

# Kapitel 4

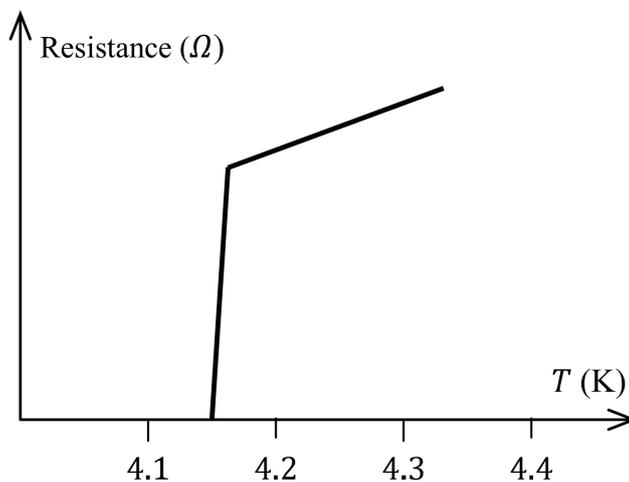
## Superconductivity

In this chapter, we shall introduce the fundamental experimental facts about superconductors and present a summary of the derivation of the BSC theory (Bardeen, Cooper and Schrieffer). This chapter is kept short due to the existence of the parallel lectures in this semester dedicated exclusively to the superconductivity.

### 4.1 Experimental results

#### 4.1.1 Zero resistance

In 1911, Kamerlingh Onnes (Nobel Prize 1913) observed that the resistance of Hg shows an abrupt drop at  $T_c = 4.15$  K (Fig. 4.1). Usually, the resistance of normal metals like



**Abbildung 4.1:** Resistance of Hg at a superconducting transition.

Cu, Ag or Na shows the following temperature dependence:

$$R(T) = R_0 + aT^2 + bT^5,$$

where  $R_0$  is proportional to the concentration of impurities in the system. The  $T^5$  contribution is due to electron-phonon scattering processes and the  $T^2$  contribution originates

from the electron-electron interaction. For a superconductor (as shown in Fig. 4.1),

$$R(T) = 0 \quad \text{for} \quad T < T_c,$$

where  $T_c$  is the critical temperature. This behavior is independent of impurities. Thus, a superconductor behaves like an *ideal metal* without impurities, which means that a system in the superconducting phase can conduct without dissipation loss. Such behavior is technologically desirable, and since decades a lot of effort has been devoted to the search for superconductors with high  $T_c$ .

Before 1986, the highest  $T_c$  was  $T_c = 23$  K for  $\text{Nb}_3\text{Ge}$ . In order to reach this low temperatures, one has to use expensive liquid helium for cooling. In 1986, Bednorz and Müller discovered that by hole doping copper oxide  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ , they could get the material superconducting at  $T_c \approx 35$  K. Following this route of doping copper oxides, in 1987  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  was shown to become superconducting at  $T_c \approx 90$  K. This set a hallmark for technical purposes since in this case one can use cheap liquid nitrogen for cooling. The highest  $T_c$  reached so far with doped cuprates is  $T_c \approx 133$  K. In 2008, a new class of high-temperature superconductors, which are based on Fe, was discovered. These superconductors were presented in one of the topical seminars.

The superconducting state is not only characterized by zero resistance, but also by other important features, which we discuss in the following.

## 4.2 Meißner effect

A superconducting material expels completely any applied external field, thus behaving like a *perfect diamagnet*. This property of a superconductor is named the Meißner effect. There is though a difference between a perfect diamagnet and the Meißner effect. In a superconductor, the magnetic field is expelled independently of the cooling procedure, either first cooling and then applying  $B$  or first applying  $B$  and then cooling (Fig. 4.2).

The superconducting state is a new state of matter. Inside the superconductor, the magnetic induction  $B$  disappears:

$$B = H + 4\pi M = 0,$$

where  $H$  is the external magnetic field.

### 4.2.0.1 Critical magnetic field

If the external magnetic field is too strong, then the superconducting state is destroyed. The dependence of the critical magnetic field  $H_c$  on temperature is given by

$$H_c(T) = H_c(0) \left[ 1 - \left( \frac{T}{T_c} \right)^2 \right],$$

where  $H_c(0)$  is the value of the critical magnetic field at zero temperature.

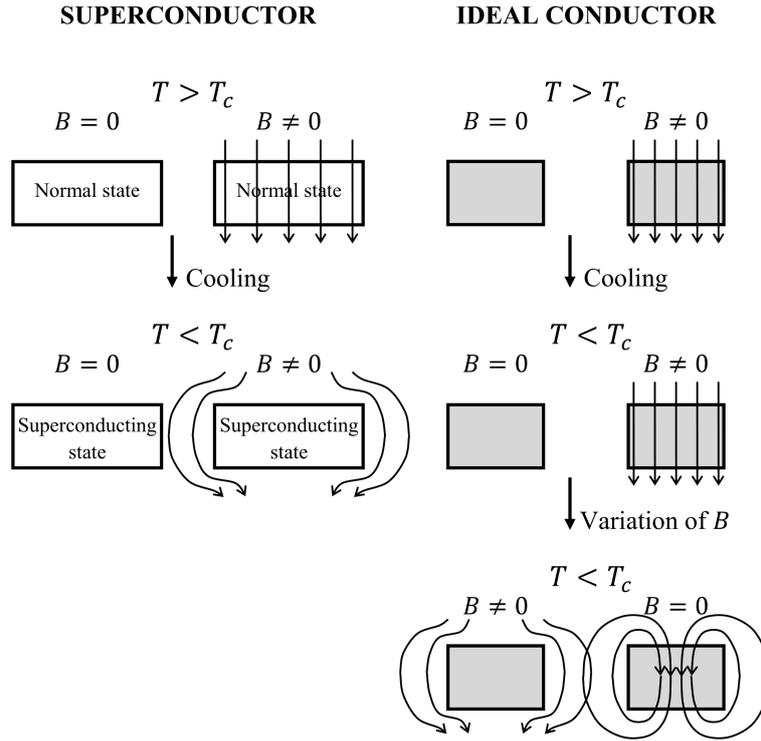


Abbildung 4.2: Superconductor *versus* ideal conductor in a magnetic field.

### 4.3 Entropy and specific heat

In the normal state, specific heat depends linearly on  $T$ ,

$$c_v^n \sim \gamma T,$$

whereas in the superconducting state the dependence is exponential:

$$c_v^s \sim e^{-\frac{\Delta}{k_B T}}.$$

This results in a discontinuity of the specific heat at  $T_c$  (Fig. 4.4).

Such behavior indicates the existence of an energy gap for thermal excitations in superconductors.

The entropy, given by

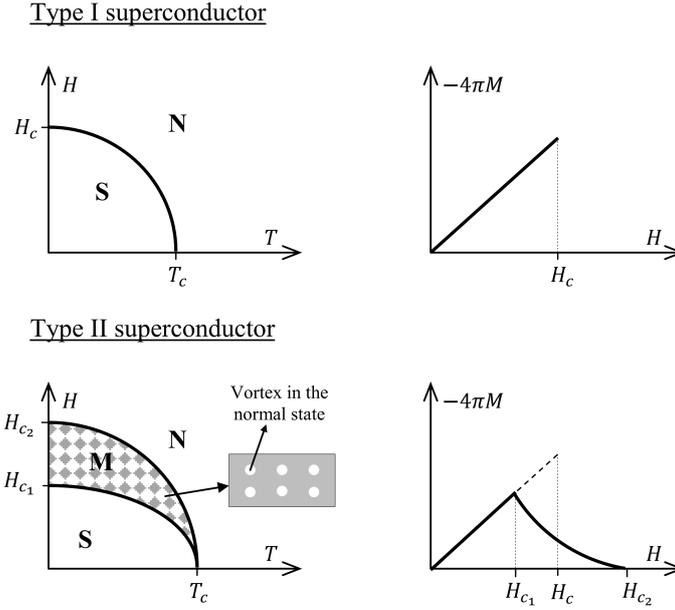
$$S(T) - S(0) = \int_0^T dT' \frac{c(T')}{T'},$$

fulfills the relation:

$$S^n(T_c) = S^s(T_c),$$

which is characteristic of second order phase transitions.

In the following sections, we shall show that



**Abbildung 4.3:** The  $H - T$  phase diagram and the  $H$ -dependence of magnetization  $M$  for either type I or type II superconductor. “S” labels the superconducting state, “N” the normal state, and “M” the mixed state.

- (i) the electron-phonon interaction in a metal can induce an attractive electron-electron interaction and
- (ii) two electrons at the Fermi sea in the presence of such an attractive interaction can build an energetically favorable bound state, the Cooper pair state.

## 4.4 Cooper pair

### 4.4.1 Retarded pair potential

In the superconducting state, the attractive interaction between electrons at the Fermi surface leads to the formation of Cooper pairs. In the traditional superconductors, the attractive electron-electron interaction is mediated by phonons via the following mechanism:

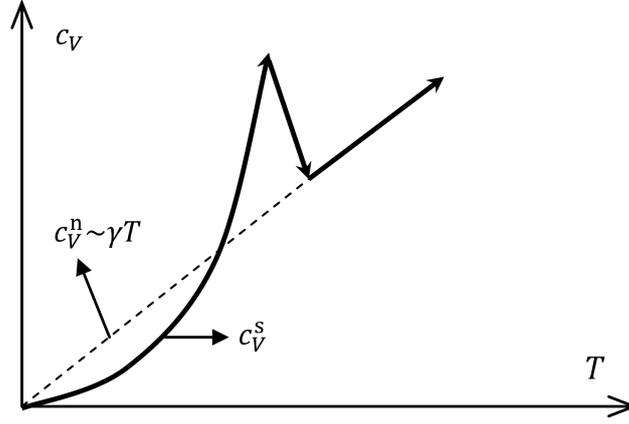
The ionic motion deforms the lattice, with a time scale  $\tau$  given by

$$\tau \sim \frac{2\pi}{\omega_D} \sim 10^{-13} \text{ s},$$

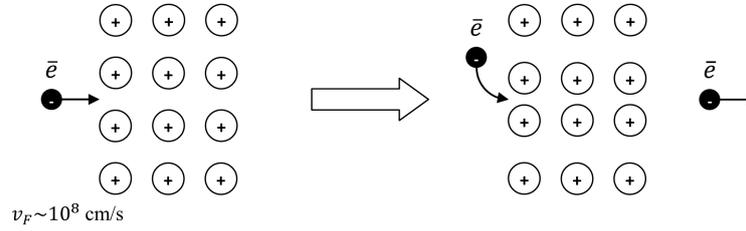
where  $\omega_D$  is the Debye frequency. During this time a conduction electron moves a distance  $v_F\tau$ :

$$v_F\tau \sim 10^8 \text{ cm/s} \cdot 10^{-13} \text{ s} \sim 1000 \text{ \AA},$$

with  $v_F$  being the Fermi velocity. A second electron can feel the “retarded” attraction of the first electron without the Coulomb repulsion playing a role.



**Abbildung 4.4:** Specific heat jump near the superconducting transition.



#### 4.4.2 Cooper instability of the Fermi sea

We consider two electrons near the Fermi surface in the presence of an attractive potential  $V(\vec{r}_1, \vec{r}_2)$ . The Schrödinger equation for this problem then reads

$$-\frac{\hbar^2}{2m} \left( \vec{\nabla}_1^2 + \vec{\nabla}_2^2 \right) \Psi(\vec{r}_1, \vec{r}_2) + V(\vec{r}_1, \vec{r}_2) \Psi(\vec{r}_1, \vec{r}_2) = (\epsilon + 2E_F) \Psi(\vec{r}_1, \vec{r}_2) \quad (4.1)$$

For a disappearing potential  $V = 0$ , the binding energy  $\epsilon = 0$  and the two-particle wavefunction is given by

$$\Phi_{V=0}(\vec{r}_1, \vec{r}_2) = \frac{1}{L^{3/2}} e^{i\vec{k}_1 \cdot \vec{r}_1} \frac{1}{L^{3/2}} e^{i\vec{k}_2 \cdot \vec{r}_2} = \frac{1}{L^3} e^{i\vec{k}(\vec{r}_1 - \vec{r}_2)}. \quad (4.2)$$

Note that here for simplification we are not considering the symmetrized form of the wavefunction. We also assume  $\vec{k}_1 = -\vec{k}_2 = \vec{k}$ .

We now consider a small  $V(\vec{r}_1, \vec{r}_2)$  and assume that  $\Psi(\vec{r}_1, \vec{r}_2)$  can in this case be taken as a linear combination of the basis functions (4.2):

$$\Psi(\vec{r}_1, \vec{r}_2) = \frac{1}{L^3} \sum_{\vec{k}} g(\vec{k}) e^{i\vec{k}(\vec{r}_1 - \vec{r}_2)}. \quad (4.3)$$

The  $\vec{k}$ -summation is here limited to a region near the Fermi surface:

$$E_F < \frac{\hbar^2 k^2}{2m} < E_F + \hbar\omega_D,$$

i.e.,

$$g(\vec{k}) = 0 \quad \text{for} \quad \begin{cases} k < k_F \\ k > \sqrt{2m(E_F + \hbar\omega_D)/\hbar} \end{cases} .$$

The Debye frequency  $\omega_D$  is much smaller than the typical Fermi energy.

#### 4.4.2.1 Self-consistent equation

By Fourier transforming the Schrödinger equation (4.1) with the ansatz (4.3) we obtain

$$\frac{\hbar^2 k^2}{m} g(\vec{k}) + \frac{1}{L^3} \sum_{\vec{k}'} g(\vec{k}') V_{\vec{k}, \vec{k}'} = (\epsilon + 2E_F) g(\vec{k}), \quad (4.4)$$

where

$$V_{\vec{k}, \vec{k}'} = \int V(\vec{r}) e^{-i(\vec{k}-\vec{k}') \cdot \vec{r}} d^3r$$

describes the scattering of pairs of electrons from  $(\vec{k}, -\vec{k})$  to  $(\vec{k}', -\vec{k}')$ . We approximate  $V_{\vec{k}, \vec{k}'}$  by an attractive constant:

$$V_{\vec{k}, \vec{k}'} = \begin{cases} -V_0 & \text{for } E_F < \frac{\hbar^2 k^2}{2m}, \frac{\hbar^2 k'^2}{2m} < E_F + \hbar\omega_D, \\ 0 & \text{otherwise.} \end{cases}$$

Then, Eq. (4.4) assumes the following form

$$\left( -\frac{\hbar^2 k^2}{m} + \epsilon + 2E_F \right) g(\vec{k}) = -\frac{V_0}{L} \sum_{\vec{k}'} g(\vec{k}') \equiv -A. \quad (4.5)$$

We insert  $g(\vec{k})$ ,

$$g(\vec{k}) = \frac{-A}{-\frac{\hbar^2 k^2}{m} + \epsilon + 2E_F}$$

into Eq. (4.5) and get

$$\frac{V_0}{L^3} \sum_{\vec{k}} \frac{A}{\frac{\hbar^2 k^2}{m} - \epsilon - 2E_F} = A,$$

$$\boxed{1 = \frac{V_0}{L^3} \sum_{\vec{k}} \frac{1}{\frac{\hbar^2 k^2}{m} - \epsilon - 2E_F}}. \quad (4.6)$$

Out of this equation we can determine the binding energy  $\epsilon$  of the electron pair.

#### 4.4.2.2 Binding energy

We substitute in Eq. (4.6) the sum over  $k$  by an integral over the energy with the help of the density of states  $N(E_F)$ :

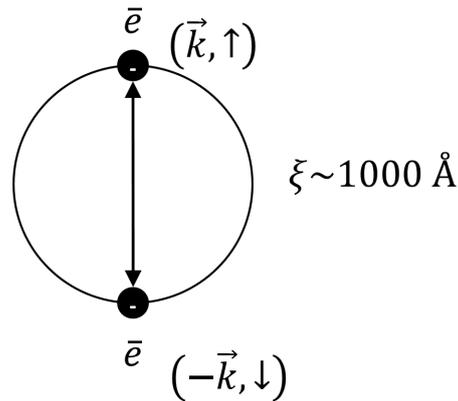
$$1 = V_0 \int_{E_F}^{E_F + \hbar\omega_D} N(E_F) \frac{dE}{2E - \epsilon - 2E_F} = \frac{1}{2} V_0 N(E_F) \ln \left( \frac{\epsilon - 2\hbar\omega_D}{\epsilon} \right).$$

Solving this equation for  $\epsilon$  gives

$$\epsilon = \frac{2\hbar\omega_D}{1 - e^{2/(V_0 N(E_F))}} \approx -2\hbar\omega_D e^{2/(V_0 N(E_F))} < 0.$$

For  $\frac{V_0}{E_F} \rightarrow 0$ , we obtain an exponentially small energy win for all  $V_0 > 0$ , which is not analytical in  $V_0$ . Therefore, the previous result cannot be obtained from perturbation theory.

The result of Cooper shows that in the presence of a (passive) Fermi sea and an infinitesimally small attractive interaction, two electrons form a bound state (see Fig. 4.5).



**Abbildung 4.5:** The Cooper pair picture. The attractive phonon-induced interaction is in real space isotropic and spin-independent. This leads to a pair wavefunction that is symmetric with respect to the spatial coordinates and antisymmetric (singlet) in the spin sector. Equivalently, the pairing in the momentum space is between electrons with  $\vec{k} \uparrow$  and  $-\vec{k} \downarrow$ .

## 4.5 BCS theory

The Cooper problem deals with the case of *two electrons* near the Fermi surface. Since electrons are indistinguishable, one has to consider a *many-body* wavefunction in order to describe *all the conduction electrons* in the superconducting state.

### 4.5.1 Hamilton operator in second quantization

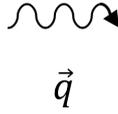
The energy of a crystal lattice can be described in terms of a certain number of harmonic oscillators, which have an equidistant energy spectrum:

$$H_{\text{ph}} = \sum_{\vec{q}s} \hbar\omega(\vec{q}, s) \left( a_{\vec{q}s}^\dagger a_{\vec{q}s} + \frac{1}{2} \right),$$

with  $a_{\vec{q}s}^\dagger$  and  $a_{\vec{q}s}$  being creation and annihilation bosonic operators:

$$\begin{aligned} [a_{\vec{q}s}, a_{\vec{q}'s'}^\dagger] &= \delta_{\vec{q}\vec{q}'} \delta_{ss'}, \\ [a_{\vec{q}s}, a_{\vec{q}'s'}] &= 0, \\ [a_{\vec{q}s}^\dagger, a_{\vec{q}'s'}^\dagger] &= 0. \end{aligned}$$

A highly excited state of a harmonic oscillator corresponds to a larger amount of phonons with energy  $\hbar\omega(q, s)$ . In the Feynman representation, a phonon can be pictured as a wavy line with an arrow (Fig. 4.6).



**Abbildung 4.6:** Feynman's representation of a phonon.

We consider the total Hamiltonian, written in a second quantization form, that describes both electrons and phonons, as well as the electron-phonon interaction:

$$H = \sum_{\vec{k}} \epsilon(\vec{k}) c_{\vec{k}}^\dagger c_{\vec{k}} + \sum_{\vec{q}} \hbar\omega_{\vec{q}} a_{\vec{q}}^\dagger a_{\vec{q}} + \sum_{\vec{k}\vec{q}} M_{\vec{q}} (a_{-\vec{q}}^\dagger + a_{\vec{q}}) c_{\vec{k}+\vec{q}}^\dagger c_{\vec{k}},$$

where  $\epsilon(\vec{k})$  is the kinetic energy of electrons,  $M_{\vec{q}}$  is the electron-phonon interaction,  $c_{\vec{k}}^\dagger$  and  $c_{\vec{k}}$  ( $a_{\vec{q}}^\dagger$  and  $a_{\vec{q}}$ ) are the fermionic (bosonic) creation and annihilation operators. The fermionic operators obey the anti-commutation relations:

$$\begin{aligned} \{c_{\vec{k}\sigma}, c_{\vec{k}'\sigma'}^\dagger\} &= \delta_{\vec{k}\vec{k}'} \delta_{\sigma\sigma'}, \\ \{c_{\vec{k}\sigma}^\dagger, c_{\vec{k}'\sigma'}^\dagger\} &= \{c_{\vec{k}\sigma}, c_{\vec{k}'\sigma'}\} = 0. \end{aligned}$$

We consider now a canonical transformation

$$H_{\text{T}} = e^{-iS} H e^{iS},$$

with  $S$  being an hermitian operator. We divide the Hamiltonian into a non-interacting part  $H_0$  and an interacting part  $H_1$ :

$$H = H_0 + H_1.$$

Then,

$$\begin{aligned}
e^{-iS} H e^{iS} &\approx \left(1 - iS - \frac{1}{2}S^2\right) H \left(1 + iS - \frac{1}{2}S^2\right) \\
&= H + i[H, S] - \frac{1}{2}[[H, S], S] + \mathcal{O}(S^3) \\
&= H_0 + H_I + i[H_0, S] + i[H_I, S] - \frac{1}{2}[[H_0, S], S] + \mathcal{O}(S^2, H_I^2).
\end{aligned}$$

We choose  $S$  so that the following equation

$$i[H_0, S] = -H_I$$

is fulfilled. With this condition, the term linear in  $H_I$  disappears in the canonically transformed Hamiltonian. Thus, we obtain

$$e^{-iS} H e^{iS} \approx H_0 + i[H_I, S] + \frac{1}{2i}[H_I, S] = H_0 + \frac{i}{2}[H_I, S].$$

By considering the explicit form of the matrix elements in the basis of  $H_0$ , it can be shown (see, for instance, Czycholl "Theoretical solid state physics") that after the canonical transformation, the original Hamiltonian results in an effective Hamiltonian of the following form

$$H = H_0 + H_{\text{IT}},$$

with

$$\begin{aligned}
H_{\text{IT}} &= \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} \sum_{\vec{q}} |M(\vec{q})|^2 \frac{\hbar\omega_{\vec{q}}}{(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{q}})^2 - (\hbar\omega_{\vec{q}})^2} \\
&\times c_{\vec{k}+\vec{q},\sigma}^\dagger c_{\vec{k}\sigma} c_{\vec{k}'-\vec{q},\sigma'}^\dagger c_{\vec{k}'\sigma'}
\end{aligned}$$

describing an effective electron-electron interaction. The matrix elements become negative and the effective interaction becomes attractive when

$$|\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}| < \hbar\omega_{\vec{q}},$$

which indicates that there is a probability of an attractive electron-electron interaction in a region near the Fermi surface, mediated by interchange of virtual phonons (Fig. 4.7).

We can simplify  $H_{\text{IT}}$  by

- (i) neglecting the  $\vec{q}$  dependence of  $V(\vec{q})$ :

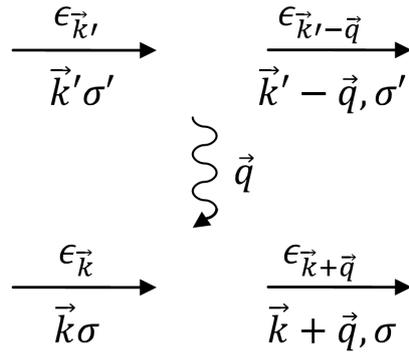
$$V(\vec{q}) = |M(\vec{q})|^2 \frac{\hbar\omega_{\vec{q}}}{(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{q}})^2 - (\hbar\omega_{\vec{q}})^2} \approx -V;$$

then,

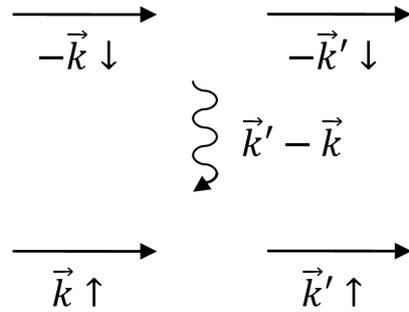
$$H_{\text{IT}} = -V \sum_{\sigma\sigma'} \sum_{\vec{k}\vec{k}'} \sum_{\vec{q}} c_{\vec{k}+\vec{q},\sigma}^\dagger c_{\vec{k}'-\vec{q},\sigma'}^\dagger c_{\vec{k}'\sigma'} c_{\vec{k}\sigma},$$

with

$$|\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}}| = |\epsilon_{\vec{k}'-\vec{q}} - \epsilon_{\vec{k}'}| \leq \hbar\omega_{\vec{q}} \leq \hbar\omega_{\text{D}}.$$



**Abbildung 4.7:** Interchange of a virtual phonon.



**Abbildung 4.8:** BSC approximation for the virtual phonon interchange.

- (ii) by taking into account only interaction between electrons with opposite momentum and spin (Fig. 4.8).

With that, we obtain the BCS Hamiltonian:

$$H = \sum_{\vec{k}\sigma} \xi_{\vec{k}} c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} - V \sum_{\vec{k}\vec{k}'} c_{\vec{k}'\uparrow}^\dagger c_{-\vec{k}'\downarrow}^\dagger c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow},$$

$$\xi_{\vec{k}} = \epsilon_{\vec{k}} - E_F.$$

This Hamiltonian can be alternatively solved by considering (1) a variational wavefunction and (2) the mean-field theory. Here we will only give a brief summary of both.

## 4.5.2 BCS wavefunction

The BCS wavefunction [Bardeen, Cooper and Schrieffer, Phys. Rev. **108**, 1175 (1957)] consists of a linear combination of unoccupied and doubly occupied states:

$$|\Psi\rangle = \prod_{\vec{k}} \left( u_{\vec{k}} + v_{\vec{k}} c_{\vec{k}\uparrow}^\dagger c_{-\vec{k}\downarrow}^\dagger \right) |0\rangle.$$

Here,  $|0\rangle$  is an "empty Fermi sphere",  $u_{\vec{k}}$  and  $v_{\vec{k}}$  are variational parameters.  $v_{\vec{k}}/u_{\vec{k}} \sim g(\vec{k})$  provides the link to the Cooper ansatz.

The BCS wavefunction has no definite particle number, but it has a definite phase. The normalization condition

$$\langle\Psi|\Psi\rangle = 1 \quad \Rightarrow \quad u_{\vec{k}}^2 + v_{\vec{k}}^2 = 1$$

is fulfilled through the parameterization

$$u_{\vec{k}}^2 = \frac{1}{2} \left( 1 + \frac{\xi_{\vec{k}}}{E_{\vec{k}}} \right), \quad v_{\vec{k}}^2 = \frac{1}{2} \left( 1 - \frac{\xi_{\vec{k}}}{E_{\vec{k}}} \right),$$

where  $E_{\vec{k}}$  is a free parameter, related to the *elementary excitations* to the BCS ground state.  $u_{\vec{k}}^2$  corresponds to the probability that a pair of states with opposite  $\vec{k}$  and  $\sigma$  is *unoccupied* while  $v_{\vec{k}}^2$  corresponds to the probability that a pair of states with opposite  $\vec{k}$  and  $\sigma$  is *occupied*. The condition of  $N = \text{const}$  can be implemented either variationally or by means of the Bogoliubov transformation.

## 4.5.3 Mean-field treatment of the Hamiltonian

The variational treatment of the BCS Hamiltonian is equivalent in this case to the mean-field treatment. Let us define the following decoupling of the interacting terms in the Hamiltonian:

$$\begin{aligned} H \rightarrow H_{\text{eff}} &= \sum_{\vec{k}\sigma} \xi_{\vec{k}} c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} - V \sum_{\vec{k}\vec{k}'} \langle c_{\vec{k}'\uparrow}^\dagger c_{-\vec{k}'\downarrow}^\dagger \rangle c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow} \\ &\quad - V \sum_{\vec{k}\vec{k}'} \langle c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow} \rangle c_{\vec{k}'\uparrow}^\dagger c_{-\vec{k}'\downarrow}^\dagger \\ &\quad + V \sum_{\vec{k}\vec{k}'} \langle c_{\vec{k}'\uparrow} c_{-\vec{k}'\downarrow} \rangle \langle c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow} \rangle; \\ H_{\text{eff}} &= \sum_{\vec{k}\sigma} \xi_{\vec{k}} c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} - \Delta^* \sum_{\vec{k}} c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow} - \Delta \sum_{\vec{k}} c_{\vec{k}'\uparrow}^\dagger c_{-\vec{k}'\downarrow}^\dagger + \frac{|\Delta|^2}{V}, \end{aligned}$$

with

$$\begin{aligned} \Delta &= V \sum_{\vec{k}'} \langle c_{-\vec{k}'\downarrow} c_{\vec{k}'\uparrow} \rangle, \\ \Delta^* &= V \sum_{\vec{k}'} \langle c_{\vec{k}'\uparrow}^\dagger c_{-\vec{k}'\downarrow}^\dagger \rangle \end{aligned} \tag{4.7}$$

being the order parameter of the superconducting phase. This effective Hamiltonian contains anomalous terms, i.e., it is not bilinear with respect to a creation operator and an annihilation operator:

$$[H_{\text{eff}}, N] \neq 0.$$

In order to diagonalize the Hamiltonian, we consider the Bogoliubov transformation:

$$\begin{aligned}\alpha_{\vec{k}} &= u_{\vec{k}}c_{\vec{k}\uparrow} - v_{\vec{k}}c_{-\vec{k}\downarrow}^\dagger, \\ \beta_{\vec{k}} &= u_{\vec{k}}c_{-\vec{k}\downarrow} + v_{\vec{k}}c_{\vec{k}\uparrow}^\dagger,\end{aligned}$$

with  $|u_{\vec{k}}|^2 + |v_{\vec{k}}|^2 = 1$ ;

$$\begin{aligned}\{\alpha_{\vec{k}}, \beta_{\vec{k}'}^\dagger\} &= 0, \\ \{\alpha_{\vec{k}}, \alpha_{\vec{k}'}^\dagger\} &= \{\beta_{\vec{k}}, \beta_{\vec{k}'}^\dagger\} = \delta_{\vec{k}\vec{k}'}.\end{aligned}$$

By choosing  $u_{\vec{k}}$  and  $v_{\vec{k}}$  as

$$u_{\vec{k}}^2 = \frac{1}{2} \left( 1 + \frac{\xi_{\vec{k}}}{\underbrace{\sqrt{\xi_{\vec{k}}^2 + |\Delta|^2}}_{E_{\vec{k}}}} \right) \quad \text{and} \quad v_{\vec{k}}^2 = \frac{1}{2} \left( 1 - \frac{\xi_{\vec{k}}}{\sqrt{\xi_{\vec{k}}^2 + |\Delta|^2}} \right),$$

$H_{\text{eff}}$  is ensured to be diagonal. These values are also obtained by considering the variational BCS wavefunction

$$H_{\text{eff}} = \sum_{\vec{k}} E_{\vec{k}} (\alpha_{\vec{k}}^\dagger \alpha_{\vec{k}} + \beta_{\vec{k}}^\dagger \beta_{\vec{k}}) + \sum_{\vec{k}} (\xi_{\vec{k}} - E_{\vec{k}}) + \frac{|\Delta|^2}{V},$$

where  $\alpha_{\vec{k}}$  and  $\beta_{\vec{k}}$  are new quasiparticles, which correspond to excitations to the BCS ground state.

#### 4.5.3.1 Gap equation

We perform statistical averaging on Eq. (4.7):

$$\Delta = V \sum_{\vec{k}} \frac{\Delta}{\sqrt{\xi_{\vec{k}}^2 + |\Delta|^2}} \left( \frac{1}{2} - f(E_{\vec{k}}) \right),$$

with

$$f(E_{\vec{k}}) = \frac{1}{e^{\beta E_{\vec{k}}} + 1};$$

$$\begin{aligned}
\Delta &= V \sum_{\vec{k}} \frac{\Delta}{E_{\vec{k}}} \left( \frac{1}{2} - \frac{1}{e^{\beta E_{\vec{k}}} + 1} \right), \\
\Delta &= \frac{V}{2} \sum_{\vec{k}} \frac{\Delta}{E_{\vec{k}}} \tanh \frac{\beta E_{\vec{k}}}{2}, \\
1 &= \frac{V}{2} \sum_{\vec{k}} \frac{1}{\sqrt{\xi_{\vec{k}}^2 + |\Delta|^2}} \tanh \frac{\beta \sqrt{\xi_{\vec{k}}^2 + |\Delta|^2}}{2}, \\
1 &= \frac{V}{2} \int_{-\hbar\omega_D}^{\hbar\omega_D} d\epsilon N(\epsilon) \frac{1}{\sqrt{\epsilon^2 + |\Delta|^2}} \tanh \frac{\beta \sqrt{\epsilon^2 + |\Delta|^2}}{2}.
\end{aligned}$$

We now focus on three limiting cases.

**Case 1:**  $T \rightarrow 0$ .

In this case, we make use of the fact that

$$\tanh \frac{\beta \sqrt{\epsilon^2 + |\Delta|^2}}{2} \xrightarrow{T \rightarrow 0} 1$$

and introduce

$$\Delta_0 \equiv \Delta(T = 0).$$

Then, the gap equation simplifies to

$$\begin{aligned}
\boxed{1} &= VN(E_F) \int_0^{\hbar\omega_D} \frac{d\epsilon}{\sqrt{\epsilon^2 + \Delta_0^2}} = VN(E_F) \operatorname{arcsinh} \frac{\epsilon}{\Delta_0} \Big|_0^{\hbar\omega_D} \\
&= \boxed{VN(E_F) \operatorname{arcsinh} \frac{\hbar\omega_D}{\Delta_0}}.
\end{aligned}$$

We get

$$\Delta_0 = \hbar\omega_D \frac{1}{\sinh \frac{1}{VN(E_F)}} \approx 2\hbar\omega_D e^{-\frac{1}{VN(E_F)}},$$

where  $N(E_F)$  is the density of states per spin. If the total density is considered, then

$$\Delta_0 \approx 2\hbar\omega_D e^{-\frac{2}{VN(E_F)}}.$$

**Case 2:**  $T \neq 0$ ,  $T \gg 1$  (high temperature).

Now,

$$\tanh \frac{\beta \sqrt{\epsilon^2 + |\Delta|^2}}{2} \approx \beta \frac{\sqrt{\epsilon^2 + |\Delta|^2}}{2}$$

and

$$1 = VN(E_F) \int_0^{\hbar\omega_D} d\epsilon \frac{\beta}{2} \frac{\sqrt{\epsilon^2 + |\Delta|^2}}{\sqrt{\epsilon^2 + |\Delta|^2}} = \beta N(E_F) \frac{\hbar\omega_D}{2}.$$

For  $T \rightarrow \infty$ , there is no trivial solution of the BCS equation (the previous equation goes into an inconsistency). This indicates that there must be a critical temperature  $T_c$ .

**Case 3:**  $T = T_c$ .

In this case,  $\Delta(T_c) = 0$  per definition. Then,

$$\begin{aligned} 1 &= VN(E_F) \int_0^{\hbar\omega_D} d\epsilon \frac{\tanh \frac{\epsilon}{2k_B T_c}}{\epsilon} \\ &= VN(E_F) \int_0^{\frac{\hbar\omega_D}{2k_B T_c}} dx \frac{\tanh x}{x}. \end{aligned}$$

Since, typically  $\hbar\omega_D \approx 300$  K and  $T_c \approx 10$  K, we can assume that

$$\frac{\hbar\omega_D}{2k_B T_c} \gg 1.$$

Then,

$$\begin{aligned} 1 &\approx VN(E_F) \left[ \ln \frac{\hbar\omega_D}{2k_B T_c} - \int_0^\infty dx \ln x (1 - \tanh^2 x) \right] \\ &= VN(E_F) \left( \ln \frac{\hbar\omega_D}{2k_B T_c} - \ln \frac{\pi}{4e^\gamma} \right), \end{aligned}$$

where  $\gamma$  is the Euler constant.

$$1 = VN(E_F) \ln \frac{1.136 \hbar\omega_D}{k_B T_c},$$

$$k_B T_c = 1.136 \hbar\omega_D e^{-\frac{1}{VN(E_F)}},$$

$$\frac{\Delta(0)}{k_B T_c} = \frac{2}{1.136} = 1.764.$$

This is a universal BCS relation.

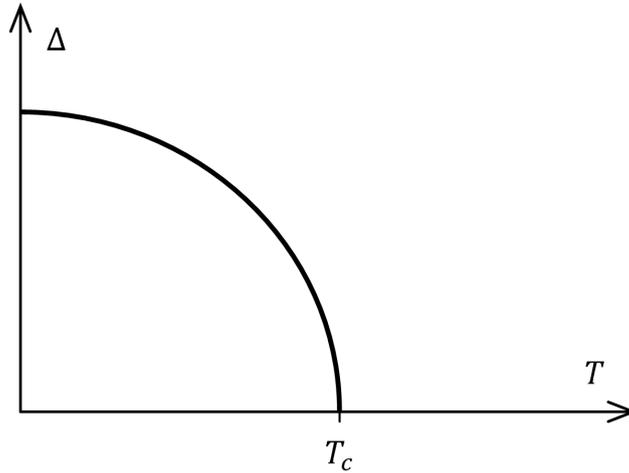
The condition for weak coupling:  $\Delta(0) \ll \hbar\omega_D$ . Since  $\hbar\omega_D \sim M^{-1/2}$ ,

$$T_c \sim \frac{1}{\sqrt{M}},$$

which is named the isotope effect. At  $T \rightarrow 0$  and  $T \rightarrow T_c$ , the order parameter behaves as (see also Fig. 4.9)

$$T \rightarrow 0 : \quad \Delta(T) = \Delta_0 - \sqrt{2\pi k_B T_c \Delta_0} e^{-\Delta_0/k_B T},$$

$$T \rightarrow T_c : \quad \Delta(T) = k_B T_c \pi \sqrt{\frac{8}{7\xi(3)}} \sqrt{1 - \frac{T}{T_c}}.$$



**Abbildung 4.9:** The order parameter  $\Delta$  as a function of temperature.

All thermodynamic properties of a BCS superconductor can be obtained from the presented BCS theory. The comparison with experiment is excellent.

