

## Chapter 4

### BCS Superfluidity

#### 4.1 Bardeen-Cooper-Schrieffer theory

The classic theory of superfluidity/superconductivity was put forth by Bardeen, Cooper, and Schrieffer in 1957 [56]. Entitled BCS theory, after its founders, the ideas presented in this seminal work were able to successfully explain almost all observed properties of conventional superconductors. We will extend BCS theory in Chapter 5 to incorporate Feshbach resonant interactions, but first it will prove instructive to review some fundamentals.

#### 4.2 Cooper pairing

The cardinal process behind superfluidity is the formation of Cooper pairs. Cooper, who originally studied the problem [57], showed that fermions, interacting above a closed Fermi sea, will show an instability towards forming pairs regardless of the weakness of the interaction, so long as the interaction remains attractive. Due to the sharpness of the Fermi surface, the main contribution to this population of paired states will arise between atoms on opposite ends of the Fermi surface. For instance, if we consider the s-wave pairing of a two spin state system ( $\uparrow, \downarrow$ ), pairs will prefer to form between atoms of  $\mathbf{k}, \uparrow$  and  $-\mathbf{k}, \downarrow$  (see Fig. 4.1). As long as the Fermi surface remains relatively sharp, it is unlikely that other combinations of pairs will form. This statement is more clearly illustrated in combination with Fig. 4.2.

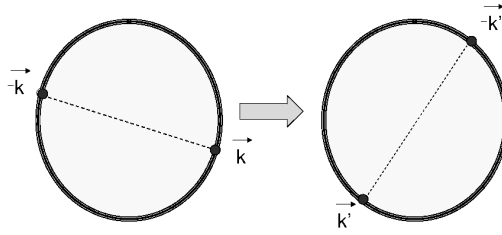


Figure 4.1: For s-wave collisions, pairs of atoms with opposite spin will form at the Fermi surface. The interior region represents the filled Fermi sea whereas the dark line around the edge shows the range of available states. In order to conserve energy the state shown on the left may scatter into any available state (right) which lies along its equipotential surface. For this example, the equipotential surface lies within the available states at the Fermi surface.

In a true many-body system, these atom pairs do not truly form bound states, but should rather be thought of as resulting from strong correlations. The energy gap, and most of the observed properties of superconductors, would be absent if it weren't for the strong correlations between these pairs. It should be noted, however, that these correlations result more from the Pauli blocking of available states within the Fermi surface than from the actual dynamical interactions. As a consequence, it is often a very good approximation to treat the system as though the interactions only occur between the Cooper pairs. This scheme may be called the BCS or pairing approximation.

### 4.3 BCS linearization and canonical transformation

Let us begin by discussing BCS theory as derived from the method of canonical transformation [58, 59]. We start with the following interacting Hamiltonian which accounts for the effects of pair-wise interactions:

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} a_{\mathbf{k}\uparrow}^{\dagger} a_{-\mathbf{k}\downarrow}^{\dagger} a_{-\mathbf{k}'\downarrow} a_{\mathbf{k}'\uparrow}, \quad (4.1)$$

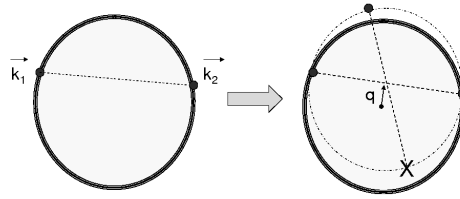


Figure 4.2: If we attempt to form a Cooper pair between  $\mathbf{k}, \uparrow$  and  $\mathbf{k}', \downarrow$ , where  $\mathbf{k} \neq -\mathbf{k}'$ , the number of states which the pair may scatter into is severely limited. This may be seen by transforming to a frame in which the pairs form with equal and opposite momentum, but with center of mass momentum  $\mathbf{q}$ . The equipotential surface is given by the dotted line and only rarely falls within the available region of states.

where  $a_{\mathbf{k}\sigma}^\dagger$  ( $a_{\mathbf{k}\sigma}$ ) are fermion creation(annihilation) operators,  $\epsilon_k = \hbar^2 k^2 / 2m$ , and  $V_{\mathbf{k}\mathbf{k}'}$  define the matrix elements of the interaction potential. A fundamental idea behind BCS theory is that the many-body wavefunction will be constructed of a phase coherent superposition of paired states

$$|\phi_N\rangle = \sum_{\mathbf{k}_1} \cdots \sum_{\mathbf{k}_{N/2}} g_{\mathbf{k}_1} \cdots g_{\mathbf{k}_{N/2}} a_{\mathbf{k}_1 \uparrow}^\dagger a_{-\mathbf{k}_1 \downarrow}^\dagger \cdots a_{\mathbf{k}_{N/2} \uparrow}^\dagger a_{-\mathbf{k}_{N/2} \downarrow}^\dagger |\varphi_0\rangle, \quad (4.2)$$

where  $g_{\mathbf{k}_{N/2}}$  is the weight of each of the  $N/2$  paired states and  $|\varphi_0\rangle$  is the vacuum ket. Because of this phase coherence, operators such as  $a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow}$  may not average to zero as they would in the normal state where the phases are at random. What's more, for a large number of particles one may assume that the fluctuations about these averages should be small. With this in mind, we rewrite the paired operator as

$$a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} = \langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \rangle + (a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} - \langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \rangle), \quad (4.3)$$

which separates the average (first term) from the fluctuations about the average (second term). Substitution of Eq. (4.3) into Eq. (4.1) results in

$$H = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} (a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger \langle a_{-\mathbf{k}'\downarrow} a_{\mathbf{k}'\uparrow} \rangle + \langle a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger \rangle a_{-\mathbf{k}'\downarrow} a_{\mathbf{k}'\uparrow}), \quad (4.4)$$

where  $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$ . We have introduced a chemical potential since the linearized Hamiltonian no longer conserves number. The chemical potential may be adjusted to gain

the desired number of atoms. We may now define the gap

$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle a_{-\mathbf{k}'\downarrow} a_{\mathbf{k}'\uparrow} \rangle. \quad (4.5)$$

For the moment, the name may seem a bit arbitrary, but this function will later be shown as equivalent to the value of the gap in the energy spectrum. The Hamiltonian may now be written as:

$$H = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} (\Delta_{\mathbf{k}} a_{\mathbf{k}\uparrow}^{\dagger} a_{-\mathbf{k}\downarrow}^{\dagger} + \Delta_{\mathbf{k}}^* a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow}). \quad (4.6)$$

This Hamiltonian may be diagonalized by an appropriate canonical transformation (see Appendix B) of the general form

$$\begin{pmatrix} a_{\mathbf{k}\uparrow} \\ a_{-\mathbf{k}\downarrow}^{\dagger} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}}^* & v_{\mathbf{k}} \\ -v_{\mathbf{k}}^* & u_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \gamma_{\mathbf{k}0} \\ \gamma_{\mathbf{k}1}^{\dagger} \end{pmatrix}, \quad (4.7)$$

where the  $\gamma$ 's are a new set of Fermi operators and the weights  $u_{\mathbf{k}}$  and  $v_{\mathbf{k}}$  must satisfy the relationship

$$|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1, \quad (4.8)$$

for the resulting transformation to remain unitary. Note that an inversion of Eq. (4.7) shows that the new operators  $\gamma$  have the net effect of mixing the spins. By inserting these substitutions into Eq. (4.6) we will recover a diagonal Hamiltonian, that is, one that only contains density type pairs of operators  $\gamma_{\mathbf{k}}^{\dagger} \gamma_{\mathbf{k}}$ , if the following condition is satisfied:

$$\Delta_{\mathbf{k}}^* v_{\mathbf{k}}^2 - \Delta_{\mathbf{k}} u_{\mathbf{k}}^2 + 2\xi_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} = 0. \quad (4.9)$$

Multiplying through by  $\Delta_{\mathbf{k}}^*/u_{\mathbf{k}}^2$  and solving the resulting quadratic equation in terms of  $\Delta_{\mathbf{k}}^* v_{\mathbf{k}}/u_{\mathbf{k}}$  we have the following condition for the coefficients

$$\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} = \frac{E_{\mathbf{k}} - \xi_{\mathbf{k}}}{\Delta_{\mathbf{k}}^*}, \quad (4.10)$$

where we define  $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$ . Equation (4.10), which is the positive root, is chosen since it corresponds to the stable minimum (as opposed to the unstable maximum)

energy solution. By combining Eq. (4.8) and Eq. (4.10) we have the following result for the value of the coefficients:

$$|v_{\mathbf{k}}|^2 = 1 - |u_{\mathbf{k}}|^2 = \frac{1}{2} \left( 1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right). \quad (4.11)$$

It should be noted that, although the phases up until now are written arbitrarily, the phase of  $u_{\mathbf{k}}$ ,  $v_{\mathbf{k}}$ , and  $\Delta_{\mathbf{k}}$  must occur so that  $\Delta_{\mathbf{k}}^* v_{\mathbf{k}}/u_{\mathbf{k}}$  is real, as implied by Eq. (4.10).

#### 4.4 The appearance of an energy gap

The resulting diagonal Hamiltonian (Eq. (4.6) written in terms of the basis defined in Eq. (4.7)) is

$$H = \sum_{\mathbf{k}} (\xi_{\mathbf{k}} - E_{\mathbf{k}}) + \sum_{\mathbf{k}} E_{\mathbf{k}} (\gamma_{\mathbf{k}0}^\dagger \gamma_{\mathbf{k}0} + \gamma_{\mathbf{k}1}^\dagger \gamma_{\mathbf{k}1}). \quad (4.12)$$

The first term gives a constant shift to the energy spectrum while the second term describes the elementary quasi-particle excitations of the system. The energy of these excitations is given by

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}, \quad (4.13)$$

so that, even at  $\xi_{\mathbf{k}} = 0$ , there remains a finite energy  $\Delta_k$  which must be invested in order to excite the system. This gap in the energy spectrum justifies our earlier labelling of  $\Delta_k$ .

#### 4.5 Populating the quasi-particles

In this diagonal representation, we may write the gap as

$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle a_{-\mathbf{k}'\downarrow} a_{\mathbf{k}'\uparrow} \rangle = - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} u_{\mathbf{k}'}^* v_{\mathbf{k}'} \langle 1 - \gamma_{\mathbf{k}'0}^\dagger \gamma_{\mathbf{k}'0} + \gamma_{\mathbf{k}'1}^\dagger \gamma_{\mathbf{k}'1} \rangle. \quad (4.14)$$

In thermal equilibrium, the quasi-particles behave as noninteracting fermions so they distribute themselves according to Fermi statistics:

$$f(E_{\mathbf{k}}) = \frac{1}{e^{\beta E_{\mathbf{k}}} + 1}. \quad (4.15)$$

By writing

$$\langle 1 - \gamma_{\mathbf{k}'0}^\dagger \gamma_{\mathbf{k}'0} + \gamma_{\mathbf{k}'1}^\dagger \gamma_{\mathbf{k}'1} \rangle = 1 - 2f(E_{\mathbf{k}'}), \quad (4.16)$$

we may convert Eq. (4.14) to the following form

$$\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh \frac{\beta E_{\mathbf{k}'}}{2}. \quad (4.17)$$

In deriving Eq. (4.17) we have used the trigonometric identity  $\tanh(x/2) = 1 - 2f(x)$ . Equation (4.17) is called the gap equation. It is often assumed that the potential is constant  $V_{\mathbf{k}\mathbf{k}'} = V$  which results in a constant gap  $\Delta_{\mathbf{k}'} = \Delta$ . This considerably simplifies the problem since a factor of  $\Delta$  may be removed from both sides of the equation resulting in

$$\frac{1}{V} = - \sum_{\mathbf{k}} \frac{\tanh(\beta E_{\mathbf{k}}/2)}{2E_{\mathbf{k}}}. \quad (4.18)$$

We may perform the same transformation on the expectation value of the number operator to derive a second equation

$$\begin{aligned} n_\sigma = \sum_{\mathbf{k}} \langle a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} \rangle &= \sum_{\mathbf{k}} |u_{\mathbf{k}}|^2 f(E_{\mathbf{k}}) + |v_{\mathbf{k}}|^2 (1 - f(E_{\mathbf{k}})) \\ &= \sum_{\mathbf{k}} \frac{1}{2} \left( 1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \tanh(\beta E_{\mathbf{k}}/2) \right). \end{aligned} \quad (4.19)$$

Equations (4.18) and (4.19) are a closed set of equations forming the foundations of BCS theory. Unfortunately, due to the form of the potential  $V_{\mathbf{k}\mathbf{k}'}$  that we have chosen, these equations will diverge. This divergence, however, may be remedied by a proper renormalization. In the case of superconductors, the divergence is often remedied by cutting the integral at the Debye energy since only a very limited shell of states about the Fermi surface are thought to contribute. However, for atomic systems, the renormalization may be performed by matching the potentials to the T-matrix describing the full 2-body scattering processes. This was explained in detail in Chapter 2.6.

## 4.6 Critical temperature

For dilute interactions, we may assume that the potential is given by  $V = 4\pi\hbar^2 a_{sc}/m$ , where  $m$  is the mass of each fermion and  $a_{sc}$  is the s-wave scattering length. At the critical point the gap vanishes,  $\Delta = 0$ , and we may solve Eqs. (4.18) and (4.19) for the critical temperature  $T_c$ . Under the assumption that  $k_F a_{sc} \ll 1$ , we find for the critical temperature:

$$\frac{T}{T_F} \approx .614e^{-\pi/(2k_F|a_{sc}|)}. \quad (4.20)$$

The exponential form of Eq. (4.20), although only approximate, shows that we must enhance the scattering in order to raise the critical temperature. For  $k_F a_{sc} \sim 1$  we have a critical temperature  $T_c/T_F \sim 0.1$ —a temperature which is accessible to modern experiments. One method to enhance the scattering, and obtain critical temperatures of this magnitude, would be by tuning the particle-particle interactions with a Feshbach resonance. In the next section, we discuss how to incorporate these resonant scattering interactions into this model.