sum_\alpha (R_\alpha^\nu U_\alpha a_\alpha^\dagger - R_\alpha^\nu N_\alpha a_{\bar\alpha})$$

Inverting this transformation, and recalling that the ground state is a quasiparticle vacuum, ρ and t may be evaluated after the three transformations have been performed.

$$\langle a_{\beta}^{\dagger} a_{\alpha} \rangle = \sum_{\nu}' (R_{\beta}^{\nu} N_{\beta})(R_{\alpha}^{\nu} N_{\alpha}) = \left(\sum_{\nu} R_{\alpha}^{\nu} R_{\beta}^{\nu} \right) N_{\alpha} N_{\beta}$$

Since R is an orthogonal transformation

$$R \tilde{R} = I \quad \text{or} \quad \sum_{\nu} R_{\alpha}^{\nu} R_{\beta}^{\nu} = \delta_{\alpha\beta}$$

so that ρ is

$$\langle a_{\beta}^{\dagger} a_{\alpha} \rangle = N_{\alpha}^{2} \delta_{\alpha\beta} \ .$$

Similarly

$$\langle a_{\bar{\beta}} a_{\alpha} \rangle = \sum_{\nu}' (R_{\beta}^{\nu} U_{\beta})(R_{\alpha}^{\nu} N_{\alpha}) = \left(\sum_{\nu} R_{\alpha}^{\nu} R_{\beta}^{\nu} \right) U_{\beta} N_{\alpha}$$

and t is

$$\langle a_{\bar{\beta}} a_{\alpha} \rangle = U_{\alpha} N_{\alpha} \delta_{\alpha\beta} \ .$$

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

$$b^\dagger_{\alpha\tau} = U_{\alpha\tau}\, a^\dagger_{\alpha\tau} - N_{\alpha\tau}\, a_{\bar{\alpha}\tau} \,. \qquad (3.96)$$

The ground state wave function is

$$|\Phi_0\rangle = \prod_{\alpha_1>0} (U_{\alpha_1 p} + N_{\alpha_1 p}\, a^\dagger_{\alpha_1 p}\, a^\dagger_{\bar{\alpha}_1 p})$$
$$\times \prod_{\alpha_2>0} (U_{\alpha_2 n} + N_{\alpha_2 n}\, a^\dagger_{\alpha_2 n}\, a^\dagger_{\bar{\alpha}_2 n})|0\rangle . \qquad (3.97)$$

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

$$H' \longrightarrow H' = H - \lambda_p N_p - \lambda_n N_n \qquad (3.98)$$

where

$$N_p = \sum_{\alpha>0} a^\dagger_{\alpha p}\, a_{\alpha p} \qquad N_n = \sum_{\alpha>0} a^\dagger_{\alpha n}\, a_{\alpha n} \qquad (3.99)$$

and λ_p and λ_n are adjusted so that

$$\langle N_p \rangle = Z \qquad \langle N_n \rangle = A - Z . \qquad (3.100)$$

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

$$H \rightarrow H' = H - (\lambda_p P_p + \lambda_n P_n) N \qquad (3.101)$$

where $\qquad N = \sum_{\alpha \tau}' a_{\alpha \tau}^{\dagger} a_{\alpha \tau} \qquad (3.102)$

and $\qquad P_\tau \qquad$ is a projection operator

$$P_\tau = |\tau \rangle \langle \tau| \qquad (3.103)$$

so that

$$P_\tau |\tau' \rangle = |\tau \rangle \langle \tau|\tau' \rangle = \delta_{\tau \tau'} |\tau \rangle . \qquad (3.104)$$

H' is obtained from H by replacing T with $T - \lambda_p P_p - \lambda_n P_n$. Note that

$$N = N_p + N_n . \qquad (3.105)$$

The density matrix is

$$\rho_{\alpha_1 \tau_1, \alpha_2 \tau_2} = N_{\alpha_1 \tau_1}^2 \delta_{\alpha_1 \alpha_2} \delta_{\tau_1 \tau_2} \qquad (3.106)$$

so that the number conservation conditions are

$$2 \sum_{\alpha > 0}' N_{\alpha p}^2 = Z \qquad 2 \sum_{\alpha > 0}' N_{\alpha n}^2 = A - Z . \qquad (3.107)$$

The pairing tensor is

$$t_{\alpha_1 \tau_1, \bar{\alpha}_2 \tau_2} = U_{\alpha_1 \tau_1} N_{\alpha_1 \tau_1} \delta_{\alpha_1 \alpha_2} \delta_{\tau_1 \tau_2} . \qquad (3.108)$$

The HF potential is

$$\Gamma_{\alpha_1 T_1, \alpha_2 T_2} = \sum_{\beta T}' \langle \alpha_1 T_1, \beta T | \mathcal{N} | \alpha_2 T_2, \beta T \rangle_A \, \mathcal{N}_{\beta T}^2 \cdot \tag{3.109}$$

Note that $\Gamma_{\alpha_1 T_1, \alpha_2 T_2} = 0$ unless $T_1 = T_2$. Neutrons contribute to the proton HF potential, and viceversa.

The pair potential is

$$\Delta_{\alpha_1 T_1, \bar{\alpha}_2 T_2} = \sum_{\substack{\beta > 0 \\ T}}' \langle \alpha_1 T_1, \bar{\alpha}_2 T_2 | \mathcal{N} | \beta T, \bar{\beta} T \rangle_A \, U_{\beta T} \, \mathcal{N}_{\beta T} \cdot \tag{3.110}$$

The pairing matrix elements vanish unless $T_1 = T_2 = T$. The only non-vanishing elements of Δ are

$$\Delta_{\alpha_1 T, \bar{\alpha}_2 T} = \sum_{\beta > 0}' \langle \alpha_1 T, \bar{\alpha}_2 T | \mathcal{N} | \beta T, \bar{\beta} T \rangle_A \, U_{\beta T} \, \mathcal{N}_{\beta T} \cdot \tag{3.111}$$

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

$$\begin{bmatrix} (\epsilon_{\alpha T} - \lambda_T) & \Delta_{\alpha T} \\ \Delta_{\alpha T} & -(\epsilon_{\alpha T} - \lambda_T) \end{bmatrix} \begin{bmatrix} U_{\alpha T} \\ -\mathcal{N}_{\alpha T} \end{bmatrix} = E_{\alpha T} \begin{bmatrix} U_{\alpha T} \\ -\mathcal{N}_{\alpha T} \end{bmatrix} \tag{3.112}$$

where $\epsilon_{\alpha T} = \mathcal{H}_{\alpha T, \alpha T}$

$$\epsilon_{\alpha T} = \langle \alpha | T | \alpha \rangle + \sum_{\beta T'}' \langle \alpha T, \beta T' | \mathcal{N} | \alpha T, \beta T' \rangle_A \, \mathcal{N}_{\beta T'}^2 \cdot \tag{3.113}$$

and $\Delta_{\alpha T} = \Delta_{\alpha T, \bar{\alpha} T}$

$$\Delta_{\alpha T} = \sum_{\beta > 0}' \langle \alpha T, \bar{\alpha} T | \mathcal{N} | \beta T, \bar{\beta} T \rangle_A \, U_{\beta T} \, \mathcal{N}_{\beta T} \cdot \tag{3.114}$$

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

$$E_{\alpha T} = \sqrt{\hat{\epsilon}_{\alpha T}^2 + \Delta_{\alpha T}^2} \tag{3.116}$$

$$U_{\alpha T}^2 = \tfrac{1}{2}(1 + \hat{\epsilon}_{\alpha T}/E_{\alpha T}) \tag{3117a}$$

$$N_{\alpha T}^2 = \tfrac{1}{2}(1 - \hat{\epsilon}_{\alpha T}/E_{\alpha T}). \tag{3.117b}$$

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

$$
\begin{aligned}
E_{\alpha p} &= E_{\alpha n} \\
U^2_{\alpha p} &= U^2_{\alpha n} \\
N^2_{\alpha p} &= N^2_{\alpha n} \\
|\Delta_{\alpha p}| &= |\Delta_{\alpha n}| \\
E_{\alpha p} &= E_{\alpha n} \\
\lambda_p &= \lambda_n
\end{aligned}
\tag{3.118}
$$

The isotopic spin subscript will be deleted for the remainder of this section.

The moments of inertia are given by [5]

$$
\mathcal{J}_x = 2 \sum_{\substack{all \ \alpha \\ \beta > 0}} \frac{|\langle \alpha | J_x | \beta \rangle|^2}{E_\alpha + E_\beta} (U_\alpha |N_\beta| - U_\beta |N_\alpha|)^2
\tag{3.119}
$$

with similar relations for $\mathcal{J}_y$ and $\mathcal{J}_z$. The multiple moments are

$$
\langle Q_{LM} \rangle = \sum_\alpha \langle \alpha | Q_{LM} | \alpha \rangle N_\alpha^2 .
\tag{3.120}
$$

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.

$$\text{Mg}^{24}$$

The asymmetric wave function has a large HF gap, and the BCS result is the trivial one.

The prolate HF state with $\Lambda = \frac{1}{2}+$, $\frac{3}{2}+$ 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 $d_{5/2}$, $d_{3/2}$, $s_{\frac{1}{2}}$. (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 d3/2 orbital is V $^2_{d3/2}$ ~ 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).

$$\text{Ar}^{36}$$

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 $V_{s\frac{1}{2}}^2 = 0.994$, $V_{d5/2}^2 = 0.974$, $V_{d3/2}^2 = 0.543$(Rosenfeld 2) and $V_{d5/2}^2 = 0.956$, $V_{s\frac{1}{2}}^2 = 0.964$, $V_{d3/2}^2 = 0.585$(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 $V^2_{d\,5/2} = 0.971$, $V^2_{s\,1/2} = 0.509$, $V^2_{d3/2} = 0.288$. Without the pf shell, a re-ordering of levels occurs. The original HF and final BCS single particle energies are considerably different.

$$\epsilon_{d5/2} = -13.340 \longrightarrow -15.099 \text{ Mev}, \quad V^2_{d5/2} = 0.972$$
$$\epsilon_{s\frac{1}{2}} = -12.377 \longrightarrow -10.470 \text{ Mev}, \quad V^2_{s\frac{1}{2}} = 0.351$$
$$\epsilon_{d3/2} = -12.048 \longrightarrow -10.755 \text{ Mev}, \quad V^2_{d3/2} = 0.367$$

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
N_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
N_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
N_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)

$\mathcal{E}_\alpha$	-11.638	-7.536	-5.583	-3.923	-0.531	1.728
$\mathcal{N}_\alpha^2$	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)

$\mathcal{E}_\alpha$	-13.547	-8.063	-5.871	-2.475	0.757	3.504
$\mathcal{N}_\alpha^2$	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 hypo-
thetical 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

$$E_{N+2} - E_N \approx E_N - E_{N-2} \ .$$

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

$$(E_{Mg26} - E_{Mg24}) - (E_{Mg24} - E_{Mg22}) = 11.25 \text{ Mev.}$$

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

$$(E_{Mg26} - E_{Mg24}) - (E_{Mg24} - E_{Mg22}) = -0.976 \text{ Mev.}$$

For $T_z = 0$ pairing the relevant quantity is

$$(E_{Al26} - E_{Mg24}) - (E_{Mg24} - E_{Na22}) = -3.750 \text{ Mev.}$$

(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: $|\alpha p, \bar{\alpha} p\rangle_{T=1}$, $|\alpha n, \bar{\alpha} n\rangle_{T=1}$, $|\alpha p, \bar{\alpha} n\rangle_{T=1}$, $|\alpha n, \bar{\alpha} p\rangle_{T=1}$, $|\alpha p, \bar{\alpha} n\rangle_{T=0}$, $|\alpha n, \bar{\alpha} p\rangle_{T=0}$. [5] 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.

$$\begin{bmatrix} b^{\dagger}_{\alpha} \\ b_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} u_{\alpha} & -\mathcal{N}_{\alpha} \\ -\mathcal{N}^{*}_{\bar{\alpha}} & u^{*}_{\bar{\alpha}} \end{bmatrix} \begin{bmatrix} a^{\dagger}_{\alpha} \\ a_{\bar{\alpha}} \end{bmatrix} \qquad (4.1)$$

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 $b^{\dagger}_{\alpha}$ and $a^{\dagger}_{\alpha}$ become two dimensional vectors

$$B^{\dagger}_{\alpha} = \begin{bmatrix} b^{\dagger}_{\alpha 1} \\ b^{\dagger}_{\alpha 2} \end{bmatrix} \qquad A^{\dagger}_{\alpha} = \begin{bmatrix} a^{\dagger}_{\alpha p} \\ a^{\dagger}_{\alpha n} \end{bmatrix} \qquad (4.2)$$

and by letting u_{α} and v_{α} become two dimensional matrices.

$$U_{\alpha} = \begin{bmatrix} u_{\alpha 11} & u_{\alpha 12} \\ u_{\alpha 21} & u_{\alpha 22} \end{bmatrix} \qquad V_{\alpha} = \begin{bmatrix} \mathcal{N}_{\alpha 11} & \mathcal{N}_{\alpha 12} \\ \mathcal{N}_{\alpha 21} & \mathcal{N}_{\alpha 22} \end{bmatrix} \qquad (4.3)$$

The counterpart of (4.1) is

$$\begin{bmatrix} B^{\dagger}_{\alpha} \\ B_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} U_{\alpha} & -V_{\alpha} \\ -V^{*}_{\bar{\alpha}} & U^{*}_{\bar{\alpha}} \end{bmatrix} \begin{bmatrix} A^{\dagger}_{\alpha} \\ A_{\bar{\alpha}} \end{bmatrix} . \qquad (4.4)$$

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 $(\mathcal{U}^\dagger \mathcal{U} = I)$

$$U_\alpha^\dagger U_\alpha + \left(V_{\bar\alpha}^\dagger V_{\bar\alpha} \right)^* = I \tag{4.6c}$$

$$U_\alpha^\dagger V_\alpha + \left(V_{\bar\alpha}^\dagger U_{\bar\alpha} \right)^* = 0. \tag{4.6d}$$

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

$$U_{\bar{\alpha}} = U_{\alpha}^{*} \qquad V_{\bar{\alpha}} = - V_{\alpha}^{*} \qquad \tag{4.7}$$

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

$$U_{\alpha} U_{\alpha}^{\dagger} + V_{\alpha} V_{\alpha}^{\dagger} = I \tag{4.8a}$$

$$U_{\alpha} V_{\alpha}^{\dagger} - V_{\alpha} U_{\alpha}^{\dagger} = 0 \tag{4.8b}$$

$$U_{\alpha}^{\dagger} U_{\alpha} + V_{\alpha}^{\dagger} V_{\alpha} = 0 \tag{4.8c}$$

$$U_{\alpha}^{\dagger} V_{\alpha} - V_{\alpha}^{\dagger} U_{\alpha} = 0 \qquad \tag{4.8d}$$

More explicitly

$$\sum_{T} (U_{\alpha \zeta_1 T} \, U_{\alpha \zeta_2 T}^{*} + N_{\alpha \zeta_1 T} \, N_{\alpha \zeta_2 T}^{*}) = \delta_{\zeta_1 \zeta_2} \tag{4.9a}$$

$$\sum_{T} (U_{\alpha \zeta_1 T} \, N_{\alpha \zeta_2 T}^{*} - N_{\alpha \zeta_1 T} \, U_{\alpha \zeta_2 T}^{*}) = 0 \tag{4.9b}$$

$$\sum_{\zeta} (U_{\alpha \zeta T_1} \, U_{\alpha \zeta T_2}^{*} + N_{\alpha \zeta T_1} \, N_{\alpha \zeta T_2}^{*}) = \delta_{T_1 T_2} \tag{4.9c}$$

$$\sum_{\zeta} (U_{\alpha \zeta T_1} \, N_{\alpha \zeta T_2}^{*} - N_{\alpha \zeta T_1} \, U_{\alpha \zeta T_2}^{*}) = 0 \qquad \tag{4.9d}$$

The quasiparticle transformation simplifies .

$$\begin{bmatrix} B_{\alpha}^{\dagger} \\ B_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} U_{\alpha} & -V_{\alpha} \\ V_{\alpha} & U_{\alpha} \end{bmatrix} \begin{bmatrix} A_{\alpha}^{\dagger} \\ A_{\bar{\alpha}} \end{bmatrix} \tag{4.10a}$$

That is

$$
\begin{bmatrix} b^\dagger_{\alpha 1} \\ b^\dagger_{\alpha 2} \\ b_{\bar{\alpha} 1} \\ b_{\bar{\alpha} 2} \end{bmatrix} = \begin{bmatrix} U_{\alpha 11} & U_{\alpha 12} & -N_{\alpha 11} & -N_{\alpha 12} \\ U_{\alpha 21} & U_{\alpha 22} & -N_{\alpha 21} & -N_{\alpha 22} \\ N_{\alpha 11} & N_{\alpha 12} & U_{\alpha 11} & U_{\alpha 12} \\ N_{\alpha 21} & N_{\alpha 22} & U_{\alpha 21} & U_{\alpha 22} \end{bmatrix} \begin{bmatrix} a^\dagger_{\alpha p} \\ a^\dagger_{\alpha n} \\ a_{\bar{\alpha} p} \\ a_{\bar{\alpha} n} \end{bmatrix} \quad (4.10b)
$$

It will be useful to list the entire set of transformations.

$$
b^\dagger_{\alpha \tau} = \sum_{\tau'} (U_{\alpha \tau \tau'} a^\dagger_{\alpha \tau'} - N_{\alpha \tau \tau'} a_{\bar{\alpha} \tau'}) \quad (4.11a)
$$

$$
b_{\alpha \tau} = \sum_{\tau'} (U^*_{\alpha \tau \tau'} a_{\alpha \tau'} - N^*_{\alpha \tau \tau'} a^\dagger_{\bar{\alpha} \tau'}) \quad (4.11b)
$$

$$
b^\dagger_{\bar{\alpha} \tau} = \sum_{\tau'} (U^*_{\alpha \tau \tau'} a^\dagger_{\bar{\alpha} \tau'} + N^*_{\alpha \tau \tau'} a_{\alpha \tau'}) \quad (4.11c)
$$

$$
b_{\bar{\alpha} \tau} = \sum_{\tau'} (U_{\alpha \tau \tau'} a_{\bar{\alpha} \tau'} + N_{\alpha \tau \tau'} a^\dagger_{\alpha \tau'}) \quad (4.11d)
$$

The inverse transformation is

$$
\begin{bmatrix} A^\dagger_\alpha \\ A_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} U^\dagger_\alpha & V^\dagger_\alpha \\ -V^T_\alpha & U^T_\alpha \end{bmatrix} \begin{bmatrix} B^\dagger_\alpha \\ B_{\bar{\alpha}} \end{bmatrix}. \quad (4.12)
$$

The set of all co-ordinates is given below.

$$
a^\dagger_{\alpha \tau} = \sum_{\tau'} (U^*_{\alpha \tau' \tau} b^\dagger_{\alpha \tau'} + N^*_{\alpha \tau' \tau} b_{\bar{\alpha} \tau'}) \quad (4.13a)
$$

$$
a_{\alpha \tau} = \sum_{\tau'} (U_{\alpha \tau' \tau} b_{\alpha \tau'} + N_{\alpha \tau' \tau} b^\dagger_{\bar{\alpha} \tau'}) \quad (4.13b)
$$

$$
a^\dagger_{\bar{\alpha} \tau} = \sum_{\tau'} (U_{\alpha \tau' \tau} b^\dagger_{\bar{\alpha} \tau'} - N_{\alpha \tau' \tau} b_{\alpha \tau'}) \quad (4.13c)
$$

$$
a_{\bar{\alpha} \tau} = \sum_{\tau'} (U^*_{\alpha \tau' \tau} b_{\bar{\alpha} \tau'} - N^*_{\alpha \tau' \tau} b^\dagger_{\alpha \tau'}) \quad (4.13d)
$$

The unitarity conditions (4.8) may also be derived from the commutation rules. For example, using (4.11a,b) we find

$$
[b^\dagger_{\alpha_1 \tau_1}, b_{\alpha_2 \tau_2}]_+ = \sum_{\tau} (U_{\alpha_1 \tau_1 \tau} U^*_{\alpha_1 \tau_2 \tau} + N_{\alpha_1 \tau_1 \tau} N^*_{\alpha_1 \tau_2 \tau}) \delta_{\alpha_1 \alpha_2}.
$$

Requiring the commutator to equal $\delta_{\alpha_1 \alpha_2} \delta_{L_1 L_2}$, we have

$$\sum_{\gamma} \left(U_{\alpha L_1 \gamma} U^*_{\alpha L_2 \gamma} + N_{\alpha L_1 \gamma} N^*_{\alpha L_2 \gamma} \right) = \delta_{L_1 L_2}$$

which is (4.9a). The set of unitarity conditions (4.8) are obtained by requiring

$$[b^\dagger_{\alpha_1 L_1}, b_{\alpha_2 L_2}]_+ = \delta_{\alpha_1 \alpha_2} \delta_{L_1 L_2} \tag{4.14a}$$

$$[b_{\alpha_1 L_1}, b_{\bar{\alpha}_2 L_2}]_+ = 0 \tag{4.14b}$$

$$[a^\dagger_{\alpha_1 T_1}, a_{\alpha_2 T_2}]_+ = \delta_{\alpha_1 \alpha_2} \delta_{T_1 T_2} \tag{4.14c}$$

$$[a_{\alpha_1 T_1}, a_{\bar{\alpha}_2 T_2}]_+ = 0 . \tag{4.14d}$$

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 $(\alpha_1, \alpha_2 > 0)$

$$\langle a^{\dagger}_{\alpha_1 \tau_1} a_{\alpha_2 \tau_2} \rangle =$$

$$\langle \sum_{\tau_1} (U^{*}_{\alpha_1 \tau_1 T_1} b^{\dagger}_{\alpha_1 \tau_1} + N^{*}_{\alpha_1 \tau_1 T_1} b_{\bar{\alpha}_1 \tau_1}) \sum_{\tau_2} (U_{\alpha_2 \tau_2 T_2} b_{\alpha_2 \tau_2} + N_{\alpha_2 \tau_2 T_2} b^{\dagger}_{\bar{\alpha}_2 \tau_2}) \rangle =$$

$$\sum_{\tau_1 \tau_2} N^{*}_{\alpha_1 \tau_1 T_1} N_{\alpha_2 \tau_2 T_2} \langle b_{\bar{\alpha}_1 \tau_1} b^{\dagger}_{\bar{\alpha}_2 \tau_2} \rangle .$$

Since $\langle b_{\bar{\alpha}_1 \tau_1} b^{\dagger}_{\bar{\alpha}_2 \tau_2} \rangle = \delta_{\alpha_1 \alpha_2} \delta_{\tau_1 \tau_2}$, the density matrix is

$$\langle a^{\dagger}_{\alpha_1 \tau_1} a_{\alpha_2 \tau_2} \rangle = \sum_{\tau} N^{*}_{\alpha_1 \tau T_1} N_{\alpha_1 \tau T_2} \delta_{\alpha_1 \alpha_2} . \qquad (4.15)$$

$$(\alpha_1, \alpha_2 > 0)$$

The non-vanishing elements are

$$\langle a^{\dagger}_{\alpha p} a_{\alpha p} \rangle = N^{*}_{\alpha 11} N_{\alpha 11} + N^{*}_{\alpha 21} N_{\alpha 21} \qquad (4.16a)$$

$$\langle a^{\dagger}_{\alpha n} a_{\alpha n} \rangle = N^{*}_{\alpha 12} N_{\alpha 12} + N^{*}_{\alpha 22} N_{\alpha 22} \qquad (4.16b)$$

$$\langle a^{\dagger}_{\alpha p} a_{\alpha n} \rangle = N^{*}_{\alpha 11} N_{\alpha 12} + N^{*}_{\alpha 21} N_{\alpha 22} \qquad (4.16c)$$

$$\langle a^{\dagger}_{\alpha n} a_{\alpha p} \rangle = N^{*}_{\alpha 12} N_{\alpha 11} + N^{*}_{\alpha 22} N_{\alpha 21} . \qquad (4.16d)$$

It is apparent that

$$\langle a^{\dagger}_{\alpha p} a_{\alpha p} \rangle \quad \text{and} \quad \langle a^{\dagger}_{\alpha n} a_{\alpha n} \rangle \quad \text{are real} \quad (4.17)$$

and

$$\langle a^{\dagger}_{\alpha p} a_{\alpha n} \rangle = \langle a^{\dagger}_{\alpha n} a_{\alpha p} \rangle^{*} . \qquad (4.18)$$

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

$$\rho^{\dagger}(\alpha) = \rho(\alpha) . \tag{4.21}$$

The elements of ρ for $\alpha < 0$ are given by

$$\langle a_{\bar{\alpha} \tau_1}^{\dagger} a_{\bar{\alpha} \tau_2} \rangle = \langle a_{\alpha \tau_1}^{\dagger} a_{\alpha \tau_2} \rangle^{*} \tag{4.22}$$

resulting in the time reversal symmetry

$$\rho(\bar{\alpha}) = \rho^{*}(\alpha) . \tag{4.23}$$

The pairing tensor may be similarly evaluated. Let $\alpha_1, \alpha_2 > 0$.

$$\langle a_{\bar{\alpha}_1 \tau_1} a_{\alpha_2 \tau_2} \rangle =$$

$$\langle \sum_{t_1} (U_{\alpha_1 t_1 \tau_1}^{*} b_{\bar{\alpha}_1 t_1} - N_{\alpha_1 \tau_1 \tau_1}^{*} b_{\alpha_1 t_1}^{\dagger}) \sum_{t_2} (U_{\alpha_2 \tau_2 \tau_2} b_{\alpha_2 t_2} + N_{\alpha_2 \tau_2 \tau_2} b_{\bar{\alpha}_2 t_2}^{\dagger}) \rangle =$$

$$\sum_{t_1 t_2} U_{\alpha_1 t_1 \tau_1}^{*} N_{\alpha_2 t_2 \tau_2} \langle b_{\bar{\alpha}_1 t_1} b_{\bar{\alpha}_2 t_2}^{\dagger} \rangle .$$

The pairing tensor is

$$\langle a_{\bar{\alpha}_1 \tau_1} a_{\alpha_2 \tau_2} \rangle = \sum_{t} U_{\alpha_1 t \tau_1}^{*} N_{\alpha_1 t \tau_2} \delta_{\alpha_1 \alpha_2} . \tag{4.24}$$
$$(\alpha_1, \alpha_2 > 0)$$

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

$$t_{\tau_1 \tau_2}(\alpha) = t_{\alpha \tau_1, \, \breve{\alpha} \tau_2} \tag{4.28}$$

and

$$t(\alpha) = \begin{bmatrix} t_{pp}(\alpha) & t_{pn}(\alpha) \\ t_{np}(\alpha) & t_{nn}(\alpha) \end{bmatrix} \tag{4.29}$$

then

$$t^{\dagger}(\alpha) = t(\alpha) \, . \tag{4.30}$$

The adjoint operation refers only to isospin co-ordinates, i.e.

$$\mathcal{L}^\dagger_{T_1 T_2}(\alpha) = \mathcal{L}^*_{\alpha T_2, \bar{\alpha} T_1} \neq \mathcal{L}^*_{\bar{\alpha} T_2, \alpha T_1} \, .$$

Since the pairing tensor is anti-symmetric

$$\langle a_{\alpha T_1} a_{\bar{\alpha} T_2} \rangle = - \langle a_{\bar{\alpha} T_2} a_{\alpha T_1} \rangle \qquad (4.31)$$

the time reversal symmetry   is

$$\mathcal{L}(\bar{\alpha}) = - \mathcal{L}^*(\alpha) \qquad (4.32)$$

where $\mathcal{L}_{T_1 T_2}(\bar{\alpha}) = \mathcal{L}_{\bar{\alpha} T_1, \alpha T_2}$.   The adjoint of the pairing

tensor is

$$\langle a^\dagger_{\alpha_1 T_1} a^\dagger_{\bar{\alpha}_2 T_2} \rangle = \langle a_{\bar{\alpha}_2 T_2} a_{\alpha_1 T_1} \rangle^* . \qquad (4.33)$$

The HF potential is

$$\Gamma_{\alpha_1 T_1, \alpha_2 T_2} =$$

$$\sum_{\substack{\beta \geq 0 \\ T_3 T_4}}^A \langle \alpha_1 T_1, \beta T_3 | \mathcal{N} | \alpha_2 T_2, \beta T_4 \rangle_A \langle a^\dagger_{\beta T_3} a_{\beta T_4} \rangle . \qquad (4.34)$$

The matrix elements of v are non-zero only if $T_1 + T_2 = T_3 + T_4$.

Therefore the diagonal – isospin elements of Γ are

$$\Gamma_{\alpha_1 T, \alpha_2 T} =$$

$$\sum_{\substack{\beta \geq 0 \\ T'}}^A \langle \alpha_1 T, \beta T' | \mathcal{N} | \alpha_2 T, \beta T' \rangle_A \langle a^\dagger_{\beta T'} a_{\beta T'} \rangle . \qquad (4.35)$$

There may also be off-diagonal – isospin elements.

$$\Gamma_{\alpha_1 T, \alpha_2 - T} =$$

$$\sum_{\beta \geq 0}^A \langle \alpha_1 T, \beta - T | \mathcal{N} | \alpha_2 - T, \beta T \rangle_A \langle a^\dagger_{\beta - T} a_{\beta T} \rangle \qquad (4.36)$$

The HF Hamiltonian is

$$\mathcal{H}_{\alpha_1 \tau_1, \alpha_2 \tau_2} = T_{\alpha_1 \tau_1, \alpha_2 \tau_2} + \Gamma_{\alpha_1 \tau_1, \alpha_2 \tau_2} \qquad (4.37)$$

Define

$$\mathcal{H}_{\tau_1 \tau_2}(\alpha) = \mathcal{H}_{\alpha \tau_1, \alpha \tau_2} . \qquad (4.38)$$

The matrix elements of T and v are real. Since $\rho_{\tau\tau}(\alpha)$ is real

$$\mathcal{H}_{pp}(\alpha) \quad \text{and} \quad \mathcal{H}_{nn}(\alpha) \qquad \text{are real.} (4.39)$$

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 $\rho_{pn}(\alpha) = \rho_{np}^*(\alpha)$

$$\mathcal{H}_{pn}(\alpha) = \mathcal{H}_{np}^*(\alpha) . \qquad (4.40)$$

Therefore the matrix

$$\mathcal{H}(\alpha) = \begin{bmatrix} \mathcal{H}_{pp}(\alpha) & \mathcal{H}_{pn}(\alpha) \\ \mathcal{H}_{np}(\alpha) & \mathcal{H}_{nn}(\alpha) \end{bmatrix} \qquad (4.41)$$

is Hermitian.

$$\mathcal{H}^\dagger(\alpha) = \mathcal{H}(\alpha) \qquad (4.42)$$

Since $\rho(\bar{\alpha}) = \rho^*(\bar{\alpha})$, the time reversal symmetry is

$$\mathcal{H}(\bar{\alpha}) = \mathcal{H}^*(\alpha) . \qquad (4.43)$$

The pair potential is

$$\Delta_{\alpha_1 T_1, \bar{\alpha}_2 T_2} =$$

$$\sum_{\substack{\beta > 0 \\ T_3 T_4}}^{1} \langle \alpha_1 T_1, \bar{\alpha}_2 T_2 | \mathcal{N} | \beta T_3, \bar{\beta} T_4 \rangle_A \langle a_{\bar{\beta} T_4} a_{\beta T_3} \rangle . \qquad (4.44)$$

For non-zero matrix elements $T_1 + T_2 = T_3 + T_4$, so that the diagonal isospin elements are

$$\Delta_{\alpha_1 T, \bar{\alpha}_2 T} =$$

$$\sum_{\beta > 0}^{1} \langle \alpha_1 T, \bar{\alpha}_2 T | \mathcal{N} | \beta T, \bar{\beta} T \rangle_A \langle a_{\bar{\beta} T} a_{\beta T} \rangle . \qquad (4.45)$$

Only protons (neutrons) contribute to the proton (neutron) pair potential. $\Delta_{\alpha_1 T, \bar{\alpha}_2 T}$ is the $|T_z| = 1$ pair potential. The $T_z = 0$ pair potential is

$$\Delta_{\alpha_1 T, \bar{\alpha}_2 - T} =$$

$$\sum_{\substack{\beta > 0 \\ T'}}^{1} \langle \alpha_1 T, \bar{\alpha}_2 - T | \mathcal{N} | \beta T', \bar{\beta} - T' \rangle_A \langle a_{\bar{\beta} - T'} a_{\beta T'} \rangle . \qquad (4.46)$$

Define

$$\Delta_{T_1 T_2}(\alpha) = \Delta_{\alpha T_1, \bar{\alpha} T_2} . \qquad (4.47)$$

Since $\langle \alpha_1 T, \alpha_2 T | \mathcal{N} | \alpha_3 T, \alpha_4 T \rangle_A =$

$$\sum_{T}^{1} \langle \tfrac{1}{2} T \tfrac{1}{2} T | T \, 2T \rangle^2 \langle \alpha_1 \alpha_2 T | \mathcal{N} | \alpha_3 \alpha_4 T \rangle_A =$$

$$\langle \alpha_1 \alpha_2 T=1 | \mathcal{N} | \alpha_3 \alpha_4 T=1 \rangle_A \quad for \ T = \pm \tfrac{1}{2} ,$$

the $|T_z| = 1$ potential is

$$\Delta_{TT}(\alpha) = \qquad (4.48)$$

$$\sum_{\beta > 0}^{1} \langle \alpha \bar{\alpha} T=1 | \mathcal{N} | \beta \bar{\beta} T=1 \rangle_A \langle a_{\bar{\beta} T} a_{\beta T} \rangle .$$

Since $\langle a_{\bar{\beta}\tau} a_{\beta\tau} \rangle$ is real

$$\Delta_{pp}(\alpha) \quad \text{and} \quad \Delta_{nn}(\alpha) \quad \text{are Real.} \qquad (4.49)$$

The $T_z = 0$ potential may be reduced to $T = 0$ and $T = 1$

components. Consider the matrix element

$$\langle \alpha_1 \tau, \alpha_2 -\tau | \mathcal{N} | \alpha_3 \tau', \alpha_4 -\tau' \rangle_A =$$

$$\sum_T \langle \tfrac{1}{2}\tau \tfrac{1}{2} -\tau | T 0 \rangle \langle \tfrac{1}{2}\tau' \tfrac{1}{2} -\tau' | T 0 \rangle \langle \alpha_1 \alpha_2 T | \mathcal{N} | \alpha_3 \alpha_4 T \rangle_A .$$

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

$$\Delta_{\tau-\tau}(\alpha) =$$

$$\tfrac{1}{2} \sum_{\substack{\beta \\ \beta>0}} \langle \alpha\bar{\alpha} T=1 | \mathcal{N} | \beta\bar{\beta} T=1 \rangle_A \{ \langle a_{\bar{\beta}-\tau} a_{\beta\tau} \rangle + \langle a_{\bar{\beta}\tau} a_{\beta-\tau} \rangle \}$$

$$+ \tfrac{1}{2} \sum_{\substack{\beta \\ \beta>0}} \langle \alpha\bar{\alpha} T=0 | \mathcal{N} | \beta\bar{\beta} T=0 \rangle_A \{ \langle a_{\bar{\beta}-\tau} a_{\beta\tau} \rangle - \langle a_{\bar{\beta}\tau} a_{\beta-\tau} \rangle \}. \qquad (4.50)$$

Since

$$\langle a_{\bar{\beta}-\tau} a_{\beta\tau} \rangle = \langle a_{\bar{\beta}\tau} a_{\beta-\tau} \rangle^* ,$$

$$\Delta_{\tau-\tau}(\alpha) = \sum_{\substack{\beta \\ \beta>0}} \langle \alpha\bar{\alpha} T=1 | \mathcal{N} | \beta\bar{\beta} T=1 \rangle_A \, Re \, \langle a_{\bar{\beta}-\tau} a_{\beta\tau} \rangle$$

$$+ i \sum_{\substack{\beta \\ \beta>0}} \langle \alpha\bar{\alpha} T=0 | \mathcal{N} | \beta\bar{\beta} T=0 \rangle_A \, Im \, \langle a_{\bar{\beta}-\tau} a_{\beta\tau} \rangle . \qquad (4.51)$$

The pair potential has the remarkable feature that its

real part describes $T = 1$ pairing while the imaginary

part describes $T = 0$ pairing. Let

$$\Delta^{T=1}_{\tau - \tau}(\alpha) = \sum_{\beta > 0} \langle \alpha \bar{\alpha}\, T=1 | \mathcal{N} | \beta \bar{\beta}\, T=1 \rangle_A \; Re \langle a_{\bar{\beta}-\tau}\, a_{\beta \tau} \rangle \qquad (4.52)$$

$$\Delta^{T=0}_{\tau - \tau}(\alpha) = \sum_{\beta > 0} \langle \alpha \bar{\alpha}\, T=0 | \mathcal{N} | \beta \bar{\beta}\, T=0 \rangle_A \; Im \langle a_{\bar{\beta}-\tau}\, a_{\beta \tau} \rangle \qquad (4.53)$$

then

$$\Delta_{\tau - \tau}(\alpha) = \Delta^{T=1}_{\tau - \tau}(\alpha) + i\, \Delta^{T=0}_{\tau - \tau}(\alpha) . \qquad (4.54)$$

Furthermore, since

$$Re \langle a_{\bar{\beta}-\tau}\, a_{\beta \tau} \rangle = Re \langle a_{\bar{\beta}\tau}\, a_{\beta -\tau} \rangle$$
$$Im \langle a_{\bar{\beta}-\tau}\, a_{\beta \tau} \rangle = - Im \langle a_{\bar{\beta}\tau}\, a_{\beta -\tau} \rangle$$

we have

$$\Delta^{T=1}_{\tau - \tau}(\alpha) = \Delta^{T=1}_{-\tau \tau}(\alpha) \qquad (4.55)$$

$$\Delta^{T=0}_{\tau - \tau}(\alpha) = - \Delta^{T=0}_{-\tau \tau}(\alpha) \qquad (4.56)$$

so that

$$\Delta_{\tau - \tau}(\alpha) = \Delta^{*}_{-\tau \tau}(\alpha) . \qquad (4.57)$$

Therefore the matrix

$$\Delta(\alpha) = \begin{bmatrix} \Delta_{pp}(\alpha) & \Delta_{pn}(\alpha) \\ \Delta_{np}(\alpha) & \Delta_{nn}(\alpha) \end{bmatrix} \qquad (4.58)$$

is self-adjoint.

$$\Delta^{\dagger}(\alpha) = \Delta(\alpha) \qquad (4.59)$$

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

$$\Delta_{\alpha \tau_1, \bar{\alpha} \tau_2} = - \Delta_{\bar{\alpha} \tau_2, \alpha \tau_1} \qquad (4.60)$$

the time reversal symmetry is

$$\Delta(\bar{\alpha}) = -\Delta^{*}(\alpha) \qquad (4.61)$$

where $\Delta_{\tau_1 \tau_2}(\bar{\alpha}) = \Delta_{\bar{\alpha}\tau_1, \alpha \tau_2}$.

The explicit expressions for the pair potentials are

$$\Delta_{pp}(\alpha) = \sum_{\beta > 0} \langle \alpha \bar{\alpha} T = 1 | \mathcal{N} | \beta \bar{\beta} T = 1 \rangle_A \langle a_{\bar{\beta}p} a_{\beta p} \rangle \qquad (4.62)$$

$$\Delta_{nn}(\alpha) = \sum_{\beta > 0} \langle \alpha \bar{\alpha} T = 1 | \mathcal{N} | \beta \bar{\beta} T = 1 \rangle_A \langle a_{\bar{\beta}n} a_{\beta n} \rangle \qquad (4.63)$$

$$\Delta_{pn}^{T=1}(\alpha) = \sum_{\beta > 0} \langle \alpha \bar{\alpha} T = 1 | \mathcal{N} | \beta \bar{\beta} T = 1 \rangle_A \, Re \langle a_{\bar{\beta}n} a_{\beta p} \rangle \qquad (4.64)$$

$$\Delta_{pn}^{T=0}(\alpha) = \sum_{\beta > 0} \langle \alpha \bar{\alpha} T = 0 | \mathcal{N} | \beta \bar{\beta} T = 0 \rangle_A \, Im \langle a_{\bar{\beta}n} a_{\beta p} \rangle \qquad (4.65)$$

where
$$\Delta_{pn}(\alpha) = \Delta_{pn}^{T=1}(\alpha) + i \, \Delta_{pn}^{T=0}(\alpha) \qquad (4.66)$$

and
$$\Delta_{np}(\alpha) = \Delta_{pn}^{*}(\alpha). \qquad (4.67)$$

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

$$\begin{bmatrix} B_{\alpha}^{+} \\ B_{\bar{\alpha}} \end{bmatrix} = \begin{bmatrix} U_{\alpha} & -V_{\alpha} \\ V_{\alpha}^{*} & U_{\alpha}^{*} \end{bmatrix} \begin{bmatrix} A_{\alpha}^{+} \\ A_{\bar{\alpha}} \end{bmatrix}.$$

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

$$\sum_C \left(U_{\alpha C T_1} \mathcal{N}^*_{\alpha C T_2} - \mathcal{N}_{\alpha C T_1} U_{\alpha C T_2} \right) = 0$$

instead of (4.9d). The pairing tensor would be

$$\langle a_{\bar\alpha T_1} a_{\alpha T_2} \rangle = \sum_C U_{\alpha C T_1} \mathcal{N}^*_{\alpha C T_2}$$

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

$$\Delta_{T-T}(\alpha) = \sum_{\beta>0} \langle \alpha \bar\alpha T=1 | \mathcal{N} | \beta \bar\beta T=1 \rangle_n \langle a_{\bar\beta -T} a_{\beta T} \rangle.$$

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)

$$H'_0 = E_0 - \lambda_p Z - \lambda_n (A - Z)$$

$$= \sum_{\alpha \geq 0, T_1 T_2} (T - \lambda_p P_p - \lambda_n P_n + \tfrac{1}{2}\Gamma)_{\alpha T_1, \alpha T_2} \langle a^+_{\alpha T_1} a_{\alpha T_2} \rangle$$

$$+ \sum_{\alpha > 0, T_1 T_2} \Delta_{\alpha T_1, \bar\alpha T_2} \langle a^+_{\alpha T_1} a^+_{\bar\alpha T_2} \rangle \qquad (4.68)$$

or by (3.38b)

$$H_o' = E_o - \lambda_p Z - \lambda_n (A-Z)$$

$$= \sum_{\alpha \geq 0, T}^{'} \langle \alpha T | T - \lambda_p P_p - \lambda_n P_n | \alpha T \rangle \langle a^\dagger_{\alpha T} a_{\alpha T} \rangle$$

$$+ \frac{1}{2} \sum_{\substack{\alpha \beta \geq 0 \\ T_1 T_2 T_3 T_4}}^{'} \langle \alpha T_1, \beta T_2 | w | \alpha T_3, \beta T_4 \rangle_A \langle a^\dagger_{\alpha T_1} a_{\alpha T_3} \rangle \langle a^\dagger_{\beta T_2} a_{\beta T_4} \rangle \quad (4.69)$$

$$+ \sum_{\substack{\alpha \beta > 0 \\ T_1 T_2 T_3 T_4}}^{'} \langle \alpha T_1, \bar{\alpha} T_2 | w | \beta T_3, \bar{\beta} T_4 \rangle_A \langle a^\dagger_{\alpha T_1} a^\dagger_{\bar{\alpha} T_2} \rangle \langle a_{\bar{\beta} T_4} a_{\beta T_3} \rangle$$

where P_T is a projection operator.

$$P_T = | T \rangle \langle T | \qquad (4.70)$$

H_2' is given by (3.39)

$$H_2' = \sum_{\alpha_1 \alpha_2 \geq 0, T_1 T_2} \hat{\mathcal{H}}_{\alpha_1 T_1, \alpha_2 T_2} N[a^\dagger_{\alpha_1 T_1} a_{\alpha_2 T_2}]$$

$$+ \sum_{\alpha_1 \alpha_2 > 0, T_1 T_2} \Delta_{\alpha_1 T_1, \bar{\alpha}_2 T_2} N[a^\dagger_{\alpha_1 T_1} a^\dagger_{\bar{\alpha}_2 T_2}] \qquad (4.71)$$

$$+ \sum_{\alpha_1 \alpha_2 > 0, T_1 T_2} \Delta^*_{\alpha_1 T_1, \bar{\alpha}_2 T_2} N[a_{\bar{\alpha}_2 T_2} a_{\alpha_1 T_1}]$$

where

$$\hat{\mathcal{H}} = \mathcal{H} - \lambda_p P_p - \lambda_n P_n . \qquad (4.72)$$

Note that

$$\hat{\mathcal{H}}_{pp}(\alpha) = \mathcal{H}_{pp}(\alpha) - \lambda_p \qquad (4.73a)$$

$$\hat{\mathcal{H}}_{nn}(\alpha) = \mathcal{H}_{nn}(\alpha) - \lambda_n \qquad (4.73b)$$

$$\hat{\mathcal{H}}_{pn}(\alpha) = \mathcal{H}_{pn}(\alpha) \qquad (4.73c)$$

$$\hat{\mathcal{H}}_{np}(\alpha) = \mathcal{H}_{np}(\alpha) . \qquad (4.73d)$$

4. Equation of Motion

The pairing parameters may be determined by the equation of motion method. It is assumed that

$$\overline{|\langle \alpha_1 \bar{\alpha}_2 T | \mathcal{N} | \beta \bar{\beta} T \rangle_A|} \ll \overline{|\langle \alpha_1 \bar{\alpha}_1 T | \mathcal{N} | \beta \bar{\beta} T \rangle_A|} \qquad (\alpha_1 \neq \alpha_2)$$

$$(4.74a)$$

so that

$$|\Delta_{\alpha_1 T_1, \bar{\alpha}_2 T_2}| \ll |\Delta_{\alpha_1 T_1, \bar{\alpha}_1 T_2}|. \qquad (\alpha_1 \neq \alpha_2) \qquad (4.74b)$$

Elements of Δ connecting different spatial orbitals are neglected. It is also assumed that

$$|\mathcal{H}_{\alpha_1 T_1, \alpha_2 T_2}| \ll |\mathcal{H}_{\alpha_1 T_1, \alpha_1 T_2}|. \qquad (\alpha_1 \neq \alpha_2) \qquad (4.75)$$

Then H_2' is simplified.

$$H_2' = \sum_{\alpha \geq 0, \, T_1 T_2} \hat{\mathcal{H}}_{T_1 T_2}(\alpha) \, N[a^\dagger_{\alpha T_1} a_{\alpha T_2}] + $$
$$\sum_{\alpha > 0, \, T_1 T_2} \left\{ \Delta_{T_1 T_2}(\alpha) \, N[a^\dagger_{\alpha T_1} a^\dagger_{\bar{\alpha} T_2}] + \Delta^{\pm}_{T_1 T_2}(\alpha) \, N[a_{\bar{\alpha} T_2} a_{\alpha T_1}] \right\}$$

$$(4.76)$$

H' has the form of an independent quasiparticle Hamiltonian if H_4' may be neglected and if

$$H_2' = \sum_{\alpha \tau} E_{\alpha \tau} \, b^\dagger_{\alpha \tau} b_{\alpha \tau}. \qquad (4.77)$$

It is therefore required that

$$[H_2', b^\dagger_{\alpha \tau}]_- = E_{\alpha \tau} b^\dagger_{\alpha \tau} \qquad (4.78a)$$

or

$$[H_2', b^\dagger_{\alpha \tau}]_- = E_{\alpha \tau} \sum_{T} (U_{\alpha \tau T} a^\dagger_{\alpha T} - N_{\alpha \tau T} a_{\bar{\alpha} T}). \qquad (4.78b)$$

The commutator may also be evaluated with (4.76).

$$[H_2', b^\dagger_{\alpha\tau}]_- = \sum_{\tau_1, \tau_2} \{\hat{\mathcal{H}}_{\tau_1 \tau_2}(\alpha) U_{\alpha\tau\tau_2} - \Delta_{\tau_1 \tau_2}(\alpha) \mathcal{N}_{\alpha\tau\tau_2}\} a^\dagger_{\alpha\tau_1}$$
$$+ \sum_{\tau_1, \tau_2} \{\Delta^\dagger_{\tau_1 \tau_2}(\alpha) U_{\alpha\tau\tau_2} + \tilde{\hat{\mathcal{H}}}_{\tau_1 \tau_2}(\bar{\alpha}) \mathcal{N}_{\alpha\tau\tau_2}\} a_{\bar{\alpha}\tau_1}. \quad (4.79)$$

The time reversal symmetry $\mathcal{H}(\bar{\alpha}) = \mathcal{H}^*(\alpha)$ and the Hermiticity of $\mathcal{H}$ result in $\tilde{\hat{\mathcal{H}}}(\bar{\alpha}) = \mathcal{H}(\alpha)$. Also $\Delta(\alpha)$ is self-adjoint. Therefore

$$[H_2', b^\dagger_{\alpha\tau}]_- = \sum_{\tau_1, \tau_2} \{\hat{\mathcal{H}}_{\tau_1 \tau_2}(\alpha) U_{\alpha\tau\tau_2} - \Delta_{\tau_1 \tau_2}(\alpha) \mathcal{N}_{\alpha\tau\tau_2}\} a^\dagger_{\alpha\tau_1}$$
$$+ \sum_{\tau_1, \tau_2} \{\Delta_{\tau_1 \tau_2}(\alpha) U_{\alpha\tau\tau_2} + \hat{\mathcal{H}}_{\tau_1 \tau_2}(\alpha) \mathcal{N}_{\alpha\tau\tau_2}\} a_{\bar{\alpha}\tau_1}. \quad (4.80)$$

Compare (4.78b) and (4.80) and equate coefficients of $a^\dagger_{\alpha\tau}$ and $a_{\bar{\alpha}\tau}$.

$$\sum_{\tau_2} \{\hat{\mathcal{H}}_{\tau_1 \tau_2}(\alpha) U_{\alpha\tau\tau_2} - \Delta_{\tau_1 \tau_2}(\alpha) \mathcal{N}_{\alpha\tau\tau_2}\} = E_{\alpha\tau} U_{\alpha\tau\tau_1} \quad (4.81a)$$

$$\sum_{\tau_2} \{\Delta_{\tau_1 \tau_2}(\alpha) U_{\alpha\tau\tau_2} + \hat{\mathcal{H}}_{\tau_1 \tau_2}(\alpha) \mathcal{N}_{\alpha\tau\tau_2}\} = -E_{\alpha\tau} \mathcal{N}_{\alpha\tau\tau_1}. \quad (4.81b)$$

In matrix form (4.81) is

$$\begin{bmatrix} \hat{\mathcal{H}}_{pp}(\alpha) & \hat{\mathcal{H}}_{pn}(\alpha) & \Delta_{pp}(\alpha) & \Delta_{pn}(\alpha) \\ \hat{\mathcal{H}}_{np}(\alpha) & \hat{\mathcal{H}}_{nn}(\alpha) & \Delta_{np}(\alpha) & \Delta_{nn}(\alpha) \\ \Delta_{pp}(\alpha) & \Delta_{pn}(\alpha) & -\hat{\mathcal{H}}_{pp}(\alpha) & -\hat{\mathcal{H}}_{pn}(\alpha) \\ \Delta_{np}(\alpha) & \Delta_{nn}(\alpha) & -\hat{\mathcal{H}}_{np}(\alpha) & -\hat{\mathcal{H}}_{nn}(\alpha) \end{bmatrix} \begin{bmatrix} U_{\alpha\tau 1} \\ U_{\alpha\tau 2} \\ -\mathcal{N}_{\alpha\tau 1} \\ -\mathcal{N}_{\alpha\tau 2} \end{bmatrix} = E_{\alpha\tau} \begin{bmatrix} U_{\alpha\tau 1} \\ U_{\alpha\tau 2} \\ -\mathcal{N}_{\alpha\tau 1} \\ -\mathcal{N}_{\alpha\tau 2} \end{bmatrix} \quad (4.82)$$

or more compactly

$$\begin{bmatrix} \hat{\mathcal{H}}(\alpha) & \Delta(\alpha) \\ \Delta(\alpha) & -\hat{\mathcal{H}}(\alpha) \end{bmatrix} \begin{bmatrix} U_\tau(\alpha) \\ -\mathcal{N}_\tau(\alpha) \end{bmatrix} = E_\tau(\alpha) \begin{bmatrix} U_\tau(\alpha) \\ -\mathcal{N}_\tau(\alpha) \end{bmatrix} \quad (4.83)$$

where $$E_\tau(\alpha) = E_{\alpha\tau} \qquad (4.84)$$

$$U_\tau(\alpha) = \begin{bmatrix} U_{\alpha\tau 1} \\ U_{\alpha\tau 2} \end{bmatrix} \qquad \mathcal{N}_\tau(\alpha) = \begin{bmatrix} \mathcal{N}_{\alpha\tau 1} \\ \mathcal{N}_{\alpha\tau 2} \end{bmatrix}. \qquad (4.85)$$

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

$$|U_{\alpha\tau 1}|^2 + |U_{\alpha\tau 2}|^2 + |\mathcal{N}_{\alpha\tau 1}|^2 + |\mathcal{N}_{\alpha\tau 2}|^2 = 1. \qquad (4.86)$$

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

$$\langle \underline{T} \rangle = 0 \qquad (4.87)$$

where $\quad \underline{T} = T_x \underline{i} + T_y \underline{j} + T_z \underline{k} \cdot \qquad (4.88)$

All components of $\underline{T}$ are to have vanishing ground state expectation values.

$$\langle T_x \rangle = \langle T_y \rangle = \langle T_z \rangle = 0 \qquad (4.89)$$

This constraint will simplify our eigenvalue equations. Since $\underline{T} = \frac{1}{2} \underline{\tau}$, the isospin operator has the second quantized form

$$\underline{T} = \frac{1}{2} \sum_{\alpha \tau_1 \tau_2} \langle \underline{\tau} \rangle_{\tau_1 \tau_2} a^+_{\alpha \tau_1} a_{\alpha \tau_2} \tag{4.90}$$

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.

$$\tau_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \tau_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \tau_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4.92}$$

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.

$$|p\rangle \sim \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |n\rangle \sim \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\langle p| \sim (1 \quad 0) \qquad \langle n| \sim (0 \quad 1) \tag{4.93}$$

The values of $\langle \tau_n \rangle_{\tau_1 \tau_2}$ are in the tables below.

$\langle \tau_x \rangle_{\tau_1 \tau_2}$

τ_1\τ_2	p	n
p	0	1
n	1	0

$\langle \tau_y \rangle_{\tau_1 \tau_2}$

τ_1\τ_2	p	n
p	0	$-i$
n	i	0

$\langle \tau_z \rangle_{\tau_1 \tau_2}$

τ_1\τ_2	p	n
p	1	0
n	0	-1

$$\tag{4.94}$$

The isospin projection conservation requirement is

$$\langle T_z \rangle = \tfrac{1}{2} \sum_\alpha^A \{ \langle a^\dagger_{\alpha p} a_{\alpha p} \rangle - \langle a^\dagger_{\alpha n} a_{\alpha n} \rangle \} = 0 . \tag{4.95}$$

It is therefore required that

$$\langle a^\dagger_{\alpha p} a_{\alpha p} \rangle = \langle a^\dagger_{\alpha n} a_{\alpha n} \rangle . \tag{4.96}$$

Consequently

$$\mathcal{H}_{pp}(\alpha) = \mathcal{H}_{nn}(\alpha) . \tag{4.97}$$

The other components of the constraint are

$$\langle T_x \rangle = \tfrac{1}{2} \sum_\alpha^A \{ \langle a^\dagger_{\alpha p} a_{\alpha n} \rangle + \langle a^\dagger_{\alpha n} a_{\alpha p} \rangle \} = 0 \tag{4.98}$$

$$\langle T_y \rangle = -\tfrac{i}{2} \sum_\alpha^A \{ \langle a^\dagger_{\alpha p} a_{\alpha n} \rangle - \langle a^\dagger_{\alpha n} a_{\alpha p} \rangle \} = 0 . \tag{4.99}$$

Since each bracket must vanish

$$\langle a^\dagger_{\alpha p} a_{\alpha n} \rangle = \langle a^\dagger_{\alpha n} a_{\alpha p} \rangle = 0 \tag{4.100}$$

and

$$\mathcal{H}_{pn}(\alpha) = \mathcal{H}_{np}(\alpha) = 0 . \tag{4.101}$$

Constraints (4.96, 4.100) are satisfied by

$$V_\alpha = \begin{bmatrix} \mathcal{N}_{\alpha 11} & \mathcal{N}_{\alpha 12} \\ \mathcal{N}^*_{\alpha 12} & -\mathcal{N}^*_{\alpha 11} \end{bmatrix} . \tag{4.102}$$

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

$$V_\alpha V_\alpha^\dagger = |Det\, V_\alpha|\, I = \{|\mathcal{N}_{\alpha 11}|^2 + |\mathcal{N}_{\alpha 12}|^2\}\, I \tag{4.104}$$

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

$$\Delta(\alpha)\Delta^\dagger(\alpha) = |Det\, \Delta(\alpha)|\, I = \{\Delta_{pp}^2(\alpha) + |\Delta_{pn}(\alpha)|^2\}\, I . \tag{4.106}$$

The eigenvalue equation (4.83)

$$\begin{bmatrix} \hat{\mathcal{H}} & \Delta \\ \Delta & -\hat{\mathcal{H}} \end{bmatrix} \begin{bmatrix} U_\tau \\ -\mathcal{N}_\tau \end{bmatrix} = E_\tau \begin{bmatrix} U_\tau \\ -\mathcal{N}_\tau \end{bmatrix}$$

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 eigen-value E_t multiply (4.83) by $\begin{bmatrix} \hat{\mathcal{H}} & \Delta \\ \Delta & -\hat{\mathcal{H}} \end{bmatrix}$.

$$\begin{bmatrix} \hat{\mathcal{H}}^2 + \Delta^2 & [\hat{\mathcal{H}}, \Delta]_- \\ -[\hat{\mathcal{H}}, \Delta]_- & \hat{\mathcal{H}}^2 + \Delta^2 \end{bmatrix} \begin{bmatrix} U_\tau \\ \mathcal{N}_\tau \end{bmatrix} = E_\tau^2 \begin{bmatrix} U_\tau \\ -\mathcal{N}_\tau \end{bmatrix}$$

$\hat{\mathcal{H}}$ 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

$$E_1^2(\alpha) = E_2^2(\alpha) = \hat{\mathcal{H}}_{pp}^2(\alpha) + \Delta_{pp}^2(\alpha) + |\Delta_{pn}(\alpha)|^2.$$

$$(4.107)$$

The positive square roots correspond to the desired eigen-vectors. The two quasiparticles $b_{\alpha 1}^{\dagger}$ and $b_{\alpha 2}^{\dagger}$ are degenerate in energy. Let

$$\hat{\mathcal{E}}(\alpha) = \hat{\mathcal{H}}_{pp}(\alpha) = \hat{\mathcal{H}}_{nn}(\alpha).$$

$$(4.108)$$

The second equality assumes

$$\lambda_p = \lambda_n.$$

$$(4.109)$$

The set of linear equations

$$
\begin{bmatrix}
(\hat{E}-E) & 0 & \Delta_{pp} & \Delta_{pn} \\
0 & (\hat{E}-E) & \Delta_{pn}^{\dagger} & -\Delta_{pp} \\
\Delta_{pp} & \Delta_{pn} & -(\hat{E}+E) & 0 \\
\Delta_{pn}^{\dagger} & -\Delta_{pp} & 0 & -(\hat{E}+E)
\end{bmatrix}
\begin{bmatrix}
U_{z1} \\
U_{z2} \\
-N_{z1} \\
-N_{z2}
\end{bmatrix}
= 0
$$

can not be solved by the usual method since all cofactors of the energy matrix vanish. Instead the eigenvectors may be found by inspection.

$$
\begin{bmatrix}
U_{11} \\
U_{12} \\
-N_{11} \\
-N_{12}
\end{bmatrix}
= K
\begin{bmatrix}
\hat{E}+E \\
0 \\
\Delta_{pp} \\
\Delta_{pn}^{*}
\end{bmatrix}
\qquad
\begin{bmatrix}
U_{21} \\
U_{22} \\
-N_{21} \\
-N_{22}
\end{bmatrix}
= K
\begin{bmatrix}
0 \\
\hat{E}+E \\
\Delta_{pn} \\
-\Delta_{pp}
\end{bmatrix}
\qquad (4.110)
$$

K is a constant of normalization. The two vectors are orthogonal. Notice that

$$
\begin{aligned}
U_{11} &= U_{22} && Real \\
U_{12} &= U_{21} = 0 && \\
N_{11} &= -N_{22} && Real \\
N_{12} &= N_{21}^{*}. && Complex
\end{aligned}
\qquad (4.111)
$$

The expressions for the density matrix and the pairing tensor are considerably simplified. Let

$$
N_{\alpha}^{2} = N_{\alpha 11}^{2} + |N_{\alpha 12}|^{2}. \qquad (4.112)
$$

$$
\langle a_{\alpha p}^{\dagger} a_{\alpha p} \rangle = \langle a_{\alpha n}^{\dagger} a_{\alpha n} \rangle = N_{\alpha}^{2} \qquad (4.113)
$$

$$\langle a^{\dagger}_{\alpha p} \, a_{\alpha n} \rangle = \langle a^{\dagger}_{\alpha n} \, a_{\alpha p} \rangle = 0 \tag{4.114}$$

$$\langle a_{\bar{\alpha} p} \, a_{\alpha p} \rangle = -\langle a_{\bar{\alpha} n} \, a_{\alpha n} \rangle = U_{\alpha 11} \, \mathcal{N}_{\alpha 11} \tag{4.115}$$

$$\langle a_{\bar{\alpha} p} \, a_{\alpha n} \rangle = \langle a_{\bar{\alpha} n} \, a_{\alpha p} \rangle^{*} = U_{\alpha 11} \, \mathcal{N}_{\alpha 12} \tag{4.116}$$

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

$$
\begin{bmatrix} b^{\dagger}_{\alpha 1} \\ b^{\dagger}_{\alpha 2} \\ b_{\bar{\alpha} 1} \\ b_{\bar{\alpha} 2} \end{bmatrix}
=
\begin{bmatrix}
U_{\alpha 11} & 0 & -\mathcal{N}_{\alpha 11} & -\mathcal{N}_{\alpha 12} \\
0 & U_{\alpha 11} & -\mathcal{N}^{*}_{\alpha 12} & \mathcal{N}_{\alpha 11} \\
\mathcal{N}_{\alpha 11} & \mathcal{N}_{\alpha 12} & U_{\alpha 11} & 0 \\
\mathcal{N}^{*}_{\alpha 12} & -\mathcal{N}_{\alpha 11} & 0 & U_{\alpha 11}
\end{bmatrix}
\begin{bmatrix} a^{\dagger}_{\alpha p} \\ a^{\dagger}_{\alpha n} \\ a_{\bar{\alpha} p} \\ a_{\bar{\alpha} n} \end{bmatrix}
\tag{4.117}
$$

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.

$$U_\alpha = \begin{bmatrix} U_{\alpha 11} & 0 \\ 0 & U_{\alpha 11} \end{bmatrix} \qquad V_\alpha = \begin{bmatrix} \mathcal{N}_{\alpha 11} & \mathcal{N}_{\alpha 12} \\ \mathcal{N}_{\alpha 12}^* & -\mathcal{N}_{\alpha 11} \end{bmatrix}$$

$$\rho(\alpha) = \begin{bmatrix} \rho_{pp}(\alpha) & 0 \\ 0 & \rho_{pp}(\alpha) \end{bmatrix} \qquad \mathcal{L}(\alpha) = \begin{bmatrix} \mathcal{L}_{pp}(\alpha) & \mathcal{L}_{pn}(\alpha) \\ \mathcal{L}_{pn}^*(\alpha) & -\mathcal{L}_{pp}(\alpha) \end{bmatrix}$$

$$\mathcal{H}(\alpha) = \begin{bmatrix} \mathcal{H}_{pp}(\alpha) & 0 \\ 0 & \mathcal{H}_{pp}(\alpha) \end{bmatrix} \qquad \Delta(\alpha) = \begin{bmatrix} \Delta_{pp}(\alpha) & \Delta_{pn}(\alpha) \\ \Delta_{pn}^*(\alpha) & -\Delta_{pp}(\alpha) \end{bmatrix}$$

$$(4.118)$$

The normalized wave function is

$$U_{\alpha 11}^2 = \tfrac{1}{2}\left(1 + \hat{\mathcal{E}}(\alpha)/E(\alpha)\right)$$

$$U_{\alpha 12}^2 = 0$$

$$\mathcal{N}_{\alpha 11}^2 = \tfrac{1}{2}\left(1 - \hat{\mathcal{E}}(\alpha)/E(\alpha)\right)\left(\Delta_{pp}(\alpha)/\Delta(\alpha)\right)^2$$

$$(Re\,\mathcal{N}_{\alpha 12})^2 = \tfrac{1}{2}\left(1 - \hat{\mathcal{E}}(\alpha)/E(\alpha)\right)\left(\Delta_{np}^{T=1}(\alpha)/\Delta(\alpha)\right)^2$$

$$(Im\,\mathcal{N}_{\alpha 12})^2 = \tfrac{1}{2}\left(1 - \hat{\mathcal{E}}(\alpha)/E(\alpha)\right)\left(\Delta_{np}^{T=0}(\alpha)/\Delta(\alpha)\right)^2$$

$$\mathcal{N}_\alpha^2 = \tfrac{1}{2}\left(1 - \hat{\mathcal{E}}(\alpha)/E(\alpha)\right) \qquad (4.119)$$

with corresponding expressions for the second eigenvector. The quasiparticle energy is

$$E(\alpha) = \sqrt{\hat{\mathcal{E}}^2(\alpha) + \Delta^2(\alpha)} \quad . \qquad (4.120)$$

For (4.119, 4.120) $\Delta^2(\alpha)$ is regarded as a one, rather than two, dimensional matrix.

$$\Delta^2(\alpha) = \Delta^2_{PP}(\alpha) + \{\Delta^{T=1}_{np}(\alpha)\}^2 + \{\Delta^{T=0}_{np}(\alpha)\}^2 \qquad (4.121)$$

The final expressions for the potentials are

$$\epsilon(\alpha) = \langle\alpha|T|\alpha\rangle + \sum_{\beta>0}\{\langle\alpha P,\beta P|\mathcal{N}|\alpha P,\beta P\rangle_A + \qquad (4.122)$$

$$\langle\alpha P,\beta n|\mathcal{N}|\alpha P,\beta n\rangle_A\}\, N_\beta^2$$

$$\Delta_{PP}(\alpha) = -\Delta_{nn}(\alpha) = \sum_{\beta>0}' \langle\alpha\bar\alpha\, T=1|\mathcal{N}|\beta\bar\beta\, T=1\rangle_A\, U_{\beta11}\, N_{\beta11} \qquad (4.123)$$

$$\Delta^{T=1}_{np}(\alpha) = \Delta^{T=1}_{pn}(\alpha) = \sum_{\beta>0}' \langle\alpha\bar\alpha\, T=1|\mathcal{N}|\beta\bar\beta\, T=1\rangle_A\, U_{\beta11}\, \mathrm{Re}\, N_{\beta12}$$

$$\Delta^{T=0}_{np}(\alpha) = -\Delta^{T=0}_{pn}(\alpha) = \sum_{\beta>0}' \langle\alpha\bar\alpha\, T=0|\mathcal{N}|\beta\bar\beta\, T=0\rangle_A\, U_{\beta11}\, \mathrm{Im}\, N_{\beta12}$$

where

$$\Delta_{np}(\alpha) = \Delta^{T=1}_{np}(\alpha) + i\, \Delta^{T=0}_{np}(\alpha) \qquad (4.124)$$

and

$$\Delta_{pn}(\alpha) = \Delta^*_{np}(\alpha). \qquad (4.125)$$

The number conservation constraint is

$$Z = A - Z = 2 \sum_{\alpha>0}' N_\alpha^2. \qquad (4.126)$$

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 $\{ N_{\alpha 11}^2, (Re\, N_{\alpha 12})^2, (Im\, N_{\alpha 12})^2 \}$ 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

$$U_{\alpha 11}\, N_{\alpha 11} = -\Delta_{pp}(\alpha) / 2\, E(\alpha)$$

$$U_{\alpha 11}\, Re\, N_{\alpha 12} = -\Delta_{np}^{T=1}(\alpha) / 2\, E(\alpha) \qquad (4.127)$$

$$U_{\alpha 11}\, Im\, N_{\alpha 12} = -\Delta_{np}^{T=0}(\alpha) / 2\, E(\alpha).$$

Substitute these expressions into (4.123).

$$\Delta_{pp}(\alpha) = -\tfrac{1}{2} \sum_{\beta > 0}' \langle \alpha\,\bar{\alpha}\, T=1 | N | \beta\bar{\beta}\, T=1 \rangle_A\, \Delta_{pp}(\beta)/E(\beta)$$

$$\Delta_{np}^{T=1}(\alpha) = -\tfrac{1}{2} \sum_{\beta > 0}' \langle \alpha\bar{\alpha}\, T=1 | N | \beta\bar{\beta}\, T=1 \rangle_A\, \Delta_{np}^{T=1}(\beta)/E(\beta) \qquad (4.128)$$

$$\Delta_{np}^{T=0}(\alpha) = -\tfrac{1}{2} \sum_{\beta > 0}' \langle \alpha\,\bar{\alpha}\, T=0 | N | \beta\bar{\beta}\, T=0 \rangle_A\, \Delta_{np}^{T=0}(\beta)/E(\beta)$$

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.

$$\langle \alpha \bar{\alpha}\, T=1 | N | \beta \bar{\beta}\, T=1 \rangle_A = -G_1$$

$$\langle \alpha \bar{\alpha}\, T=0 | N | \beta \bar{\beta}\, T=0 \rangle_A = -G_0$$

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

$$\langle a^{\dagger}_{\alpha p} a_{\alpha p} \rangle = \langle a^{\dagger}_{\alpha n} a_{\alpha n} \rangle$$

$$\sum_{\tau}' \Gamma_{\alpha\tau,\alpha\tau} \langle a^{\dagger}_{\alpha\tau} a_{\alpha\tau} \rangle = 2 \Gamma_{pp}(\alpha) \langle a^{\dagger}_{\alpha p} a_{\alpha p} \rangle .$$

Similarly $\Delta_{pp}(\alpha) = - \Delta_{nn}(\alpha)$ and $\langle a^{\dagger}_{\alpha p} a^{\dagger}_{\bar{\alpha} p} \rangle = - \langle a^{\dagger}_{\alpha n} a^{\dagger}_{\bar{\alpha} n} \rangle$ so that

$$\sum_{\tau}' \Delta_{\alpha\tau,\bar{\alpha}\tau} \langle a^{\dagger}_{\alpha\tau} a^{\dagger}_{\bar{\alpha}\tau} \rangle = 2 \Delta_{pp}(\alpha) \langle a^{\dagger}_{\alpha p} a^{\dagger}_{\bar{\alpha} p} \rangle .$$

Finally $\Delta_{pn}(\alpha) = \Delta^{*}_{np}(\alpha)$ and $\langle a^{\dagger}_{\alpha p} a^{\dagger}_{\bar{\alpha} n} \rangle = \langle a^{\dagger}_{\alpha n} a^{\dagger}_{\bar{\alpha} p} \rangle^{*}$ and

$$\sum_{\tau}' \Delta_{\alpha\tau,\bar{\alpha}-\tau} \langle a^{\dagger}_{\alpha\tau} a^{\dagger}_{\bar{\alpha}-\tau} \rangle = 2 \operatorname{Re} \{ \Delta_{np}(\alpha) \langle a^{\dagger}_{\alpha n} a^{\dagger}_{\bar{\alpha} p} \rangle \} =$$

$$2 \{ \Delta^{T=1}_{np}(\alpha) \operatorname{Re} \langle a^{\dagger}_{\alpha n} a^{\dagger}_{\bar{\alpha} p} \rangle - \Delta^{T=0}_{np}(\alpha) \operatorname{Im} \langle a^{\dagger}_{\alpha n} a^{\dagger}_{\bar{\alpha} p} \rangle \} .$$

Collecting terms we have

$$H_0' = E_0 - \lambda A = 2 \Big\{ \sum_{\alpha > 0}' \big(T_{pp}(\alpha) - \lambda + \tfrac{1}{2} \Gamma_{pp}(\alpha) \big) N_\alpha^2 +$$

$$\sum_{\alpha > 0}' \big(\Delta_{pp}(\alpha) U_{\alpha 11} N_{\alpha 11} + \Delta^{T=1}_{np}(\alpha) U_{\alpha 11} \operatorname{Re} N_{\alpha 12} + \Delta^{T=0}_{np}(\alpha) U_{\alpha 11} \operatorname{Im} N_{\alpha 12} \big) \Big\}$$

(4.129)

or

$$H_0' = E_0 - \lambda A = 2 \Big\{ \sum_{\alpha > 0}' \langle \alpha | T - \lambda | \alpha \rangle N_\alpha^2 +$$

$$\sum_{\alpha\beta > 0}' \big(\langle \alpha p, \beta p | \mathcal{N} | \alpha p, \beta p \rangle_A + \langle \alpha p, \beta n | \mathcal{N} | \alpha p, \beta n \rangle_A \big) N_\alpha^2 N_\beta^2 +$$

$$\sum_{\alpha\beta > 0}' \langle \alpha \bar{\alpha} \, T=1 | \mathcal{N} | \beta \bar{\beta} \, T=1 \rangle_A \, U_{\alpha 11} N_{\alpha 11} U_{\beta 11} N_{\beta 11} +$$

$$\sum_{\alpha\beta > 0}' \langle \alpha \bar{\alpha} \, T=1 | \mathcal{N} | \beta \bar{\beta} \, T=1 \rangle_A \, U_{\alpha 11} \operatorname{Re} N_{\alpha 12} U_{\beta 11} \operatorname{Re} N_{\beta 12} +$$

(4.130)

$$\sum_{\alpha\beta > 0}' \langle \alpha \bar{\alpha} \, T=0 | \mathcal{N} | \beta \bar{\beta} \, T=0 \rangle_A \, U_{\alpha 11} \operatorname{Im} N_{\alpha 12} U_{\beta 11} \operatorname{Im} N_{\beta 12} \Big\}$$

where

$$\lambda = \lambda_p = \lambda_n .$$

(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

$$t_{\alpha\beta} = t_{\alpha\bar{\alpha}}\, \delta_{\bar{\alpha}\beta} \tag{4.132b}$$

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.

$$\rho_{\alpha_1 \tau_1, \, \alpha_2 \tau_2} \qquad\qquad t_{\alpha_1 \tau_1, \, \alpha_2 \tau_2}$$

$\alpha_1\tau_1$ \ $\alpha_2\tau_2$	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	$\rho_{pp}(\alpha)$

$\alpha_1\tau_1$ \ $\alpha_2\tau_2$	αp	αn	$\bar{\alpha} p$	$\bar{\alpha} n$
αp	0	0	$t_{pp}(\alpha)$	$t_{pn}(\alpha)$
αn	0	0	$t_{pn}^{*}(\alpha)$	$-t_{pp}(\alpha)$
$\bar{\alpha} p$	$-t_{pp}(\alpha)$	$-t_{pn}^{*}(\alpha)$	0	0
$\bar{\alpha} n$	$-t_{pn}(\alpha)$	$t_{pp}(\alpha)$	0	0

where

$$\rho_{pp}(\alpha) = N_{\alpha 11}^{2} + |N_{\alpha 12}|^{2} \qquad\qquad t_{pp}(\alpha) = U_{\alpha 11}\, N_{\alpha 11}$$
$$t_{pn}(\alpha) = U_{\alpha 11}\, N_{\alpha 12}^{*}$$

The canonical representation is obtained by finding a basis in which the matrix

$$t(\alpha) = \begin{bmatrix} t_{pp}(\alpha) & t_{pn}(\alpha) \\ t_{pn}^{*}(\alpha) & -t_{pp}(\alpha) \end{bmatrix}$$

is diagonal. The eigenvalue equation is

$$t(\alpha)\, \underline{C}(\alpha) = t_{c}(\alpha)\, \underline{C}(\alpha) \tag{4.133a}$$

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
$$U_\alpha = U_{\alpha 11} \tag{4.136}$$
$$N_\alpha = \left[N_{\alpha 11}^2 + |N_{\alpha 12}|^2 \right]^{1/2}$$

then
$$t_c^2(\alpha) = (U_\alpha N_\alpha)^2. \tag{4.137}$$

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
$$\begin{bmatrix} C_{\alpha 1} \\ C_{\alpha 2} \end{bmatrix} = K \begin{bmatrix} t_{pp}(\alpha) + t_c(\alpha) \\ t_{pn}^\dagger(\alpha) \end{bmatrix}. \tag{4.139}$$

The normalized vector is
$$C_{\alpha 1} = \left[\frac{1}{2}(1 + N_{\alpha 11}/N_\alpha) \right]^{1/2}$$
$$C_{\alpha 2} = \left[\frac{1}{2}(1 - N_{\alpha 11}/N_\alpha) \right]^{1/2} e^{-i\theta} \tag{4.140}$$

where $\theta = \mathrm{Tan}^{-1}(\mathrm{Im}\ v_{\alpha 12} / \mathrm{Re}\ v_{\alpha 12})$.

Let
$$t_c(\alpha) = U_\alpha N_\alpha \tag{4.141}$$

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

$$\mathcal{L}(\bar{\alpha})\,\underline{C}(\bar{\alpha}) = \mathcal{L}_c(\bar{\alpha})\,\underline{C}(\bar{\alpha}).\tag{4.142}$$

Since $t(\bar{\alpha}) = -t^*(\alpha)$, the solution is

$$\underline{C}(\bar{\alpha}) = \underline{C}^*(\alpha)\tag{4.143}$$

$$\mathcal{L}_c(\bar{\alpha}) = -\mathcal{L}_c(\alpha)\tag{4.144}$$

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

$$\mathcal{L}(\alpha) = \begin{bmatrix} \mathcal{L}_c(\alpha) & 0 \\ 0 & -\mathcal{L}_c(\alpha) \end{bmatrix}\tag{4.146}$$

$$\mathcal{L}(\bar{\alpha}) = -\mathcal{L}(\alpha).\tag{4.147}$$

Since $t_{ij}(\alpha) = t_{\alpha i,\,\bar{\alpha} j}$ (see 4.28) the components of the rotated matrix $t(\alpha)$ have the meaning

$$\mathcal{L}_c(\alpha) = \begin{cases} \mathcal{L}_{11}(\alpha) = \mathcal{L}_{\alpha 1,\,\bar{\alpha}1} \\ -\mathcal{L}_{22}(\alpha) = -\mathcal{L}_{\alpha 2,\,\bar{\alpha}2} \end{cases}$$

Also $t_{ij}(\bar{\alpha}) = t_{\bar{\alpha} i,\,\alpha j}$ (see 4.32 ff) so that

$$\mathcal{L}_c(\alpha) = \begin{cases} -\mathcal{L}_{11}(\bar{\alpha}) = -\mathcal{L}_{\bar{\alpha}1,\,\alpha 1} \\ \mathcal{L}_{22}(\bar{\alpha}) = \mathcal{L}_{\bar{\alpha}2,\,\alpha 2} \end{cases}$$

Consequently the pairing tensor has the canonical form.

$$C_{\alpha_1 C_1, \alpha_2 C_2}$$

$\alpha_1 C_1$ \ $\alpha_2 C_2$	$\alpha 1$	$\bar{\alpha} 1$	$\alpha 2$	$\bar{\alpha} 2$
$\alpha 1$	0	$C_c(\alpha)$	0	0
$\bar{\alpha} 1$	$-C_c(\alpha)$	0	0	0
$\alpha 2$	0	0	0	$-C_c(\alpha)$
$\bar{\alpha} 2$	0	0	$C_c(\alpha)$	0

(4.148)

Since $\rho(\alpha)$ is diagonal and doubly degenerate the density matrix remains diagonal in the rotated basis with the same representation.

$$\rho(\alpha) = \begin{bmatrix} N_\alpha^2 & 0 \\ 0 & N_\alpha^2 \end{bmatrix}.$$

(4.149)

Therefore the new basis does indeed furnish the canonical representation. Consider the various limiting cases.

a) $|T_z| = 1$ pairing $\qquad (N_{\alpha 12} = 0)$ (4.150)

$\qquad C_{\alpha 1} = 1$

$\qquad C_{\alpha 2} = 0$

b) $|T_z| = 0$ pairing $\qquad (N_{\alpha 11} = 0)$ (4.151)

$\qquad C_{\alpha 1} = \sqrt{1/2}$

$\qquad C_{\alpha 2} = \sqrt{1/2}\, e^{-i\theta}$

c) $T = 1$ pairing $\quad (N_{\alpha 11} = N_{\alpha 12} = Real)$ (4.152)

$\qquad C_{\alpha 1} = \left[\frac{1}{2}(1 + \sqrt{1/2}) \right]^{1/2}$

$\qquad C_{\alpha 2} = \left[\frac{1}{2}(1 - \sqrt{1/2}) \right]^{1/2}$

d) $T = 0$ pairing $\quad (N_{\alpha 11} = Re\, N_{\alpha 12} = 0)$ (4.153)

$\qquad C_{\alpha 1} = \sqrt{1/2}$

$\qquad C_{\alpha 2} = -\sqrt{1/2}\, i$

The density matrix and pairing tensor may be reproduced by a new set of quasiparticle operators.

$$b^\dagger_{\alpha 1} = U_\alpha\, a^\dagger_{\alpha 1} - N_\alpha\, a_{\bar\alpha 1}$$
$$b^\dagger_{\alpha 2} = U_\alpha\, a^\dagger_{\alpha 2} + N_\alpha\, a_{\bar\alpha 2}$$
$$b^\dagger_{\bar\alpha 1} = U_\alpha\, a^\dagger_{\bar\alpha 1} + N_\alpha\, a_{\alpha 1}$$
$$b^\dagger_{\bar\alpha 2} = U_\alpha\, a^\dagger_{\bar\alpha 2} - N_\alpha\, a_{\alpha 2}$$

(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.

(4.156)

$$| \Phi_0 \rangle = \prod_{\alpha > 0} (U_\alpha - N_\alpha\, a^\dagger_{\alpha 2}\, a^\dagger_{\bar\alpha 2})(U_\alpha + N_\alpha\, a^\dagger_{\alpha 1}\, a^\dagger_{\bar\alpha 1}) | 0 \rangle$$

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

$$C_{\alpha 1}^2 - C_{\alpha 2}^2 = N_{\alpha 11} / N_\alpha$$
$$2 C_{\alpha 1} C_{\alpha 2} = N_{\alpha 12} / N_\alpha$$

and using $a^\dagger_k\, a^\dagger_k | 0 \rangle = 0$, we find

$$|\Phi_0\rangle = \prod_{\alpha>0} \{ U_{\alpha 11}(U_{\alpha 11} + N_{\alpha 11} a^\dagger_{\alpha p} a^\dagger_{\bar\alpha p}$$

$$- N_{\alpha 11} a^\dagger_{\alpha n} a^\dagger_{\bar\alpha n} + N^*_{\alpha 12} a^\dagger_{\alpha p} a^\dagger_{\bar\alpha n} + N_{\alpha 12} a^\dagger_{\alpha n} a^\dagger_{\bar\alpha p})$$

$$+ (N^2_{\alpha 11} + |N_{\alpha 12}|^2) a^\dagger_{\alpha p} a^\dagger_{\alpha n} a^\dagger_{\bar\alpha p} a^\dagger_{\bar\alpha n} \} |0\rangle . \qquad (4.157)$$

$(|\Phi_0\rangle$ 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 $v_{jm}^2 \neq v_{jm'}^2$,
$\epsilon_{jm} \neq \epsilon_{jm'}$ ($m \neq m'$). 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 $v_{\alpha 11} = \text{Re } v_{\alpha 12}$ and $\Delta_{pp}(\alpha) = \Delta_{np}^{T=1}(\alpha)$.

$$S^{32}$$

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 $\hbar^2/2J$ 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 NDK3 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)

$E(\alpha)$	-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)

$E(\alpha)$	-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)

$E(\alpha)$	-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)

$E(\alpha)$	-11.373	-7.740	-4.822	-4.286	-0.685	1.638
$(Im \, N_{\alpha 12})^2$	$(-)0.975$	$(+)0.746$	$(+)0.185$	$(-)0.079$	$(-)0.011$	$(-)0.014$
$\Delta_{np}^{T=0}(\alpha)$	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)

$E(\alpha)$	-13.477	-8.417	-5.186	-2.756	0.739	3.654
$(Im \, N_{\alpha 12})^2$	$(-)0.990$	$(+)0.810$	$(+)0.173$	$(-)0.022$	$(-)0.004$	$(-)0.005$
$\Delta_{np}^{T=0}(\alpha)$	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}: $N_{\alpha 11} = Re \, N_{\alpha 12} = \Delta_{pp}(\alpha) = \Delta_{np}^{T=1}(\alpha) = 0$.
The sign of $Im \, N_{\alpha 12}$ is given in parentheses before $(Im \, N_{\alpha 12})^2$.
$U_{\alpha 11} > 0$.

Table 4.7: 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
$E(\alpha)$	- 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

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2. A. Goswami, Nucl. Phys. <u>60</u>, 228 (1964).

3. A. Goswami and L.S. Kisslinger, Phys. Rev. <u>140</u>, B26 (1965).

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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 <u>26B</u>, 260 (1968).

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8. The wave function may also be expressed as

$$|\Phi_0\rangle = \prod_{\alpha > 0} (U_{\alpha 11} + N_{\alpha 11}\, a^\dagger_{\alpha p} a^\dagger_{\bar{\alpha} p} + N^*_{\alpha 12}\, a^\dagger_{\alpha p} a^\dagger_{\bar{\alpha} n})$$

$$\times (U_{\alpha 11} - N_{\alpha 11}\, a^\dagger_{\alpha n} a^\dagger_{\bar{\alpha} n} + N_{\alpha 12}\, a^\dagger_{\alpha n} a^\dagger_{\bar{\alpha} p})|0\rangle .$$

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

$$\frac{|\langle \alpha \beta T | \mathcal{N} | \alpha' \beta T \rangle_A|}{|\langle \alpha \bar{\alpha}' T | \mathcal{N} | \beta \bar{\beta} T \rangle_A|} << \frac{|\langle \alpha \beta T | \mathcal{N} | \alpha \beta T \rangle_A|}{|\langle \alpha \bar{\alpha} T | \mathcal{N} | \beta \bar{\beta} T \rangle_A|}$$

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 $a_{\bar{\alpha}}$

$$b^{+}_{\alpha} = U_{\alpha} a^{+}_{\alpha} - N_{\alpha} a_{\bar{\alpha}}$$

(special)

we permit each quasiparticle to be a linear combination of all particle creation and annihilation operators.

$$b^{+}_{i} = \sum_{j} \left(U_{ij} a^{+}_{j} + V_{ij} a_{j} \right)$$

(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

$$b_i^\dagger = \sum_j (U_{ij} a_j^\dagger + V_{ij} a_j) \qquad (5.1a)$$

$$b_i = \sum_j (U_{ij}^* a_j + V_{ij}^* a_j^\dagger) \qquad (5.1b)$$

or

$$\begin{bmatrix} b^\dagger \\ b \end{bmatrix} = \begin{bmatrix} U & V \\ V^* & U^* \end{bmatrix} \begin{bmatrix} a^\dagger \\ a \end{bmatrix} \qquad (5.2)$$

where a and 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

$$\begin{bmatrix} a^\dagger \\ a \end{bmatrix} = \begin{bmatrix} \tilde{U}^* & \tilde{V} \\ \tilde{V}^* & \tilde{U} \end{bmatrix} \begin{bmatrix} b^\dagger \\ b \end{bmatrix} \qquad (5.3)$$

or

$$a_j^\dagger = \sum_i (U_{ij}^* b_i^\dagger + V_{ij} b_i) \qquad (5.4a)$$

$$a_j = \sum_i (U_{ij} b_i + V_{ij}^* b_i^\dagger). \qquad (5.4b)$$

The unitarity conditions are ($XX^\dagger = I$)

$$U U^\dagger + V V^\dagger = I \qquad (5.5a)$$

$$U \tilde{V} + V \tilde{U} = 0 \qquad (5.5b)$$

and ($X^\dagger X = I$)

$$U^\dagger U + (V^\dagger V)^* = I \qquad (5.5c)$$

$$U^\dagger V + (V^\dagger U)^* = 0. \qquad (5.5d)$$

That is

$$\sum_j (U_{cj} U_{kj}^* + V_{cj} V_{kj}^*) = \delta_{ck} \tag{5.6a}$$

$$\sum_j (U_{cj} V_{kj} + V_{cj} U_{kj}) = 0 \tag{5.6b}$$

$$\sum_j (U_{jc}^* U_{jk} + V_{jc} V_{jk}^*) = \delta_{ck} \tag{5.6c}$$

$$\sum_j (U_{jc} V_{jk} + V_{jc} U_{jk}^*) = 0 \ . \tag{5.6d}$$

These relations may also be obtained by requiring the particle and quasiparticle operators to satisfy the Fermion commutation rules. Substituting (5.1) into

$$[b_c^\dagger, b_k]_+ = \delta_{ck} \tag{5.7a}$$

$$[b_c^\dagger, b_k^\dagger]_+ = [b_c, b_k]_+ = 0 \tag{5.7b}$$

results in (5.6a,b). Substituting (5.4) into

$$[a_c^\dagger, a_k]_+ = \delta_{ck} \tag{5.8a}$$

$$[a_c^\dagger, a_k^\dagger]_+ = [a_c, a_k]_+ = 0 \tag{5.8b}$$

results in (5.6c,d).

The reference state $|\Phi_0\rangle$ is defined as a quasiparticle vacuum. Therefore

$$b_c |\Phi_0\rangle = 0 \ . \quad (all \ c) \tag{5.9}$$

Since $[b_i, b_i]_+$ vanishes, $b_i b_i = 0.$ Therefore a solution to (5.9) is

$$|\Phi_0\rangle = C \prod_c b_c |0\rangle \tag{5.10}$$

where C is a constant of normalization.

3. The Hamiltonian

The Hamiltonian is

$$H' = H - \lambda N \tag{5.11}$$

$$= \sum_{ij} \langle i | T - \lambda | j \rangle a_i^\dagger a_j + \frac{1}{4} \sum_{ijk\ell} \langle ij | \mathcal{N} | k\ell \rangle_A \, a_i^\dagger a_j^\dagger a_\ell a_k$$

where

$$N = \sum_i a_i^\dagger a_i \tag{5.12a}$$

$$\lambda = \lambda_p P_p + \lambda_n P_n \tag{5.12b}$$

$$P_\tau = | \tau \rangle \langle \tau |. \tag{5.12c}$$

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

$$N_\tau = \sum_k^\prime a_{k\tau}^\dagger a_{k\tau} \tag{5.13b}$$

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

$$H_0' = \sum_{ij} (T - \lambda + \tfrac{1}{2} \Gamma)_{ij} \rho_{ji} + \frac{1}{2} \sum_{ij} \Delta_{ij} t_{ji}^\dagger \tag{5.15}$$

$$H_2' = \sum_{ij} (\mathcal{H} - \lambda)_{ij} N[a_i^\dagger a_j] + \frac{1}{2} \sum_{ij} \Delta_{ij} N[a_i^\dagger a_j^\dagger] \tag{5.16}$$

$$+ \frac{1}{2} \sum_{ij} \Delta_{ij}^\dagger N[a_i a_j]$$

$$H_4' = \frac{1}{4} \sum_{ijk\ell} \langle ij | \mathcal{N} | k\ell \rangle_A N[a_i^\dagger a_j^\dagger a_\ell a_k]. \tag{5.17}$$

ρ is the density matrix.

$$\rho_{ji} = \langle a^{\dagger}_{i} a_{j} \rangle \qquad (5.18)$$

$$\rho^{\dagger} = \rho \qquad (5.19)$$

t is the pairing tensor.

$$t_{ji} = \langle a_{i} a_{j} \rangle \qquad (5.20)$$

$$t^{*}_{ji} = \langle a^{\dagger}_{j} a^{\dagger}_{i} \rangle \qquad (5.21)$$

$$\tilde{t} = -t \qquad (5.22)$$

Γ is the HF potential.

$$\Gamma_{ij} = \sum_{k\ell} \langle ik | \mathcal{N} | j\ell \rangle_{A} \, \rho_{\ell k} \qquad (5.23)$$

$$\Gamma^{\dagger} = \Gamma \qquad (5.24)$$

$\mathcal{H}$ is the HF Hamiltonian.

$$\mathcal{H}_{ij} = T_{ij} + \Gamma_{ij} \qquad (5.25)$$

$$\mathcal{H}^{\dagger} = \mathcal{H} \qquad (5.26)$$

Δ is the pair potential.

$$\Delta_{ij} = \frac{1}{2} \sum_{k\ell} \langle ij | \mathcal{N} | k\ell \rangle_{A} \, t_{k\ell} \qquad (5.27)$$

$$\Delta^{*}_{ij} = \frac{1}{2} \sum_{k\ell} \langle k\ell | \mathcal{N} | ij \rangle_{A} \, t^{*}_{k\ell} \qquad (5.28)$$

$$\tilde{\Delta} = -\Delta \qquad (5.29)$$

The expectation values and normal orderings are with respect to a reference state, which is chosen to be the quasiparticle vacuum. It follows that

$$\langle b^\dagger_k b^\dagger_\ell \rangle = \langle b_k b_\ell \rangle = \langle b^\dagger_k b_\ell \rangle = 0 \qquad (5.30)$$

$$\langle b_k b^\dagger_\ell \rangle = \delta_{k\ell} \qquad (5.31)$$

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).

$$\rho_{ji} = \sum_k V_{ki} V^*_{kj} \qquad (5.32a)$$

or $$\rho = V^\dagger V . \qquad (5.32b)$$

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

$$t_{ji} = \sum_k U_{ki} V^*_{kj} \qquad (5.33a)$$

or $$t = V^\dagger U . \qquad (5.33b)$$

4. Hartree - Fock - Bogoliubov Equations

The Hamiltonian will acquire the desired form of an independent quasiparticle Hamiltonian if H_4' (the quasiparticle interactions) may be neglected and if

$$H_2' = \sum_k E_k b_k^\dagger b_k .$$

(5.34)

The problem therefore is to choose U and V so that (5.34) is satisfied. The commutator $\left[H_2', b_k^\dagger \right]_-$ may be evaluated with (5.34)

$$\left[H_2', b_k^\dagger \right]_- = E_k b_k^\dagger$$

(5.35)

or $\quad \left[H_2', b_k^\dagger \right]_- = E_k \sum_i \left(U_{ki} a_i^\dagger + V_{ki} a_i \right).$ (5.36)

Alternatively, (5.16) may be used.

$$\left[H_2', b_k^\dagger \right]_- = \sum_{ij} \left\{ (\mathcal{H} - \lambda)_{ij} U_{kj} + \Delta_{ij} V_{kj} \right\} a_i^\dagger$$
$$+ \sum_{ij} \left\{ \Delta_{ij}^\dagger U_{kj} + (\lambda - \tilde{\mathcal{H}})_{ij} V_{kj} \right\} a_i$$

(5.37)

Equate the coefficients of $a_i^\dagger$ and a_i in (5.36) and (5.37).

$$\sum_j \left\{ (\mathcal{H} - \lambda)_{ij} U_{kj} + \Delta_{ij} V_{kj} \right\} = E_k U_{ki}$$

(5.38a)

$$\sum_j \left\{ \Delta_{ij}^\dagger U_{kj} + (\lambda - \tilde{\mathcal{H}})_{ij} V_{kj} \right\} = E_k V_{ki}$$

(5.38b)

Let

$$\underline{U}_k = \begin{bmatrix} U_{k1} \\ U_{k2} \\ \vdots \\ U_{kN} \end{bmatrix} \qquad \underline{V}_k = \begin{bmatrix} V_{k1} \\ V_{k2} \\ \vdots \\ V_{kN} \end{bmatrix}$$

(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.

$$\mathcal{K}^\dagger = \mathcal{K} \qquad E_K = Real \tag{5.45}$$

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 ($\Delta = 0$), 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 $\begin{bmatrix} (\lambda - \tilde{\mathcal{H}}) & \Delta^t \\ \Delta & (\mathcal{H} - \lambda) \end{bmatrix}$.

Since $\mathcal{H}$ is Hermitian and Δ is antisymmetric

$$A \mathcal{K} A = -\mathcal{K}^* . \tag{5.47}$$

Complex conjugate (5.44).

$$\mathcal{K}^* \underline{X}_k^* = E_k \underline{X}_k^*$$

Substitute (5.47).

$$-A \mathcal{K} A \underline{X}_k^* = E_k \underline{X}_k^*$$

Since

$$A^2 = 1 \qquad (5.48)$$

multiplying through by A gives

$$\mathcal{K} A \underline{X}_k^* = -E_k A \underline{X}_k^* . \qquad (5.49)$$

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

$$[H_2', b_K]_- = -E_k b_k . \qquad (5.50)$$

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 $\qquad (5.51)$

$$\mathcal{L} = H_0' - \sum_k' E_k \left\{ \sum_j' (U_{kj}^* U_{kj} + V_{kj}^* V_{kj}) - 1 \right\}$$

and

$$H_0' = \sum_{ijm} (T - \lambda)_{ij} \, V_{mi} V_{mj}^* \, +$$

$$\frac{1}{2} \sum_{ijk\ell mn} N_{ijk\ell} \, V_{mi} V_{mk}^* \, V_{nj} V_{n\ell}^* \, + \tag{5.52}$$

$$\frac{1}{4} \sum_{ijk\ell mn} N_{ijk\ell} \, U_{mj}^* V_{mi} U_{n\ell} V_{nk}^* \, .$$

Unfortunately the resulting energy matrix is

$$\begin{bmatrix} \mathcal{H} & \frac{1}{2} \Delta \\ \frac{1}{2} \Delta^\dagger & 0 \end{bmatrix}$$

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.

$$1 \le i, j, k, \ell, p \le N$$
$$1 \le m, n, r, s, q \le 2N$$
$$\bar{i} = i + N, \text{etc.}$$

Let $\quad \underline{A}^\dagger = \begin{bmatrix} \underline{q}^\dagger \\ \underline{q} \end{bmatrix} \qquad \underline{A} = \begin{bmatrix} \underline{q} \\ \underline{q}^\dagger \end{bmatrix}$. $\qquad$ (5.54)

Then the generalized particle density matrix is

$$R_{mn} = \langle A_n^t A_m \rangle . \tag{5.55}$$

It may be verified that

$$R = \begin{bmatrix} \rho & t \\ t^\dagger & 1-\tilde{\rho} \end{bmatrix} . \tag{5.56}$$

For example $R_{ij} = \langle A_j^t A_i \rangle = \langle a_j, a_i^t \rangle =$
$\langle \delta_{ij} - a_i^t a_j \rangle = (1-\tilde{\rho})_{ij}$. Alternatively one
may define

$$\underline{B}^t = \begin{bmatrix} \underline{b}^t \\ \underline{b} \end{bmatrix} \qquad \underline{B} = \begin{bmatrix} \underline{b} \\ \underline{b}^t \end{bmatrix} . \tag{5.57}$$

The generalized quasiparticle density matrix is

$$G_{mn} = \langle B_n^t B_m \rangle . \tag{5.58}$$

Noting (5.30 - 5.31)

$$G = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} . \tag{5.59}$$

Let $\quad X = \begin{bmatrix} U & V \\ V^* & U^* \end{bmatrix} . \tag{5.60}$

Then the quasiparticle transformation (5.2) is

$$\underline{B}^t = X \underline{A}^t \qquad B_m^t = \sum_n X_{mn} A_n^t \tag{5.61}$$

and the inverse transformation is

$$\underline{A}^t = X^t \underline{B}^t \qquad A_n^t = \sum_m X_{mn}^* B_m^t . \tag{5.62}$$

Then R is easily evaluated.

$$\langle A_n^\dagger A_m \rangle = \sum_{rs} X_{sn}^* X_{rm} \langle B_s^\dagger B_r \rangle$$

Substitute G.

$$R_{mn} = \sum_{k} X_{\bar{k}n}^* X_{\bar{k}m} \tag{5.63}$$

R is symmetrical in U and V.

$$R = \begin{bmatrix} V^\dagger V & V^\dagger U \\ U^\dagger V & U^\dagger U \end{bmatrix} \tag{5.64}$$

This form of R is equivalent to (5.56). For example, $U^\dagger U = 1 - (V^\dagger V)^* = 1 - \rho^* = 1 - \tilde{\rho}$. 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

$$H_o' = Tr\left[(T - \lambda + \tfrac{1}{2}\Gamma)\rho + \tfrac{1}{2}\Delta L^\dagger\right]. \tag{5.65}$$

Define
$$\hat{T} = \begin{bmatrix} T & 0 \\ 0 & -\tilde{T} \end{bmatrix} \quad \hat{\lambda} = \begin{bmatrix} \lambda & 0 \\ 0 & -\lambda \end{bmatrix}. \tag{5.66}$$

Since H_o' is real; T, H, ρ are Hermitian; Δ, 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 $\hat{\Gamma}$

$$\hat{\Gamma}_{mn} = \sum_{rs} \hat{\mathcal{N}}_{mr,ns} R_{sr} \tag{5.67}$$

where $\hat{v}$ remains to be defined. Choose

$$\hat{N}_{ijk\ell} = \tfrac{1}{2} N_{ijk\ell} \qquad \hat{N}_{\bar{i}\bar{j}\bar{k}\bar{\ell}} = \tfrac{1}{2} N_{k\ell ij}$$

$$\hat{N}_{ij k \bar{\ell}} = -\tfrac{1}{2} N_{i\ell k j} \qquad \hat{N}_{\bar{i}\bar{j} k \ell} = -\tfrac{1}{2} N_{k j i \ell}$$

$$\hat{N}_{i\bar{j}\bar{k}\ell} = -\tfrac{1}{2} N_{ik j \ell} \qquad \hat{N}_{\bar{i}j k \bar{\ell}} = -\tfrac{1}{2} N_{j\ell i k} \qquad (5.68)$$

all other components of $\hat{v}$ being zero.[3] Then

$$\hat{\Gamma} = \begin{bmatrix} (\Gamma - \tfrac{1}{2} V) & \Delta \\ \Delta^\dagger & -(\tilde{\Gamma} - \tfrac{1}{2} \tilde{V}) \end{bmatrix} \qquad (5.69)$$

where $\qquad V_{ij} = \sum_{k} N_{ik jk}$. $\qquad\qquad (5.70)$

Let $\qquad \hat{V} = \begin{bmatrix} V & 0 \\ 0 & -\tilde{V} \end{bmatrix} \qquad\qquad (5.71)$

and $\qquad \hat{\mathcal{J}} = \hat{T} - \hat{\lambda} + \tfrac{1}{2} \hat{V} \qquad\qquad (5.72)$

then $\qquad \mathcal{K} = \hat{\mathcal{J}} + \hat{\Gamma}$. $\qquad\qquad (5.73)$

Substitute into $H_o{}'$.

$$H_o{}' = \tfrac{1}{4} Tr\left[(2\hat{\mathcal{J}} + \hat{\Gamma} - \tfrac{1}{2}\hat{V})R + 2(T-\lambda) + \Gamma \right]$$

Fortunately $Tr\left[-\tfrac{1}{2}\hat{V} R + \Gamma \right] = Tr\left[\tfrac{1}{2} V \right]$,

so that all dependence on ρ, L is eliminated.

$$H_o{}' = \tfrac{1}{2} Tr\left[(\hat{\mathcal{J}} + \tfrac{1}{2}\hat{\Gamma})R + \tfrac{1}{4} V + (T-\lambda) \right] \qquad (5.74a)$$

or $\qquad H_o{}' = \tfrac{1}{2} \sum_{mn} \hat{\mathcal{J}}_{mn} R_{nm} + \tfrac{1}{4} \sum_{mnrs} \hat{N}_{mnrs} R_{sn} R_{rm}$

$$+ \tfrac{1}{8} \sum_{k\ell} N_{k\ell k\ell} + \tfrac{1}{2} \sum_{k} (T-\lambda)_{kk} \qquad (5.74b)$$

This expression is similar in form to that obtained in

HF theory.

$$H_0 = \sum_{ij}' T_{ij} \, \rho_{ji} + \frac{1}{2} \sum_{ijkl}' N_{ijkl} \, \rho_{lj} \, \rho_{ki}$$

The variational principle is

$$\frac{\partial \mathcal{L}}{\partial X_{\bar{p}q}^*} = 0 \tag{5.75}$$

where

$$\mathcal{L} = H_0' - \sum_m' \mathcal{E}_m \left(\sum_n' X_{mn}^* X_{mn} - 1 \right) \tag{5.76}$$

and

$$H_0' = \frac{1}{2} \sum_{Kmn} \hat{T}_{mn} X_{\bar{K}m}^* X_{\bar{K}n} + \frac{1}{4} \sum_{Kemnrs} \hat{N}_{mnrs} X_{\bar{K}n}^* X_{\bar{K}s} X_{\bar{\rho}m}^* X_{\bar{\rho}r}$$

$$+ \frac{1}{8} \sum_{ke} N_{kekl} + \frac{1}{2} \sum_{K}' (T - \lambda)_{KK} \, . \tag{5.77}$$

Performing the variation we find

$$\sum_n' K_{qn} X_{\bar{p}n} = E_{\bar{p}} X_{\bar{p}q} \tag{5.78a}$$

or

$$K \, \underline{X}_{\bar{p}} = E_{\bar{p}} \, \underline{X}_{\bar{p}} \tag{5.78b}$$

where

$$E_{\bar{p}} = 2 \, \mathcal{E}_{\bar{p}} \, . \tag{5.79}$$

By the argument following (5.46) we find

$$K \, \underline{X}_p = E_p \, \underline{X}_p \tag{5.80}$$

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 $\qquad R = (X^*)^\dagger G (X^*)$. $\hspace{3cm}$ (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

$$R^2 = R \hspace{3cm} (5.83)$$

and $\qquad Tr \, R = N$. $\hspace{3cm}$ (5.84)

Inspection of (5.56) shows that (5.84) is automatically satisfied. (5.83) implies

$$\rho - \rho^2 = C C^\dagger \hspace{3cm} (5.85)$$

$$\rho C = C \tilde{\rho} \ . \hspace{3cm} (5.86)$$

For zero pairing (5.85) reduces to the HF relation $\rho^2 = \rho$.

If ρ and C are given, one may ask whether it is possible to determine the co-ordinates of the quasiparticle transformation. The adjoint of (5.9) is

$$< \Phi_0 | \, b_k^\dagger = 0 \ . \hspace{3cm} (5.87)$$

Consequently

$$< b_k^\dagger \, a_j > = < b_k^\dagger \, a_j^\dagger > = 0 \ .$$

Substituting (5.1a)

$$\sum_i (U_{ki} < a_i^\dagger \, a_j > + V_{ki} < a_i \, a_j >) = 0$$

$$\sum_i (U_{ki} < a_i^\dagger \, a_j^\dagger > + V_{ki} < a_i \, a_j^\dagger >) = 0$$

we find

$$\sum_i \left(\rho_{ji} U_{ki} + \mathcal{L}_{ji} V_{ki} \right) = 0$$

$$\sum_i \left(\mathcal{L}^\dagger_{ji} U_{ki} + (1-\tilde{\rho})_{ji} V_{ki} \right) = 0 .$$

The matrix equation is

$$R \, \underline{X}_k = 0 . \qquad\qquad (5.88)$$

$\underline{X}_k$ 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)

$$ARA = A(X^*)^\dagger A A G A A (X^*) A .$$

It may be verified that

$$A X^* A = X \qquad A(X^*)^\dagger A = X^\dagger \qquad AGA = 1 - G .$$

Consequently $\qquad ARA = X^\dagger (1-G) X .$

Since $X^\dagger X = 1$

$$ARA = 1 - R^* . \qquad\qquad (5.89)$$

Complex conjugate (5.88).

$$R^* \underline{X}_k^* = 0$$

Substitute (5.89).

$$ARA \, \underline{X}_k^* = \underline{X}_k^*$$

Since $A^2 = 1$

$$R A \underline{X}_k^* = A \underline{X}_k^* . \qquad (5.90)$$

$A\underline{X}_k^*$ are the eigenvectors of R corresponding to eigen-
values of 1. Recall that $A\underline{X}_k^*$ are also the eigenvectors
of $\mathcal{H}$ 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.

$$b_k \mid \Phi_o \rangle = 0$$

If
$$b_k' = \sum_\ell \mathcal{U}_{k\ell} \, b_\ell$$

where $\mathcal{U}$ is an arbitrary unitary transformation, then

$$b_k' \mid \Phi_o \rangle = 0 .$$

This is reminiscent of our conclusion in III.6 that
a rotation in particle space followed by a special quasi-
particle 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 $H_2^{\bullet}$ 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.

$$b_\alpha = \begin{cases} a_\alpha & e_\alpha = 0 \\ a_\alpha^\dagger & e_\alpha = 1 \end{cases}$$

The reference state is defined by

$$b_\alpha \, | \Phi_o \rangle = 0 \, .$$

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. $H_2^{\bullet}$ (5.16) may be written as

$$H_2' = \tfrac{1}{2} \sum_{mn} \mathcal{K}_{mn} \, N[A_m^\dagger A_n] \, . \tag{5.91}$$

Substitute the inverse transformation (5.62).

$$H_2' = \tfrac{1}{2} \sum_{mnrs} \mathcal{K}_{mn} \, X_{rm}^* \, X_{sn} \, N[B_r^\dagger B_s]$$

or

$$H_2' = \tfrac{1}{2} \sum_{rs} \left[(X^*) \mathcal{K} (X^*)^\dagger \right]_{rs} N[B_r^\dagger B_s] \tag{5.92}$$

H_2' acquires the desired form if X is chosen so that $(X^*) \, \mathcal{K} \, (X^*)^+$ is diagonal. It is therefore required that

$$(X^*) \, \mathcal{K} \, (X^*)^\dagger = E \qquad (5.93)$$

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

$$H_2' = \frac{1}{2} \sum_r E_r \, N[\, B_r^\dagger \, B_r \,].$$

Since $E_{\overline{k}} = -E_k$

and $-N[\, b_k b_k^\dagger \,] = N[\, b_k^\dagger b_k \,] = b_k^\dagger b_k$

we arrive at

$$H_2' = \sum_k E_k \, b_k^\dagger b_k \,.$$

5. Symmetries of the HFB Solutions

If S is a symmetry of the Hamiltonian H, then

$$[H, S]_- = 0, \qquad (5.94)$$

We have partitioned H as

$$H = H_0 + H_2 + H_4.$$

It may not be true that

$$[H_2, S]_- = 0 \qquad (5.95a)$$

or equivalently

$$[K, S]_- = 0. \qquad (5.95b)$$

If S commutes with H (5.94) and leaves the reference state invariant

$$S|\Phi_0\rangle = |\Phi_0\rangle \qquad (5.96a)$$

or $\qquad [R, S]_- = 0 \qquad (5.96b)$

then S commutes with K (5.95), and S is termed a "self-consistent symmetry." If a self-consistent symmetry is introduced into R, then 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

$$P\left\{\begin{matrix} a_K^\dagger \\ a_K \end{matrix}\right\} P^{-1} = \pm \left\{\begin{matrix} a_K^\dagger \\ a_K \end{matrix}\right\} \tag{5.98a}$$

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 $\quad P|0\rangle = |0\rangle \tag{5.98c}$

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.

$$\rho = \begin{bmatrix} \rho_{++} & 0 \\ 0 & \rho_{--} \end{bmatrix} \qquad \mathcal{L} = \begin{bmatrix} \mathcal{L}_{++} & 0 \\ 0 & \mathcal{L}_{--} \end{bmatrix} \tag{5.100a}$$

Since the two nucleon interaction conserves the parity of

the two particle state, $\mathcal{H}$ and Δ have the same structure.

$$\mathcal{H} = \begin{bmatrix} \mathcal{H}_{++} & 0 \\ 0 & \mathcal{H}_{--} \end{bmatrix} \qquad \Delta = \begin{bmatrix} \Delta_{++} & 0 \\ 0 & \Delta_{--} \end{bmatrix} \qquad (5.100b)$$

The energy matrix has the form

$$\mathcal{K} = \begin{bmatrix} \mathcal{H}_{++} - \lambda & 0 & \Delta_{++} & 0 \\ 0 & \mathcal{H}_{--} - \lambda & 0 & \Delta_{--} \\ \Delta_{++}^{\dagger} & 0 & \lambda - \tilde{\mathcal{H}}_{++} & 0 \\ 0 & \Delta_{--}^{\dagger} & 0 & \lambda - \tilde{\mathcal{H}}_{--} \end{bmatrix} . \qquad (5.100c)$$

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

$$\mathcal{J}\,|N\ell J m T\rangle \equiv |\overline{N\ell J m T}\rangle = (-1)^{J-m+\ell}\,|N\ell J-m\,T\rangle . \qquad (5.101)$$

(We choose $\langle \Gamma|\ell m_\ell\rangle = Y_{\ell m_\ell}$. 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 $m - \tfrac{1}{2}$ = even integer, the second containing states with $m - \tfrac{1}{2}$ = odd integer. Denote the sets respectively by $\{|K\rangle\}$ and $\{|\bar{K}\rangle\}$. More specifically $\{|K\rangle\}$ is composed of states with

$$m = \cdots -7/2, -3/2, \; 1/2, \; 5/2, \cdots \qquad\qquad |K\rangle \qquad (5.102a)$$

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

$$1 \leqslant i, j, k, \ell \leqslant N/2$$
$$1 \leqslant m, n, r, s \leqslant N$$
$$\bar{k} = k + N/2, \, etc. \tag{5.102d}$$

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

$$u_{jk} = U_{jk} \qquad\qquad v_{jk} = V_{j\bar{k}} \tag{5.104}$$

$$\bar{u}_{jk} = U_{\bar{j}\bar{k}} \qquad\qquad \bar{v}_{jk} = V_{\bar{j}k} .$$

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.

$$\rho = \begin{bmatrix} \rho & 0 \\ 0 & \bar{\rho} \end{bmatrix} = \begin{bmatrix} \bar{V}^\dagger \bar{V} & 0 \\ 0 & V^\dagger V \end{bmatrix} \tag{5.107}$$

$$t = \begin{bmatrix} 0 & \tau \\ \bar{\tau} & 0 \end{bmatrix} = \begin{bmatrix} 0 & \bar{V}^\dagger \bar{U} \\ V^\dagger U & 0 \end{bmatrix} \tag{5.108}$$

where

$$\rho_{iJ} = \rho_{iJ} \qquad \tau_{iJ} = t_{i\bar{J}}$$

$$\bar{\rho}_{iJ} = \rho_{\bar{i}\bar{J}} \qquad \bar{\tau}_{iJ} = t_{\bar{i}J} . \tag{5.109}$$

Since the two nucleon interaction conserves angular momentum projection ($m_i + m_J = m_K + m_\ell$ for $N_{iJK\ell}$), the HF Hamiltonian and the pair potential follow the partitioning of ρ and t .

$$\mathcal{H} = \begin{bmatrix} \mathcal{H} & 0 \\ 0 & \bar{\mathcal{H}} \end{bmatrix} \qquad \Delta = \begin{bmatrix} 0 & \Delta \\ \bar{\Delta} & 0 \end{bmatrix} \tag{5.110}$$

where
$$\mathcal{H}_{ij} = \mathcal{H}_{ij} \qquad \Delta_{ij} = \Delta_{ij} \tag{5.111}$$

$$\bar{\mathcal{H}}_{ij} = \mathcal{H}_{\bar{i}\bar{j}} \qquad \bar{\Delta}_{ij} = \Delta_{\bar{i}j} .$$

The elements of the HF Hamiltonian (5.23, 5.25) are

$$\mathcal{H}_{ij} = T_{ij} + \sum_{k\ell}' \left\{ \langle ik | \mathcal{N} | j\ell \rangle_A \rho_{\ell k} + \langle i\bar{k} | \mathcal{N} | j\bar{\ell} \rangle_A \bar{\rho}_{\ell k} \right\} \tag{5.112}$$

$$\bar{\mathcal{H}}_{ij} = T_{ij} + \sum_{k\ell}' \left\{ \langle ik | \mathcal{N} | j\ell \rangle_A \bar{\rho}_{\ell k} + \langle i\bar{k} | \mathcal{N} | j\bar{\ell} \rangle_A \rho_{\ell k} \right\}$$

where we have used $T_{\bar{i}\bar{j}} = T_{ij}$ and $\langle \bar{i}\bar{j} | \mathcal{N} | \bar{k}\bar{\ell} \rangle_A = \langle ij | \mathcal{N} | k\ell \rangle_A$. The expression for the pair potential (5.27) simplifies.

$$\Delta_{mn} = \tfrac{1}{2} \sum_{k\ell}' \langle mn | \mathcal{N} | k\bar{\ell} \rangle_A \, t_{k\bar{\ell}} + \tfrac{1}{2} \sum_{k\ell}' \langle mn | \mathcal{N} | \bar{k}\ell \rangle_A \, t_{\bar{k}\ell}$$

Since t is anti-symmetric and $\langle mn | \mathcal{N} | \bar{k}\ell \rangle_A = -\langle mn | \mathcal{N} | \ell\bar{k} \rangle_A$, the second sum equals the first sum.

$$\Delta_{mn} = \sum_{k\ell}' \langle mn | \mathcal{N} | k\bar{\ell} \rangle_A \, t_{k\bar{\ell}} \tag{5.113}$$

The non-vanishing components of Δ are $\Delta_{i\bar{j}}$ and $\Delta_{\bar{i}j}$.

$$\Delta_{i\bar{j}} = \sum_{k\ell}' \langle i\bar{j} | \mathcal{N} | k\bar{\ell} \rangle_A \, t_{k\ell}$$

$$\bar{\Delta}_{ij} = \sum_{k\ell}' \langle i\bar{j} | \mathcal{N} | k\bar{\ell} \rangle_A \, \tilde{t}_{k\ell} \tag{5.114}$$

The $\mathcal{K}$ matrix (5.42) has the form

$$\begin{bmatrix} \mathcal{H}-\lambda & 0 & 0 & \Delta \\ 0 & \bar{\mathcal{H}}-\lambda & \bar{\Delta} & 0 \\ 0 & \bar{\Delta}^\dagger & \lambda-\tilde{\mathcal{H}} & 0 \\ \Delta^\dagger & 0 & 0 & \lambda-\tilde{\bar{\mathcal{H}}} \end{bmatrix} \tag{5.115}$$

so that the HFB equations (5.41) decouple into two sets.

$$\begin{bmatrix} H-\lambda & \Delta \\ \Delta^\dagger & \lambda-\tilde{\bar{H}} \end{bmatrix} \begin{bmatrix} \underline{u}_K \\ \underline{v}_K \end{bmatrix} = E_K \begin{bmatrix} \underline{u}_K \\ \underline{v}_K \end{bmatrix}$$

$$\begin{bmatrix} \bar{H}-\lambda & \bar{\Delta} \\ \bar{\Delta}^\dagger & \lambda-\tilde{H} \end{bmatrix} \begin{bmatrix} \bar{u}_K \\ \bar{v}_K \end{bmatrix} = E_{\bar{K}} \begin{bmatrix} \bar{u}_K \\ \bar{v}_K \end{bmatrix} \qquad (5.116)$$

Consequently the new set of quasiparticle co-ordinates has the form of (5.103). Therefore, choosing the quasi-particle transformation to be a linear combination of the set $\{a^\dagger_K\}$ 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_0' and H_2' which are valid whenever $C_{ij} = C_{\bar{i}\bar{j}} = \Delta_{ij} = \Delta_{\bar{i}\bar{j}} = 0$ (see equations 3.35 - 3.40).

We now restrict our attention to systems with time-reversal degeneracy. This is achieved by relating $\bar{\mathcal{U}}$ to $\mathcal{U}$ and $\bar{\mathcal{V}}$ to $\mathcal{V}$. The usual convention is

$$\bar{u} = u \qquad \bar{v} = -v.$$

Instead we determine the phases by

$$b^\dagger_{\bar{j}} = \mathcal{J} b^\dagger_j \mathcal{J}^{-1}. \qquad (5.117a)$$

Since
$$\mathcal{J} \begin{Bmatrix} a^\dagger_K \\ a_K \end{Bmatrix} \mathcal{J}^{-1} = + \begin{Bmatrix} a^\dagger_{\bar{K}} \\ a_{\bar{K}} \end{Bmatrix} \qquad (5.117b)$$

$$\mathcal{J} \begin{Bmatrix} a^\dagger_{\bar{K}} \\ a_{\bar{K}} \end{Bmatrix} \mathcal{J}^{-1} = - \begin{Bmatrix} a^\dagger_K \\ a_K \end{Bmatrix}$$

and since $\mathcal{J}$ is anti-linear, we find

$$\mathcal{J} b_J^\dagger \mathcal{J}^{-1} = \sum_K (u_{JK}^* a_{\bar{K}}^\dagger - v_{JK}^* a_K). \qquad (5.117c)$$

Compare to (5.106c). The phases are

$$\bar{u}_{JK} = u_{JK}^* \qquad \bar{v}_{JK} = -v_{JK}^* . \qquad (5.117d)$$

It then follows that

$$\mathcal{J} \left\{ \begin{array}{c} b_J^\dagger \\ b_J \end{array} \right\} \mathcal{J}^{-1} = + \left\{ \begin{array}{c} b_{\bar{J}}^\dagger \\ b_{\bar{J}} \end{array} \right\} \qquad (5.117e)$$

$$\mathcal{J} \left\{ \begin{array}{c} b_{\bar{J}}^\dagger \\ b_{\bar{J}} \end{array} \right\} \mathcal{J}^{-1} = - \left\{ \begin{array}{c} b_J^\dagger \\ b_J \end{array} \right\} .$$

Therefore

$$\mathcal{J} b_J b_{\bar{J}} \mathcal{J}^{-1} = (\mathcal{J} b_J \mathcal{J}^{-1})(\mathcal{J} b_{\bar{J}} \mathcal{J}^{-1}) = -b_{\bar{J}} b_J = b_J b_{\bar{J}} . \qquad (5.117f)$$

The ground state wave function is

$$|\Phi_0\rangle = \prod_{J>0} b_J b_{\bar{J}} |0\rangle . \qquad (5.117g)$$

Since

$$\mathcal{J} |0\rangle = |0\rangle \qquad (5.117h)$$

we have

$$\mathcal{J} |\Phi_0\rangle = \prod_{J>0} \mathcal{J} b_J b_{\bar{J}} \mathcal{J}^{-1} |0\rangle = \prod_{J>0} b_J b_{\bar{J}} |0\rangle$$

so that $|\Phi_0\rangle$ is invariant under time-reversal.

$$\mathcal{J} |\Phi_0\rangle = |\Phi_0\rangle \qquad (5.117i)$$

Therefore time-reversal is a self-consistent symmetry.

The quasiparticle transformations (5.106) become

$$b_J^+ = \sum_k (U_{JK} \, a_K^+ + V_{JK} \, a_{\bar{K}}) \qquad (5.118a)$$

$$b_{\bar{J}} = \sum_k (U_{JK} \, a_{\bar{K}} - V_{JK} \, a_K^+) \qquad (5.118b)$$

and

$$b_{\bar{J}}^+ = \sum_k (U_{JK}^* \, a_{\bar{K}}^+ - V_{JK}^* \, a_K) \qquad (5.118c)$$

$$b_J = \sum_k (U_{JK}^* \, a_K + V_{JK}^* \, a_{\bar{K}}^+) . \qquad (5.118d)$$

The unitarity conditions (5.5) are

$$U \, U^+ + V \, V^+ = I \qquad (5.119a)$$
$$U \, V^+ - V \, U^+ = O \qquad (5.119b)$$
$$U^+ U + V^+ V = I \qquad (5.119c)$$
$$U^+ V - V^+ U = O . \qquad (5.119d)$$

The density matrix (5.107) is

$$\rho = (V^+ V)^* \qquad \text{or} \qquad \rho_{JL} = \sum_k V_{KL}^* \, V_{KJ} \qquad (5.120)$$

with the time-reversal symmetry

$$\bar{\rho} = \rho^* . \qquad (5.121)$$

Clearly ρ is self-adjoint.

$$\rho^+ = \rho \qquad (5.122)$$

The pairing tensor (5.108) is

$$\tau = -(V^+ U)^* \qquad \text{or} \qquad \tau_{JL} = -\sum_k U_{KL}^* \, V_{KJ} \qquad (5.123)$$

with the time-reversal symmetry

$$\bar{\tau} = -\tau^* . \qquad (5.124)$$

Also, since τ is antisymmetric (see 5.109)

$$\bar{\tau} = -\tilde{\tau} . \qquad (5.125)$$

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

$$H_{ij} = T_{ij} + \sum_{k\ell} \left\{ \langle ik|\nu|j\ell \rangle_A \rho_{\ell k} + \langle i\bar{k}|\nu|j\bar{\ell} \rangle_A \rho_{\ell k}^* \right\} \tag{5.129}$$

with the time-reversal symmetry

$$\bar{H} = H^* . \tag{5.130}$$

Since H is Hermitian

$$H^{\dagger} = H . \tag{5.131}$$

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

$$\begin{bmatrix} H-\lambda & \Delta \\ \Delta & \lambda-H \end{bmatrix} \begin{bmatrix} \underline{u}_k \\ \underline{v}_k \end{bmatrix} = E_k \begin{bmatrix} \underline{u}_k \\ \underline{v}_k \end{bmatrix}. \tag{5.135}$$

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

$$\begin{bmatrix} H^*-\lambda & -\Delta^* \\ -\Delta^* & \lambda-H^* \end{bmatrix} \begin{bmatrix} \bar{u}_k \\ \bar{v}_k \end{bmatrix} = E_{\bar{k}} \begin{bmatrix} \bar{u}_k \\ \bar{v}_k \end{bmatrix}.$$

Rewriting

$$\begin{bmatrix} H^*-\lambda & \Delta^* \\ \Delta^* & \lambda-H^* \end{bmatrix} \begin{bmatrix} \bar{u}_k \\ -\bar{v}_k \end{bmatrix} = E_{\bar{k}} \begin{bmatrix} \bar{u}_k \\ -\bar{v}_k \end{bmatrix}$$

and complex conjugating

$$\begin{bmatrix} H-\lambda & \Delta \\ \Delta & \lambda-H \end{bmatrix} \begin{bmatrix} \bar{u}_k^* \\ -\bar{v}_k^* \end{bmatrix} = E_{\bar{k}} \begin{bmatrix} \bar{u}_k^* \\ -\bar{v}_k^* \end{bmatrix}$$

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

$$R_y(\pi)\,|\,\bar{\Phi}_0\rangle = K\,|\,\bar{\Phi}_0\rangle.$$ (5.136c)

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

$$R_z(\theta)\,|Jm\rangle = e^{-im\theta}\,|Jm\rangle$$ (5.137a)

The particle operators transform as

$$R_z(\theta)\begin{Bmatrix} a^\dagger_{Jm} \\ a_{\overline{Jm}} \end{Bmatrix} R_z^{-1}(\theta) = e^{-im\theta} \begin{Bmatrix} a^\dagger_{Jm} \\ a_{\overline{Jm}} \end{Bmatrix}$$ (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 $(m-\tfrac{1}{2})$ = even integer and the states $\{|\bar{K}\rangle\}$ have $(m-\tfrac{1}{2})$ = odd integer, they transform under $R_Z(\pi)$ as

$$R_z(\pi)\begin{Bmatrix} a^\dagger_K \\ a_{\bar{K}} \end{Bmatrix} R_z^{-1}(\pi) = -i \begin{Bmatrix} a^\dagger_K \\ a_{\bar{K}} \end{Bmatrix}$$

$$R_z(\pi)\begin{Bmatrix} a^\dagger_{\bar{K}} \\ a_K \end{Bmatrix} R_z^{-1}(\pi) = +i \begin{Bmatrix} a^\dagger_{\bar{K}} \\ a_K \end{Bmatrix}.$$ (5.137c)

The quasiparticle operators (5.118) therefore transform as

$$R_z(\pi)\begin{Bmatrix} b^\dagger_J \\ b_{\bar{J}} \end{Bmatrix} R_z^{-1}(\pi) = -i \begin{Bmatrix} b^\dagger_J \\ b_{\bar{J}} \end{Bmatrix}$$

$$R_z(\pi)\begin{Bmatrix} b^\dagger_{\bar{J}} \\ b_J \end{Bmatrix} R_z^{-1}(\pi) = +i \begin{Bmatrix} b^\dagger_{\bar{J}} \\ b_J \end{Bmatrix}.$$ (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 $\quad R_z(\theta)\, |0\rangle = |0\rangle$ \hfill (5.137f)

we have

$$R_z(\pi)\, |\Phi_o\rangle = \prod_{j>0} R_z(\pi)\, b_j\, b_{\bar{j}}\, R_z^{-1}(\pi)|0\rangle = \prod_{j>0} b_j\, b_{\bar{j}}\, |0\rangle$$

so that $|\Phi_o\rangle$ is invariant under $R_z(\pi)$.

$$R_z(\pi)\, |\Phi_o\rangle = |\Phi_o\rangle \tag{5.138}$$

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

$$R_z(\theta) \begin{Bmatrix} b^{\dagger}_j \\ b_{\bar{j}} \end{Bmatrix} R_z^{-1}(\theta) = e^{-im\theta} \begin{Bmatrix} b^{\dagger}_j \\ b_{\bar{j}} \end{Bmatrix} \tag{5.139a}$$

$$R_z(\theta) \begin{Bmatrix} b^{\dagger}_{\bar{j}} \\ b_j \end{Bmatrix} R_z^{-1}(\theta) = e^{+im\theta} \begin{Bmatrix} b^{\dagger}_{\bar{j}} \\ b_j \end{Bmatrix} .$$

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

$$R_z(\theta)\,|\Phi_o\rangle = \prod_{j>0} R_z(\theta)\,b_j\,b_{\bar{j}}\,R_z^{-1}(\theta)\,|0\rangle = \prod_{j>0} b_j\,b_{\bar{j}}\,|0\rangle$$

so that $|\Phi_o\rangle$ is invariant under $R_z(\theta)$.

$$R_z(\theta)\,|\Phi_o\rangle = |\Phi_o\rangle \qquad (\text{for all } \theta) \qquad (5.139c)$$

Therefore axial symmetry is a self-consistent symmetry. The components of R and $\mathcal{K}$ have the structure

$$\rho_{ij} = \tau_{ij} = \mathcal{K}_{ij} = \Delta_{ij} = 0 \qquad (5.140)$$

$$\text{unless } m_i = m_j\,.$$

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

$$(M_{\tau_1 \tau_2})_{ij} = M_{i\tau_1,\,j\tau_2} \qquad (5.141)$$

where $M_{\tau_1 \tau_2}$ is a sub-matrix of M. The quasiparticle co-ordinates are

$$\mathcal{U} = \begin{bmatrix} \mathcal{U}_{pp} & \mathcal{U}_{pn} \\ \mathcal{U}_{np} & \mathcal{U}_{nn} \end{bmatrix} \qquad V = \begin{bmatrix} V_{pp} & V_{pn} \\ V_{np} & V_{nn} \end{bmatrix}. \qquad (5.142)$$

The unitarity conditions (5.119) are

$$\sum_{\tau} \left(\mathcal{U}_{c_1 \tau} \, \mathcal{U}^{\dagger}_{c_2 \tau} + V_{c_1 \tau} \, V^{\dagger}_{c_2 \tau} \right) = \delta_{c_1 c_2} \qquad (5.143a)$$

$$\sum_{\tau} \left(\mathcal{U}_{c_1 \tau} \, V^{\dagger}_{c_2 \tau} - V_{c_1 \tau} \, \mathcal{U}^{\dagger}_{c_2 \tau} \right) = 0 \qquad (5.143b)$$

$$\sum_{c} \left(\mathcal{U}^{\dagger}_{c \tau_1} \, \mathcal{U}_{c \tau_2} + V^{\dagger}_{c \tau_1} \, V_{c \tau_2} \right) = \delta_{\tau_1 \tau_2} \qquad (5.143c)$$

$$\sum_{c} \left(\mathcal{U}^{\dagger}_{c \tau_1} \, V_{c \tau_2} - V^{\dagger}_{c \tau_1} \, \mathcal{U}_{c \tau_2} \right) = 0 \; . \qquad (5.143d)$$

The reduced density matrix and pairing tensor are

$$\rho = \begin{bmatrix} \rho_{pp} & \rho_{pn} \\ \rho_{np} & \rho_{nn} \end{bmatrix} \qquad \tau = \begin{bmatrix} \tau_{pp} & \tau_{pn} \\ \tau_{np} & \tau_{nn} \end{bmatrix}. \qquad (5.144)$$

Since ρ and τ are self-adjoint

$$\begin{aligned} \rho^{\dagger}_{pp} &= \rho_{pp} & \tau^{\dagger}_{pp} &= \tau_{pp} \\ \rho^{\dagger}_{pn} &= \rho_{np} & \tau^{\dagger}_{pn} &= \tau_{np} & (5.145) \\ \rho^{\dagger}_{nn} &= \rho_{nn} & \tau^{\dagger}_{nn} &= \tau_{nn} \; . \end{aligned}$$

The density matrix is evaluated with (5.120).

$$\rho_{\tau_1 \tau_2} = \sum_{c} \left(V^{\dagger}_{c \tau_1} \, V_{c \tau_2} \right)^{*} \qquad (5.146)$$

The various components are

$$\begin{aligned} \rho_{pp} &= \left(V^{\dagger}_{pp} \, V_{pp} + V^{\dagger}_{np} \, V_{np} \right)^{*} \\ \rho_{pn} &= \left(V^{\dagger}_{pp} \, V_{pn} + V^{\dagger}_{np} \, V_{nn} \right)^{*} & (5.147) \\ \rho_{np} &= \left(V^{\dagger}_{pn} \, V_{pp} + V^{\dagger}_{nn} \, V_{np} \right)^{*} \\ \rho_{nn} &= \left(V^{\dagger}_{pn} \, V_{pn} + V^{\dagger}_{nn} \, V_{nn} \right)^{*} \; . \end{aligned}$$

Similarly the pairing tensor is given by (5.123)

$$\mathcal{T}_{\tau_1 \tau_2} = - \sum_{c}^{\prime} \left(V^{\dagger}_{c \tau_1} \, \mathcal{U}_{c \tau_2} \right)^{*} \tag{5.148}$$

so that

$$\tilde{\mathcal{T}}_{pp} = - \left(V^{\dagger}_{pp} \, \mathcal{U}_{pp} + V^{\dagger}_{np} \, \mathcal{U}_{np} \right)^{*}$$

$$\mathcal{T}_{pn} = - \left(V^{\dagger}_{pp} \, \mathcal{U}_{pn} + V^{\dagger}_{np} \, \mathcal{U}_{nn} \right)^{*} \tag{5.149}$$

$$\mathcal{T}_{np} = - \left(V^{\dagger}_{pn} \, \mathcal{U}_{pp} + V^{\dagger}_{nn} \, \mathcal{U}_{np} \right)^{*}$$

$$\mathcal{T}_{nn} = - \left(V^{\dagger}_{pn} \, \mathcal{U}_{pn} + V^{\dagger}_{nn} \, \mathcal{U}_{nn} \right)^{*} .$$

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

$$\mathcal{H}^{\dagger}_{pp} = \mathcal{H}_{pp} \qquad\qquad \Delta^{\dagger}_{pp} = \Delta_{pp}$$

$$\mathcal{H}^{\dagger}_{pn} = \mathcal{H}_{np} \qquad\qquad \Delta^{\dagger}_{pn} = \Delta_{np} \tag{5.151}$$

$$\mathcal{H}^{\dagger}_{nn} = \mathcal{H}_{nn} \qquad\qquad \Delta^{\dagger}_{nn} = \Delta_{nn} .$$

The HF Hamiltonian (5.129) has matrix elements

$$\left(\mathcal{H}_{\tau_1 \tau_2} \right)_{ij} = T_{i \tau_1, j \tau_2} + \sum_{\substack{k \ell \\ \tau_3 \tau_1}}^{\prime} \left\{ \langle i \tau_1, k \tau_3 | \nu | j \tau_2, \ell \tau_4 \rangle_A \left(\rho_{\tau_4 \tau_3} \right)_{\ell k} \right.$$

$$\left. + \langle i \tau_1, \bar{k} \tau_3 | \nu | j \tau_2, \bar{\ell} \tau_4 \rangle_A \left(\rho_{\tau_4 \tau_3} \right)^{*}_{\ell k} \right\} . \tag{5.152}$$

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

$$(H_{TT})_{ij} = T_{ij} + \sum_{K\ell T'} \{ \langle iT, KT'|N|jT, \ell T'\rangle_A \, (\rho_{T'T'})_{\ell K}$$

$$+ \langle iT, \bar{K}T'|N|jT, \bar{\ell}T'\rangle_A \, (\rho_{T'T'})^*_{\ell K} \} \tag{5.153}$$

and the off-diagonal -isospin elements are

$$(H_{T-T})_{ij} = \sum_{K\ell} \{ \langle iT, K-T|N|j-T, \ell T\rangle_A \, (\rho_{T-T})_{\ell K}$$

$$+ \langle iT, \bar{K}-T|N|j-T, \bar{\ell}T\rangle_A \, (\rho_{T-T})^*_{\ell K} \} . \tag{5.154}$$

The pair potential (5.114) has elements

$$(\Delta_{T_1 T_2})_{ij} = \sum_{\substack{K\ell \\ T_3 T_4}} \langle iT_1, jT_2|N|KT_3, \bar{\ell}T_4\rangle_A \, (\tau_{T_3 T_4})_{K\ell} . \tag{5.155}$$

The $|T_z| = 1$ pair potential is Δ_{TT} . Only protons (neutrons) may contribute to the proton (neutron) pair potential.

$$(\Delta_{TT})_{ij} = \sum_{K\ell} \langle iT, \bar{j}T|N|KT, \bar{\ell}T\rangle_A \, (\tau_{TT})_{K\ell} \tag{5.156}$$

Since

$$\langle iT, jT|N|KT, \ell T\rangle_A =$$

$$\sum_T \langle \tfrac{1}{2}T \tfrac{1}{2}T|T \, 2T\rangle^2 \, \langle ijT|N|K\ell T\rangle_A =$$

$$\langle ijT=1|N|K\ell T=1\rangle_A \quad for \quad T = \pm \tfrac{1}{2}$$

the $|T_z| = 1$ potential is

$$(\Delta_{TT})_{ij} = \sum_{K\ell} \langle i\bar{j}T=1|N|K\bar{\ell}T=1\rangle_A \, (\tau_{TT})_{K\ell} . \tag{5.157}$$

The $T_z = 0$ pair potential is Δ_{T-T} .

$$(\Delta_{T-T})_{ij} = \sum_{K\ell T'} \langle iT, \bar{j}-T|N|KT', \bar{\ell}-T'\rangle_A \, (\tau_{T'-T'})_{K\ell} \tag{5.158}$$

It may be separated into $T = 0$ and $T = 1$ components. Consider the matrix element

$$\langle iT, j-\tau | \mathcal{N} | k\tau', \ell-\tau' \rangle_A =$$

$$\sum_T \langle \tfrac{1}{2}\tau\,\tfrac{1}{2}-\tau | T\,0 \rangle \langle \tfrac{1}{2}\tau'\,\tfrac{1}{2}-\tau' | T\,0 \rangle \langle ij\,T | \mathcal{N} | k\ell\,T \rangle_A .$$

The product of the Clebsch-Gordon coefficients is evaluated in the table below.

	$T = 0$	$T = 1$
$\tau' = \tau$	$1/2$	$1/2$
$\tau' = -\tau$	$-1/2$	$1/2$

Therefore the $T_Z = 0$ potential is

$$(\Delta_{\tau-\tau})_{ij} = \tfrac{1}{2} \sum_{k\ell} \langle ij\,T=1 | \mathcal{N} | k\ell\,T=1 \rangle_A (\mathcal{C}_{\tau-\tau} + \mathcal{C}_{-\tau\tau})_{k\ell}$$

$$+ \tfrac{1}{2} \sum_{k\ell} \langle ij\,T=0 | \mathcal{N} | k\ell\,T=0 \rangle_A (\mathcal{C}_{\tau-\tau} - \mathcal{C}_{-\tau\tau})_{k\ell} . \tag{5.159}$$

Since $\mathcal{C}_{-\tau\tau} = \mathcal{C}^{\dagger}_{\tau-\tau}$

$$(\Delta_{\tau-\tau})_{ij} = \tfrac{1}{2} \sum_{k\ell} \langle ij\,T=1 | \mathcal{N} | k\ell\,T=1 \rangle_A (\mathcal{C}_{\tau-\tau} + \mathcal{C}^{\dagger}_{\tau-\tau})_{k\ell} \tag{5.160}$$

$$+ \tfrac{1}{2} \sum_{k\ell} \langle ij\,T=0 | \mathcal{N} | k\ell\,T=0 \rangle_A (\mathcal{C}_{\tau-\tau} - \mathcal{C}^{\dagger}_{\tau-\tau})_{k\ell} .$$

The $T = 1$ and $T = 0$ components of the $T_Z = 0$ pair potential are

$$(\Delta^{T=1}_{\tau-\tau})_{ij} = \tfrac{1}{2} \sum_{k\ell} \langle ij\,T=1 | \mathcal{N} | k\ell\,T=1 \rangle_A (\mathcal{C}_{\tau-\tau} + \mathcal{C}^{\dagger}_{\tau-\tau})_{k\ell} \tag{5.161}$$

$$(\Delta^{T=0}_{\tau-\tau})_{ij} = -\tfrac{1}{2}i \sum_{k\ell} \langle ij\,T=0 | \mathcal{N} | k\ell\,T=0 \rangle_A (\mathcal{C}_{\tau-\tau} - \mathcal{C}^{\dagger}_{\tau-\tau})_{k\ell} \tag{5.162}$$

so that

$$\Delta_{\tau - \tau} = \Delta_{\tau - \tau}^{T=1} + \iota \Delta_{\tau - \tau}^{T=0} \quad . \tag{5.163}$$

Since
$$\left\{ \begin{array}{l} (\tau_{\tau - \tau} + \tau_{\tau - \tau}^{\dagger}) \\ -\iota (\tau_{\tau - \tau} - \tau_{\tau - \tau}^{\dagger}) \end{array} \right\} \quad \text{are Hermitian}$$

and
$$\langle \iota \bar{j} \, T | N | \bar{k} \bar{\ell} \, T \rangle_A = \langle j \iota \, T | N | \ell \bar{k} \, T \rangle_A ,$$

the $T = 1$ and $T = 0$ potentials are Hermitian.

$$(\Delta_{\tau - \tau}^{T=1})^{\dagger} = \Delta_{\tau - \tau}^{T=1} \tag{5.164}$$

$$(\Delta_{\tau - \tau}^{T=0})^{\dagger} = \Delta_{\tau - \tau}^{T=0} \tag{5.165}$$

From (5.159) we note that

$$\Delta_{\tau - \tau}^{T=1} = \Delta_{-\tau \tau}^{T=1} \tag{5.166}$$

$$\Delta_{\tau - \tau}^{T=0} = - \Delta_{-\tau \tau}^{T=0} \tag{5.167}$$

which verifies that

$$\Delta_{\tau - \tau}^{\dagger} = \Delta_{-\tau \tau} \quad . \tag{5.168}$$

$\iota \Delta_{\tau - \tau}^{T=0}$ is anti-Hermitian. If the quasiparticle transformation is restricted to real parameters, it follows that

$$(\Delta_{\tau - \tau}^{T=0})_{KK} = 0 \quad . \tag{5.169}$$

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)

$$(\Delta_{\tau-\tau}^{T=1})_{ij} = \frac{1}{2} \sum_{kl} \langle i \bar{j}\, T=1 | \mathcal{N} | k \bar{l}\, T=1 \rangle_A (\tau_{\tau-\tau} + \tilde{\tau}_{\tau-\tau})_{kl}$$

$$(\Delta_{\tau-\tau}^{T=0})_{ij} = -\frac{1}{2} i \sum_{kl} \langle i \bar{j}\, T=0 | \mathcal{N} | k \bar{l}\, T=0 \rangle_A (\tau_{\tau-\tau} - \tilde{\tau}_{\tau-\tau})_{kl} .$$

Since $(\gamma_{\tau-\tau} - \tilde{\zeta}_{\tau-\tau})_{\kappa\ell}$ is antisymmetric

$$\tilde{\Delta}_{\tau-\tau}^{T=0} = - \Delta_{\tau-\tau}^{T=0}$$

so that

$$\left(\Delta_{\tau-\tau}^{T=0}\right)_{KK} = 0$$

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

$$e^{i \underline{J} \cdot \theta} |\Phi_0\rangle = |\Phi_0\rangle .$$

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

$$e^{i \underline{I} \cdot \theta} |\Phi_0\rangle = |\Phi_0\rangle .$$

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 $e^{i \underline{I} \cdot \theta}$.

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 HFS 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 $\quad \tau_{pn} = \tau_{pn}^R + i\,\tau_{pn}^I$. $\tag{5.171}$

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

$$\mathcal{H}_{pp}, \; \Delta_{pp}, \; \Delta_{pn}^{T=1}, \; \Delta_{pn}^{T=0} \qquad \text{are} \tag{5.176}$$

    a) real

    b) symmetric.

Δ_{pn} is also symmetric. The components of $\mathcal{H}$ and Δ are

$$(\mathcal{H}_{pp})_{ij} = T_{ij} + \sum_{k\ell T} \{ \langle ip, k\,T | \mathcal{N} | jp, \ell\,T \rangle_A + \tag{5.177}$$

$$\langle ip, \bar{k}\,T | \mathcal{N} | jp, \bar{\ell}\,T \rangle_A \} (\rho_{pp})_{k\ell}$$

$$(\Delta_{pp})_{ij} = \sum_{k\ell} \langle i\,\bar{j}\,T=1 | \mathcal{N} | k\,\bar{\ell}\,T=1 \rangle_A \; (\zeta_{pp})_{k\ell} \tag{5.178}$$

$$(\Delta_{pn}^{T=1})_{ij} = \sum_{k\ell} \langle i\,\bar{j}\,T=1 | \mathcal{N} | k\,\bar{\ell}\,T=1 \rangle_A \; (\zeta_{pn}^{R})_{k\ell} \tag{5.179}$$

$$(\Delta_{pn}^{T=0})_{ij} = \sum_{k\ell} \langle i\,\bar{j}\,T=0 | \mathcal{N} | k\,\bar{\ell}\,T=0 \rangle_A \; (\zeta_{pn}^{I})_{k\ell} \; . \tag{5.180}$$

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

$$\begin{bmatrix} \mathcal{U}_{pp} \\ \mathcal{U}_{pn} \\ \mathcal{V}_{pp} \\ \mathcal{V}_{pn} \end{bmatrix} = \begin{bmatrix} Real \\ 0 \\ Real \\ Complex \end{bmatrix}$$

(5.183)

are a set of eigenvectors with eigenvalues E_1, then

$$\begin{bmatrix} \mathcal{U}_{np} \\ \mathcal{U}_{nn} \\ \mathcal{V}_{np} \\ \mathcal{V}_{nn} \end{bmatrix} = \begin{bmatrix} \mathcal{U}_{pn} \\ \mathcal{U}_{pp}^* \\ \mathcal{V}_{pn} \\ -\mathcal{V}_{pp} \end{bmatrix}$$

(5.184a)

are a set of eigenvectors with eigenvalues

$$E_2 = E_1 .$$

(5.184b)

This may be seen by writing out the components of the eigenvalue equation $\mathcal{K}\tilde{X} = \tilde{X}E$, 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 $\mathcal{C}$ have the form (5.170).

The symmetries (5.170) have been introduced to ensure that

$$\langle \underline{T} \rangle = 0 .$$

(5.185a)

This constraint is satisfied if

$$\text{Tr} \, \rho_{pn} = \text{Tr} \, \rho_{np} = 0$$

$$\text{Tr} \, \rho_{pp} = \text{Tr} \, \rho_{nn} \quad .$$

(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).

$$\rho^\dagger = \rho \qquad\qquad [\rho, \tau]_- = 0$$

$$\tau^\dagger = \tau \qquad\qquad \tau^2 = \rho(1-\rho)$$

Since ρ and τ are Hermitian and commute they may be diagonalized by the same unitary transformation .

$$\rho \rightarrow u^\dagger \rho u$$

$$\tau \rightarrow u^\dagger \tau u \qquad\qquad (5.186)$$

In the rotated single particle basis ρ and τ are diagonal and real. Since

$$\rho = \begin{bmatrix} \rho & 0 \\ 0 & \rho^* \end{bmatrix} \qquad \tau = \begin{bmatrix} 0 & \tau \\ -\tau^* & 0 \end{bmatrix} \qquad (5.187)$$

the density matrix and pairing tensor in the rotated basis have the form

$$\rho = \begin{bmatrix} \begin{matrix} \rho_{\alpha\alpha} & 0 \\ 0 & \rho_{\alpha\alpha} \end{matrix} & \begin{matrix} & 0 & \end{matrix} \\ 0 & \begin{matrix} \rho_{\beta\beta} & 0 \\ 0 & \rho_{\beta\beta} \end{matrix} \\ & & \ddots \end{bmatrix} \qquad (5.188)$$

$$\tau = \begin{bmatrix} \begin{matrix} 0 & \tau_{\alpha\bar{\alpha}} \\ -\tau_{\alpha\bar{\alpha}} & 0 \end{matrix} & \begin{matrix} & 0 & \end{matrix} \\ 0 & \begin{matrix} 0 & \tau_{\beta\bar{\beta}} \\ -\tau_{\beta\bar{\beta}} & 0 \end{matrix} \\ & & \ddots \end{bmatrix} . \qquad (5.189)$$

The time-reversal symmetries are

$$\rho_{\bar{\alpha}\bar{\alpha}} = \rho_{\alpha\alpha} \qquad \text{(5.190a)}$$

$$L_{\bar{\alpha}\alpha} = -L_{\alpha\bar{\alpha}} \,. \qquad \text{(5.190b)}$$

From the last unitarity condition we have

$$|L_{\alpha\bar{\alpha}}| = \sqrt{\rho_{\alpha\alpha}(1-\rho_{\alpha\alpha})} \,. \qquad \text{(5.191)}$$

ρ is real and diagonal. L is real and has non-vanishing elements only between time-reversed states. This representation of ρ and L is termed the canonical representation, and the single particle states $|\alpha\rangle$, $|\beta\rangle \cdots$ 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 $L_{\alpha\bar{\alpha}}$ may be complex. Since they work with L (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.

$$\rho_{ji} = \langle a^{\dagger}_{i} a_{j} \rangle \qquad \tau_{ji} = \langle a_{\bar{i}} a_{j} \rangle$$

If $a^{\dagger}_{i}$ transforms as

$$a^{\dagger}_{\alpha} = \sum_{k} D^{\alpha}_{k} a^{\dagger}_{k}$$

then a_i transforms as

$$a_\alpha = \sum_k D_k^{\alpha}{}^* a_k$$

and $a^+_i a_j$ transforms as

$$a^+_\alpha a_\beta = \sum_{k\ell} D_k^\alpha a^+_k a_\ell D_\ell^{\beta}{}^* \qquad (5.192a)$$

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

$$a_{\bar{\alpha}} a_\beta = \sum_{k\ell} D_k^\alpha a_{\bar{k}} a_\ell D_\ell^{\beta}{}^* \qquad (5.192b)$$

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 .

$$\mathcal{H}_{\alpha\beta} = \sum_{k\ell} D_k^\alpha \mathcal{H}_{k\ell} D_\ell^{\beta}{}^* \qquad (5.192c)$$

$$\Delta_{\alpha\beta} = \sum_{k\ell} D_k^\alpha \Delta_{k\ell} D_\ell^{\beta}{}^* \qquad (5.192d)$$

The generalized density matrix R (5.56) separates into blocks.

$$R(\alpha) = \begin{bmatrix} \rho_{\alpha\alpha} & 0 & 0 & \tau_{\alpha\bar{\alpha}} \\ 0 & \rho_{\alpha\alpha} & -\tau_{\alpha\bar{\alpha}} & 0 \\ 0 & -\tau_{\alpha\bar{\alpha}} & 1-\rho_{\alpha\alpha} & 0 \\ \tau_{\alpha\bar{\alpha}} & 0 & 0 & 1-\rho_{\alpha\alpha} \end{bmatrix} \qquad (5.193)$$

The quasiparticle co-ordinates are eigenvectors of R with eigenvalues of 0 (5.88).

$$\begin{bmatrix} \rho_{\alpha\alpha} & t_{\alpha\bar{\alpha}} \\ t_{\alpha\bar{\alpha}} & 1-\rho_{\alpha\alpha} \end{bmatrix} \begin{bmatrix} U_\alpha \\ -N_\alpha \end{bmatrix} = 0 \qquad \begin{bmatrix} \rho_{\alpha\alpha} & -t_{\alpha\bar{\alpha}} \\ -t_{\alpha\bar{\alpha}} & 1-\rho_{\alpha\alpha} \end{bmatrix} \begin{bmatrix} U_{\bar{\alpha}} \\ -N_{\bar{\alpha}} \end{bmatrix} = 0 \qquad (5.194)$$

where $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (5.195)$

$$U_\alpha = U_{\alpha\alpha} \qquad\qquad U_{\bar{\alpha}} = \bar{U}_{\alpha\alpha}$$
$$N_\alpha = -V_{\alpha\alpha} \qquad\qquad N_{\bar{\alpha}} = -\bar{V}_{\alpha\alpha}$$

The co-ordinates may be chosen real with the phase

$$U_{\bar{\alpha}} = U_\alpha = Real \qquad\qquad\qquad\qquad (5.196)$$
$$N_{\bar{\alpha}} = -N_\alpha = Real .$$

The quasiparticle transformations are

$$b_\alpha^\dagger = U_\alpha a_\alpha^\dagger - N_\alpha a_{\bar{\alpha}} \qquad\qquad\qquad (5.197)$$

$$b_{\bar{\alpha}}^\dagger = U_\alpha a_{\bar{\alpha}}^\dagger + N_\alpha a_\alpha .$$

This is simply the special quasiparticle transformation.
We may conclude that the ground state wave function (ρ, t)
may always be given by the special transformation in the
canonical basis. $|\Phi_o\rangle$ may always be given in the form

$$|\Phi_o\rangle = \prod_{\alpha > 0} (U_\alpha + N_\alpha a_\alpha^\dagger a_{\bar{\alpha}}^\dagger) |o\rangle . \qquad\qquad (5.198)$$

The density matrix and pairing tensor are

$$\rho_{\alpha\alpha} = N_\alpha^2 \qquad\qquad t_{\alpha\bar{\alpha}} = U_\alpha N_\alpha . \qquad\qquad (5.199)$$

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
transformations:

$$B_{gen} = U_2 \, B_{sp} \, U_1 \tag{5.200}$$

where

U_1: Rotation in particle space

$$a^\dagger_\alpha = \sum_K D^\alpha_K \, a^\dagger_K \tag{5.201}$$

B_{sp}: Special Bogoliubov quasiparticle transformation

$$b^\dagger_\alpha = U_\alpha \, a^\dagger_\alpha - N_\alpha \, a_{\bar\alpha} \tag{5.202}$$

U_2: Rotation in quasiparticle space

$$b^\dagger_\nu = \sum_\alpha R^\nu_\alpha \, b^\dagger_\alpha \tag{5.203}$$

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

$$D^{\bar\beta}_K = D^\beta_K \tag{5.204}$$

and

$$\mathcal{U}_{\beta K} = U_\beta \, D^\beta_K \qquad V_{\beta K} = - N_\beta \, D^\beta_K \cdot \tag{5.205}$$

The components of (5.135) are

$$\sum_{K_2} (\mathcal{H}'_{K_1 K_2} U_\beta - \Delta_{K_1 K_2} N_\beta) D^\beta_{K_2} = E_\beta U_\beta D^\beta_{K_1} \tag{5.206a}$$

$$\sum_{K_2} (\mathcal{H}'_{K_1 K_2} N_\beta + \Delta_{K_1 K_2} U_\beta) D^\beta_{K_2} = - E_\beta N_\beta D^\beta_{K_1} \tag{5.206b}$$

where $\quad \mathcal{H}' = \mathcal{H} - \lambda \cdot \tag{5.207}$

Multiply (5.206a) by $\quad N_\alpha D^\alpha_{K_1} \quad$ and sum on K_1.

$$\mathcal{H}'_{\alpha\beta} U_\beta N_\alpha - \Delta_{\alpha\beta} N_\alpha N_\beta = E_\beta U_\beta N_\alpha \, \delta_{\alpha\beta}$$

Multiply (5.206b) by $\quad U_\alpha D^\alpha_{K_1} \quad$ and sum on K_1.

$$\mathcal{H}'_{\alpha\beta} U_\alpha N_\beta + \Delta_{\alpha\beta} U_\alpha U_\beta = - E_\beta U_\alpha N_\beta \, \delta_{\alpha\beta}$$

Add the last two equations.

$$\mathcal{H}'_{\alpha\beta} (U_\alpha N_\beta + U_\beta N_\alpha) + \Delta_{\alpha\beta} (U_\alpha U_\beta - N_\alpha N_\beta) = 0 \tag{5.208}$$

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 $N_\beta D^\alpha_{k_1}$ and summing on K_1.

$$H'_{\alpha\beta} N_\beta^2 + \Delta_{\alpha\beta} U_\beta N_\beta = -E_\beta N_\beta^2 \delta_{\alpha\beta}$$

Exchange the indices α and β, recalling that H and Δ are symmetric.

$$H'_{\alpha\beta} N_\alpha^2 + \Delta_{\alpha\beta} U_\alpha N_\alpha = -E_\alpha N_\alpha^2 \delta_{\alpha\beta}$$

By subtracting, we arrive at the HB equations.

$$H'_{\alpha\beta}(N_\alpha^2 - N_\beta^2) + \Delta_{\alpha\beta}(U_\alpha N_\alpha - U_\beta N_\beta) = 0 \qquad (5.209)$$

The relationship between the HFB and HB-BCS formalisms is now transparent. Both provide the ground state wavefunction 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.

$$D = \begin{bmatrix} \mathcal{D} & O \\ O & \mathcal{D} \end{bmatrix} \qquad (5.210a)$$

where $\qquad \mathcal{D}^{\alpha}_{\kappa} = D^{\alpha p}_{\kappa p} = D^{\alpha n}_{\kappa n} .$ $\qquad (5.210b)$

Since ρ_{pp} is real and symmetric

$\qquad \mathcal{D} \qquad$ is real and orthogonal . $\qquad (5.210c)$

The density matrix is

$$\rho^{(\alpha)} = \begin{bmatrix} \rho_{pp}(\alpha) & O \\ O & \rho_{pp}(\alpha) \end{bmatrix} . \qquad (5.211a)$$

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 $\alpha \neq \beta$.)

$$\tau(\alpha) = \begin{bmatrix} \tau_{pp}(\alpha) & \tau_{pn}(\alpha) \\ \tau_{pn}^{*}(\alpha) & -\tau_{pp}(\alpha) \end{bmatrix} \qquad (5.211b)$$

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 $\quad |\alpha\rangle = \sum_K' \mathcal{D}_K^\alpha |K\rangle$.

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 $\quad |\bar{\alpha}\rangle = \sum_K' \mathcal{D}_K^\alpha |\bar{K}\rangle$.

Because $\{|\alpha_c\rangle\}$ form a complete orthonormal set, Δ may be expressed as

$$(\Delta_{T_1 T_2})_{K\ell} = \sum_{\alpha_c > 0}' \langle K T_1, \ell T_2 | \mathcal{N} | \alpha_c \bar{\alpha}_c \rangle_A \, t_{\alpha_c \bar{\alpha}_c} \tag{5.214}$$

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

$$(\Delta_{pn})_{K\ell} = \tfrac{1}{2} \sum_{\alpha_c > 0}' \langle K\ell\, T{=}1 | \mathcal{N} | \alpha\bar{\alpha}\, T{=}1 \rangle_A \left(C_p^\alpha C_n^{\alpha\,*} + C_p^{\alpha\,*} C_n^\alpha \right) t_{\alpha_c \bar{\alpha}_c}$$
$$+ \tfrac{1}{2} \sum_{\alpha_c > 0}' \langle K\ell\, T{=}0 | \mathcal{N} | \alpha\bar{\alpha}\, T{=}0 \rangle_A \left(C_p^\alpha C_n^{\alpha\,*} - C_p^{\alpha\,*} C_n^\alpha \right) t_{\alpha_c \bar{\alpha}_c}. \tag{5.215}$$

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

$$(\Delta_{pn})_{k\ell} = \sum_{\alpha c > 0} \langle K\bar{\ell} \; T=1 | \mathcal{N} | \alpha \bar{\alpha} \; T=1\rangle_A \; C_P^\alpha \; C_n^\alpha \; \mathcal{I}_{\alpha_c \bar{\alpha}_c}$$

and all elements of the $T = 0$ potential vanish. Implicit in these proofs is the fact that $\mathcal{D}_K^\alpha$ is independent of isospin.

If ρ and $\mathcal{I}$ are given by (5.211) then the eigenvectors of R are given by (4.117)

$$\begin{bmatrix} b_{\alpha 1}^\dagger \\ b_{\alpha 2}^\dagger \\ b_{\bar{\alpha}1} \\ b_{\bar{\alpha}2} \end{bmatrix} = \begin{bmatrix} U_{\alpha 11} & 0 & -\mathcal{N}_{\alpha 11} & -\mathcal{N}_{\alpha 12} \\ 0 & U_{\alpha 11} & -\mathcal{N}_{\alpha 12}^* & \mathcal{N}_{\alpha 11} \\ \mathcal{N}_{\alpha 11} & \mathcal{N}_{\alpha 12} & U_{\alpha 11} & 0 \\ \mathcal{N}_{\alpha 12}^* & -\mathcal{N}_{\alpha 11} & 0 & U_{\alpha 11} \end{bmatrix} \begin{bmatrix} a_{\alpha p}^\dagger \\ a_{\alpha n}^\dagger \\ a_{\bar{\alpha}p} \\ a_{\bar{\alpha}n} \end{bmatrix} \qquad (5.216)$$

plus the time-reversed set.

$$U_{\alpha 11}, \; \mathcal{N}_{\alpha 11} = \text{Real} \qquad (5.217)$$

The density matrix and pairing tensor are (see 4.112 - 4.116, 5.147)

$$\rho_{pp}(\alpha) = \mathcal{N}_\alpha^2 \equiv \mathcal{N}_{\alpha 11}^2 + |\mathcal{N}_{\alpha 12}|^2 \qquad (5.218)$$

$$\mathcal{I}_{pp}(\alpha) = U_{\alpha 11} \mathcal{N}_{\alpha 11} \qquad (5.219)$$

$$\mathcal{I}_{pn}(\alpha) = U_{\alpha 11} \mathcal{N}_{\alpha 12}^* . \qquad (5.220)$$

$\mathcal{I}^2(\alpha)$ is diagonal.

$$\mathcal{I}^2(\alpha) = (U_\alpha \mathcal{N}_\alpha)^2 I \qquad (5.221)$$

where $U_\alpha \equiv U_{\alpha 11} .$ $\qquad (5.222)$

U_α is given by

$$|U_\alpha| = \sqrt{\zeta^2(\alpha)/\rho(\alpha)}$$ (5.223a)

or by

$$|U_\alpha| = \sqrt{1 - \rho_{PP}(\alpha)} \; .$$ (5.223b)

We choose $U_\alpha > 0$. (5.224)

Then $\mathcal{N}_{\nu 11}$ and $\mathcal{N}_{\alpha 12}$ 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.

$$b^\dagger_\nu = \sum_\alpha (U_{\nu\alpha} \, a^\dagger_\alpha + V_{\nu\alpha} \, a_{\bar\alpha})$$ (5.225)

Inverting (5.201) and substituting into (5.118) we find

$$b^\dagger_\nu = \sum_{\alpha k} (U_{\nu k} \, D^{\alpha *}_k \, a^\dagger_\alpha + V_{\nu k} \, D^{\alpha *}_k \, a_{\bar\alpha}) \, .$$

Comparing the last two equations we obtain

$$U_{\nu\alpha} = \sum_k U_{\nu k} \, D^{\alpha *}_k \qquad V_{\nu\alpha} = \sum_k V_{\nu k} \, D^{\alpha *}_k \; .$$ (5.226)

Combining (5.202, 5.203), we have a third expression for $b^\dagger_\nu$ in terms of the canonical basis.

$$b^\dagger_\nu = \sum_\alpha (R^\nu_\alpha \, U_\alpha \, a^\dagger_\alpha - R^\nu_\alpha \, \mathcal{N}_\alpha \, a_{\bar\alpha})$$

Comparing with (5.225), the matrix R may be evaluated.

$$R^\nu_\alpha = U_{\nu\alpha} / U_\alpha$$ (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

$$b^{\dagger}_{\nu 1} = \sum_{\alpha 1} R^{\nu 1}_{\alpha 1} \, b^{\dagger}_{\alpha 1} \tag{5.228}$$

$$b^{\dagger}_{\nu 2} = \sum_{\alpha 2} R^{\nu 2}_{\alpha 2} \, b^{\dagger}_{\alpha 2} \, .$$

That is

$$R^{\nu 1}_{\alpha 2} = R^{\nu 2}_{\alpha 1} = 0 . \tag{5.229}$$

Furthermore the two sets transform by the same rotation, so that R has the form

$$R = \begin{bmatrix} \mathcal{R} & 0 \\ 0 & \mathcal{R} \end{bmatrix} \tag{5.230}$$

where

$$\mathcal{R}^{\nu}_{\alpha} = R^{\nu 1}_{\alpha 1} = R^{\nu 2}_{\alpha 2} \, . \tag{5.231}$$

Comparing (5.183) and (5.216) $\mathcal{R}$ may be evaluated.

$$\mathcal{R}^{\nu}_{\alpha} = (\mathcal{U}_{pp})_{\nu\alpha} / \, U_{\alpha} \tag{5.232}$$

Since R is unitary and $\mathcal{U}_{pp}$ and U_{α} are real

$$\mathcal{R} \quad \text{is real and orthogonal} \, . \tag{5.233}$$

To recapitulate, for generalized isospin pairing the general transformation may be expressed as the product of three transformations.

1. Rotation in particle space

$$
\begin{bmatrix} \underline{a}^{\dagger}_{\alpha p} \\ \underline{a}^{\dagger}_{\alpha n} \\ \underline{a}_{\bar{\alpha} p} \\ \underline{a}_{\bar{\alpha} n} \end{bmatrix} = \begin{bmatrix} \mathcal{D} & 0 & 0 & 0 \\ 0 & \mathcal{D} & 0 & 0 \\ 0 & 0 & \mathcal{D} & 0 \\ 0 & 0 & 0 & \mathcal{D} \end{bmatrix} \begin{bmatrix} \underline{a}^{\dagger}_{k p} \\ \underline{a}^{\dagger}_{k n} \\ \underline{a}_{\bar{k} p} \\ \underline{a}_{\bar{k} n} \end{bmatrix}
\tag{5.234}
$$

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

$$
(\mathcal{U}_{11})_{\beta\alpha} = U_{\alpha 11}\, \delta_{\alpha\beta}
$$

$$
(\mathcal{V}_{11})_{\beta\alpha} = N_{\alpha 11}\, \delta_{\alpha\beta}
\tag{5.236}
$$

$$
(\mathcal{V}_{12})_{\beta\alpha} = N_{\alpha 12}\, \delta_{\alpha\beta}
$$

and $U_{\alpha 11}, N_{\alpha 11} = Real$

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 $\mathcal{t}$ 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, $\mathcal{t}$) 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.)

```
8.3 ——————— oblate
6.8 ——————— oblate


3.6 ——————— prolate

                                        1.1 ——————— oblate
                                        0.6 ——————— prolate
 0 ——————— asymmetric                   0 ——————— asymmetric

        HF            Mg²⁴            HFB
_____

9.0 ——————— oblate


5.3 ——————— prolate

                                   3.2 ——————— prolate


 0 ——————— asymmetric          0 ——————— asymmetric

                              -2.0 ——————— oblate

        HF            S³²              HFB
_____
```
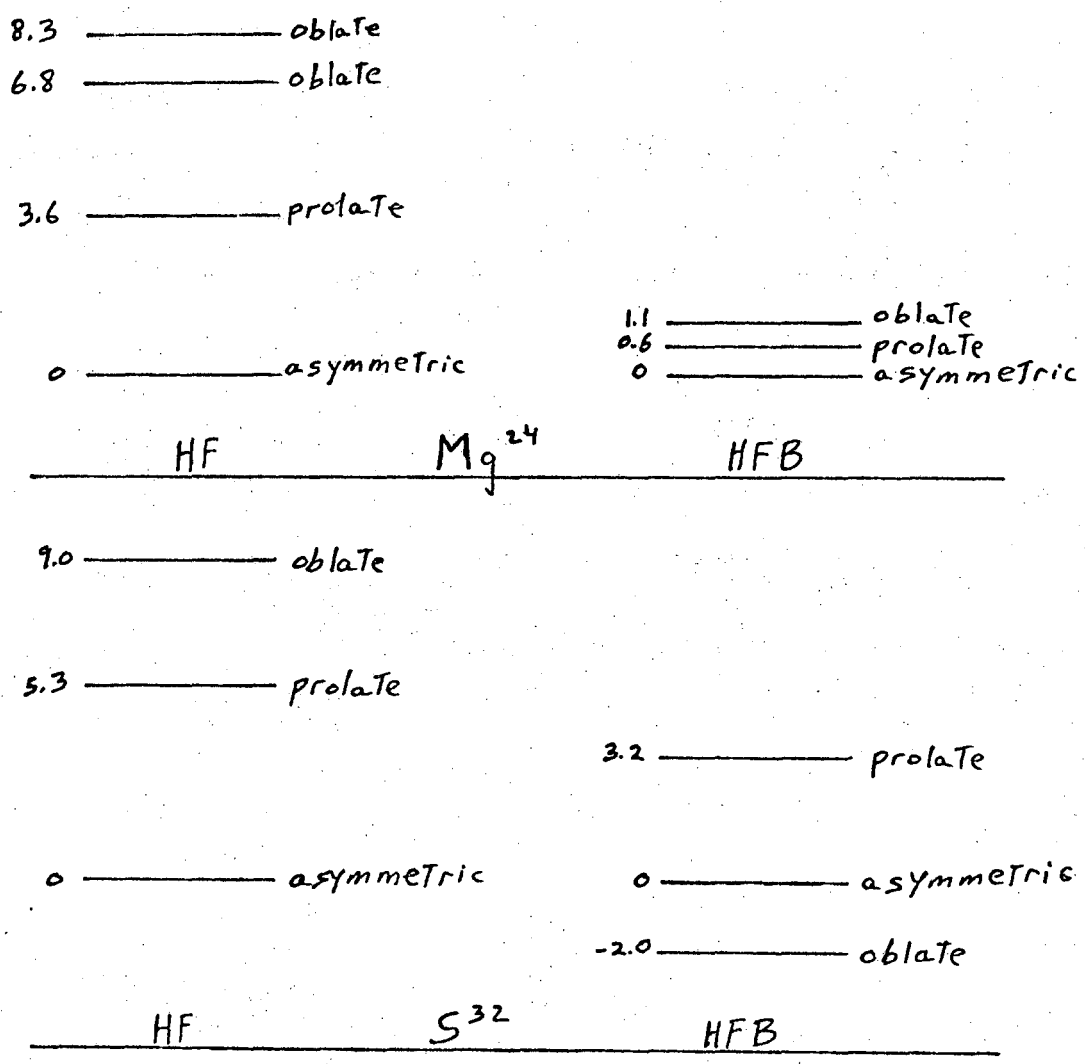
Very often BCS wave – functions based on different HF intrinsic states converge to the same HFB limit. The HFB equations therefore alleviate a major difficulty of the HF theory: having too many intrinsic states from which to choose the physically relevant one. Also discrepancies between the different 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 $\mathcal{N}_\alpha^2$. (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 quasi-particle 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 $\Omega, \pi = \frac{1}{2}, +$ 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 quasi-
particle 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 $|\Phi_b\rangle$ 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 $|\Phi_o\rangle$, 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 $3\frac{1}{2}$ to $8\frac{1}{2}$ 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, 5.13-19.

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. $\mathcal{R}_q^\nu$, a square matrix.

4. $(Im \underline{v}_{\alpha12})^2$, a column vector. In parentheses is given

   the sign of $Im v_{\alpha12}$. Since there is no T = 1 pairing,

   $v_{\alpha11}$ = Re $v_{\alpha12}$ = 0. $u_{\alpha11}$ is real and positive; it is

   given by $u_{\alpha11} = [1- (Im v_{\alpha12})^2]^{1/2}$.

5. $\mathcal{D}_k^\alpha$, a square matrix.

The Fermi energy, λ, is also given. (Mev).

Tables 5.11 - 5.19. HFB T = 0 pair potentials, $\Delta_{pn}^{T=0}$, in canonical

basis $|\alpha\rangle$. $\Delta_{pp} = \Delta_{pn}^{T=1}$ = 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 (O)	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 (O)								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

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 (O2)	T = 0	-2.207	-150.041	-0.5	-96.5		6.13
		Prolate (O3)	T = 0	-6.050	-147.808	0.14	110.5		4.91
	Rosenfeld 2	Prolate (O2)	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 (O2)	T = 0	-14.375	-138.733	3.1	-84.0	0.035	4.74
	NDKB 2	Prolate (O2,S)	T = 0	-8.359	-146.853	24.9	-72.0	0.282	4.71

c

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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 (O1, O3)	T = 0	-1.385	-212.901	-1.5	-95.8		5.89	
	Rosenfeld 2	Oblate (O2,O3)	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-O)	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 (O)	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 (O)	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	

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(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

$$\lambda = -6.582$$

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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.)

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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	.303	.595	-.323
(-).992	.521	.845	.061	.030	.091	.032
(+).998	.846	-.521	.085	.012	-.069	.011

$$\lambda = -6.871$$

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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 ($\Delta_{pn}^{T = 0}$) 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 ($\Delta^{T=0}_{pn}$) 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 $\left(\Delta_{pn}^{T=0} \right)$ 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 ($\Delta^{T = 0}_{pn}$) 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

$$\frac{E_{PAIR} \ (NDKB \ 2) - E_{PAIR} \ (NDKB \ 1)}{E_{PAIR} \ (NDKB \ 1)}$$

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

References to Chapter 5

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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 inter-
preted 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)

ACKNOWLEDGEMENTS