Pairing Correlations in Nuclei

1 The Seniority Scheme

We consider N particles in a single $(2j+1)$-fold degenerate j-shell interacting a monopole pairing force. If we place this j-shell at zero energy, the corresponding Hamiltonian is of the form:

$$H = -G \sum_{mm'>0} a_m^+ a_{\tilde{m}}^+ a_{\tilde{m}'} a_{m'} = -G S_+ S_-, \tag{1}$$

with

$$S_+ = \sum_{m>0} a_m^+ a_{\tilde{m}}^+, \qquad S_- = (S_+)^+ . \tag{2}$$

Here $a_m = a_{jm}, \quad a_{\tilde{m}} = (-)^{j-m} a_{-m}, \;\; \Omega = j + \frac{1}{2}$. For each of the Ω pairs of levels $(m, -m)$ with $m > 0$ we introduce the operators

$$s_+^{(m)} = a_m^\dagger a_{\tilde{m}}^\dagger, \tag{3}$$

$$s_-^{(m)} = a_{\tilde{m}} a_m, \tag{4}$$

$$s_0^{(m)} = \frac{1}{2}\left(a_m^\dagger a_m + a_{\tilde{m}}^\dagger a_{\tilde{m}} - 1\right), \tag{5}$$

The operators $s_\pm = s_x \pm i s_y$ are the raising and the lowering operators of a fictitious angular momentum $\mathbf{s}$, which we will call *quasi-spin*. It has nothing to do with real spin, but group theory greatly facilitates the exact diagonalization of the Hamiltonian.These operators have the commutation relations of the group SU(2)

$$[s_+, s_-] = 2 s_0, \tag{6}$$

$$[s_0, s_+] = s_+, \tag{7}$$

$$[s_0, s_-] = -s_-, \tag{8}$$

Furthermore, we can see from the definition of $s_0^{(m)}$ that it has the eigenvalues $\pm\frac{1}{2}$ depending on whether the pair $(m, -m)$ is full or empty. The vector $\mathbf{s}^{(m)}$, therefore, has a spin of $\frac{1}{2}$ angular momentum for 0 or 2 particles in the j-level. If only one particle is present, all the components of $\mathbf{s}^{(m)}$ are zero, so that $\mathbf{s}^{(m)}$ has spin zero in this subspace.

The total quasi-spin vector $\mathbf{S}$ is defined by

$$\mathbf{S} = \sum_{m>0} \mathbf{s}^{(m)}. \tag{9}$$

or

$$S_+ = \sum_{m>0} s_+^{(m)} = \sum_{m>0} a_m^\dagger a_{\bar{m}}^\dagger = \sqrt{\frac{\Omega}{2}} \left[a^\dagger a^\dagger\right]_{J=0}, \tag{10}$$

$$S_0 = \frac{1}{2}\sum_m a_m^\dagger a_m - \frac{1}{2}\Omega = \frac{1}{2}(\hat{N} - \Omega), \tag{11}$$

In particular we have for the pair

$$C^\dagger = \frac{1}{\sqrt{\Omega}} S_+ \tag{12}$$

$$\left[C, C^\dagger\right] = \frac{1}{\Omega}\left[S_-, S_+\right] = 1 - \frac{\hat{N}}{\Omega}, \tag{13}$$

this means: for $N \ll \Omega$ the operators $C, C^\dagger$ behave like bosons.

The pairing Hamiltonian (1) has the form:The Hamiltonian in the single j-shell with a monopole force has the form

$$\hat{H} = -GS_+S_- = -G\left(\mathbf{S}^2 - S_0^2 + S_0\right). \tag{14}$$

The eigenfunctions can be classified by the quantum numbers of the quasispin S, S_0, or S, N:

$$\hat{H}|S, N\rangle = E|S, N\rangle \tag{15}$$

with (S_0 is determined by the paritcle number N)

$$E(S, N) = -G\left(S(S+1) - \frac{1}{4}(N-\Omega)^2 + \frac{1}{2}(N-\Omega)\right). \tag{16}$$

The maximal value of S is $\frac{1}{2}\Omega$ (Ω small quasispins with $s = \frac{1}{2}$) and the minimal value is

$$S \geq |S_0| = \frac{1}{2}|\Omega - N|. \tag{17}$$

Instead of S we introduce the quantum numer *seniority*

$$S = \frac{1}{2}(\Omega - s), \qquad s = \Omega - 2S \tag{18}$$

The lowest state is given by the maximal S, i.e. by $S = \Omega/2$, i.e. $s = 0$.

Steps in S by 1 correspond to

$$S = \frac{\Omega}{2}, \frac{\Omega}{2} + 1, \frac{\Omega}{2} + 2, \dots \tag{19}$$
$$s = 0, 2, 4, \dots$$

and the corresponding spectrum:

$$E(s, N) = \frac{G\Omega}{2} \left(s - N - \frac{1}{2\Omega}(s(s-2) - N(N-2)) \right) \tag{20}$$

The ground state corresponds to $s = 0$ with the energy

$$E(0, N) = -G\Omega \frac{N}{2} \left(1 - \frac{N-2}{2\Omega} \right) \tag{21}$$

The excitation energies are independent on N:

$$E(s, N) - E(0, N) = G\Omega \frac{s}{2} \left(1 - \frac{s-2}{2\Omega} \right) \tag{22}$$

The wave function of the vacuum state is

$$|-\rangle = |s = 0, N = 0\rangle = |S = \frac{\Omega}{2}, S_0 = -\frac{\Omega}{2}\rangle. \tag{23}$$

The application of S_+ leads to $N = 2$ or $S_0 = -\frac{\Omega}{2}$. This means the exact ground state is

$$|\Psi_0(N)\rangle = |s = 0, N\rangle \propto (S_+)^{N/2}|-\rangle = (\sum_{m>0} a_m^\dagger a_{\tilde{m}}^\dagger)^{N/2}|-\rangle \propto \left(C^\dagger\right)^{N/2}|-\rangle \tag{24}$$

This is a highly correlated state, a condensate of S-pairs, in the limit of $\Omega \gg N$, a boson condensate.

How can we write express this wave function as product state. We can write

$$|\Psi_0\rangle \propto \hat{P}^N \exp(\eta S_+)|-\rangle = \hat{P}^N \sum_n \frac{\eta^n}{n!}(S_+)^n|-\rangle \tag{25}$$

where $\hat{P}^N$ projects onto good particle number N. The "intrinsic function" can be written as a product

$$\exp(\eta S_+)|-\rangle = \exp(\eta \sum_{m>0} a_m^\dagger a_{\tilde{m}}^\dagger)|-\rangle = \prod_{m>0}(1 + \eta a_m^\dagger a_{\tilde{m}}^\dagger)|-\rangle \tag{26}$$

and after normalization as ($\eta = v/u$)

$$|BCS\rangle = \prod_{m>0}(u + va_m^\dagger a_{\tilde{m}}^\dagger)|-\rangle \quad \text{with} \quad u^2 + v^2 = 1, \tag{27}$$
$$\propto \prod_{m>0}(ua_m - va_{\tilde{m}}^\dagger)(ua_{\tilde{m}} + va_m^\dagger)|-\rangle = \prod_m \alpha_m|-\rangle,$$

where we have introduced quasiparticles

$$\alpha_m^\dagger = ua_m^\dagger - va_{\tilde{m}} \tag{28}$$
$$\alpha_{\tilde{m}}^\dagger = ua_{\tilde{m}}^\dagger + va_m \tag{29}$$

with the Fermion communtation relations

$$\left\{\alpha_m, \alpha_{m'}^\dagger\right\} = \delta_{mm'}, \qquad \{\alpha_m, \alpha_{m'}\} = 0 \tag{30}$$

Note: In intrisic BCS-state is a product state, a quasiparticle vacuum

$$\alpha_m|BCS\rangle = \alpha_m \prod_{m'} \alpha_{m'}|-\rangle = 0 \quad \text{for all values of} \quad m \tag{31}$$

Expressed in terms of particles, we see that is a complicated linear combination and it violates particle number

$$|BCS\rangle = \prod_{m>0}(u + va_m^\dagger a_{\tilde{m}}^\dagger)|-\rangle \tag{32}$$
$$\propto \left(1 + \eta \sum_{m>0} a_m^\dagger a_{\tilde{m}}^\dagger + \eta^2 \sum_{mm'>0} a_m^\dagger a_{\tilde{m}}^\dagger a_{m'}^\dagger a_{\tilde{m}'}^\dagger + \ldots \eta^\Omega a_j^\dagger a_{j-1}^\dagger a_{j-2}^\dagger .. a_{-j+1}^\dagger a_{-j}^\dagger\right)|-\rangle \tag{33}$$

However after symmetry restauration, we obtain the exact ground state

$$|\Psi_0\rangle \propto \hat{P}^N|BCS\rangle \tag{34}$$

So far, the parameter η (i.e. the BCS-occupation numbers u,v) are free. Since the BCS-state violates particle number, we try to optimize is by the requirement, that the average particle number has the proper value:

$$\langle BCS|\hat{N}|BCS\rangle = 2\sum_{m>0} v^2 = N \tag{35}$$

How did we get this relation? We work in the quasiparticle space and transform the operator. First we invert the relations

$$a_m^\dagger = u\alpha_m^\dagger + v\alpha_{\tilde{m}} \tag{36}$$

$$a_{\tilde{m}}^\dagger = u\alpha_{\tilde{m}}^\dagger - v\alpha_m \tag{37}$$

and obtain:

$$\langle BCS|\hat{N}|BCS\rangle = \langle BCS|\sum_{m>0} a_m^\dagger a_m + a_{\tilde{m}}^\dagger a_{\tilde{m}}|BCS\rangle \tag{38}$$

$$= \langle BCS|\sum_{m>0}\left(v^2 a_{\tilde{m}} a_{\tilde{m}}^\dagger + v^2 a_m a_m^\dagger\right)|BCS\rangle = \sum_{m>0} 2v^2 \tag{39}$$

This means, that the occupations are completely determined by the particle number

$$v = \sqrt{\frac{N}{2\Omega}}, \qquad u = \sqrt{1 - \frac{N}{2\Omega}} \tag{40}$$

The distribution of particle numbers is given by

$$|BCS\rangle = \sum_{N'=0}^{2\Omega} c_{N'}|N'\rangle \tag{41}$$

where $|N'\rangle$ are normalized states with fixed particle number N. We obtain

$$\langle BCS|\hat{P}^N|BCS\rangle = |c_N|^2. \tag{42}$$

The BCS-energy is given by

$$E_{\mathrm{BCS}}^{(N)} = -G\Omega\frac{N}{2}\left(1 - \frac{N}{2\Omega} + \frac{N}{2\Omega^2}\right). \tag{43}$$

This expression agrees for large N up to order $1/\Omega$ with the exact formula on Eq. (21). Therefore, we see that the BCS ansatz is a good approximation, well suited to treat the nuclear pairing correlations.

The uncertainty in the particle number can also be obtained as

$$(\Delta N)^2 := \langle \mathrm{BCS}|\hat{N}^2|\mathrm{BCS}\rangle - N^2 = 4\Omega u^2 v^2 \tag{44}$$

or

$$\frac{\Delta N}{N} = \frac{1}{\sqrt{N}}\sqrt{2 - \frac{N}{\Omega}}. \tag{45}$$

2 The BCS-Model

2.1 The BCS Wave Function

The applicability of the seniority model is not limited to j^N configurations. The model can be generalized. Far away form closed shells, however, where nuclei are deformed and the levels more or less uniformly separated, the seniority model breaks down completely. However, the idea of the BCS-ansatz, to take treat pairing correlations in a generalized mean field model breaking particle number symmetry can be generalized:

This method no longer provides an exact solution of the eigenvalue problem, but like the Hartree-Fock method, it can be derived from a variational principle with the special BCS-ansatz (Bardeen, Cooper, and Schrieffer, 1957):

$$|\mathrm{BCS}\rangle = \prod_{k>0}(u_k + v_k a_k^+ a_{\tilde{k}}^+)|-\rangle, \tag{46}$$

where u_k and v_k represent variational parameters. The product runs only over half the configuration space, as indicated by $k > 0$. For each state $k > 0$ there exists a "conjugate state" $\tilde{k} < 0$ and the states $(k, \tilde{k})$ generate the whole single-particle space.

The v_k^2 and u_k^2 represent the probability that a certain pair state $(k, \tilde{k})$ is or is not occupied, which has to be determined in such a way that the corresponding energy has a minimum. They are not, however, independent, as the norm of the state requires

$$u_k^2 + v_k^2 = 1. \tag{47}$$

In many cases, especially if the Hamiltonian is invariant under time reversal, the conjugate state can be chosen as the time-reversed state

$$|\tilde{k}\rangle = \mathcal{T}|k\rangle. \tag{48}$$

An example is a spherical basis:

$$|k\rangle = |nljm\rangle, \qquad |\tilde{k}\rangle = (-)^{(j-m)}|nlj-m\rangle, \qquad m > 0. \tag{49}$$

The $|\mathrm{BCS}\rangle$ state is a superposition of different numbers of pairs and has no longer a sharp particle number. The product can be written as

$$|\mathrm{BCS}\rangle \propto |-\rangle + \sum_{k>0} \frac{v_k}{u_k} a_k^+ a_{\tilde{k}}^+ |-\rangle + \frac{1}{2}\sum_{k>0} \frac{v_k v_{k'}}{u_k u_{k'}} a_k^+ a_{\tilde{k}}^+ a_{k'}^+ a_{\tilde{k}'}^+ |-\rangle + \ldots \tag{50}$$

This is actually a great disadvantage in nuclear physics. In solid state physics, where $N \simeq 10^{23}$, the violation of particle number has no influence on any physical quantity. In nuclei, however, the violation of the invariance corresponding to the particle number in many cases give rise to serious errors. One then has to unse improved methods to deal ith such problems (projection to good particle number etc.)

To give an impression of the flexibility of the ansatz (46), we rewrite it in a different way: It can be expressed by a *generalized pair creation operator* (2)

$$A^+ = \sum_{k>0} \frac{v_k}{u_k} a_k^+ a_{\tilde{k}}^+ \tag{51}$$

as

$$|\mathrm{BCS}\rangle \propto \exp(A^+)|-\rangle = \sum_{\nu=0}^{\infty} \frac{1}{\nu!}(A^+)^\nu|-\rangle. \tag{52}$$

The component having the particle number N is therefore $(A^+)^{N/2}$. This corresponds to the seniority zero state ($s = 0$) of Eq. (25).

2.2 The BCS-Equations

We assume that a many-body system is described by the Hamiltonian

$$\hat{H} = \sum_k \epsilon_k a_k^+ a_k + \frac{1}{4} \sum_{k_1 k_2 \gtrless 0} \bar{v}_{k_1 k_2 k_3 k_4} a_{k_1}^+ a_{k_2}^+ a_{k_4} a_{k_3}. \tag{53}$$

where we assume $\epsilon_{\tilde{k}} = \epsilon_k$. The parameters u and v of the trial wave function (46) are determined by variation of the energy. However, this variation is *restricted* by the subsidiary condition that the expectation value of the particle number has the desired value N

$$\langle \mathrm{BCS}|\hat{N}|\mathrm{BCS}\rangle = 2\sum_{k>0} v_k^2 = N \tag{54}$$

This can be achieved by adding the term $-\lambda\hat{N}$ to the variational Hamiltonian

$$\hat{H}' = \hat{H} - \lambda\hat{N}. \tag{55}$$

The *Lagrange multiplier* λ is fixed by the number condition (54). It is called the *chemical potential* or the *Fermi energy* because it represents the increase

of the energy $E = \langle \mathrm{BCS}|\hat{H}|\mathrm{BCS}\rangle$ for a change in the particle number

$$\lambda = \frac{dE}{dN}. \tag{56}$$

To see this, we use the fact that the expectation value of $\hat{H}'$ is a minimum with respect to an arbitrary variation of the BCS wave function (46). One special variation is a change of the parameter λ. Therefore we get

$$\frac{d}{d\lambda'}\left\{\langle \mathrm{BCS}(\lambda')|\hat{H}|\mathrm{BCS}(\lambda')\rangle - \lambda\langle \mathrm{BCS}(\lambda')|\hat{N}|\mathrm{BCS}(\lambda')\rangle\right\}_{\lambda=\lambda'} = 0. \tag{57}$$

or

$$\frac{dE}{d\lambda} = \lambda\frac{dN}{d\lambda}. \tag{58}$$

In the following we will always use $\hat{H}'$ instead of $\hat{H}$. For the calculation of the actual energy, however, we have to remember that we have to add the term λN at the end.

From (46) and (53), we gain for the BCS expectation value of $\hat{H}'$:

$$\langle \mathrm{BCS}|\hat{H}'|\mathrm{BCS}\rangle = \sum_k (\epsilon_k - \lambda)v_k^2 + \frac{1}{2}\sum_{kk'>0} \bar{v}_{k\tilde{k}k'\tilde{k}'}u_k v_k u_{k'} v_{k'}. \tag{59}$$

Here we have neglected the term $\frac{1}{2}\sum_{kk'} \bar{v}_{kk'kk'}v_k^2 v_{k'}^2$ because it contributes to the mean field, and therefore it should be already taken into account in the single particle energies. Since the BCS wave function is completely determined by the parameters v_k and the condition (47) the variation

$$\delta\langle \mathrm{BCS}|\hat{H}'|\mathrm{BCS}\rangle = 0 \tag{60}$$

yields

$$\left(\frac{\partial}{\partial v_k} + \frac{\partial u_k}{\partial v_k}\frac{\partial}{\partial u_k}\right)\langle \mathrm{BCS}|\hat{H}'|\mathrm{BCS}\rangle = 0. \tag{61}$$

After differentiating we finally obtain the set of BCS equations

$$2(\epsilon_k - \lambda)u_k v_k + \Delta_k(u_k^2 - v_k^2) = 0, \qquad k > 0. \tag{62}$$

and the gap parameters (for real matrix elements)

$$\Delta_k = \sum_{k'>0} \bar{v}_{k\tilde{k}k'\tilde{k}'}u_{k'}v_{k'}. \tag{63}$$

For fixed values of $\epsilon_k - \lambda$ and Δ_k, (47) and (62) yield two quadratic equations for u_k^2 and v_k^2, respectively, having the solutions:

$$\left.\begin{matrix} u_k^2 \\ v_k^2 \end{matrix}\right\} = \frac{1}{2}\left(1 \pm \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta_k^2}}\right). \tag{64}$$

Thus the variational principle (60) yields the set of equations (63) and (64). Together with the *particle-number condition*

$$2\sum_{k>0} v_k^2 = N \tag{65}$$

they allow the calculation of the BCS parameters u_k, v_k. In general, these equations are nonlinear and have to be solved by interation.

For discussion of the properties of these equations it is often useful to insert (64) into (63) and obtain the so-called *gap equation*

$$\Delta_k = \frac{1}{2}\sum_{k'>0} \bar{v}_{k\tilde{k}k'\tilde{k}'} \frac{\Delta_{k'}}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta_k^2}}. \tag{66}$$

For all practical cases, the BCS-equations have to be solved on a computer and the question arises of ow many levels one should include for such calculations, that is, we have to investigate which states contribute most to the sum appearing in the gap equation (66). For this purpose, let us first consider the gap Δ_k for a state close to the Fermi level. In this case the main contributions to the sum come from states in the vicinity of the Fermi level. The reason for this is that (i) in this case the expression $\Delta_k/(\epsilon_k - \lambda)^2 + \Delta_k^2)^{1/2} \simeq 1$ ($\epsilon_k \simeq \lambda$), and (ii) the matrix elements $\bar{v}_{k\tilde{k}k'\tilde{k}'}$ for $k' \simeq k$ (strongly overlapping wave functions) are larger than the other matrix elements.

Conversely, if k is far from the Fermi surface, all the terms in the sum of Eq. (66) are small. for $k' \simeq k$, the overlap of the wave functions is still large, but the factor $\Delta_k/(\epsilon_k - \lambda)^2 + \Delta_k^2)^{1/2}$ is now small because of $(\epsilon_k - \lambda)^2 \gg \Delta_k^2$. For states k' at the Fermi surface it is just the other way around, since the matrix elements are very small (k and k' usually belonging to different principal quantum numbers).

The effect of the pairing force is therefore restricted to the neighborhood of the Fermi surface, that is, only there is Δ_k different from zero. We may now understand why it might be a valid approximation to take a constant pairing force in the vicinity of the Fermi, socalled *pairing window* $|\epsilon_k - \lambda| < \Lambda$.

The restriction of the pairing to the vicinity of the Fermi level is also the reason that neutrons and protons can be treated separately (at least for heavy nuclei). For nuclei with $A \sim 150$, the neutron excess $(N - Z) \geq 20$. The neutron and proton levels close to the Fermi energy, therefore, have very small overlap compared to that of protons or neutrons alone. Therefore, neglecting the proton-neutron-pairing, the total wave function may be represented as a product of the proton and neutron functions:

$$|\mathrm{BCS}\rangle = \prod_{k_1>0} (u_{k_1}^{(p)} + v_{k_1}^{(p)} a_{k_1}^{(p)\dagger} a_{\tilde{k}_1}^{(p)\dagger}) \prod_{k_2>0} (u_{k_2}^{(n)} + v_{k_2}^{(n)} a_{k_2}^{(n)\dagger} a_{\tilde{k}_2}^{(n)\dagger})|-\rangle. \tag{67}$$

2.3 BCS for a Monopole Pairing Force

As we have seen the pure pairing force provides a very simple and powerful model for the description of pairing properties in nuclei. It is therefore widely used in the BCS description of nuclei. In the following, we therefore present the most important formulae of this theory for this special case.

The Hamiltonian here has the form

$$\hat{H}' = \sum_k (\epsilon_k - \lambda) a_k^+ a_k - G \sum_{kk'>0} a_k^+ a_{\tilde{k}}^+ a_{\tilde{k}'} a_{k'}. \tag{68}$$

with the expectation value

$$\langle \mathrm{BCS}|\hat{H}'|\mathrm{BCS}\rangle = \sum_k (\epsilon_k - \lambda) v_k^2 - \frac{\Delta^2}{G}. \tag{69}$$

In this case the gap parameter Δ does not depend on k:

$$\Delta = G \sum_{k>0}^{\Lambda} u_k v_k. \tag{70}$$

The $v_k^2 = \langle \mathrm{BCS}|a_k^\dagger a_k|\mathrm{BCS}\rangle$ are the *occupation probabilities* for the different single-particle states.

Again, we see that in the limit $G \to 0$, that is, $\Delta \to 0$, the $v_k^2 = 1$ for occupied levels and $v_k^2 = 0$ for unoccupied ones. In this case v_k^2 is a step function, whereas for $\Delta \neq 0$ the step function is somewhat smeared out. Due to the interaction, particles are scattered from below to avove the Fermi

surface. This yields a partial depletion of the states below and a partial filling of the states above the Fermi level. The *gap equation* takes the simple form

$$\Delta = G\sum_{k>0}^{\Lambda}\frac{\Delta}{2\sqrt{(\epsilon_k-\lambda)^2+\Delta^2}}. \tag{71}$$

where the sum runs over the Λ-shell only. The gap equation always has the trivial solution $\Delta = 0$, that is $u_k v_k = 0$, which for no or sufficient weak pairing force in the only solution. However, for

$$\frac{1}{2}G\sum_{k>0}^{\Lambda}\frac{1}{|\epsilon_k-\lambda|} > 1 \tag{72}$$

there exists a second nontrivial solution $\Delta > 0$. This always happens if the pairing force is sufficiently strong or if the Λ-shell is sufficiently large. However, this sharp transition is a consequence of particle number violation and it is somewhat smeared out in more extended theories For an infinite system, particle number violation is neglegible, and the transition is always sharp.

On the other hand, the gap equation can also be used to determine the strength G of the pairing force since, and, as we have already said, Δ can be determined empirically from the odd-even effect. It still, however, depends on the "cutoff" Λ.

In realistic application one uses nowadays very often a zero range pairing force

$$V_{pp}(\mathbf{r}_1-\mathbf{r}_2) = -V_0\delta(\mathbf{r}_1-\mathbf{r}_2), \tag{73}$$

. It can be shown, that in this case one also needs a cutoff. This can be see most easily, when we try to solve the gap equation in nuclear matter:

$$\Delta(k) = \int_0^{\infty}\frac{k'^2dk'}{2\pi^2}v(k,k')\frac{\Delta(k')}{2\sqrt{(\epsilon(k')-\lambda)^2+\Delta^2(k')}}, \tag{74}$$

For the zero range force the interaction is a constant in momentum space. Considering that the kinetic energy is proportional to k^2, we find that the integral diverges. Only for forces with a finite range, like the Gogny force of Gaussian shape, the integral converges and one does not need a cutoff.

It most of the applications with a delta force in the pairing channel one uses a cutoff Λ (rather arbitrarily) and adjusts the strength V_0 in such a way,

that the gap at the Fermi surface corresponds to the experimental odd-even mass difference.

2.4 Bogoliubov Quasi-particles and Excited States

The main advantage of writing the ground state in the form (46) and (50) is that despite being very similar to the exact ground state of the seniority model (condensate of pairs), and therefore containing correlations between pairs of particles, $|\text{BCS}\rangle$ can at the same time be written as a product state of a new type of fermions, the *Bogoliubov quasi-particles*. The concept of quasi-particles as a general concept in many-body physics will be discussed later in the lecture about Hartree-Fock-Bogoliubov theory. In fact, as we have seen in the case of a single j-shell we have

$$|BCS\rangle \propto \prod_k \alpha_k |-\rangle \tag{75}$$

with

$$\alpha_k^\dagger = u_k a_k^\dagger - v_k a_{\tilde{k}}, \tag{76}$$

$$\alpha_{\tilde{k}}^\dagger = u_k a_{\tilde{k}}^\dagger + v_k a_k. \tag{77}$$

and the following Fermion communtation relations hold

$$\left\{\alpha_k, \alpha_{k'}^\dagger\right\} = \delta_{kk'}, \qquad \{\alpha_k, \alpha_{k'}\} = 0, \tag{78}$$

where we have used (49) and the usual phase convention

$$u_{\tilde{k}} = u_k > 0, \quad v_{\tilde{k}} = -v_k < 0 \qquad \text{for} \quad k > 0. \tag{79}$$

From Eqs. (76) and (64) we see that a quasi-particle has some properties of a bare particle and some of a bare hole: Above the Fermi surface (v_k^2 small) it is nearly a particle, while below the Fermi surface (u_k^2 small) it is nearly a hole.

We see from (76) that by using a the trick of a linear a *"Bogoliubov" transformation,* we have achieved a representation of the ground state of pairwise *interacting* particles in terms of a gas of *non-interacting* quasi-particles. The price we have to pay is that the transformation (76) clearly does not conserve

particle number because we mix creation and annihilation operators. If we assume that not only the ground state is well represented by a product states of quasi-particles, but also *excited states* then the Hamiltonian $\hat{H}_{qp}$, which corresponds to this gas of non-interacting quasi-particles, is given by

$$\hat{H}_{qp} = \langle \mathrm{BCS}|\hat{H}'|\mathrm{BCS}\rangle + \sum_{k \gtrless 0} E_k \alpha_k^\dagger \alpha_k, \tag{80}$$

where the constant $\langle \hat{H}' \rangle$ takes account of the fact that we have

$$\alpha_k|\mathrm{BCS}\rangle = 0 \qquad \text{for all} \quad k \gtrless 0, \tag{81}$$

therefore $\hat{H}_{qp}$ has the right ground state expectations value. The quasi-particle energies E_k are a straightforward generalization of the definition of those for real particles (further details will be discussed in the HFB-lecture)

$$E_k = \langle \mathrm{BCS}|\alpha_k \hat{H}' \alpha_k^\dagger|\mathrm{BCS}\rangle - \langle \mathrm{BCS}|\hat{H}'|\mathrm{BCS}\rangle = \sqrt{(\epsilon_k - \lambda)^2 + \Delta_k^2}. \tag{82}$$

The one-quasiparticle states

$$\alpha_{k_1}^\dagger|\mathrm{BCS}\rangle = a_{k_1}^\dagger \prod_{k \neq k_1 > 0} (u_k + v_k a_k^+ a_{\tilde{k}}^+)|-\rangle, \tag{83}$$

$$\alpha_{\tilde{k}_1}^\dagger|\mathrm{BCS}\rangle = a_{\tilde{k}_1}^\dagger \prod_{k \neq k_1 > 0} (u_k + v_k a_k^+ a_{\tilde{k}}^+)|-\rangle \tag{84}$$

obviously have the energy $\langle \hat{H}' \rangle + E_k$. They are a superposition of states with odd particle number and describe a nucleus with an odd number of nucleons. According to the quantum number k_1 this state can be either the ground state or an excited state.

The two-quasiparticle states

$$\alpha_{k_1}^\dagger \alpha_{k_2}^\dagger|\mathrm{BCS}\rangle = a_{k_1}^\dagger a_{k_2}^\dagger \prod_{k \neq k_1, k_2 > 0} (u_k + v_k a_k^+ a_{\tilde{k}}^+)|-\rangle, \qquad k_2 \neq \tilde{k}_1 \tag{85}$$

$$\alpha_{k_1}^\dagger \alpha_{\tilde{k}_1}^\dagger|\mathrm{BCS}\rangle = (-v_k + u_k a_{k_1}^+ a_{\tilde{k}_1}^+) \prod_{k \neq k_1 > 0} (u_k + v_k a_k^+ a_{\tilde{k}}^+)|-\rangle, \qquad k_2 \neq \tilde{k}_1 \tag{86}$$

have the energy $\langle \hat{H}' \rangle + E_{k_1} + E_{k_2}$. They describe excited states in the even system. In this case one pair is broken and the excitation energy is

$$E_{k_1} + E_{k_2} \geq 2\Delta. \tag{87}$$

The first excited state in the even system thus lies at least 2Δ higher than the ground state.

In *the odd system* with the ground state k_0 ($\tilde{\epsilon}_{k_0} \backsimeq 0$), the excitation energy is

$$E_k - E_{k_0} = \sqrt{(\epsilon_k - \lambda)^2 + \Delta^2} - \Delta. \tag{88}$$

For small excitation energy ($\epsilon_k - \lambda \ll \Delta$) we therefore find a high level density in these odd systems.

We also can explain the odd-even mass difference by the following consideration: The ground state energies E_N^{GS} are given for any N by

$$E_{N+2}^{GS} = E_N^{GS} + 2\lambda, \quad E_{N+1}^{GS} = E_N^{GS} + \lambda + E_{k_0}. \tag{89}$$

and therefore the odd-even mass difference is given by

$$\frac{1}{2}\left\{(E_{N+1}^{GS} - E_N^{GS}) - (E_N^{GS} - E_{N-1}^{GS})\right\} = E_{k_0} \simeq \Delta \tag{90}$$

Eq. (90) is often exploited to determine the gap empirically from the measured binding energies. It has been found that on the average the gap follows the relation $\Delta = 12/\sqrt{A}$ as a function of teh nucleon number A.

The above considerations give a qualitative understanding of the structure of many states in the superfluid nuclei. There remain, however, a few important points to take into account in a more detailed investigation:

2.4.1 (i) The Chemical Potential

The chemical potential λ is determined in such a way that the average particle number in the BCS ground state has the correct value. With the same λ, we find for a one-quasiparticle state $|k\rangle = \alpha_k^\dagger|\mathrm{BCS}\rangle$

$$\langle k|\hat{N}|k\rangle = N + u_k^2 - v_k^2. \tag{91}$$

This is $N \pm 1$ only for levels k which are far away from the Fermi surface. For the levels in the vicinity of the Fermi surface the average particle number is wrong. Since the energy depends strongly on the average particle number, one should re-adjust the chemical potential λ for the different levels in odd nuclei and also for the excited states in even nuclei. As long as we have not done this, we should use the operator $\hat{H}' = \hat{H} - \lambda\hat{N}$ instead of $\hat{H}$ for

the calculation of excitation energies (as we have done so far). This can, for instance, be seen if we correct for the wrong particle number in the state $|k\rangle$:

$$E^k_{N+1} = \langle k|\hat{H}|k\rangle + \frac{dE}{dN}(N+1-\langle k|\hat{N}|k\rangle) \tag{92}$$

$$= \langle k|\hat{H}-\lambda\hat{N}|k\rangle + \frac{dE}{dN}(N+1) \tag{93}$$

$$= (E^{GS}_{N+1}-\lambda N) + E_k + \lambda(N+1) \tag{94}$$

$$= E^{GS}_{N+1} + E_k + \lambda \tag{95}$$

2.4.2 (ii) The Blocking Effect

The occupation probabilities v_k^2 of the BCS ground state (64) were determined by the variational principle. The ground state of an odd system is described by the wave function

$$\alpha^\dagger_{k_1}|\mathrm{BCS}\rangle = a^\dagger_{k_1}\prod_{k\neq k_1}(u_k + v_k a^+_k a^+_{\tilde{k}})|-\rangle, \tag{96}$$

The unpaired particle sits in the level k_1 and blocks this level. The Pauli principle prevents this level from participating in the scattering process of nucleons caused by the pairing correlations. The level k_1 always stays occupied and the level $\tilde{k}_1$ always stays empty. Only for $k \neq k_1$ do we have $v_k^2 = v_{\tilde{k}}^2$. Using the blocked wave function as a trial wave function in the variational principle, we find the same equations for v_k^2 as before. The only difference is that in the calculation of the gap one level is *blocked:*

$$\Delta = G\sum_{k\neq k_1} u_k v_k. \tag{97}$$

i.e. the level k_1 has to be excluded from the sum because it cannot contribute to the pairing energy. The chemical potetial is determined by

$$N = 1 + 2\sum_{k\neq k_1} v_k^2. \tag{98}$$

Similar equations hold for the case of a higher number of blocked levels, as in the case of two-quasiparticle excitations.

The change in Δ and in the u_k's and v_k's is called *blocking effect.* These blocking correlations are of the order Ω^{-1} amd can often be neglected. However, the correction may be large in some cases. this can happen particularly

for deformed nuclei where, although there may be 20 levels in the spectrum, only 4 or 5 contribute appreciably to the sum of Eq. (63). Clearly the blocking of one or two such levels in such a case has a big effect so that one cannot simply equate the excitation energy of the excited state and subtract it from the vacuum energy. For two-quasiparticle states the corrected energy ($\simeq 1.4$ MeV) is always smaller than the quasi-particle energy ($\simeq 1.7$ MeV), but much larger than the free-particle energy ($\simeq 0.15$ MeV). One problem that arises in this corrected theory, in which the v_k's can be appreciably different in the ground state and the excited states, is that these states are no longer automatically orthogonal, although sometimes a different quantum number, such as the spin or the parity, guarantees the orthogonality. In particular, two-quasiparticle states of spin 0^+ are not orthogonal to the ground state in such cases.

3 Hartree-Bogoliubov Theory

3.1 General Bogoliubov Transformation

The basic idea of any quasi-particle concept is to represent the ground state $|\Phi\rangle$ of a nucleus as a *vacuum* with respect to *quasi-particles*. Here we use the so-called Bogoliubov quasi-particles.

One can define quasiparticles also in the Hartree-Fock case:

$$\alpha_m^+ = a_m^+ \quad \text{for} \quad \epsilon_k > \epsilon_F, \qquad \alpha_i^+ = a_i \quad \text{for} \quad \epsilon_i \leq \epsilon_F \tag{99}$$

with the quasiparticle vaccum

$$|\Phi\rangle = \prod_{i=1}^{A} a_i^\dagger |-\rangle \quad \text{and} \quad \alpha_k \, |\Phi\rangle = 0, \qquad \text{for all} \;\; k \lesseqgtr 0 \tag{100}$$

where (for arbitrary basis states $|l\rangle$)

$$a_k^\dagger = \sum_l D_{kl} c_l^\dagger \tag{101}$$

BCS quasi-particles $\alpha_k^\dagger = u_k a_k^\dagger - v_k a_{\tilde{k}}^\dagger$

$$\alpha_k^\dagger = u_k a_k^\dagger - v_k a_{\tilde{k}}^\dagger \tag{102}$$

are linear combinations of creation and annihilation operators.

The Bogoliubov *quasi-particle operators* generalize this concept:

$$\beta_k^\dagger = \sum_l U_{lk} c_l^\dagger + V_{lk} c_l \tag{103}$$

The indices k and l both run over the whole configuration space ($k = 1, \ldots, M$). The Hermitian conjugation of this equation gives us the operator β_k. We therefore have a transformation of the operators

$$\mathfrak{c} = (c_1^\dagger \ldots c_M^\dagger, c_1 \ldots c_M) \rightarrow \mathfrak{b} = (\beta_1^\dagger \ldots \beta_M^\dagger, \beta_1 \ldots \beta_M) \tag{104}$$

which acts in a $2M$-dimensional space:

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix} \tag{105}$$

or

$$\mathfrak{b}^\dagger = \mathcal{W}^\dagger \mathfrak{c}^\dagger \tag{106}$$

with

$$\mathcal{W} = \begin{pmatrix} U & V^* \\ V & U^*. \end{pmatrix} \tag{107}$$

The coefficients U, V are not completely arbitrary. We require the new operators β_k^+, β_k obey Fermion commutation relations as the old ones. This restricts the matrix $\mathcal{W}$ to being unitary.

$$\mathcal{W}^+\mathcal{W} = 1 \qquad \text{and} \qquad \mathcal{W}\mathcal{W}^+ = 1. \tag{108}$$

or

$$\begin{aligned} U^+U + V^+V = 1, \qquad & UU^+ + V^*V^T = 1, \\ U^TV + V^TU = 0, \qquad & UV^+ + V^*V^T = 0. \end{aligned} \tag{109}$$

and we can invert

$$\mathfrak{c}^\dagger = \mathcal{W}\mathfrak{b}^\dagger \tag{110}$$

3.2 The Quasiparticle-vacuum

The ground state of the many-body system $|\Phi\rangle$ shall be represented as the vacuum with respect to these quasi-particles. It is therefore defined by:

$$\beta_k|\Phi\rangle = 0 \qquad \text{for all} \qquad k = 1 \ldots M. \tag{111}$$

We call wave functions which fulfill these conditions for a complete set of quasi-particle operators as called HFB wave functions.

3.3 The Density Matrix and the Pairing Tensor

We now define a generalize density matrix (*Valatin-density*) of dimension $2M \times 2M$:

$$\mathcal{R}_{ll'} = \begin{pmatrix} \langle\Phi|c_{l'}^\dagger c_l|\Phi\rangle & \langle\Phi|c_{l'}c_l|\Phi\rangle \\ \langle\Phi|c_{l'}^\dagger c_l^\dagger|\Phi\rangle & \langle\Phi|c_{l'}c_l^\dagger|\Phi\rangle \end{pmatrix} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix}. \tag{112}$$

in particle space. The quantities ρ and κ are called the *normal* and *abnormal density* (or *density matrix* and *pairing tensor*), and are given by

$$\rho_{ll'} = \langle\Phi|c^\dagger_{l'}c_l|\Phi\rangle, \qquad \kappa_{ll'} = \langle\Phi|c_{l'}c_l|\Phi\rangle, \tag{113}$$

or in matrix notation

$$\rho = V^*V^T, \qquad \kappa = V^*U^T = -UV^+. \tag{114}$$

ρ is Hermitian ($\rho^+ = \rho$) and κ is skew symmetric ($\kappa^T = -\kappa$).

We transform the Valatin density to quasiparticle-space

$$\mathcal{W}^+\mathcal{R}\mathcal{W} = \begin{pmatrix} \langle\Phi|\beta^\dagger_{k'}\beta_k|\Phi\rangle & \langle\Phi|\beta_{k'}\beta_k|\Phi\rangle \\ \langle\Phi|\beta^\dagger_{k'}\beta^\dagger_k|\Phi\rangle & \langle\Phi|\beta_{k'}\beta^\dagger_k|\Phi\rangle \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{115}$$

$\mathcal{R}$ is Hermitian and idempotent:

$$\mathcal{R}^+ = \mathcal{R} \qquad \text{and} \qquad \mathcal{R} = \mathcal{R}^2. \tag{116}$$

and diagonal in the quasiparticle-basis. We obtain the relations

$$\rho^2 - \rho = -\kappa\kappa^+, \qquad \rho\kappa = \kappa\rho^* \tag{117}$$

3.4 The Bloch-Messiah Theorem

Using the relations (117) Bloch and Messiah have shown that the unitary matrix $\mathcal{W}$ can be decomposed into a product of three matrices of a very special form:

$$\mathcal{W} = \begin{pmatrix} D & 0 \\ 0 & D^* \end{pmatrix} \cdot \begin{pmatrix} \bar{U} & \bar{V} \\ \bar{V} & \bar{U} \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & C^* \end{pmatrix}. \tag{118}$$

or

$$U = D\bar{U}C, \qquad V = D^*\bar{V}C. \tag{119}$$

D and C are unitary matrices and $\bar{U}$, $\bar{V}$ are real matrices of the dimension $M \times M$ containing essentially only the values 0 and 1 in the diagonal and up

to a string of 2×2 matrices along the diagonal:

$$U = \begin{bmatrix} 0 & & & & & & & \\ & \cdot & & 0 & & 0 & & 0 \\ & & 0 & & & & & \\ & 0 & & \boxed{\begin{matrix} u_1 & 0 \\ 0 & u_1 \end{matrix}} & & 0 & & 0 \\ & & & & \cdot & & & \\ & 0 & & 0 & & \boxed{\begin{matrix} u_n & 0 \\ 0 & u_n \end{matrix}} & & 0 \\ & & & & & & 1 & \\ & 0 & & 0 & & 0 & & \cdot \\ & & & & & & & & 1 \end{bmatrix} \tag{120}$$

$$V = \begin{bmatrix} 1 & & & & & & & \\ & \cdot & & 0 & & 0 & & 0 \\ & & 1 & & & & & \\ & 0 & & \boxed{\begin{matrix} 0 & v_1 \\ -v_1 & 0 \end{matrix}} & & 0 & & 0 \\ & & & & \cdot & & & \\ & 0 & & 0 & & \boxed{\begin{matrix} 0 & v_n \\ -v_n & 0 \end{matrix}} & & 0 \\ & & & & & & 0 & \\ & 0 & & 0 & & 0 & & \cdot \\ & & & & & & & & 0 \end{bmatrix} \tag{121}$$

Its meaning is that the general Bogoliubov transformation $\mathfrak{c}^\dagger \to \mathfrak{b}^\dagger$ can be decomposed into three parts:

$$\left.\begin{matrix} c & \to & a \\ c^\dagger & \to & a^\dagger \end{matrix}\right\} \quad \to \quad \left\{\begin{matrix} \alpha & \to \beta \\ \alpha^\dagger & \to \beta^\dagger \end{matrix}\right. \tag{122}$$
$$D \qquad \bar{U}, \bar{V} \qquad C$$

(i) a unitary transformation of the particle operators $c^\dagger$ among themselves as in the HF case:

$$a_k^\dagger = \sum_l D_{lk} c_l^\dagger. \tag{123}$$

It defines a new basis is called the *canonical basis*.

(ii) a *special Bogoliubov transformation*, which distinguishes between *paired* levels ($u_p > 0, v_p > 0$)

$$\begin{aligned} \alpha_p^+ &= u_p a_p^+ - v_p a_{\bar{p}} \\ \alpha_{\bar{p}}^+ &= u_p a_{\bar{p}}^+ + v_p a_p \end{aligned} \tag{124}$$

xwhere $(p, \bar{p})$ are defined by the 2×2 boxes and *blocked* levels which are either occupied ($v_i = 1, u_i = 0$) or empty ($v_m = 0, u_m = 1$):

$$\begin{aligned} \alpha_i^+ &= a_i \ , \qquad \alpha_m^+ = a_m^+, \\ \alpha_i \ &= a_i^+, \qquad \alpha_m \ = a_m. \end{aligned} \tag{125}$$

(iii) a *unitary transformation of the quasi-particle operators* α_k^+ among themselves

$$\beta_k^+ = \sum_{k'} C_{k'k} \alpha_{k'}^+ \tag{126}$$

The decomposition (118) defines fully occupied levels (i), completely empty levels (m), and paired levels (p) with canonical conjugate states $p, \bar{p}$. Often, but not always, time reversal symmetry is canonical conjugation.

Using the Bloch-Messiah decomposition, we find

$$\rho = D\bar{V}^2 D^+, \qquad \kappa = D\bar{U}\bar{V}D^T. \tag{127}$$

ρ is diagonal in the canonical basis. The eigenvalues of ρ are the occupation probabilities v_k^2 and the eigenvectors D_k are the wave functions in the canonical basis. At the same time, κ is in its canonical form: it decomposes into 2×2 matrices:

$$\begin{pmatrix} 0 & u_k v_k \\ -u_k v_k & 0 \end{pmatrix}. \tag{128}$$

Many theories developed originally in the HF picture of pure Slater determinants ($\rho^2 = \rho$) can be immediately generalized to the HFB case with pairing correlations simply by working in the $2M$-dimensional formalism with the super-matrix $\mathcal{R}$.

3.5 The HFB Wave Function

The HFB wave function is defined by (111). It can be written as

$$|\Phi\rangle = \prod_k \beta_k |-\rangle. \tag{129}$$

If k runs over all values $k = 1 \ldots M$. In many cases, however, such a function vanishes identically. In a HF state, for instance, the product can run only over the annihilation operators of all hole states

$$|HF\rangle = \prod_i \alpha_i |-\rangle = \prod_i a_i^+ |-\rangle. \tag{130}$$

In cases of blocking, we therefore have to represent it in the canonical basis:

$$|\Phi\rangle = \prod_i {}' \alpha_i |-\rangle = \prod_i a_i^+ \prod_p (u_p + v_p a_p^+ a_{\bar{p}}^+) |-\rangle. \tag{131}$$

where $\prod'$ runs over all paired $(p, \bar{p})$ and all occupied (i) levels. Therefore, depending on whether the number of occupied levels i is even or odd, the function $|\Phi\rangle$ is a superposition of states with an even and an odd particle number (*number parity).* It is evident that a wave function $|\Phi\rangle$ with even number parity can only describe a system with an even particle number and vice versa.

3.6 The HFB Equations

We give three ways to derive the HFB-equations:

3.6.1 Derivation from the Thouless Theorem

We assume that $|\Phi\rangle$ is an approximation for the exact ground state of the Hamiltonian

$$\hat{H} = \sum_{l_1 l_2} \epsilon_{l_1 l_2} c_{l_1}^+ c_{l_2} + \frac{1}{4} \sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2 l_3 l_4} c_{l_1}^+ c_{l_2}^+ c_{l_4} c_{l_3} \tag{132}$$

and use the variational principle of Ritz. The trial wave functions are the set of all generalized product states $|\Phi\rangle$ of the HFB type. As in the BCS

model these wave functions violate particle number. We have to use the Hamiltonian $\hat{H}' = \hat{H} - \lambda\hat{N}$. For simplicity we use in the following only $\hat{H}$. Starting from the variational principle

$$\delta \frac{\langle\Phi|\hat{H}|\Phi\rangle}{\langle\Phi|\Phi\rangle} = 0, \tag{133}$$

we have to investigate small variations $|\delta\Phi\rangle$ in the vicinity of the solution. We use a theorem of Thouless and express the function $|\Phi'\rangle = |\Phi\rangle + |\delta\Phi\rangle$, which is not orthogonal to $|\Phi\rangle$ by:

$$|\Phi'\rangle = \exp\left(\sum_{k<k'} Z_{kk'}\beta_k^+\beta_{k'}^+\right)|\Phi\rangle. \tag{134}$$

In contrast to the coefficients U_{lk} and V_{lk} which obey unitarity relations, the variables $Z_{kk'}$ (with $k < k'$) are independent variables. The solution $|\Phi\rangle$ of the variational equation corresponds to $Z_{kk'} = 0$. For infinitesimal variations, we expand up to second order. Using the quasi-particle representation for the Hamiltonian

$$\hat{H} = H^0 + \sum_{k_1k_2} H^{11}_{k_1k_2}\beta_{k_1}^+\beta_{k_2} + \sum_{k_1<k_2}(H^{20}_{k_1k_2}\beta_{k_1}^+\beta_{k_2}^+) + h.c.) + H_{int}. \tag{135}$$

and find

$$\frac{\langle\Phi'|\hat{H}|\Phi'\rangle}{\langle\Phi'|\Phi'\rangle} = H^0 + \begin{pmatrix} H^{20*} & H^{20}\end{pmatrix}\begin{pmatrix} Z \\ Z^*\end{pmatrix} + \frac{1}{2}\begin{pmatrix} Z^* & Z\end{pmatrix}\begin{pmatrix} A & B \\ B^* & A^*\end{pmatrix}\begin{pmatrix} Z \\ Z^*\end{pmatrix}. \tag{136}$$

where the index of the vectors and the matrixes runs over all pairs ($k < k'$) and

$$\begin{aligned} H^0 &= \langle\Phi|\hat{H}|\Phi\rangle, & A_{kk'll'} &= \langle\Phi|[\beta_{k'}\beta_k,[\hat{H},\beta_l^+\beta_{l'}^+]]|\Phi\rangle, \\ H^{20}_{kk'} &= \langle\Phi|[\beta_{k'}\beta_k,\hat{H}]|\Phi\rangle, & B_{kk'll'} &= -\langle\Phi|[\beta_{k'}\beta_k,[\hat{H},\beta_{l'}\beta_l]]|\Phi\rangle, \end{aligned} \tag{137}$$

Eq. (136) gives a quadratic approximation of the multidimensional energy surface in the vicinity of $|\Phi\rangle$. The variation with respect to $Z^*_{kk'}$ yields

$$\frac{\partial}{\partial Z^*_{kk'}}\frac{\langle\Phi'|\hat{H}|\Phi'\rangle}{\langle\Phi'|\Phi'\rangle} = H^{20}_{kk'} = 0, \tag{138}$$

which means that the linear terms H^{20} vanish at the stationary point. To see, whether this is a minimum or a saddle point, the quadratic terms must be investigated the matrix

$$\mathcal{S} = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \tag{139}$$

is called the *stability matrix* (or *curvature tensor*). At a minimum it has to be positive definite.

The variational equations are not affected by a C-transformation of the quasi-particles among themselves. The requirement $H^{20} = 0$ determines, therefore, only the first two of the Bloch-Messiah transformations. The third transformation can be used to diagonalize H^{11}. Together with Eq. (138), this corresponds to the diagonalization of the super-matrix

$$\begin{pmatrix} H^{11} & H^{20} \\ -H^{20*} & -H^{11*} \end{pmatrix} = \begin{pmatrix} \langle\Phi|\{[\beta_k, \hat{H}], \beta^+_{k'}\}|\Phi\rangle & \langle\Phi|\{[\beta_k, \hat{H}], \beta_{k'}\}|\Phi\rangle \\ \langle\Phi|\{[\beta^+_k, \hat{H}], \beta^+_{k'}\}|\Phi\rangle & \langle\Phi|\{[\beta^+_k, \hat{H}], \beta_{k'}\}|\Phi\rangle \end{pmatrix} \tag{140}$$

in the space of the basis operators c_l, c^+_l this matrix has the form

$$\mathcal{H} = \mathcal{W} \begin{pmatrix} H^{11} & H^{20} \\ -H^{20*} & -H^{11*} \end{pmatrix} \mathcal{W}^+ = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \tag{141}$$

with

$$h_{ll'} = \langle\Phi|\{[c_l, H], c^+_{l'}\}|\Phi\rangle \qquad \text{and} \qquad \Delta_{ll'} = \langle\Phi|\{[c_l, H], c_{l'}n\}|\Phi\rangle. \tag{142}$$

Applying Wick's theorem, we find

$$h = \epsilon + \Gamma - \lambda, \qquad \Gamma_{ll'} = \sum_{qq'} \bar{v}_{lq'l'q}\rho_{qq'}, \qquad \Delta_{ll'} = \sum_{q<q'} \bar{v}_{ll'qq'}\kappa_{qq'}. \tag{143}$$

We are left with a diagonalization problem for the matrix $\mathcal{H}$, the so-called HFB *equations*:

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}_k = \begin{pmatrix} U \\ V \end{pmatrix}_k E_k. \tag{144}$$

where the columns U_k and V_k of the matrices U and V determine the quasi-particle operators β^+_k (103). In the basis corresponding to the operators β_k,

both matrices $\mathcal{H}$ and $\mathcal{R}$ are diagonal. We therefore get as an equivalent condition:

$$[\mathcal{H}, \mathcal{R}] = 0, \tag{145}$$

The Hamiltonian (135) now takes the form

$$\hat{H} = H^0 + \sum_k E_k \beta_k^+ \beta_k + \hat{H}_{int}. \tag{146}$$

H_{int} contains the terms H^{40}, H^{31}, and H^{22}. These terms are neglected in the HFB approach. In this case, H is diagonal. Its eigenstates are the quasi-particle vacuum $|\Phi\rangle$ (with the eigenvalue H^0), one-quasi-particle states

$$|\Phi_k\rangle = \beta_k^+ |\Phi\rangle, \tag{147}$$

with the eigenvalues $H^0 + E_k$, two-quasi-particle states, and so on. The excited states to $|\Phi\rangle$ are states with an even number of quasi-particles. The states with odd number of quasi-particles describe the neighboring nuclei with mass numbers $(A \pm 1)$.

3.6.2 From the Wick Theorem

Let us give a different derivation which shows some interesting aspects of the theory and requires less calculations. Using the theorem of Wick, we expand the Hamiltonian in normal order $(: :)$ with respect to the ground state $|\Phi\rangle$. We then get for the one-particle operator

$$\begin{aligned} c_1^+ c_2 &= \langle \Phi | c_1^+ c_2 | \Phi \rangle + : c_1^+ c_2 : \\ &= \rho_{21} + : c_1^+ c_2 : \end{aligned} \tag{148}$$

and for the two-particle operator

$$\begin{aligned} c_1^+ c_2^+ c_4 c_3 = {} & \rho_{31}\rho_{42} - \rho_{32}\rho_{41} + \kappa_{12}^* \kappa_{34} \\ & + \rho_{31} : c_2^+ c_4 : + \rho_{42} : c_1^+ c_3 : - (3 \leftrightarrow 4) \\ & + \kappa_{12}^* : c_4 c_3 : + \kappa_{34} : c_1^+ c_3^+ : \\ & + : c_1^+ c_2^+ c_4 c_3 : . \end{aligned} \tag{149}$$

Using the definitions (143) for Γ and Δ we immediately find

$$H = H^0 + \frac{1}{2} : \begin{pmatrix} c^+ & c \end{pmatrix} \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} c \\ c^+ \end{pmatrix} : + \frac{1}{4} \sum_{1234} \bar{v}_{1234} : c_1^+ c_2^+ c_4 c_3 : . \tag{150}$$

The last term contains only products of four-quasi-particle operators. It corresponds to H^{40}, H^{31}, and H^{22} in the quasi-particle representation.

3.6.3 From Density Functional Theory

Density functional theory of superfluid systems starts from an energy functional, which depends on two densities, or on the Valatin density

$$E[\rho, \kappa] = E[\mathcal{R}]$$

Now we carry out a variation with respect to $\mathcal{R}$. Of course, the matrix elements are not independent variables, because we require $\mathcal{R}$ to correspond to a generalized Slater determinat $|\Phi\rangle$, which means that we have to carry out the variation with the constraint $\mathcal{R}^2 = \mathcal{R}$, wich is added with a matrix Λ of Lagrangeparameters

$$\delta(E[\mathcal{R}] - \mathrm{Tr}(\Lambda(\mathcal{R}^2 - \mathcal{R})) = 0.$$

or

$$\begin{aligned} \mathrm{Tr}\left((\frac{\delta E}{\delta \mathcal{R}}\delta\mathcal{R} - \Lambda\delta\mathcal{R}\mathcal{R} - \Lambda\mathcal{R}\delta\mathcal{R} - *\delta\mathcal{R}\right) = 0, \\ \mathrm{Tr}\left((\mathcal{H} - \mathcal{R}\Lambda - \Lambda\mathcal{R} - *)\delta\mathcal{R}\right) = 0, \end{aligned}$$

.

Here we have introduced the mean field Hamiltonian

$$\mathcal{H} = \frac{\delta E}{\delta \mathcal{R}^*} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}.$$

with

$$h = \frac{\delta E}{\delta \hat{\rho}^*}, \qquad \Delta = \frac{\delta E}{\delta \hat{\kappa}^*},$$

From the variational equation we find

$$\mathcal{H} - \mathcal{R}\Lambda - \Lambda\mathcal{R} - * = 0.$$

Multiplying this by $\mathcal{R}$ from the left and from the right we find

$$\begin{aligned} \mathcal{H}\mathcal{R} - \mathcal{R}\Lambda\mathcal{R} = 0, \\ \mathcal{R}\mathcal{H} - \mathcal{R}\Lambda\mathcal{R} = 0. \end{aligned}$$

or

$$[\mathcal{H},\mathcal{R}] = 0$$

This means that $\mathcal{R}$ and $\mathcal{H}$ diagonal in the same basis. Since $\mathcal{R}$ is diagonalized by the HFB wave functions $\mathcal{W}$, this is also true for the matrix $\mathcal{H}$, which means that we have the HFB-equations.

3.7 Properties of the HFB Equations

The HFB equations are a $2M$-dimensional set of non-linear equations. They show more or less the same properties as the HF equations. They have to be solved by iteration and we have the theorem of self-consistent symmetries.

Differences to the HF equations are

- The chemical potential has to be determined by the average particle number
- We have two densities ρ and κ and two selfconsistent potentials Γ and Δ.
- The dimension is twice as big

The equations have a symmetry:

$$\mathcal{H}\mathcal{W} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix}. \quad (151)$$

To each quasiparticle energy E_k with the eigenfunction (U_k, V_k) there exists an eigenvalue $-E_k$ with the eigenvector (V_k^*, U_k^*). An exchange of these two eigenvectors corresponds to a replacement of one operator β_k^+ by β_k and vice versa. It is forbidden to choose E_k and $-E_k$ at the same time (otherwise it is impossible to fulfill the Fermi commutation relations for the operators β, β^+). Therefore, we have to decide for each k ($k = 1 \ldots M$) whether one takes the eigenvalue E_k with the eigenvector (U_k, V_k) or the eigenvalue $-E_k$ with the eigenvector (V_k^*, U_k^*). This choice has a clear correspondence in the HF-case, where one has to decide, whether the level k is occupied or empty in the HF-wave function.

Usually one chooses only positive eigenvalues $E_k > 0$, because in this case the quasiparticle vaccum $|\Phi_0\rangle$ has the lowest energy. In most cases (but not

always) this corresponds to a fully paired state. In order to see, if this is true, one can use the Bloch-Messiah theorem and determine the canonical basis by diagonalization of the density matrix $\rho = V^* V^\intercal$.

For a fully paired state we have $|\Phi_0\rangle = \beta_1 \dots \beta_M |-\rangle$ with even number parity. It is a vacuum with respect to the operators $(\beta_1 \dots \beta_M)$. Starting with this ground state for an even system we can construct a wave function in an odd system, i.e. a one-quasiparticle state

$$|\Phi_1\rangle = \beta_1^+ \, |\Phi_0\rangle \tag{152}$$

It is a vacuum with respect to the operators $(\tilde{\beta}_1 \dots \tilde{\beta}_M)$ with

$$\tilde{\beta}_1 = \beta_1^+, \;\; \tilde{\beta}_2 = \beta_2, \;\; \dots \;\; \tilde{\beta}_M = \beta_M. \tag{153}$$

The exchange of a quasi-particle creation operator β_1^+ with the corresponding annihilation operator β_1 means that we have replaced columns 1 in the matrices U and V by the corresponding columns in the matrices V^*, U^*:

$$(U_{l1}, V_{l1}) \quad \Longleftrightarrow \quad (V_{l1}^*, U_{l1}^*) \tag{154}$$

Thus, by making such a replacement, we change the number parity of the corresponding vacuum and go over to a one-quasi-particle state. This can be continued. Starting form the fully paired ground state we can come to many-quasi-particle states by simply interchanging the corresponding columns in the HFB coefficients. With this trick we represent *quasi-particle excitations* as HFB *vacua* for properly defined new quasi-particle operators.

Of course, the transformations C, $\bar{U}$, $\bar{V}$, and D of Eq. (118) are changed by the replacement, because the canonical basis for $|\Phi_1\rangle$ is, in general, different form that for $|\Phi_0\rangle$. Only in cases where the C transformation is equal to unity (i.e., if $|\Phi_1\rangle = \alpha_1^+ |\Phi_0\rangle$) do the two wave functions have the same canonical basis.

For the paired levels $(k, \bar{k})$ in the canonical basis we calculate the matrix element of H^{20} in the canonical basis. It has to vanish and we find

$$u_k v_k (h_{kk} + h_{\bar{k}\bar{k}}) + \Delta_{k\bar{k}} (u_k^2 - v_k^2) = 0, \tag{155}$$

As shown in the BCS-model the solution of this equation is

$$\left.\begin{matrix} u_k^2 \\ v_k^2 \end{matrix}\right\} = \frac{1}{2} \left(1 \pm \frac{\epsilon_\kappa - \lambda}{\sqrt{(\epsilon_\kappa - \lambda)^2 + \Delta_{k\bar{k}}^2}} \right) . \text{ with} \qquad \epsilon_\kappa = \frac{1}{2}(h_{kk} + h_{\bar{k}\bar{k}}) \tag{156}$$

Note, h_{kk} and $\Delta_{k\bar{k}}$ diagonal and skew-diagonal matrix elements. Neither the matrix $h_{kk'}$, nor the matrix $\Delta_{kk'}$ is diagonal in the canonical basis. In many cases one has and additional symmetries, such as time-reversal which guarantees that the matrices h and Δ have block structure

$$h = \begin{pmatrix} h_{++} & 0 \\ 0 & h_{--} \end{pmatrix}, \qquad \text{and} \qquad \Delta = \begin{pmatrix} 0 & \Delta_{+-} \\ -\Delta_{+-}^{\intercal} & 0 \end{pmatrix}. \tag{157}$$

In this case the HFB-matrix can be reduced to half dimension:

$$\begin{pmatrix} h_{++} & \Delta_{+-} \\ \Delta_{+-}^{\dagger} & -h_{--}^{*} \end{pmatrix}. \tag{158}$$

3.8 The Pairing-plus-Quadrupole Model

From general considerations of the theory of effective forces in nuclei one finds that the effective interactions in the *ph*-channel are different from those in the *pp*-channel.

(i) The interaction between the particles can be summed up, as a first approach, by an average spherical single-particle potential which is localized in space and breaks the translational invariance.

(ii) In open shell nuclei, there are two types of additional correlations: long-range *ph*-correlations can be taken into account by a deformation of the mean field. At this point the rotational symmetry is lost.

(iii) Short-range *pp*-correlations are treated by a self-consistent pairing potential Δ which violates number symmetry.

These three aspects are included most simply in the pairing-plus-quadrupole model. The average spherical potential is approximated by a spherical single particle energies ϵ_k^0.The remaining residual interaction has two parts, one contributing to Γ (which here is only that part of the field going beyond the spherical part already contained in the single-particle energies ϵ^0), and the second which contributes to Δ.

Both parts are chosen to be separable in the appropriate indices.

$$H = \sum_k \epsilon_k^0 c_k^+ c_k - \frac{\chi}{2} \sum_{\mu=-2}^{2} : Q_\mu^+ Q_\mu : -GP^+P, \tag{159}$$

with the quadrupole operator

$$Q_\mu = \sum_{kk'} \langle k|r^2 Y_{2\mu}|k'\rangle \, c_k^+ c_{k'}, \tag{160}$$

and the creation operator for a Cooper pair

$$P^+ = \sum_{k>0} c_k^+ c_{\tilde{k}}^+. \tag{161}$$

The actual values of the force constants χ and G are adjusted to experimental data.

Working in a basis symmetric with respect to the signature operation $R_x = \exp(i\pi j_x)$. we find a HFB single-particle Hamiltonian of the form:

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}. \tag{162}$$

where

$$h = h^0 - \frac{1}{2}\sum_{\mu=-2}^{2} q_\mu (Q_\mu^+ + Q_\mu) - \lambda, \qquad \text{with} \quad q_\mu = \chi \langle \Phi | Q_\mu | \Phi \rangle \tag{163}$$

and $\Delta = G\langle \Phi|P^+|\Phi\rangle$ is a multiple of the unity matrix. The deformation parameters q_μ and the gap parameter Δ depend on the solution $|\Phi\rangle$, that is of ρ and κ. They have to be determined by iteration, or by - what is equivalent in the case of separable forces - minimizing the energy $E(q_\mu, \Delta)$ with respect to these parameters. Choosing the principal axis of the density distribution as the axis of our coordinate frame implies $q_1 = q_{-1} = 0$ and $q_2 = q_{-2}$. For a pure pairing force, since Δ is a multiple of unity and invariant under the first Bloch-Messiah transformation. To determine the transformation D it is therefore sufficient to diagonalize the self-consistent field:

$$h = \epsilon^0 + \Gamma = \epsilon^0 - q_0 Q_0 - q_2(Q_2 + Q_{-2}). \tag{164}$$

This is exactly a Nilsson Hamiltonian for fixed deformation parameters q_0 and q_2. The canonical basis in this case is therefore the Nilsson basis with the eigenvalues ϵ_k. In this basis the HFB equations split into 2×2 matrices:

$$\begin{pmatrix} \epsilon_k - \lambda & \Delta \end{pmatrix}, \begin{pmatrix} u_k \\ v_k \end{pmatrix} = \begin{pmatrix} u_k \\ v_k \end{pmatrix} E_k \tag{165}$$

which have the BCS solutions.

To summarize, then, the complete solution of the HFB equations in the pairing-plus-quadrupole model corresponds to a Nilsson diagonalization with variable deformation parameters q_0 and q_2, a subsequent BCS calculation with constant gap parameter $\Delta = p_0$, and a minimization of the total energy

$$E(q_0, q_2, \Delta) = \langle \Phi | H | \Phi \rangle = \sum_k \epsilon_k v_k^2 + \frac{1}{2\chi}(q_0^2 + 2q_2^2) - \frac{\Delta^2}{G} \tag{166}$$

This force explains the Nilsson model with BCS occupation probabilities very nicely and by a suitable choice of the constants G and χ one can reproduce all its results. We have to emphasize, however, that it is only a model constructed for certain phenomena, namely quadrupole deformations and monopole pairing correlations and the interplay between these degrees of freedom. For these phenomena it contains all the gross features of a more realistic approach.

3.9 HFB-theory in the continuum

For exotic nuclei with a large neutron excess the Fermi level of neutrons comes close to the continuum limit. If BCS-correlations produce a scattering of pairs aroud the Fermi surface, we will have partially occupied levels in the continuum. Within BCS-theory these are independent particles and form a gas, which evaporates and the nucleus is no longer stable. In fact, this is only an artifact of the BCS-model. Dobaczewski, Flocard and Treiner could show that in a full HFB-theory we will still have a bound system as long as the chemical potential is negative, i.e. below the continuum limit.

Treating the continuum properly, we have to work in r-space. In this case the HFB-equations are integro-differential equations and the solutions have to fulfill proper boundary conditions. In many applications one uses zero-range forces in the *ph*-channel (e.g. Skyrme forces) as well as in the *pp*-channel. Neglecting spin- and isospin degrees of freedom the potentials $\Gamma(\mathbf{r})$ and $\Delta(\mathbf{r})$ are local and one is left with differential equations of the form

$$\begin{pmatrix} \frac{\mathbf{p}^2}{2m} + \Gamma(\mathbf{r}) - \lambda & \Delta(\mathbf{r}) \\ \Delta(\mathbf{r}) & -\frac{\mathbf{p}^2}{2m} - \Gamma(\mathbf{r}) + \lambda \end{pmatrix} \begin{pmatrix} U(\mathbf{r}) \\ V(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} U(\mathbf{r}) \\ V(\mathbf{r}) \end{pmatrix} E. \tag{167}$$

In the assymptotic region ($r \to \infty$) the potentials Γ and Δ vanish and we

find

$$-\frac{\hbar^2}{2m}\Delta U(r) = (\lambda + E)U(r) \tag{168}$$

$$-\frac{\hbar^2}{2m}\Delta V(r) = (\lambda - E)U(r) \tag{169}$$

It has the asymptotic solutions:

$$U(r)\sim \begin{cases} \cos(k_u r + \delta_u) & \text{for } \lambda + E > 0 \\ \exp(-\kappa_u r) & \text{for } \lambda + E < 0 \end{cases} \tag{170}$$

$$V(r)\sim \begin{cases} \cos(k_v r + \delta_u) & \text{for } \lambda - E > 0 \\ \exp(-\kappa_v r) & \text{for } \lambda - E < 0 \end{cases} \tag{171}$$

with $k_u = \sqrt{2m(\lambda + E)}$, $\kappa_u = \sqrt{-2m(\lambda + E)}$, $k_v = \sqrt{2m(\lambda - E)}$, $\kappa_v = \sqrt{-2m(\lambda - E)}$. For $\lambda > 0$, the entire spectrum is continous. For $\lambda < 0$ only the part of the spectrum with $E > -\lambda$ has a continuum, but for $E < -\lambda$ the spectrum is discrete and the wave functions decay exponentially. We choose only positive E-values and in the case of $\lambda < 0$ we have $\lambda - E < 0$ and therefore for all energies exponentially decaying $V(r)$-functions. The density

$$\rho(\mathbf{r}) = \sum_{E_k<|\lambda|.} |V_k(\mathbf{r})|^2 + \int\limits_{E>|\lambda|} g(E)dE|V_E(\mathbf{r})|^2 \tag{172}$$

is a sum over the discrete part of the spectrum and an integral over continuous part of the spectrum with the level density $g(E)$. Since all the functions $V_k(\mathbf{r})$ and $V_E(\mathbf{r})$ decay exponentially, the density of the system is localized. Of course, we have to include a cutoff Λ for zero-range pairing forces, but this does not influence the fact that the system is bound.

Of course, there is a question left: As we have seen the full HFB-function can be written in the canonical basis as a BCS-function and we find definitely canonical levels with $\epsilon_\kappa = h_{kk} > 0$ which are partially occupied. Why can it happen, that the system is still stable, although simple BCS-theory leads to an unstable solution in such a case. The answer is, that in the canonical basis h is not diagonal, neither Δ. The canonical levels $\epsilon_\kappa = h_{kk}$ do not correspond to eigenstates of h and they are not occupied by independent particles forming a gas. One needs the third transformation in the Bloch-Messiah theorem to get to the independent quasiparicles with energyy E. This additional mixing brings additional binding. The deeply bound states

at the bottom of the average potential Γ lead to large positive quasi-particle enegies and to narrow resonances in the continuum.