# The BCS theory

#### 3.1 The BCS wavefunction

To deal with realistic situations, the degenerate model of Section 2.4 has to be generalized for more realistic applications than those discussed in Chapter 2. We need to consider not only the case where several nucleons outside a closed shell occupy non-degenerate single-particle levels, but also the situation where the matrix elements  $G_{\nu\nu'}$  of the pairing interaction are not necessarily equal. There is no analytical method for finding the energy levels and wavefunctions of the more general pairing Hamiltonian defined in equation (2.28) but the BCS method gives the solution to this problem in the mean-field approximation (Bardeen, Cooper and Schrieffer (1957a,b)).

One way to generalize the ground-state wavefunction of the degenerate model discussed in Chapter 2 is to define an operator

$$B^{\dagger} = \sum_{\nu} g_{\nu} a^{\dagger}_{\nu} a^{\dagger}_{\bar{\nu}}, \qquad (3.1)$$

which creates a correlated pair of nucleons analogous to a Cooper pair. The coefficients  $g_{\nu}$  specify its structure. In a spherical nucleus the binding is strongest for an s-pair with total angular momentum zero. In this case the pair-creation operator can be written in terms of the operators  $P_i^{\dagger}$  defined in equation (2.16)

$$B^{\dagger} = \sum_{j} g_{j} P_{j}^{\dagger}.$$
(3.2)

A completely antisymmetric state  $\Phi_n$  with *n* pairs outside a closed inert core  $|0\rangle$  is approximated by

$$\Phi_n = N_n (B^{\dagger})^n |0\rangle, \qquad (3.3)$$

where  $N_n$  is a normalization constant. The wavefunction (3.3) can be used as a trial wavefunction in a variational principle and the coefficients  $g_j$  treated as variational parameters (de Gennes (1966)). The wavefunction (3.3) is not very easy to work with. One can consider instead a generating function

$$\Phi = C \Pi_{\nu>0} (1 + e^{i\phi} g_{\nu} a^{\dagger}_{\nu} a^{\dagger}_{\bar{\nu}}) |0\rangle, \qquad (3.4)$$

where C is chosen so that  $\Phi$  is normalized. In equation (3.4)  $\nu$  refers to the quantum numbers of the single-particle states  $|j, m\rangle$  and  $\bar{\nu}$  to the time-reversed states  $(-1)^{j-m}|j-m\rangle$  (see Appendix A, Section A.2).

The product in equation (3.4) is over  $\nu > 0$ , where the notation indicates that only a single term is included for each pair of degenerate levels. For example, in a spherical nucleus the product is taken only over positive values of the magnetic quantum numbers *m*. Negative values of *m* are included automatically because  $a_{\nu}^{\dagger} a_{\overline{\nu}}^{\dagger}$  creates a pair in the state  $\nu$  and its time reverse  $\overline{\nu}$ . The state  $\Phi$  is not an eigenstate of the particle number. However the state  $\Phi_n$  can be projected out of  $\Phi$  by picking out the coefficient of  $\exp(in\phi)$  in the expansion of (3.4) (see equations (4.45), (4.46) and subsequent discussion).

The BCS wavefunction is obtained by writing  $\Phi$  in a slightly different way by incorporating the normalization constant into the product (see Appendix G, Section G.4)

$$\Phi = \prod_{\nu > 0} \left( U_{\nu} + V_{\nu} \, a_{\nu}^{\dagger} \, a_{\bar{\nu}}^{\dagger} \right) |0\rangle, \qquad (3.5)$$

with

$$V_{\nu}/U_{\nu} = e^{i\phi}g_{\nu}, \quad |U_{\nu}|^2 + |V_{\nu}|^2 = 1.$$
 (3.6)

In general the coefficients  $U_{\nu}$  and  $V_{\nu}$  are complex but in Sections 3.2–3.7 they are taken to be real quantities restricted only by the normalization condition in equation (3.6), which ensures that  $\Phi$  is normalized to unity. The phase  $\phi$  will reemerge in Section 3.8 and will play an important role as a gauge angle (see also Chapters 1, 4 and Appendix I). The wavefunction  $\Phi$  was introduced by Bardeen, Cooper and Schrieffer (1957a) in their fundamental paper on superconductivity.

The wavefunction  $\Phi$  does not have a definite number of particles, but it can be written as a linear combination of the normalized eigenstates  $\Phi_n$  with the particle number N = 2n

$$\Phi=\sum_n a_n \Phi_n.$$

The average number of particles is

$$\langle N \rangle = 2 \langle n \rangle = 2 \sum_{\nu > 0} |V_{\nu}|^2, \qquad (3.7)$$

and the width  $\Delta N$  of the probability distribution  $|a_n|^2$  is given by

$$(\Delta N)^{2} = \langle N^{2} \rangle - \langle N \rangle^{2} = 4 \sum_{\nu > 0} |U_{\nu}|^{2} |V_{\nu}|^{2}.$$
 (3.8)

To estimate  $\Delta N$  assume that the single nucleon states  $|\nu\rangle$  (i.e. the states  $|jm\rangle$  with positive *m*) have an average spacing *d* and are partially occupied over an energy range  $2\Delta$ . Then

$$(\Delta N)^2 \simeq 2 \ \Delta/d \simeq \langle N_p \rangle \tag{3.9}$$

where  $\langle N_p \rangle$  is the average number of particles occupying single-particle levels with energy lying in this energy range.

In a superconductor  $\langle N_p \rangle \gg 1$  so that

$$\langle N \rangle > \langle N_p \rangle \gg \Delta N \gg 1.$$
 (3.10)

Typical numbers are  $\langle N_p \rangle \simeq 10^{16}$ ,  $\Delta N \sim 10^8$ . In these circumstances the probability distribution of the number of pairs has a very sharp maximum, but  $a_n$  still has a rather smooth dependence on n in the sense that

$$a_n \approx a_{n+p},\tag{3.11}$$

if p is not too large. This result means that expectation values of simple operators can be calculated accurately with the wavefunction  $\Phi$ . Suppose F conserves particle number. Then

$$\langle \Phi | F | \Phi \rangle = \sum |a_{N/2}|^2 \langle N | F | N \rangle.$$
(3.12)

If  $\langle N|F|N \rangle$  is slowly varying on the scale of  $\Delta N$ , then N may be replaced by its average value  $\langle N \rangle = N^*$ , and the matrix element taken outside the summation so that

$$\langle \Phi | F | \Phi \rangle \approx \langle N^* | F | N^* \rangle,$$
 (3.13)

In the same way if F acting on a state with N particles gives a state with N + 2 particles then

$$\langle \Phi | F | \Phi \rangle = \sum_{N} a_{(\frac{N+2}{2})}^{*} a_{(\frac{N}{2})} \langle N+2|F|N \rangle$$

$$\approx \sum_{N} |a_{N/2}|^{2} \langle N^{*}+2|F|N^{*} \rangle$$

$$\approx \langle N^{*}+2|F|N^{*} \rangle.$$

$$(3.14)$$

The situation in a nucleus is different because in a typical case  $\langle N_p \rangle \simeq 10$ and  $\Delta N \sim 3$ . The relations (3.10) are not very well satisfied and the formulae (3.13) and (3.14) are not so accurate. They are, however, still useful for making semi-quantitative estimates. If more accurate values are needed then there are two ways to proceed. Either the number projected wavefunctions  $\Phi_n$  must be used, or the particle number fluctuations in  $\Phi$  must be taken into account (see Chapter 4 and Appendix I, Section I.4, see also Appendix J). Both procedures lead to equivalent results (see Section 6.6). The number projected wavefunctions  $\Phi_n$  have exactly the form of equation (3.3) with  $g_\nu = V_\nu/U_\nu$  (see Section 4.2).

#### 3.2 The energy

The best wavefunction  $\Phi_n$  of the form (3.3) is obtained by minimizing the expectation value  $\langle \Phi_n | H | \Phi_n \rangle$  with respect to the coefficients  $g_v$ . When using the wavefunction  $\Phi$  the procedure is different because the number of particles is not fixed. The expectation value  $\langle \Phi | H | \Phi \rangle$  has to be minimized with a constraint that the average number of particles has a definite value. This can be done by minimizing

$$\langle \Phi | H - \lambda N | \Phi \rangle, \tag{3.15}$$

where  $\lambda$  is a Lagrange multiplier. Physically  $\lambda$  is the Fermi energy. The Hamiltonian *H* contains the single-particle term and the pairing interaction defined in equation (2.28) and is

$$H = \sum_{\nu > 0} \varepsilon_{\nu} (a_{\nu}^{\dagger} a_{\nu} + a_{\bar{\nu}}^{\dagger} a_{\bar{\nu}}) - \sum_{\nu \nu' > 0} G_{\nu \nu'} P_{\nu}^{\dagger} P_{\nu'}.$$
 (3.16)

The expectation value of  $H - \lambda N$  can be calculated in a straightforward way using equation (3.5) for  $\Phi$ . The result is

$$\langle \Phi | H - \lambda N | \Phi \rangle = \sum_{\nu > 0} 2V_{\nu}^{2}(\varepsilon_{\nu} - \lambda) - \sum_{\nu\nu' > 0} G_{\nu\nu'} U_{\nu} V_{\nu} U_{\nu'} V_{\nu'} - \sum_{\nu > 0} G_{\nu\nu} | V_{\nu} |^{4}.$$
(3.17)

Here we have used the relations

$$\langle \Phi | P_{\nu}^{\dagger} | \Phi \rangle = \langle \Phi | P_{\nu} | \Phi \rangle = U_{\nu} V_{\nu}, \qquad (3.18)$$

where  $U_{\nu}$  and  $V_{\nu}$  are taken to be real and positive.

The last term proportional to  $|V_{\nu}|^4$  in equation (3.17) is essentially a Hartree– Fock self-consistent field contribution to the single-particle energy. Its main effect is to give a small renormalization of the single-particle energies. It complicates the theory without giving any important physical effects and is usually neglected because the aim of the simple BCS theory is to focus on the effects of pairing (see Appendix G, Section G.3). We omit it in the subsequent discussions. Any more general interaction would have other Hartree–Fock contributions.

The stationary condition with respect to variations of  $U_{\nu}$  and  $V_{\nu}$ 

$$\delta \langle \Phi | H - \lambda | \Phi \rangle = 0$$

with the constraint  $U_{\nu}\delta U_{\nu} + V_{\nu}\delta V_{\nu} = 0$ , coming from the normalization condition on  $U_{\nu}$  and  $V_{\nu}$ , leads to the equation

$$2(\varepsilon_{\nu} - \lambda)U_{\nu}V_{\nu} - \sum_{\nu'>0} G_{\nu\nu'}(U_{\nu}^2 - V_{\nu}^2)U_{\nu'}V_{\nu'} = 0.$$
(3.19)

This equation can be simplified by setting

$$U_{\nu} = \sin \theta_{\nu}, \quad V_{\nu} = \cos \theta_{\nu}, \tag{3.20}$$

where  $0 \le \theta_{\nu} \le \pi/2$  so that  $U_{\nu} \ge 0$  and  $V_{\nu} \ge 0$ . This representation was used by Anderson (1958) in his paper on collective excitations in superconductors.

The normalization condition for  $U_{\nu}$  and  $V_{\nu}$  is satisfied automatically by this choice and

$$2U_{\nu}V_{\nu} = \sin 2\theta_{\nu}, \qquad |U_{\nu}|^2 - |V_{\nu}|^2 = \cos 2\theta_{\nu}. \tag{3.21}$$

Then the variational equations (3.17) reduce to

$$2(\varepsilon_{\nu} - \lambda) \tan 2\theta_{\nu} = \sum_{\nu' > 0} G_{\nu\nu'} \sin 2\theta_{\nu'}.$$
 (3.22)

Equation (3.22) can be written in the form

$$\tan 2\theta_{\nu} = \frac{\Delta_{\nu}}{\varepsilon_{\nu} - \lambda},\tag{3.23}$$

with

$$\Delta_{\nu} = \frac{1}{2} \sum_{\nu'>0} G_{\nu\nu'} \sin 2\theta_{\nu'} = \sum_{\nu'>0} G_{\nu\nu'} U_{\nu'} V_{\nu'}.$$
(3.24)

The angles  $\theta_{\nu}$  are real and lie in the range  $0 \le \theta_{\nu} \le \pi/2$ . Hence the  $\Delta_{\nu}$  are real and positive if  $G_{\nu\nu'} > 0$ .

Equations (3.23) is equivalent to the relations

$$\sin 2\theta_{\nu} = \frac{\Delta_{\nu}}{E_{\nu}}, \qquad \cos 2\theta_{\nu} = \frac{(\varepsilon_{\nu} - \lambda)}{E_{\nu}}, \qquad (3.25)$$

where

$$E_{\nu} = \sqrt{(\varepsilon_{\nu} - \lambda)^2 + \Delta_{\nu}^2} > 0.$$
(3.26)

We also have

$$|U_{\nu}^{2}| = \frac{1}{2} \left( 1 + \frac{\varepsilon_{\nu} - \lambda}{E_{\nu}} \right), \qquad |V_{\nu}^{2}| = \frac{1}{2} \left( 1 - \frac{\varepsilon_{\nu} - \lambda}{E_{\nu}} \right). \tag{3.27}$$

Note that  $|V_{\nu}|^2 > \frac{1}{2}$  if the state  $\varepsilon_{\nu}$  is below the Fermi level  $\lambda$ . Inserting equations (3.25) into equations (3.24) leads to

$$\Delta_{\nu} = \frac{1}{2} \sum_{\nu'>0} \frac{G_{\nu'\nu} \Delta_{\nu'}}{\sqrt{(\varepsilon_{\nu'} - \lambda)^2 + \Delta_{\nu'}^2}} .$$
(3.28)

These equations have to be solved simultaneously with

$$N = \langle N \rangle \approx \sum_{\nu > 0} \left[ 1 - \frac{\varepsilon_{\nu} - \lambda}{\sqrt{(\varepsilon_{\nu} - \lambda)^2 + \Delta_{\nu}^2}} \right],$$
(3.29)

which can be considered as an equation for the Fermi energy  $\lambda$ . This condition comes from the constraint that the mean number of particles in  $\Phi$  should equal the actual number N in the system. The minimum value of the energy which corresponds to the above set of variational equations is

$$\langle E \rangle = \sum_{\nu>0} 2|V_{\nu}|^2 \varepsilon_{\nu} - \frac{1}{4} \sum_{\mu\nu>0} G_{\mu\nu} \frac{\Delta_{\mu}}{E_{\mu}} \frac{\Delta_{\nu}}{E_{\nu}}.$$
 (3.30)

An important special case is the constant pairing model, where the pairing matrix elements are  $G_{\mu\nu} = G$  for single-particle states  $\mu$  and  $\nu$  lying in a certain range around the Fermi level, and are zero if  $\mu$  or  $\nu$  lie outside that range. In this case the  $\Delta_{\nu} = \Delta$  are all equal and the set of equations (3.28) reduces to a single equation

$$1 = \frac{G}{2} \sum_{\nu > 0} \frac{1}{\sqrt{(\varepsilon_{\nu} - \lambda)^2 + \Delta^2}} = \frac{G}{2} \sum_{\nu} \frac{1}{E_{\nu}}.$$
 (3.31)

This is the well-known gap equation which is the starting point of much of the theory of pairing in nuclei. The total energy equation (3.30) simplifies to

$$\langle E \rangle = 2 \sum_{\nu > 0} |V_{\nu}|^2 \varepsilon_{\nu} - \frac{\Delta^2}{G}.$$
(3.32)

The mean square fluctuation in the nucleon number (3.8) is

$$(\Delta N)^2 = \sum_{\nu > 0} \frac{\Delta^2}{E_{\nu}^2}.$$
 (3.33)

An alternative approach to BCS theory is given in Appendix G.

#### 3.3 Excited states and quasiparticles

The wavefunction  $\Phi$  is a linear combination of states with an even number of particles and is appropriate as an approximation to the ground state of a system

with N even. A possible trial wavefunction for an odd nucleus with a single nucleon in the state  $\mu$  is

$$\Phi_{\mu} = \Pi_{\nu > 0, \nu \neq \mu} (U_{\nu} + V_{\nu} a_{\overline{\nu}}^{\dagger} a_{\nu}^{\dagger}) a_{\mu}^{\dagger} |0\rangle.$$
(3.34)

The expectation value of  $(H - \lambda N)$  in this state can be obtained from equation (3.17) by replacing the term  $2 |V_{\nu}|^2 (\varepsilon_{\mu} - \lambda)$  in the sum over single-particle energies by  $(\varepsilon_{\mu} - \lambda)$  and by omitting the terms with  $\nu$  or  $\nu'$  equal to  $\mu$  in the potential energy terms. The result reduces to

$$\langle \Phi_{\mu}|H - \lambda N|\Phi_{\mu}\rangle - \langle \Phi|H - \lambda N|\Phi\rangle = E_{\mu}, \qquad (3.35)$$

where  $E_{\mu}$  is given by equation (3.26). It is the energy needed to place an odd particle in the state  $\mu$ . The actual situation is more complicated because the argument assumes that adding the extra particle does not change  $\Delta_{\nu}$  or  $\lambda$ . In fact there are changes in both equation (3.28) and equation (3.29) which determine  $\Delta_{\nu}$  and  $\lambda$ . The term  $\nu = \mu$  is omitted in equation (3.28), and in equation (3.29) *N* must be replaced by N + 1 and the term  $\nu = \mu$  omitted in the sum on the righthand side. For a system like a superconductor, where the fluctuations are small, the changes in  $\lambda$  and  $\Delta_{\mu}$  are negligible but in a nucleus they can be important. The changes in excitation energies and wavefunctions due to the fact that the state  $\mu$  is occupied by a single nucleon are called 'blocking effects'.

If blocking effects are neglected, then the wavefunction  $\Phi_{\mu}$  defined in equation (3.34) can be written in another way by introducing quasiparticle creation and annihilation operators by the Valatin (1958)–Bogoliubov (1958a,b) transformations

$$\alpha^{\dagger}_{\mu} = U_{\mu}a^{\dagger}_{\mu} - V_{\mu}a_{\bar{\mu}}, \qquad (3.36a)$$

$$\alpha^{\dagger}_{\bar{\mu}} = U_{\mu}a^{\dagger}_{\bar{\mu}} + V_{\mu}a_{\mu}, \qquad (3.36b)$$

$$\alpha_{\bar{\mu}} = U_{\mu}a_{\bar{\mu}} + V_{\mu}a_{\mu}^{+}, \qquad (3.36c)$$

$$\alpha_{\mu} = U_{\mu}a_{\mu} - V_{\mu}a_{\bar{\mu}}^{+}.$$
 (3.36*d*)

In a spherical nucleus the coefficients  $(U_{\mu}, V_{\mu})$  should depend on *j* but not on *m*. Using the phases introduced in equation (2.22), equation (3.36*a*) can be written as

$$\alpha_{jm}^{\dagger} = U_j a_{jm}^{\dagger} - V_j (-1)^{j-m} a_{j-m}.$$
(3.37*a*)

Equation (3.36b) becomes

$$(-1)^{j+m}\alpha_{j-m}^{\dagger} = (-1)^{j+m}U_j a_{j-m}^{\dagger} + V_j a_{jm}.$$
(3.37b)

These two equations are consistent for both positive and negative m.

The quasiparticle operators in equations (3.37) have the properties

$$\Phi_{\mu} = \alpha_{\mu}^{+} \Phi , \qquad (3.38a)$$

$$\alpha_{\mu}\Phi = 0 , \qquad (3.38b)$$

$$\{\alpha_{\mu}, \alpha_{\nu}^{+}\} = \delta_{\mu\nu}. \tag{3.38c}$$

The operators  $\alpha^{\dagger}_{\mu}$  and  $\alpha_{\mu}$  obey fermion commutation relations and are called quasiparticle creation and annihilation operators. Because of condition (3.38*b*)  $\Phi$  is the quasiparticle vacuum state, and  $\Phi_{\mu}$  defined by equation (3.38*a*) is a onequasiparticle state with a quasiparticle in the state  $\mu$ . The quasiparticle energy is

$$E_{\mu} = \sqrt{(\varepsilon_{\mu} - \lambda)^2 + \Delta^2} , \qquad (3.39)$$

its minimum value being  $\Delta$ .

The wavefunction  $\Phi$  gives an approximate description of the ground state of an even (open shell) nucleus. The one-quasiparticle state  $\alpha^{\dagger}_{\mu} \Phi$  is an approximation to a state of an odd nucleus. The two-quasiparticle state

$$\Phi_{\mu\nu} = \alpha^{\dagger}_{\mu} \alpha^{\dagger}_{\nu} \Phi, \qquad (3.40)$$

with excitation energy

$$E_{\mu} + E_{\nu} \ge 2\Delta, \tag{3.41}$$

is an approximation to an excited state of an even nucleus.

Thus BCS theory with constant pairing predicts that there is an energy gap of at least  $2\Delta$  between the ground state and the two-quasiparticle states. For a metal, this implies that electrons can move without resistance, provided the temperature is low so the probability of collisions with an energy exchange of  $2\Delta$  is low (see Chapter 1, see also discussion end Section 1.2). The system is then said to be in a superconducting state. In the nuclear case the relation (3.41) implies, for example, that the moment of inertia of a deformed system is considerably smaller than the rigid value, provided that the angular momentum is low so that the effect of the Coriolis force is smaller than  $2\Delta$  (see Chapter 6).

The concept of a quasiparticle state is simple only if blocking effects are neglected and the values of  $\Delta$  and  $\lambda$  are kept constant for the ground state and for excited states. Blocking effects become more and more important as more quasiparticles are excited and in the end are responsible for the phase transition from the superconducting to the normal phase when the temperature, magnetic field or angular velocity are increased beyond critical values. As the temperature of a superconductor is increased, more and more quasiparticles are excited and the pairing gap  $2\Delta$  is reduced because of blocking. As the pairing gap is reduced it is easier to excite quasiparticles. At the critical temperature the blocking effects are catastrophic, the pairing gap goes to zero and superconductivity disappears (see Fig. 1.15).

## 3.4 The mean-field Hamiltonian

The single-particle states in the Hartree–Fock theory are eigenstates of the meanfield Hamiltonian. The mean-field potential in this Hamiltonian describes the average interaction of a nucleon with all the other nucleons in the nucleus. In the same way it is possible to introduce a mean field to describe the average pairing interaction. In what follows we give a heuristic approach which is specific for the BCS model with a constant pairing strength.

The procedure is to introduce a pair-potential which is analogous to the Hartree–Fock self-consistent field (see also Appendix G)

$$V_{\text{pair}} = -\Delta(P^{\dagger} + P) \quad \text{with} \quad \Delta = G\langle P^{\dagger} \rangle = G\langle P \rangle.$$
 (3.42)

In this equation  $\langle P^{\dagger} \rangle$  is shorthand for  $\langle \Phi_0 | P^{\dagger} | \Phi_0 \rangle$  and  $P^{\dagger}$  is the pair-creation operator

$$P^{\dagger} = \sum_{\nu>0} a^{\dagger}_{\nu} a^{\dagger}_{\bar{\nu}}.$$
(3.43)

With the sign convention of Section 3.2,  $\Delta$  and  $\langle P^{\dagger} \rangle = \langle P \rangle^*$  are real and positive. A notable feature of the pair-potential (3.42) is that it does not conserve particle number. This is not unexpected because the BCS ground state does not have a good particle number in any case.

The mean-field Hamiltonian is

$$h' = \sum_{\nu>0} (\varepsilon_{\nu} - \lambda) (a_{\nu}^{\dagger} a_{\nu} + a_{\bar{\nu}}^{\dagger} a_{\bar{\nu}}) - \Delta (P^{\dagger} + P).$$
(3.44)

When h' is written in terms of the quasiparticle operators (3.36) it reduces to

$$h' = \sum_{\nu} E_{\nu} (\alpha_{\nu}^{\dagger} \alpha_{\nu} + \alpha_{\bar{\nu}}^{\dagger} \alpha_{\bar{\nu}}) + h_0, \qquad (3.45)$$

where  $E_{\nu}$  are the quasiparticle energies,  $\alpha_{\nu}^{\dagger}$ ,  $\alpha_{\nu}$  are the quasiparticle creation and annihilation operators and  $h_0$  is a constant. The quasiparticle operators (3.36) satisfy Fermi commutation relations. Hence (see (A.69))

$$[h', \alpha_{\nu}^{\dagger}] = E_{\nu} \alpha_{\nu}^{\dagger} \quad \text{and} \quad [h', \alpha_{\nu}] = -E_{\nu} \alpha_{\nu}. \quad (3.46)$$

Substituting the expression (3.44) for h' and (3.36) for  $\alpha_{\nu}^{\dagger}$  we find that (3.44) and (3.45) are consistent provided  $U_{\nu}$  and  $V_{\nu}$  satisfy the matrix equations

$$\begin{pmatrix} \varepsilon_{\nu} - \lambda & \Delta \\ \Delta & -(\varepsilon_{\nu} - \lambda) \end{pmatrix} \begin{pmatrix} U_{\nu} \\ V_{\nu} \end{pmatrix} = E_{\nu} \begin{pmatrix} U_{\nu} \\ V_{\nu} \end{pmatrix}.$$
 (3.47)

The positive eigenvalue of equation (3.47) is the quasiparticle energy

$$E_{\nu} = \sqrt{(\varepsilon_{\nu} - \lambda)^2 + \Delta^2},$$

and the coefficients  $(U_{\nu}, V_{\nu})$  satisfy

$$\Delta V_{\nu} = (E_{\nu} - (\varepsilon_{\nu} - \lambda)) U_{\nu}.$$

Combining this with the normalization condition  $(U_v^2 + V_v^2) = 1$  gives

$$U_{\nu}^{2} - V_{\nu}^{2} = \frac{2(\varepsilon_{\nu} - \lambda)}{\Delta} U_{\nu} V_{\nu}, \qquad (3.48)$$

which is consistent with equations (3.21) and (3.25) (see Appendix G).

We conclude this section with some general remarks about mean-field potentials. Suppose h' includes a deformation potential as well as a pairing potential. A possible form is

$$h' = \sum_{\nu>0} (\varepsilon_{\nu} - \lambda) (a_{\nu}^{\dagger} a_{\nu} + a_{\bar{\nu}}^{\dagger} a_{\bar{\nu}}) - K \langle Q \rangle Q - G (\langle P^{\dagger} \rangle P + \langle P \rangle P^{\dagger}).$$
(3.49)

The first term in (3.49) contains the single-particle energies in a spherical potential. The second is a quadrupole deformation field proportional to a quadrupole moment operator Q of the nucleons in occupied orbitals. It arises from an effective quadrupole–quadrupole interaction between nucleons and is self-consistent in the sense that it is proportional to the average quadrupole moment of the nucleus (Bohr and Mottelson (1975)). The first two terms in (3.49) together correspond to the Nilsson shell-model potential for a deformed nucleus (Nilsson (1955), Nilsson and Ragnarsson (1995)). The third term is the pairing potential.

The total energy of a nucleus with mean-field Hamiltonian (3.49) is

$$\langle (H - \lambda N) \rangle = \sum (\varepsilon_{\nu} - \lambda) \langle N_{\nu} \rangle - \frac{1}{2} K \langle Q \rangle \langle Q \rangle - G \langle P^{\dagger} \rangle \langle P \rangle.$$
(3.50)

The factor  $\frac{1}{2}$  in the second term arises because the quadrupole–quadrupole force is a two-body effective interaction and the term  $-K\langle Q\rangle \langle Q\rangle$  counts the energy of each pair twice. A similar argument explains the relation between the coefficients of the pairing terms in the mean field and in the total energy.

#### 3.5 The correlation energy

The pair-correlation energy of a many-particle system is the difference between the energies with and without pairing. If the pairing strength is constant, the energy including pair correlations is

$$E_{\rm p} = \sum_{\nu > 0} 2|V_{\nu}|^2 \varepsilon_{\nu} - \Delta^2 / G, \qquad (3.51)$$

while the energy without correlations is

$$E_0 = \sum_{\nu > 0} 2|V_{\nu}^0|^2 \varepsilon_{\nu}.$$
 (3.52)

The occupation probabilities  $|V_{\nu}^{0}|^{2}$  in equation (3.52) are unity below the Fermi level and zero above. In both equations (3.51) and (3.52) the Fermi energy  $\varepsilon_{\rm F}$  has to be chosen to give the correct number of particles. The correlation energy is

$$E_{\rm corr} = E_{\rm p} - E_0.$$
 (3.53)

This energy must be negative if the pairing correlations are to be stable. The correlation energy can also be written as

$$E_{\rm corr} = E_{\rm s} - \Delta^2 / G \tag{3.54}$$

where

$$E_{\rm s} = \sum_{\nu>0} 2(|V_{\nu}|^2 - |V_{\nu}^0|^2)\varepsilon_{\nu}.$$
(3.55)

The correlation energy can be estimated in a closed form when the singleparticle levels which contribute to the pairing are uniformly spaced between  $\varepsilon_{\rm F} - \Lambda$  and  $\varepsilon_{\rm F} + \Lambda$  and the pairing strength is constant in this range and zero outside. We choose  $\varepsilon_{\rm F} = 0$  and denote the single-particle level density by g. The level v and its time reverse  $\bar{v}$  are degenerate so the density of levels with v > 0 is g/2. Note that for a uniform level distribution g/2 = 1/d, where d is the energy difference between two successive levels (see Fig. 2.3). The gap equation (3.31) can be written as an integral equation

$$\frac{gG}{4} \int_{-\Lambda}^{\Lambda} \frac{\mathrm{d}\varepsilon}{\sqrt{\varepsilon^2 + \Delta^2}} = 1, \qquad (3.56)$$

provided that the gap parameter  $\Delta$  is large compared with the spacing of singleparticle levels ( $g\Delta \gg 1$ ). The integral can be evaluated to give

$$\frac{gG}{2}\sinh^{-1}(\Lambda/\Delta) = 1.$$
(3.57)

This equation yields a formula for the gap parameter

$$\Delta = \Lambda / \sinh(2/gG) \approx 2\Lambda e^{-2/gG}, \qquad (3.58)$$

where the last formula is valid in the weak coupling limit  $2/gG \gg 1$  or  $\Delta \ll \Lambda$ . With the same approximation the single-particle part of the correlation energy is given by

$$E_{\rm s} = \frac{g}{2} \left[ \int_{-\Lambda}^{\Lambda} \left( 1 - \frac{\varepsilon}{\sqrt{\varepsilon^2 + \Delta^2}} \right) \varepsilon d\varepsilon - 2 \int_{-\Lambda}^{0} \varepsilon d\varepsilon \right]$$
$$= \frac{g}{2} \left[ \Lambda^2 - \Lambda \sqrt{\Lambda^2 + \Delta^2} \right] + \Delta^2 / G$$
$$\approx \Delta^2 / G - g \Delta^2 / 4, \quad \text{if} \quad \Lambda \gg \Delta. \tag{3.59}$$

Substituting this expression in equation (3.54) gives the BCS expression for the correlation energy

$$E_{\rm corr} = -g \frac{\Delta^2}{4} . \tag{3.60}$$

In the case of a uniform level (g = 2/d) distribution  $E_{\text{corr}} = -\Delta^2/2d$ .

At this stage we give some estimates of the parameters in equation (3.58). The total level density for neutrons and protons for a nucleus with N = Z in the Fermi gas model is

$$g_{\rm n} + g_{\rm p} = \frac{3A}{2\varepsilon_{\rm F}} \approx \frac{A}{25} \,\mathrm{MeV}^{-1},\tag{3.61}$$

making use of the Fermi energy  $\varepsilon_{\rm F} = 37$  MeV. Empirical evidence shows that the value given in equation (3.61) is an underestimate. A better estimate which takes surface effects into account (see Chapter 9 and Appendix B) is  $g_{\rm n} + g_{\rm p} = A/16 \,\text{MeV}^{-1}$  (see Bohr and Mottelson (1969), Bortignon, Bracco and Broglia (1998)). In this section we use

$$g_{\rm n} = N/16 \,{\rm MeV^{-1}}, \qquad g_{\rm p} = Z/16 \,{\rm MeV^{-1}},$$
(3.62)

for the neutron and proton level densities (see Section 8.2).

The monopole pairing force constants used in the rare earth region to reproduce the empirical value of the pairing gap are (Nilsson and Ragnarsson (1995), see also equation (2.27))

$$G_{\rm n} = 20.5/A \,{\rm MeV}, \qquad G_{\rm p} = 26/A \,{\rm MeV}.$$
 (3.63)

The parameter combination in the gap equation (3.58) is 2/gG. In the rare earth region this combination does not have a strong *A* dependence and the values for neutrons and protons are

$$2/(g_{\rm n}G_{\rm n}) = 2.7, \qquad 2/(g_{\rm p}G_{\rm p}) = 2.9.$$
 (3.64)

They are consistent with the weak coupling limit (3.58). Bohr and Mottelson (1975) choose  $\Lambda = \hbar \omega_c$  where  $\hbar \omega_c = 41 A^{-1/3}$  MeV is the major shell spacing in the harmonic oscillator shell model. For a nucleus with A = 160 we have  $\Lambda = 7.6$  MeV which leads to a gap parameter  $\Delta_n = 1.0$  MeV for neutrons. The

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global empirical formula given in equation (1.28) gives  $\Delta_n = 0.95$  MeV which is close to the value calculated from the gap equation.

For the same mass number the numerical values of the terms in (3.59) for one type of particle are

$$\Delta^2/G \approx 7.8 \,\mathrm{MeV}, \qquad g \Delta^2/4 \approx 1.5 \,\mathrm{MeV},$$

where the values of  $G_n$  and  $g_n$  from equations (3.63) and (3.62) have been used. In this last equation the empirical value N = 0.6A was used.

The total pairing energy  $\Delta^2/G$  is quite large but in the correlation energy it is partially cancelled by a similar term describing the fact that, in the BCS ground state, particles moving in levels close to the Fermi energy are partially excited across the Fermi surface, in keeping with the fact that  $V_{\nu}^2$  changes smoothly from 1 to 0 around  $\lambda$ , being equal to  $\frac{1}{2}$  at the Fermi energy. The overall result  $E_{\rm corr} \approx$  $-g\Delta^2/4 \approx -1.5$  MeV, corresponds to a considerably smaller (in absolute value) contribution.

#### 3.6 Pairing correlations in the wavefunction

If the nucleus has many nucleons outside closed shells the pairing interaction can produce strong correlations in the wavefunction. The matrix element

$$\alpha_0 = \langle \Phi | P^{\dagger} | \Phi \rangle \tag{3.65}$$

of the pair addition operator  $P^{\dagger}$  is non-zero and gives a measure of the pair correlations in the BCS wavefunction. The operator  $P^{\dagger}$  increases the number of particles by 2 and, according to the arguments in Section 3.1,

$$\alpha_0 = \langle \Phi | S_+ | \Phi \rangle \approx \langle N^* + 2 | P^\dagger | N^* \rangle. \tag{3.66}$$

The matrix element (3.65) can be easily calculated and the result is

$$\alpha_0 = \sum_{\nu > 0} U_{\nu} V_{\nu} = \frac{\Delta}{2} \sum_{\nu > 0} \frac{1}{E_{\nu}} = \frac{\Delta}{G}.$$
(3.67)

Because  $U_{\nu}V_{\nu}$  is peaked at the Fermi energy, one can replace the state dependent value of this quantity by 1/2. Consequently  $2\alpha_0 = \Omega$ .

Thus, the quantity  $\alpha_0$  can be used to give an estimate of the number of correlated pairs in the BCS ground state.

In the rare earth region ( $A \sim 170$ )  $G_{\rm n} \approx 0.12$  MeV,  $G_{\rm p} \approx 0.15$  MeV and  $\Delta_{\rm n} \approx \Delta_{\rm p} \approx 0.92$  MeV and the pairing-correlation parameters for neutrons and protons are estimated as

$$(\alpha_0)_n \approx 8,$$
  $(\alpha_0)_p \approx 6.$  (3.68)

Thus the number of correlated neutron and proton pairs is small, and pairing is a relatively weak effect in nuclei. Consequently, one expects that pairing fluctuations, which play a minor role in macroscopic systems, become important in nuclei (see Chapter 5 and Section 8.4).

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#### 3.7 The degenerate model in the BCS approximation

The pairing model with degenerate single-particle levels was solved analytically by the quasi-spin method in Section 2.4. Expressions were given for the energy levels, wavefunctions, and pair-distortion matrix elements. In this section we test the accuracy of the BCS method by comparing the BCS approximation with the exact results of the quasi-spin approach (see also Appendix H).

The exact ground-state energy of a system with an even number of particles is given in equation (2.39) as

$$E_{\rm ex} = N\varepsilon - \frac{1}{4}GN(2\Omega - N + 2), \qquad (3.69)$$

where  $2\Omega$  is the degeneracy of the level with energy  $\varepsilon$ . To obtain the BCS approximation to the ground-state energy we note that, as all the single-particle energies  $\varepsilon_{\nu}$  are equal, the quasiparticle energies  $E_{\nu}$  and occupation probabilities  $|V_{\nu}|^2$  are independent of  $\nu$ . The gap equation (3.31) reduces to a simple algebraic equation for the quasiparticle energy

$$E = \sqrt{(\varepsilon - \lambda)^2 + \Delta^2} = \frac{1}{2}\Omega G.$$
(3.70)

The constraint (3.7) on the total particle number gives the BCS occupation probability

$$V^2 = \frac{N}{2\Omega}.$$
(3.71)

The Fermi energy and gap parameter are given by

$$\varepsilon - \lambda = \frac{1}{2}G(\Omega - N), \quad \Delta^2 = \frac{1}{4}G^2N(2\Omega - N).$$
 (3.72)

Using these in equation (3.32) for the BCS ground-state energy we get

$$E_{\rm BCS} = N\varepsilon - \frac{1}{4}GN(2\Omega - N). \tag{3.73}$$

To assess the accuracy of the BCS method one can look at the ratio

$$\frac{E_{\rm ex} - E_{\rm BCS}}{E_{\rm ex} - N\varepsilon} = \frac{2}{2\Omega - N + 2}.$$
(3.74)

As an example, one can consider the case of <sup>116</sup>Sn where there are N = 16 valence neutrons occupying the orbits  $g_{7/2}$ ,  $h_{11/2}$ ,  $d_{5/2}$ ,  $d_{3/2}$  and  $s_{1/2}$  (see Fig. 10.2). If all these levels are assumed to be degenerate then  $\Omega = 16$  and the ratio (3.74) is 0.11 or 11%.

The first excited states in the exact solution are the seniority v = 2 states while in the BCS method they are the two-quasiparticle states. The excitation energy is  $\Delta E = G\Omega$  in both cases. The pair-transfer amplitude is the BCS pair-distortion parameter (3.67)

$$\alpha_0 = \Delta/G = \frac{1}{2}\sqrt{N(2\Omega - N)},$$

which agrees well with (2.57) if N and  $\Omega$  are reasonably large. For the <sup>116</sup>Sn example the ratio  $\alpha_0/\langle N+2, 0|P^+|N, 0\rangle$  is equal to  $(16/18)^{1/2} = 0.94$ , implying a 6% error of the BCS estimate. However, the measurable quantity is the ratio of the two-particle transfer cross-sections. In this case, the ratio is 16/18 = 0.89, corresponding again to an 11% error. Note that if one considers the Hartree–Fock self-consistent field contribution in equation (3.17), (3.73) becomes  $E_{\text{BCS}} = NE - \frac{1}{4}GN(2\Omega - N + N/\Omega)$ . The ratio (3.74) is equal to  $(2 - N/\Omega)/(2\Omega - N + 2)$  (Lawson (1980)) which has the value 0.06 for  $\Omega = N = 16$ .

### 3.8 Gauge invariance

There is a close analogy between the BCS wavefunction for a system with pairing and the Hartree–Fock wavefunction of a deformed nucleus (Bes and Broglia (1966)). In both cases there is a broken symmetry, which is the topic of discussion of the next chapter, and which is briefly touched upon in this section. First we recall some properties of a deformed Hartree–Fock wavefunction.

The Hartree–Fock method approximates the ground-state wavefunction of a nucleus by a Slater determinant which minimizes the expectation value of the Hamiltonian (see Appendix A). The nuclear Hamiltonian is rotationally invariant and its exact eigenstates are also eigenstates of angular momentum. On the other hand, in many cases, the Hartree–Fock state is deformed and is not an angular momentum eigenstate. Symmetry is broken because the Hartree–Fock wavefunction has a lower symmetry than the original Hamiltonian. Rotational symmetry is still present in the sense that there are many degenerate solutions of the Hartree–Fock equations. Rotating one solution yields another with the same energy. States with definite angular momentum, which are approximations to the states in the lowest rotational band of the nucleus, can be projected out of a deformed Hartree–Fock wavefunction. The Hartree–Fock state is called the intrinsic state of the rotational band (Nilsson (1955), Bohr and Mottelson (1975), see equation (3.50)).

The BCS wavefunction has analogous properties. The pairing Hamiltonian conserves particle number and if N is the particle number operator

$$[N, H] = 0 \text{ or } U^{\dagger}(\chi) H U(\chi) = 1,$$
 (3.75)

where the unitary gauge operator is defined as

$$U(\chi) = e^{-iN\chi/2}.$$
 (3.76)

The relations (3.75) express the fact that *H* is invariant for rotations in gauge space. The general BCS wavefunction is

$$\Phi = \Pi_{\nu>0}(U_{\nu} + \mathrm{e}^{\mathrm{i}\phi}V_{\nu}a_{\nu}^{\dagger}a_{\bar{\nu}}^{\dagger})|0\rangle, \qquad (3.77)$$

where  $U_{\nu}$  and  $V_{\nu}$  are chosen to be real. The gauge operator acting on  $\Phi$  gives

$$U(\chi)\Phi = \prod_{\nu>0} (U_{\nu} + e^{i(\phi-\chi)} V_{\nu} a_{\nu}^{\dagger} a_{\bar{\nu}}^{\dagger}) |0\rangle.$$
(3.78)

The BCS state  $\Phi$  does not have a definite particle number and can be called a 'deformed state in gauge space'. The angle  $\phi$  specifies the orientation of the BCS state  $\Phi$  in gauge space and  $U(\chi)$  rotates it through an angle  $\chi$  in that space. Invariance of H for rotations in gauge space implies that the energy expectation value is independent of  $\phi$  or  $\chi$ . The BCS wavefunction (3.77) can be thought of as being deformed in gauge space. The  $\alpha_0$  in equation (3.65) gives a measure of the deformation. For this reason it is sometimes called the pair-distortion parameter.

As discussed in Section 3.1 the BCS state can be written as a linear combination of normalized states  $\Phi_n$  with a definite number of pairs n = N/2,

$$\Phi = \sum a_n \mathrm{e}^{\mathrm{i}n\phi} \Phi_n. \tag{3.79}$$

Projection of a state with definite particle number *n* means to pick out the component  $\Phi_n$  from  $\Phi$ . It is the term with coefficient proportional to  $e^{in\phi}$  in the expansion (3.79).

The gauge angle  $\chi$  is the conjugate variable to the number *n* of pairs. One can transform from a pair number to a gauge angle representation by making a Fourier transformation (see discussion after equation (4.46), Section 4.2)

$$\Phi(\chi) = \sum_{n} e^{in\phi} \Phi_{n}.$$
 (3.80)

Then the gauge angle  $\chi$  is a dynamical variable conjugate to the number of pairs *n*. In the gauge angle representation the operator can be written as

$$n = -i\frac{\partial}{\partial\chi}.$$
 (3.81)

There is an uncertainty relation between  $\chi$  and *n* 

$$\Delta \chi \Delta n \sim 1, \tag{3.82}$$

which has to be understood with the same qualifications as for the angle – angular momentum uncertainty relation because  $\chi$  is restricted to the range  $0 \le \chi < 2\pi$ . These subjects are taken up in further detail in the next chapter (see also Appendix I).

#### 3.9 Matrix elements of one-body operators

Formulae for matrix elements of one-body operators in the BCS theory are derived in Lane (1964), Kisslinger and Sorensen (1963), Rowe (1970), Bes and Sorensen (1969), Ring and Schuck (1980), Bohr and Mottelson (1975). For completeness we summarize some of the important results here. In second

quantization the one-body operator  $\hat{F}$  is

$$F = \sum_{\mu\nu} \langle \mu | F | \nu \rangle a_{\mu}^{\dagger} a_{\nu}.$$
(3.83)

Expressing the particle-creation and annihilation operators in terms of quasiparticle operators this equation becomes

$$F = \sum_{\mu\nu} \langle \mu | F | \nu \rangle \left( U_{\mu} \alpha_{\mu}^{\dagger} + V_{\mu} \alpha_{\bar{\mu}} \right) \left( U_{\nu} \alpha_{\nu} + V_{\nu} \alpha_{\bar{\nu}}^{\dagger} \right)$$
$$= F_{0qp} + F_{1qp} + F_{2qp} + F_{2qp}^{\dagger}.$$
(3.84)

Here

$$F_{0qp} = \sum_{\nu} \langle \nu | F | \nu \rangle V_{\nu}^{2},$$
  

$$F_{1qp} = \sum_{\mu\nu} \langle \mu | F | \nu \rangle \left( U_{\mu} U_{\nu} \alpha_{\mu}^{\dagger} \alpha_{\nu} - V_{\mu} V_{\nu} \alpha_{\bar{\nu}}^{\dagger} \alpha_{\bar{\mu}} \right),$$
  

$$F_{2qp} = \sum_{\mu\nu} \langle \mu | F | \nu \rangle U_{\mu} V_{\nu} \alpha_{\mu}^{\dagger} \alpha_{\bar{\nu}}^{\dagger},$$
(3.85)

where the Bogoliubov amplitudes  $U_{\nu}$  and  $V_{\nu}$  are real.

The operator  $F_{0qp}$  does not depend on the quasiparticle operators and may have a non-zero expectation value in the BCS vacuum state  $|BCS\rangle$ . The  $F_{1qp}$  operator has matrix elements between one-quasiparticle states while the operators  $F_{2qp}$ and  $F_{2qp}^{\dagger}$  create and annihilate pairs of quasiparticles respectively.

When the operator F has the time-reversal properties  $(\tau^{-1}F\tau)^{\dagger} = -cF$  then the analysis carried out in Appendix A, Section A.2 shows that

$$\langle \bar{\mu}|F|\bar{\nu}\rangle = -c\langle \nu|F|\mu\rangle$$
 and  $\langle \mu|F|\bar{\nu}\rangle = c\langle \nu|F|\bar{\mu}\rangle.$  (3.86)

Using these relations we get

$$F_{0qp} = \sum_{\nu>0} V_{\nu}^{2} \left( \langle \nu | F | \nu \rangle + \langle \bar{\nu} | F | \bar{\nu} \rangle \right) = \sum_{\nu>0} V_{\nu}^{2} (1-c) \langle \nu | F | \nu \rangle.$$
(3.87)

The expression for  $F_{1qp}$  can be simplified by making a change of summation variables  $\bar{\nu} \rightarrow \mu$  and  $\bar{\mu} \rightarrow \nu$  in the second term. It reduces to

$$F_{1qp} = \sum_{\mu\nu} \langle \mu | F | \nu \rangle \left( U_{\mu} U_{\nu} \alpha_{\mu}^{\dagger} \alpha_{\nu} + c V_{\mu} V_{\nu} \alpha_{\nu}^{\dagger} \alpha_{\nu} \right).$$
(3.88)

In a similar way

$$F_{2qp} = \sum_{\mu > \nu} \left( U_{\nu} V_{\mu} - c U_{\mu} V_{\nu} \right) \langle \mu | F | \bar{\nu} \rangle \alpha_{\mu}^{\dagger} \alpha_{\nu}^{\dagger}.$$
(3.89)

Matrix elements of F between states with the same number of quasiparticles or with quasiparticle number differing by 2 can be calculated from these

expressions. Pair correlations can enhance or suppress matrix elements depending on the time-reversal properties of the operator.

One example is the influence of pairing correlations on matrix elements of single-particle multipole operators in one-quasiparticle states in a spherical nucleus. The reduced matrix element of the operator  $F_{\lambda\mu}$  in a quasiparticle state  $\bar{j}$  is related to the corresponding single-particle reduced matrix element by

$$\langle \bar{j} \| F_{\lambda} \| \bar{j} \rangle = \left( U_j^2 + c V_j^2 \right) \langle j \| F_{\lambda} \| j \rangle.$$
(3.90)

The quadrupole operator  $Q_{2\mu}$  is time-even and has c = -1. Hence quadrupole matrix elements in one-quasiparticle states are modified by a factor  $\left(U_j^2 - V_j^2\right)$ . This factor is positive if the quasiparticle state is above the Fermi level and negative if it is below. On the other hand the magnetic moment operator  $M_{1\mu}$  is time-odd, has c = 1 and the corresponding factor is  $\left(U_j^2 + V_j^2\right) = 1$ . Thus the magnetic moment of a quasiparticle state is the same as for a particle state.

Another example is the effect of pairing on the moment of inertia of a deformed nucleus. The cranking moment of inertia in a nucleus with pairing is (Belyaev (1959), Migdal (1959), Bohr and Mottelson (1975))

$$\mathcal{I} = 2\hbar^2 \sum_{\mu\nu} \frac{|\langle \mu\nu| j_y |BCS\rangle|^2}{E_\mu + E_\nu},$$
(3.91)

where the sum is taken over two-quasiparticle states. Using the relation between two-quasiparticle matrix elements and particle matrix elements we have

$$|\langle \mu \nu | j_y | BCS \rangle|^2 = |\langle \mu | j_y | \bar{\nu} \rangle|^2 \left( U_\mu V_\nu - U_\nu V_\mu \right)^2$$
(3.92)

because  $j_y$  is a time-odd operator and c = 1. The cranking formula gives a moment of inertia equal to the rigid value when there are no pairing correlations. Pairing correlations reduce the moment of inertia partly because the energy denominators are increased (the quasiparticle excitation energies are larger than the corresponding particle excitations) and partly because the two-quasiparticle matrix elements of  $j_y$  are smaller than the corresponding particle matrix elements.

#### 3.10 Pairing and isospin

An important nuclear symmetry property manifests itself in the conservation of isospin: a nuclear state is characterized by the total isospin quantum number as well as by the total angular momentum, the number of pairs of particles, etc. The existence of the isospin symmetry requires that the Hamiltonian describing the nuclear system should be invariant under rotations in isospace. The isospin symmetry is violated by a pairing interaction acting only between identical nucleons,

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as was the case considered in the previous sections. Thus an invariant pairing force must, in addition to the nn and pp terms, contain pn components. One may distinguish between an isoscalar (T = 0) and an isovector (T = 1) pairing interaction. The isoscalar pairing interaction acts only between np pairs coupled to T = 0. The isovector interaction has equal matrix elements between pp, np and nn pairs coupled to T = 1 (see e.g. Bohr (1968), Nathan (1968), Bayman *et al.* (1969), Bes *et al.* (1977), Dussel *et al.* (1970), Garrido *et al.* (1999)).

Parikh (1965) gave an exact solution of the pairing problem for a system of neutrons and protons in a degenerate single-particle level interacting with an isovector pairing force by generalizing the quasi-spin methods using identical nucleons. The role of the seniority v is played by two quantum numbers, namely the seniority itself and the reduced isospin t (which is the isospin of the unpaired nucleons). Within each representation (v, t), the states are labelled by the total number of nucleons N, the total isospin T and its z-component  $T_z$ . The energy eigenvalues are given by

$$E(v, t; N, T) = -\frac{G_1}{2} \left[ N\left(\Omega - \frac{N-6}{4}\right) - v\left(\Omega - \frac{v-6}{4}\right) + t(t+1) - T(T+1) \right]$$
(3.93)

This expression reduces to equation (2.39) in the case of identical nucleons by putting T = N/2 and t = v/2. If v = 0 only even (odd) values of T are allowed if the number of pairs is even (odd).

## 3.10.1 T = 0 and T = 1 pairing co-existence

All the discussion in the previous sections of this chapter relate to isovector pairing. The strength of the two-body nucleon–nucleon interaction is comparable in T = 0 and T = 1 states so there is no *a priori* reason why pairing should be more important for isovector pairs than for isoscalar pairs. To give an idea of the issues involved we refer to a selection of the many papers written on this subject.

Engel *et al.* (1997) examined the possible co-existence of isovector and isoscalar pairing in an exactly solvable model. They considered a degenerate model with a Hamiltonian containing both isovector (T = 1, S = 0) and isoscalar pairing (T = 0, S = 1) pairing. The Hamiltonian contains a parameter x which fixes the relative strengths of the isovector and isoscalar pairing; x = -1 is pure isovector pairing, x = 1 is pure isoscalar while for x = 0 the isovector and isoscalar strengths are equal. They calculated the overlap between the exact ground state and the pure isovector spin-singlet paired state as a function of x in a T = 0 nucleus with an even number of pairs. They found that there is a

relatively sharp phase transition as x increases through zero. The ground state is a rather pure isovector paired state for x < 0 and changes to an isoscalar paired state as x increases through zero. There is a strong mixing for x = 0 and for this value of x the Hamiltonian has Wigner SU(4) supermultiplet symmetry.

Goodman (1998) solved the isospin generalized BCS and Hartree–Fock– Bogoliubov equations for the ground states of even–even N = Z nuclei with mass numbers A = 76-96. His calculations included both isovector and isoscalar pairing. He found a transition from isovector pairing at the beginning of the isotope sequence to isoscalar pairing near the middle of the sequence. These results indicate that T = 0 and T = 1 pairing can co-exist and that T = 0 pairing can be dominant in some nuclei. This result is consistent with the findings of Engel *et al.* (1997). In a recent paper Bes *et al.* (2000) found a more general class of solutions to the BCS equations in the presence of isovector and isoscalar pairing correlations.

One indication of np pairing comes from the Wigner energy. This is an additional binding energy of an N = Z nucleus relative to its neighbours which appears as a spike in the isobaric mass parabola as a function of  $T_3 = |N - Z|/2$ . Satula et al. (1997a) used a standard form for the Wigner energy and extracted its parameters from experimental binding energies. Then they made shell model calculations in the s-d and p-f shells using standard interactions which include both T = 1 and T = 0 components. The parameters of the Wigner energy extracted from the shell model binding energies fit the experimental values (see also Goriely et al. (2001, 2002)). The authors repeated the shell model calculations with the T = 0 components removed. By comparing the results of the two calculations they found that most of the Wigner energy in the shell model calculations comes from the T = 0 neutron-proton interaction and that the interaction between deuteron-like (J = 1) and 'stretched'  $(J_{max})$  pairs are of comparable importance. Within this context, it may be possible to create a T = 0 nuclear vortex (see Appendix K, and Ramon Wyss, Key Topics in Nuclear Structure, Abstracts, Paestum 23-27 May 2004, p. 73, as well as Satula and Wyss (2001a) and Frauendorf and Sheikh (2000)).

Satula and Wyss (1997b) studied the competition between T = 0 and T = 1pairing in  $N \approx Z$  nuclei in a cranked mean field calculation (see also Satula and Wyss (2001b)). They found that the sudden phase transition between T = 0 and T = 1 pairing is a generic feature of the BCS approximation for N = Z nuclei. This phase transition is smeared out if a good particle number is projected out by the Lipkin (1960), Nogami (1964) method. Then the T = 0 and T = 1 pairing correlations can co-exist even at non-zero rotational frequencies. For  $N \neq Z$  nuclei T = 0 and T = 1 pairing correlations can co-exist even in the BCS approximation but are confined to a narrow region along the N = Z line. The additional binding arising from these correlations can be viewed as a microscopic origin of the Wigner energy in even nuclei.

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