Chapter 6

Superconductivity

Before we start with the theoretical treatment of superconducitvity, we review some of the charactistic experimental facts, in order to gain an overall picture of this striking manifestation of quantum mechanics on a macrosocpic scale.

We start with an experimental result that gives the name of this phenomenon, namely with the rather abrupt change in resistivity at a temperature $T = T_c$ called the *critical temperature*. At temperatures above T_c, the metal is in the *normal*

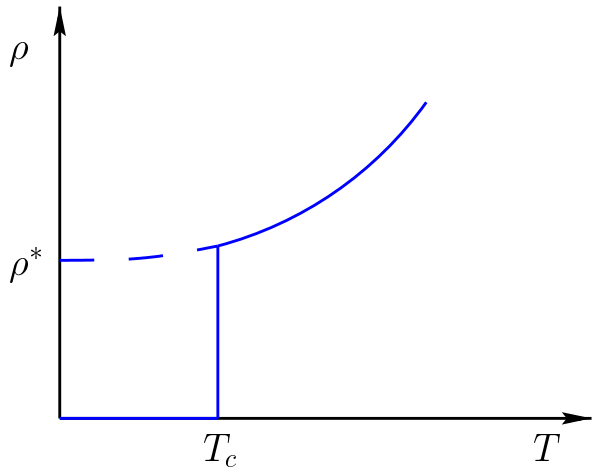

Figure 6.1: Schematic representation of the resistivity of a metal with a transition to a superconducting phase at T_c.

state, where $\rho(T) \sim T^2$ at low enough temperatures in the case of a Fermi liquid. In the absence of the transition, the resistivity extrapolates in general to a finite value as $T \to 0$, the *residual resisitivity*, that arises due to the presence of impurities. This is schematically shown in Fig. 6.1, where the residual resistivity is denoted ρ^*. In the case of a superconductor, however, the resisitivity vanishes at $T = T_c$ and no dissipation is present anymore for $T < T_c$. Accompanying this change in the resistivity, there is also a feature in the specific heat c_V that is common to phase transitions. At temperatures $T > T_c$ the specific heat (actually the electronic

contribution to it) decreases linearly with decreasing temperature, as expected for Fermi liquids. We have already seen in the case of the Fermi gas in Sec. 4.3.3 that this is a consequence of the Fermi-Dirac statistics. At T_c, however, there is a singularity in c_V that manifests experimentally as a jump, as shown in Fig. 6.2. At

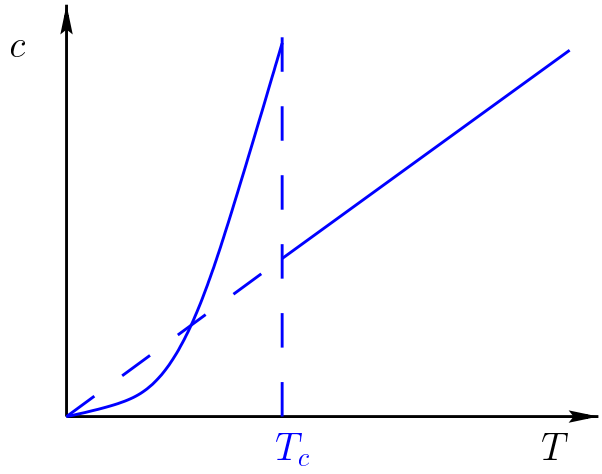

Figure 6.2: Schematic representation of the specific heat of a metal with a transition to a superconducting phase at T_c.

low temperatures the specific heat decreases exponentially,

$$c_V \sim \exp\left(-\frac{a}{T}\right) . \tag{6.1}$$

Since we have seen in (4.258), the specific heat is associated with the density of states at the Fermi energy. An exponential decrease is then a signal of an energy gap in the electronic spectrum.

Also in the presence of a magnetic field a number of remarkable phenomena are observed. Perhaps the most striking one is the fact that superconductors show perfect diamagnetism, a phomenon known under the name of *Meißner effect*. In normal metals the applied magnetic field and the total magnetic field B are proportional with the magnetic permeability as a porportionality constant. At low enough temperatures and aplied magnetic field H in the superconducting phase, however, the field B inside the sample vanishes, as shown in Fig. 6.3 *a*). In the H, T plane, the phase diagram shows a line $H_c(T)$ separating the superconducting and the normal

phases. Both features correspond to so-called type I superconductors.

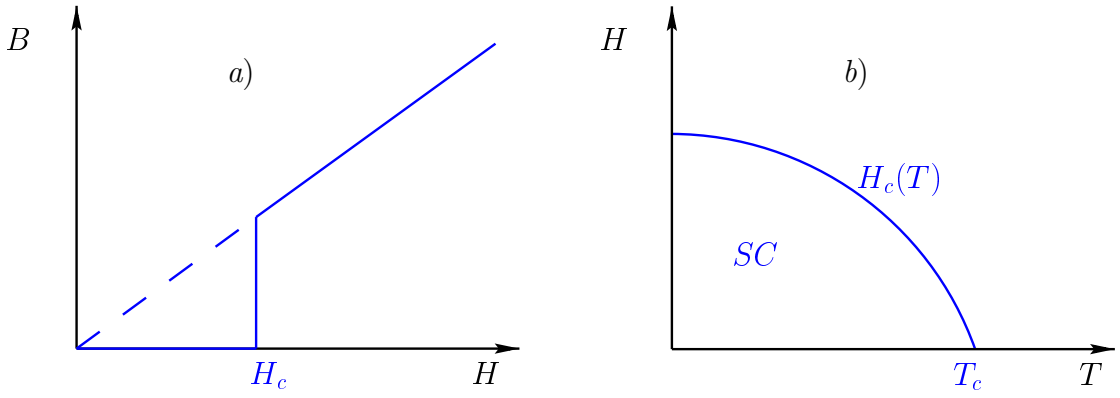

Figure 6.3: Magnetic properties of type I superconductors.

Type II superconductors, on the other hand, show a more complex behavior, with the Meißner phase below a magnetic field $H_{c1}(T)$ (Fig. 6.4*a*) and a new phase for $H_{c1}(T) < H < H_{c2}(T)$ (Fig. 6.4*b*) , where the magnetic field penetrates the sample in the form of *flux tubes* that build an array called *Abrikosov lattice*.

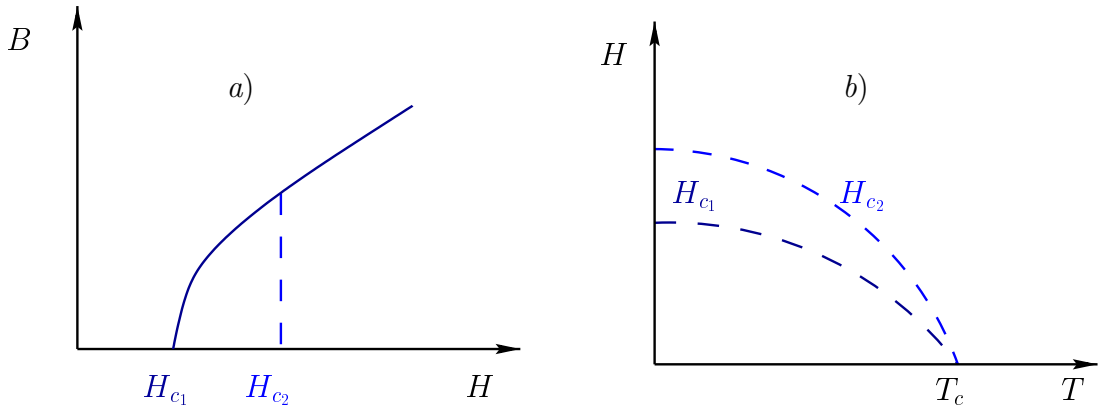

Figure 6.4: Magnetic properties of type II superconductors.

We will discuss first a phenomenological theory due to Ginzburg and Landau, that starting with general considerations for phase transitions will be able to describe consistently many of the features discussed above. Later, we discuss electron-phonon coupling and the *BCS-theory* due to Bardeen, Cooper and Schrieffer, that will give us a microscopic insight into the mechanism of superconductivity.

6.1 Ginzburg-Landau theory

This phenomelogical theory is a special case of the general theory for phase transitions developed by Landau. In this frame, we consider the free energy F as a functional of a field that should describe the possible phases of the system. This *order parameter* ψ has the property of being zero in the high temeprature phase, where the new order is still not established, and $\psi \neq 0$ below T_c, where the new phase appears. The order parameter should be such that it contains information relevant to the ordered phase. In the case of superconductivity, we consider that the new phase can be described by a wave function, and hence it will have in general a real and an imaginary part. We say then, that the order parameter has two *components*. In the general frame of the theory of phase transitions, the number of components of the order parameter will determine in general the major features of the transition. For example, in the case of a ferromagnet, if the system is isotropic in spin space, the order parameter will be a vector with three components.

6.1.1 Free energy without magnetic field

We consider first the form that the free energy is supposed to have without taking into account a magnetic field. We assume that close to the phase transition, the free energy should be a functional of ψ with ψ small so that an expansion in powers of it can be performed. Since the free energy is a real quantity, it will depend only on the modulus of the order parameter. We assume the following form for the free energy.

$$\begin{aligned} F[\psi] &= F_n(T) + \frac{1}{V}\int \mathrm{d}^3x \left\{ a\,\frac{T-T_c}{T_c}\mid \psi(\boldsymbol{x})\mid^2 + \frac{b}{2}\mid \psi(\boldsymbol{x})\mid^4 + \cdots \right. \\ &\qquad \left. + \frac{\hbar^2}{2m}\mid \boldsymbol{\nabla}\psi(\boldsymbol{x})\mid^2 + \cdots \right\}, \end{aligned} \tag{6.2}$$

where $F_n(T)$ is the contribution for the normal state, that we assume to be continuous and analytical across the transition. Furthermore, $\cdots$ represent higher order terms that in principle could be included. However, nowadays we know through *renormalization group* arguments that these terms are *irrelevant* for the *critical properties* of the phase transition.

In order to have a physical understanding of the parameters entering the free energy, let us consider the case where $\mid \psi(\boldsymbol{x}) \mid$ is homogeneous, i.e. it does not depend on position. Then, we can regard F as a potential depending only on $\mid \psi \mid$. For $\mid \psi \mid$ very small we need only to consider the term of order $\mathcal{O}(\mid \psi \mid^2)$. Taking

$a > 0$, we have a free energy that behaves as shown in Fig. 6.5 close to $\mid \psi \mid = 0$.

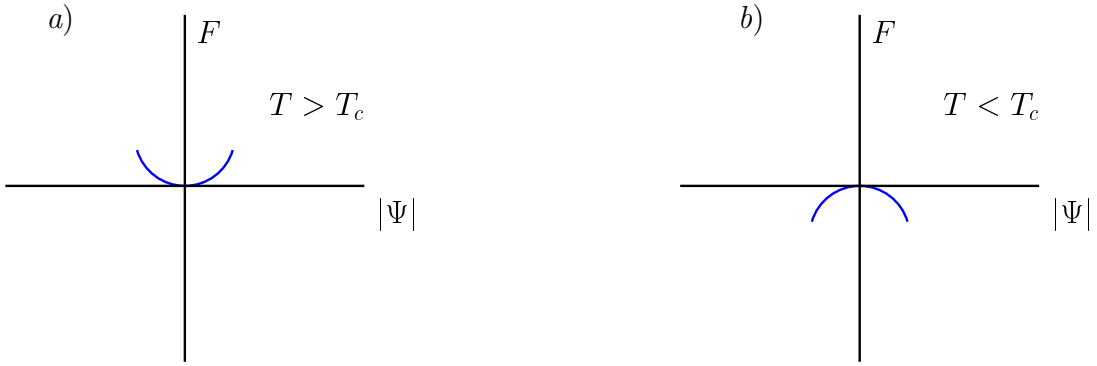

Figure 6.5: Free energy close to $\mid \psi \mid = 0$ for $a > 0$.

Since the physical state corresponds to the minimum of the free energy, Fig. 6.5 shows that by the choice $a > 0$, the phase at $T > T_c$ corresponds to a vanishing order paramter, whereas for $T < T_c$ such a state is unstable. If the expansion in powers of $\mid \psi(\boldsymbol{x}) \mid$ is cut at the fourth order, then, we should have $b > 0$ in order to have a stable system.

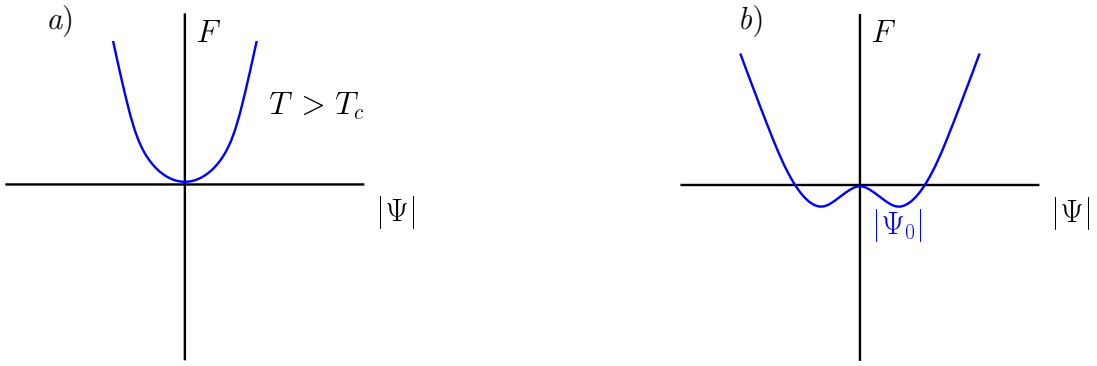

Figure 6.6: Free energy close to $\mid \psi \mid = 0$ for $a > 0$ and $b > 0$.

Figure 6.6 shows that for $b > 0$ and $T < T_c$, the minimum of the free energy is at a finite value of $\mid \psi \mid$, such that a non-vanishing order parameter characterizes the low temperature region. Finally, the gradient term in (6.2) allows in principle for non-homogenous solutions but since the constants in front of it are positive, the homogeneous solutions will lead to a lower free energy and will be therefore prefered.

Since, as we stated previously, the physical state is the one for which the free energy is at its minumum, and since with the argument above, the homogeneous

case leads to a lower free energy, we only need to minimize

$$F\left[\psi\right] \;\rightarrow\; a\,\frac{T-T_c}{T_c}\;\mid\psi\mid^2+\frac{b}{2}\mid\psi\mid^4\,, \tag{6.3}$$

in order to have a quantitative estimate of the order parameter, such that the value of the order parameter is determined by the equation

$$\frac{\partial F}{\partial\mid\psi\mid} \;=\; 2\mid\psi\mid\left[a\,\frac{T-T_c}{T_c}+b\mid\psi\mid^2\right]=0\,. \tag{6.4}$$

Since we already fixed $a, b > 0$, for $T > T_c$ the minimum is at $\mid\psi\mid = 0$, as shown by Fig. 6.6. If we recall the fact that the order parameter has actually a phase, in the two-dimensional space of the order parameter, the free energy has revolution symmetry. Then, the order parameter is zero and the free energy is given by the the normal state contribution in (6.2). On the other hand, for $T < T_c$, we have the solution

$$\mid\psi\mid \;=\; \sqrt{\frac{a\,(T_c-T)}{bT_c}}\,, \tag{6.5}$$

showing that the order parameter can be expressed as

$$\mid\psi\mid\sim\,(T_c-T)^{\beta}\;\;, \tag{6.6}$$

with β a *critical exponent* that in the Ginzburg-Landau theory has the value $\beta = 1/2$.

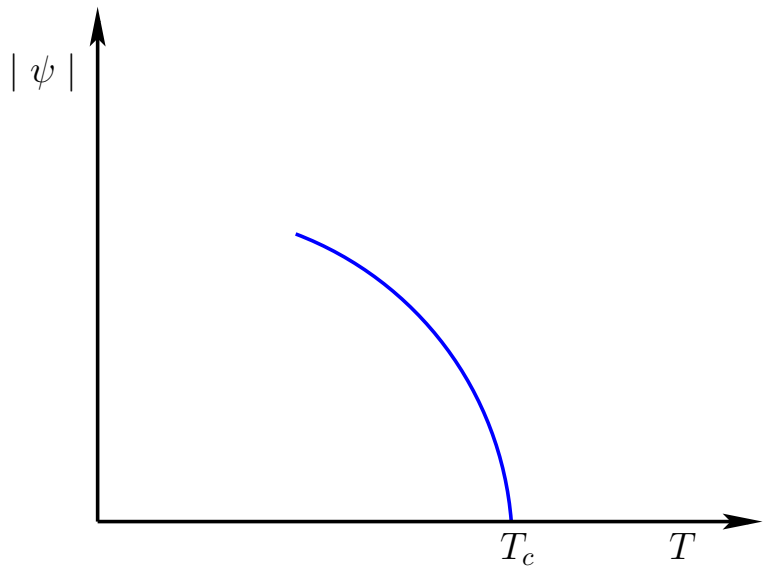

Figure 6.7: Order parameter for temperatures close to T_c.

Once the free energy is obtained, we can calculate the specific heat, as

$$c_V = -T\left(\frac{\partial^2 F}{\partial T^2}\right)\,. \tag{6.7}$$

Inserting (6.4) into (6.2), and carrying out the derivatives, we have

$$\left.\frac{c_V^{sc}-c_V^n}{T}\right|_{T_c}=\frac{a^2}{bT_c^2}\,, \tag{6.8}$$

where the superscript *sc* refers to the superconducting phase, whereas n to the normal one. Thus, the phenomenological theory leads to a jump of the specific heat, as observed experimentally. Actually, in phase transitions of *second order* as the one to a superconducting state, the specific heat shows either a divergence or a cusp at T_c. The result obtained here is the one correponding to so-called *mean-field theories*. In superconductors, the *critical region*, i.e. the region where divergencies in different quantities are observed is very small, of the order of $\mid T-T_c \mid /T_c \sim 10^{-5}$, such that in conventional experiments only the mean-field behavior is observed. However, in magnetic systems also presenting phase transitions, the deviations from mean-field behavior can be clearly seen.

6.1.2 Free energy with magnetic field

In the case a magnetic field is applied, we have to postulate the form in which it couples to the order parameter. It is useful in this case, to recall how a magnetic field couples to a charged particle. From the lectures in mechanics and electrodynamics, we know that in the presence of a magnetic field $\boldsymbol{B}$, a particle with charge e the Hamiltonian reads

$$H=\frac{1}{2m}\left(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A}\right)^2\,, \tag{6.9}$$

where $\boldsymbol{A}$ is the vector potential fulfilling $\boldsymbol{B}=\boldsymbol{\nabla}\times\boldsymbol{A}$. We therefore adopt a similar form for the coupling of the magnetic field to the order parameter, such that the free energy reads now

$$\begin{aligned} F\left[\psi\right] &= F_n(T)+\frac{1}{V}\int \mathrm{d}^3x\left\{a\,\frac{T-T_c}{T_c}\mid\psi\left(\boldsymbol{x}\right)\mid^2+\frac{b}{2}\mid\psi\left(\boldsymbol{x}\right)\mid^4\right. \\ &\quad +\frac{1}{2m}\left|\left[\frac{\hbar}{i}\boldsymbol{\nabla}-\frac{e^*}{c}\boldsymbol{A}\left(\boldsymbol{x}\right)\right]\psi\left(\boldsymbol{x}\right)\right|^2 \\ &\quad \left.+\frac{1}{8\pi}\boldsymbol{B}^2\right\}\,. \end{aligned} \tag{6.10}$$

The first line of the equation above contains those parts that were already taken into account in the absence of a magnetic field, for a homogeneous order parameter. The second line gives the modification of the term in (6.2) that took into account the contributions due to inhomogeneities of the order parameter. It looks like the momentum for a quantum mechanical particle of mass m and charge e^*, in the presence of a magnetic field. This term is clearly *gauge invariant*, since a change in $\boldsymbol{A}$ of the form

$$\boldsymbol{A}\left(\boldsymbol{x}\right)\rightarrow\boldsymbol{A}\left(\boldsymbol{x}\right)+\boldsymbol{\nabla}\Lambda\left(\boldsymbol{x}\right) \tag{6.11}$$

is compensated by a corresponding change in the phase of the order parameter

$$\psi\left(\boldsymbol{x}\right) \rightarrow \psi\left(\boldsymbol{x}\right) \exp\left[i\frac{e^*}{\hbar c}\Lambda\left(\boldsymbol{x}\right)\right] . \tag{6.12}$$

The third line in (6.10) takes into account the energy due to the magnetic field.

Once we have the free energy, we have to determine the values of the fields by minimizing it. Since in this case we are dealing with functions, we have to perform a variation of functions, as done in mechanics when deducing the Euler-Lagrange equations of motions. This can be done by carrying out a functional derivative. Since this was possibly not shown in other lectures, let us give a definition, which can be directly applied. For a functional $F[\psi]$, the funtional derivative is defined as

$$\int \mathrm{d}^d x \, \frac{\delta F}{\delta\psi\left(\boldsymbol{x}\right)} f\left(\boldsymbol{x}\right) \;=\; \lim_{\epsilon\rightarrow 0}\frac{1}{\epsilon}\Big\{F\left[\psi+\epsilon f\right]-F\left[\psi\right]\Big\} , \tag{6.13}$$

where $f\left(\boldsymbol{x}\right)$ is an arbitrary function. The free energy (6.10) has to be varied with respect to $\boldsymbol{A}$, ψ, and ψ^*. Let us consider first the variation with respect to $\boldsymbol{A}$, with $i = x$, y, or z, of the last term in (6.10).

$$\int \mathrm{d}^3 x \, \frac{\delta F}{\delta\psi\left(\boldsymbol{x}\right)} f\left(\boldsymbol{x}\right) \;\rightarrow\; \lim_{\epsilon\rightarrow 0}\frac{1}{\epsilon}\left\{\int \mathrm{d}^3 x\, \boldsymbol{B}^2\left[\boldsymbol{A}+\epsilon\boldsymbol{f}\right]-\int \mathrm{d}^3 x\, \boldsymbol{B}^2\left[\boldsymbol{A}\right]\right\} , \tag{6.14}$$

where we introduced an arbitrary vector $\boldsymbol{f}$. Since

$$\boldsymbol{B}\left[\boldsymbol{A}+\epsilon\boldsymbol{f}\right] \;=\; \boldsymbol{\nabla}\times\boldsymbol{A}+\epsilon\boldsymbol{\nabla}\times\boldsymbol{f} , \tag{6.15}$$

we have

$$\begin{aligned}
(6.14) \;&=\; 2\int \mathrm{d}^3 x\, \boldsymbol{B}\cdot\boldsymbol{\nabla}\times\boldsymbol{f} = 2\int \mathrm{d}^3 x\, B^i\, \varepsilon^{ijk}\frac{\partial f^k}{\partial x^j} \\
&=\; -2\varepsilon^{ijk}\int \mathrm{d}^3 x\, \frac{\partial B^i}{\partial x^j} f^k = 2\varepsilon^{kji}\int \mathrm{d}^3 x\, \frac{\partial B^i}{\partial x^j} f^k \\
&=\; \int \mathrm{d}^3 x\, 2\boldsymbol{\nabla}\times\boldsymbol{B}\cdot\boldsymbol{f} .
\end{aligned} \tag{6.16}$$

In a similar way we can perform the other functional derivatives, leading to

$$\frac{1}{4\pi}\boldsymbol{\nabla}\times\boldsymbol{B} \;=\; \frac{\hbar e^*}{2mc}\left[\psi^*\left(\frac{1}{i}\boldsymbol{\nabla}-\frac{e^*}{\hbar c}\boldsymbol{A}\right)\psi+\psi\left(-\frac{1}{i}\boldsymbol{\nabla}-\frac{e^*}{\hbar c}\boldsymbol{A}\right)\psi^*\right] . \tag{6.17}$$

Since in general

$$\boldsymbol{\nabla}\times\boldsymbol{B} \;=\; \frac{4\pi}{c}\boldsymbol{j} , \tag{6.18}$$

we see that a magnetic field induces a current due to the order parameter, such that

$$\boldsymbol{j}_s = \frac{\hbar e^*}{2m}\left[\psi^*\left(\frac{1}{i}\boldsymbol{\nabla}-\frac{e^*}{\hbar c}\boldsymbol{A}\right)\psi+\psi\left(-\frac{1}{i}\boldsymbol{\nabla}-\frac{e^*}{\hbar c}\boldsymbol{A}\right)\psi^*\right] . \tag{6.19}$$

is called the *supercurrent density* .

By considering the variation of the free energy with respect to the order parameter, or its complex conjugate, another equation is obtained,

$$\frac{1}{2m}\left(\frac{\hbar}{i}\boldsymbol{\nabla}-\frac{e^*}{c}\boldsymbol{A}\right)^2\psi+a\,\frac{T-T_c}{T_c}\,\psi+b\mid\psi\left(\boldsymbol{x}\right)\mid^2\psi=0\;. \tag{6.20}$$

Equation (6.17) and (6.20) constitute the Ginzburg-Landau equations for a superconductor. In the following we consider some of the consequences of the Ginzburg-Landau equations.

Superfluid density, superfluid velocity, and critical current

Consider a thin superconductor, such that the space dependence needs only to be assumed one-dimensional:

$$\psi=\psi_0\,\mathrm{e}^{iqx}\;. \tag{6.21}$$

Assume also that no magnetic field is present ($\boldsymbol{A}=0$). Then, eq. (6.20) becomes

$$\frac{\hbar^2q^2}{2m}\,\psi_0+a\,\frac{T-T_c}{T_c}\,\psi_0+b\,\psi_0^3=0\;. \tag{6.22}$$

There are again two solution, the trivial one $\psi_0=0$ for $T>T_c$ and

$$\psi_0=\sqrt{\frac{a(T_c-T)}{bT_c}-\frac{\hbar^2q^2}{2mb}}\;, \tag{6.23}$$

for $T<T_c$. On the other hand, from (6.19) we can calculate the supercurrent density in this case

$$j_s=e^*\frac{\hbar q}{m}\,\psi_0^2\equiv e^*\,v_s\,\rho_s\;, \tag{6.24}$$

where we have defined the *superfluid velocity* $v_s=\hbar q/m$ and the *superfluid density* $\rho_s=\psi_0^2$. Since ψ_0 can be only real, eq. (6.23) shows that the supercurrent density can only reach a maximal value called the *critical current* j_c. Beyond this value, the metal has only normal conduction.

Meißner effect and penetration depth

Let us consider a homogeneous superconductor, such that the superfluid density can be considered constant in space. The whole space dependence is the in the phase of the order parameter,

$$\psi=\psi_0\,\exp\left[i\varphi\left(\boldsymbol{x}\right)\right]\;. \tag{6.25}$$

If a magnetic fiels is present, then the supercurrent density is given by

$$\boldsymbol{j}_s = \frac{\hbar e^*}{m}\,\rho_s\,\boldsymbol{\nabla}\varphi\,(\boldsymbol{x}) - \frac{e^{*2}}{mc}\,\rho_s \boldsymbol{A}\,(\boldsymbol{x}) \ . \tag{6.26}$$

Since the curl of a scalar is zero, we have

$$\boldsymbol{\nabla}\times\boldsymbol{j}_s = -\frac{e^{*2}}{mc}\,\rho_s\boldsymbol{B} \ . \tag{6.27}$$

This equation is called *London equation*. It was formulated by London empirically, in order to explain the Meißner effect. In fact, once we arrive at it, since on the other hand eq. (6.18) also relates $\boldsymbol{B}$ and $\boldsymbol{j}_s$, and $\boldsymbol{\nabla}\cdot\boldsymbol{B}=0$, we have

$$\begin{aligned}\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{B}) &= \boldsymbol{\nabla}\,(\boldsymbol{\nabla}\cdot\boldsymbol{B}) - \boldsymbol{\nabla}^2\boldsymbol{B} = -\boldsymbol{\nabla}^2\boldsymbol{B} \\ &= \frac{4\pi}{c}\,\boldsymbol{\nabla}\times\boldsymbol{j}_s = -\frac{4\pi e^{*2}}{mc^2}\,\rho_s\boldsymbol{B} \ .\end{aligned} \tag{6.28}$$

From here we see that a length scale is present in the problem, namely

$$\lambda_L = \sqrt{\frac{mc^2}{4\pi e^{*2}\rho_s}} \ , \tag{6.29}$$

called the *London penetration depth*. The name becomes clear by solving the equation

$$\boldsymbol{\nabla}^2\boldsymbol{B} = \frac{1}{\lambda_L^2}\,\boldsymbol{B} \ . \tag{6.30}$$

Let us assume that the superconductor is occupying the half-space $x>0$, and the magnetic field is parallel to the surface of the superconductor. Then, the differential equation becomes a one-dimensional one with a solution

$$\boldsymbol{B}(x) = \boldsymbol{B}_0\,\mathrm{e}^{-x/\lambda_L} \ , \tag{6.31}$$

where $\boldsymbol{B}_0$ is the magnetic field at the surface of the superconductor. Here we see that when a magnetic field is present, supercurrents are induced that shield the magnetic field in the interior of a superconductor. In fact, London equation (6.27) shows that these currents produce a magnetic field opposed to the applied one.

Flux quantization

We consider here a superconducting ring as shown in Fig. 6.8

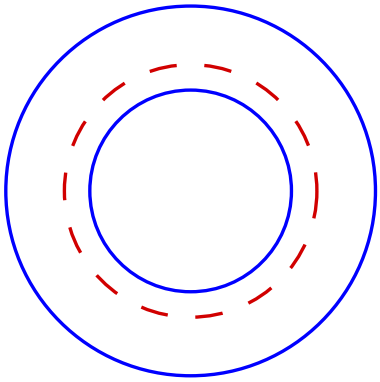

Figure 6.8: Superconducting ring with a contour (red dashed line) deep in the interior of the superconductor.

Deep in the interior of the superconductor, the magnetic field is completely screened out, and therefore, supercurrents should be absent there. This means that on the red dashed line in Fig. 6.8 $\boldsymbol{j}_s = 0$, or equivalently,

$$\oint_C \boldsymbol{j}_s \cdot \mathrm{d}\boldsymbol{\ell} = 0 \tag{6.32}$$

Using (6.26), we have

$$0 \;=\; \frac{\hbar e^*}{m}\rho_s \oint_C \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\boldsymbol{\ell} - \frac{e^{*2}}{mc}\rho_s \oint_C \boldsymbol{A}\cdot \mathrm{d}\boldsymbol{\ell}\;, \tag{6.33}$$

but on the one hand, we ask the wavefunction to be single-valued, and hence

$$\oint_C \boldsymbol{\nabla}\varphi \cdot \mathrm{d}\boldsymbol{\ell} = 2\pi n\;, \tag{6.34}$$

with n integer. On the other hand,

$$\oint_C \boldsymbol{A}\cdot \mathrm{d}\boldsymbol{\ell} = \int_S \boldsymbol{B}\cdot \mathrm{d}\boldsymbol{S} = \Phi_S\;, \tag{6.35}$$

is the magnetic flux through the ring. We see then, that the magnetic flux is quantized

$$\Phi_S = n\frac{2\pi\hbar c}{e^*} = n\Phi_0\;, \tag{6.36}$$

in units of the flux quantum

$$\Phi_0 = \frac{hc}{e^*}\;. \tag{6.37}$$

6.2 Electron-phonon coupling

The previous discussion of the phenomenon of superconductivity did not make any reference to the mechanism that leads to its appearance. In order to come closer to a microscopic understanding of superconductivity we should mention a decisive experimental finding, namely the *isotope effect*, where the critical temperature varies as

$$T_c \sim M^{-\alpha} \ , \tag{6.38}$$

with M the mass of the ions, and $\alpha \sim 1/2$. Such a relationship, points to the fact that phonons play an important role for a system that becomes superconducting.

Here we will consider a Hamiltonian introduced by Fröhlich, who actually predicted the isotope effect before its observation.

$$H_F = H_{el} + H_{ph} + H_{el-ph} \ , \tag{6.39}$$

where

$$H_{el} = \sum_{\boldsymbol{k}} \epsilon\left(\boldsymbol{k}\right) \ f^\dagger_{\boldsymbol{k}} f_{\boldsymbol{k}} \tag{6.40}$$

describes the electronic part. Here it is assumed that the role of Coulomb interaction is not important for the phenomenon of superconductivity, such that $\epsilon\left(\boldsymbol{k}\right)$ describes some band-structure, that takes into account the Coulomb interaction in the frame of a Fermi liquid theory. The phonons are described by

$$H_{ph} = \sum_{\boldsymbol{q}} \hbar\omega_{\boldsymbol{q}} \left(b^\dagger_{\boldsymbol{q}} b_{\boldsymbol{q}} + \frac{1}{2} \right) \ , \tag{6.41}$$

i.e. harmonic oscillators with a dispersion $\omega_{\boldsymbol{q}}$.

For the coupling of electrons and phonons we can take the following simple picture. First we consider acoustic phonons since they are always present, such that our discussion remains general. We consider further those phonons that produce a local change of the ionic density, and hence, directly couple to the density of electrons. Let us describe such a change in ionic potential with a field $D\left(\boldsymbol{x}\right)$, such that

$$H_{el-ph} \ = \ \int \mathrm{d}^3x \, \hat{\psi}^\dagger_\alpha\left(\boldsymbol{x}\right) \ D\left(\boldsymbol{x}\right) \ \hat{\psi}_\alpha\left(\boldsymbol{x}\right) \ . \tag{6.42}$$

Changes in the ionic density correspond to displacement fields $\boldsymbol{u}\left(\boldsymbol{x}\right)$ with

$$D\left(\boldsymbol{x}\right) = \boldsymbol{\nabla} \cdot \boldsymbol{u}\left(\boldsymbol{x}\right) \ , \tag{6.43}$$

corresponding to local dilatations and contractions. This means that we need only to consider longitudinal phonons, i.e. with $\boldsymbol{u} \sim \boldsymbol{q}$, where $\boldsymbol{q}$ is the wavevector of the

phonon. From the relation between creation and annihilation of phonon quanta and the displacemente fields (2.43), we can obtain the following relationship.

$$\boldsymbol{u}\left(\boldsymbol{x}\right) = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{q}}\frac{\boldsymbol{q}}{\mid \boldsymbol{q} \mid}\left(\frac{\hbar}{2M\omega_{\boldsymbol{q}}}\right)^{\frac{1}{2}}\left[b_{\boldsymbol{q}}\,\exp\left(i\boldsymbol{q}\cdot\boldsymbol{x}\right)+b_{\boldsymbol{q}}^{\dagger}\,\exp\left(-i\boldsymbol{q}\cdot\boldsymbol{x}\right)\right] \quad (6.44)$$

From here we can then calculate the field D using (6.43), and the fact that for an acoustic phonon, $\omega_{\boldsymbol{q}} = v_s\, q$, with v_s the sound velocity.

$$D\left(\boldsymbol{x}\right) = \frac{i}{\sqrt{N}}\sum_{\boldsymbol{q}}\left(\frac{\hbar q}{2Mv_s}\right)^{\frac{1}{2}}\left[b_{\boldsymbol{q}}\,\exp\left(i\boldsymbol{q}\cdot\boldsymbol{x}\right)-b_{\boldsymbol{q}}^{\dagger}\,\exp\left(-i\boldsymbol{q}\cdot\boldsymbol{x}\right)\right]\ . \quad (6.45)$$

For the electronic field operators, we use an expansion in Bloch states

$$\begin{aligned}\hat{\psi}_{\alpha}\left(\boldsymbol{x}\right) &= \sum_{\boldsymbol{k}} f_{\boldsymbol{k}\alpha}\, u_{\boldsymbol{k}}\left(\boldsymbol{x}\right)\,\exp\left(i\boldsymbol{k}\cdot\boldsymbol{x}\right)\ ,\\ \hat{\psi}_{\beta}^{\dagger}\left(\boldsymbol{x}\right) &= \sum_{\boldsymbol{k}} f_{\boldsymbol{k}\beta}^{\dagger}\, u_{\boldsymbol{k}}^{*}\left(\boldsymbol{x}\right)\,\exp\left(-i\boldsymbol{k}\cdot\boldsymbol{x}\right)\ .\end{aligned} \quad (6.46)$$

Then, the electron-phonon interaction looks as follows.

$$\begin{aligned}H_{el-ph} &= \frac{i}{\sqrt{N}}\sum_{\boldsymbol{q}}\left(\frac{\hbar q}{2Mv_s}\right)^{\frac{1}{2}}\left\{b_{\boldsymbol{q}}\sum_{\boldsymbol{k}\boldsymbol{k}'} f_{\boldsymbol{k}\alpha}^{\dagger} f_{\boldsymbol{k}'\alpha}\right.\\ &\quad\left.\times\int \mathrm{d}^3x\, u_{\boldsymbol{k}}^{*}\left(\boldsymbol{x}\right)\, u_{\boldsymbol{k}'}\left(\boldsymbol{x}\right)\,\exp\left[i\left(\boldsymbol{q}-\boldsymbol{k}+\boldsymbol{k}'\right)\cdot\boldsymbol{x}\right]-h.c.\right\}\\ &= i\sum_{\boldsymbol{k},\boldsymbol{q}} D_{\boldsymbol{q}}\left(b_{\boldsymbol{q}}\, f_{\boldsymbol{k}+\boldsymbol{q},\alpha}^{\dagger} f_{\boldsymbol{k},\alpha} - b_{\boldsymbol{q}}^{\dagger}\, f_{\boldsymbol{k}-\boldsymbol{q},\alpha}^{\dagger} f_{\boldsymbol{k},\alpha}\right)\ ,\end{aligned} \quad (6.47)$$

where in going to the last line, we restricted ourselves to a model on the lattice, where Wannier functions as in (4.334) are taken, such that no further k-dependence appears in $D_{\boldsymbol{q}}$.

Finally, we can write the full Hamiltonian as

$$\begin{aligned}H_F &= \sum_{\boldsymbol{k}}\epsilon\left(\boldsymbol{k}\right)\, f_{\boldsymbol{k}}^{\dagger} f_{\boldsymbol{k}} + \sum_{\boldsymbol{q}}\hbar\omega_{\boldsymbol{q}}\left(b_{\boldsymbol{q}}^{\dagger} b_{\boldsymbol{q}}+\frac{1}{2}\right)\\ &\quad +i\sum_{\boldsymbol{k},\boldsymbol{q}} D_{\boldsymbol{q}}\left(b_{\boldsymbol{q}}\,\rho_{\boldsymbol{q}}^{\dagger} - b_{\boldsymbol{q}}^{\dagger}\,\rho_{\boldsymbol{q}}\right)\ ,\end{aligned} \quad (6.48)$$

where

$$\rho_{\boldsymbol{q}} = \sum_{\boldsymbol{k},\alpha} f_{\boldsymbol{k}-\boldsymbol{q},\alpha}^{\dagger} f_{\boldsymbol{k},\alpha} = \rho_{-}^{\dagger}\boldsymbol{q} \quad (6.49)$$

is an electron-density operator.

6.2.1 Effective electron-electron interaction

In the following we will see that it is possible to extract an effective electron-electron interaction from the electron-phonon interaction. This can be normally achieved, when the different degrees of freedom appear in bilinear forms and the coupling between different kinds of excitations is linear. This can be easily shown in a *path-integral formalism*. Here, we will restrict ourselves to work in the frame of second quantization and use a canonical transformation. A canonical transformation is one in which the canonical commutation relations of operators is preserved.

We start with an antiunitary operator S, i.e. $S^\dagger = -S$, such that $\exp S$ is unitary. By performing a unitary transformation, all physical quantities remain unchanged. Applied on the Hamiltonian, we transform it as follows

$$\begin{aligned} \tilde{H}_F &= \mathrm{e}^{-S}\, H_F\, \mathrm{e}^{S} \\ &= H_F + [H_F, S] + \frac{1}{2!}\left[[H_F, S], S\right] + \frac{1}{3!}\left[[[H_F, S], S], S\right] + \cdots \end{aligned} \tag{6.50}$$

For the choice of S, we look at the diagramatic representation of the electron-phonon interaction in (6.48). There, a phonon is created or annihilated in a

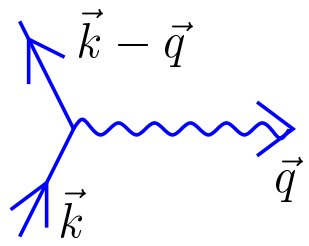

Figure 6.9: Diagramatic representation of the electron-phonon coupling in eq. (6.48).

scattering process with an electron. However, after a phonon is e.g. created, it can be annihilated by another scattering process with an electron. The corresponding diagram is shown in Fig. 6.10. Thus, a phonon is exchanged by two electrons

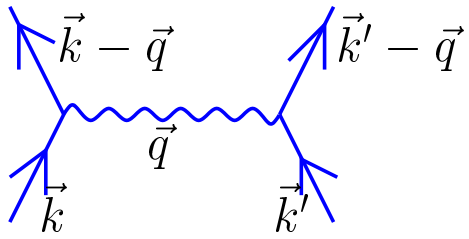

Figure 6.10: Effective electron-electron interaction throught the exchange of a phonon.

giving rise to an effective interaction. Such a process can occur only in second order

in the electron-phonon interaction or in higher orders. Therefore, the canonical transformation should be chosen in such a way that contributions from the electron-phonon interaction are cancelled in first order. Let us write H_F as

$$H_F = H_0 + \lambda H_{el-ph} \, , \tag{6.51}$$

such that

$$\begin{aligned} \tilde{H}_F &= \mathrm{e}^{-S} \, H_F \, \mathrm{e}^{S} \\ &= H_0 + \lambda H_{el-ph} + [H_0, S] + \lambda \, [H_{el-ph}, S] \\ &\quad + \frac{1}{2} \, [[H_0 + \lambda H_{el-ph}, S] \, , S] + \cdots \end{aligned} \tag{6.52}$$

In the case that

$$\lambda H_{el-ph} + [H_0, S] = 0 \, , \tag{6.53}$$

$S \sim \mathcal{O}(\lambda)$, implying that $\tilde{H}_F$ has no term linear in λ. Let us consider now the possible matrix elements of the condition above for states $\mid m >$ that are eingenstates of H_0.

$$\begin{aligned} \lambda < n \mid H_{el-ph} \mid m > &= < n \mid [S, H_0] \mid m > \\ &= (E_m - E_n) < n \mid S \mid m > \, , \end{aligned} \tag{6.54}$$

leading to

$$< n \mid S \mid m > = \lambda \, \frac{< n \mid H_{el-ph} \mid m >}{(E_m - E_n)} \, , \tag{6.55}$$

such that we have S in the basis that diagonalizes H_0. Once we have S, we can consider the first non-vanishing correction to H_0. In the next order in λ we have

$$\lambda \, [H_{el-ph}, S] + \frac{1}{2} \, [[H_0, S] \, , S] = \lambda \, [H_{el-ph}, S] - \frac{\lambda}{2} \, [H_{el-ph}, S] \, . \tag{6.56}$$

Therefore, we need now to consider the matrix elements of $[H_{el-ph}, S]$. Let us look first at $H_{el-ph} S$.

$$\begin{aligned} < n \mid H_{el-ph} S \mid m > &= \sum_{\ell} < n \mid H_{el-ph} \mid \ell >< \ell \mid S \mid m > \\ &= \lambda \sum_{\ell} \frac{< n \mid H_{el-ph} \mid \ell >< \ell \mid H_{el-ph} \mid m >}{(E_m - E_\ell)} \, . \end{aligned} \tag{6.57}$$

Since the phenomena we are interested in occur at very low temperatures, we restrict the states we consider to zero-phonon states, the one-phonon state being only reached virtually. This means that in the expression above we have for a particular phonon mode,

$$\begin{aligned} (6.57) \;\rightarrow\; & \frac{< 0 \mid H_{el-ph} \mid 1_{\boldsymbol{q}} >< 1_{\boldsymbol{q}} \mid H_{el-ph} \mid 0 >}{(E_m - E_\ell)} \\ &= D_{\boldsymbol{q}}^2 \sum_{\boldsymbol{k}, \boldsymbol{k}'} f_{\boldsymbol{k}'}^{\dagger} \, f_{\boldsymbol{k}' - \boldsymbol{q}} f_{\boldsymbol{k} - \boldsymbol{q}}^{\dagger} \, f_{\boldsymbol{k}} \frac{1}{\epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k} - \boldsymbol{q}} - \hbar \omega_{\boldsymbol{q}}} \, . \end{aligned} \tag{6.58}$$

Now we consider SH_{el-ph}. In this case we have

$$\begin{aligned} < n \mid SH_{el-ph} \mid m > &= \sum_{\ell} < n \mid S \mid \ell >< \ell \mid H_{el-ph} \mid m > \\ &= \lambda \sum_{\ell} \frac{< n \mid H_{el-ph} \mid \ell >< \ell \mid H_{el-ph} \mid m >}{(E_\ell - E_n)} \\ &\rightarrow D_{\boldsymbol{q}}^2 \sum_{\boldsymbol{k},\boldsymbol{k}'} f_{\boldsymbol{k}'}^\dagger f_{\boldsymbol{k}'-\boldsymbol{q}} f_{\boldsymbol{k}-\boldsymbol{q}}^\dagger f_{\boldsymbol{k}} \frac{1}{\epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}-\boldsymbol{q}} + \hbar\omega_{\boldsymbol{q}}} \quad (6.59) \end{aligned}$$

Putting all the contributions together, we obtain an effective electron-electron interaction of the form

$$H_{el-el} = \sum_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}'} W_{\boldsymbol{k}\boldsymbol{q}} f_{\boldsymbol{k}'}^\dagger f_{\boldsymbol{k}'+\boldsymbol{q}} f_{\boldsymbol{k}-\boldsymbol{q}}^\dagger f_{\boldsymbol{k}} \,, \quad (6.60)$$

with

$$W_{\boldsymbol{k}\boldsymbol{q}} = \frac{D_{\boldsymbol{q}}^2 \hbar\omega_{\boldsymbol{q}}}{\left(\epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{q}}\right)^2 - \hbar^2\omega_{\boldsymbol{q}}^2} \,. \quad (6.61)$$

This means that for a small region around the Fermi energy with $\mid \epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{q}} \mid < \hbar\omega_{\boldsymbol{q}}$, an attractive interaction among electrons arises mediated by phonons. One could then roughly argue that a new bound state consisting of two fermions could appear, such that the bound pair would have bosonic character, and hence, similarly to ^{4}He, a superfluid phase could appear. Since in this case the pair would be charged, superconductivity would take place. That such a bound state can occur even in the presence of many electrons, is the subject of the theory by Bardeen, Cooper ans Schrieffer.

6.3 The BCS theory

After we have seen that the electron-phonon coupling gives rise to an effective attractive interaction between electrons, the idea that pairs will form becomes natural. The theory developed by Bardeen, Cooper and Schrieffer (BCS), allows for a calculation of several features related to the transition to superconductivity like the isotope effect, and also features related to the ground-state like the opening of a gap in the one-particle excitation spectrum. Although the full developement of the consequences of the BCS-theory lie beyond the scope of these lectures, we should mention that this theory is one of the most predictive theories in solid state physics.

The following features should be taken into account, when discussing pairing.

i) As shown by (6.61), there is an attractive interaction for states with energy $\mid \epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{q}} \mid < \delta \sim \hbar\omega_D$, where ω_D is the Debye frequency, that gives the

characteristic phonon frequency of the system (see Sec. 2.3)

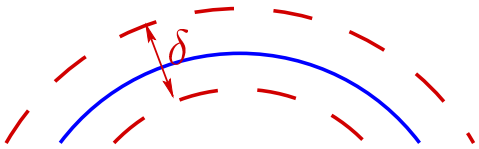

Figure 6.11: Shell around the Fermi surface with an attractive interaction.

ii) Pairs with total momentum zero and total spin zero. The states would be $\mid k >= \mid \boldsymbol{k}, \sigma >$, $\mid -k >= \mid -\boldsymbol{k}, -\sigma >$. As can be seen in Fig. 6.12, such states can be realized on the whole Fermi sphere and have therefore a high density of states. Since electrons are $S - \frac{1}{2}$ particles, a pair can be in a state with

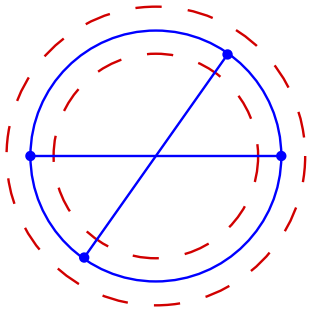

Figure 6.12: All states diametrically opposed can form time-reversal invariant pairs

total spin $S = S_1 + S_2 = 0$ or 1. If $S = 0$ one speaks of singlet pairing and if $S = 1$ triplet pairing.

The Hamiltonian introduced by Bardeen, Cooper, and Schrieffer (BCS) is restricted to the conditions mentioned above.

$$H_{BCS} = \sum_{\boldsymbol{k},\sigma} \epsilon\left(\boldsymbol{k}\right) f^{\dagger}_{\boldsymbol{k},\sigma} f_{\boldsymbol{k},\sigma} + \frac{1}{2} \sum_{k,k'} W_{kk'} f^{\dagger}_{k} f^{\dagger}_{-k} f_{-k'} f_{k'} \ , \tag{6.62}$$

where

$$W_{kk'} = \begin{cases} < 0 & \text{for } \mid \epsilon\left(\boldsymbol{k}\right) - E_F \mid < \frac{\delta}{2} \text{ and } \mid \epsilon\left(\boldsymbol{k'}\right) - E_F \mid < \frac{\delta}{2} \\ 0 & \text{otherwise} \end{cases} \tag{6.63}$$

This is still an interacting Hamiltonian and, hence in general difficult to solve. However, the following equalities will prove to be useful.

$$\begin{aligned} f_{-k} f_{k} &= < f_{-k} f_{k} > + \left(f_{-k} f_{k} - < f_{-k} f_{k} > \right) \\ f^{\dagger}_{k} f^{\dagger}_{-k} &= < f^{\dagger}_{k} f^{\dagger}_{-k} > + \left(f^{\dagger}_{k} f^{\dagger}_{-k} - < f^{\dagger}_{k} f^{\dagger}_{-k} > \right) \ . \end{aligned} \tag{6.64}$$

Such a decomposition of operators, makes explicit the picture that when a certain type of order is established, the operators can be viewed as a *mean-field* (first terms

in eqs. (6.64)) and fluctuations around it. This mean-field is in the case of superconductivity of a rather strange nature. In the normal state, $< f_{-k} f_k >=< f_k^\dagger f_{-k}^\dagger >= 0$, since it is an expectation number of operators that change the number of particles in the system. On the other hand, if it happens to be non-zero, we have $< f_k^\dagger f_{-k}^\dagger >=< f_{-k} f_k >^*$, and hence, this field is complex. From these characteristics, we can identify it with the order parameter we had in the phenomenological treatment above. However, if $< f_{-k} f_k > \neq 0$, then the new state is one without a definite number of particles. Although we do not show this here, let us mention that this is directly related to the fact that gauge invariance is broken.

After the remarks above, let us use the relations (6.64) to express the interaction term, but neglecting terms quadratic in fluctuations (second terms in eqs. (6.64)) . We have then,

$$\begin{aligned} f_k^\dagger f_{-k}^\dagger f_{-k'} f_{k'} &\simeq < f_k^\dagger f_{-k}^\dagger >< f_{-k'} f_{k'} > \\ &\quad + < f_k^\dagger f_{-k}^\dagger > \left(f_{-k'} f_{k'} - < f_{-k'} f_{k'} > \right) \\ &\quad + \left(f_k^\dagger f_{-k}^\dagger - < f_k^\dagger f_{-k}^\dagger > \right) < f_{-k'} f_{k'} > \\ &= f_k^\dagger f_{-k}^\dagger \, \psi_{k'} + \psi_k^* \, f_{-k'} f_{k'} - \psi_k^* \psi_{k'} \, , \end{aligned} \tag{6.65}$$

where we defined

$$\psi_k \equiv < f_{-k} f_k > \ . \tag{6.66}$$

After such an approximation, and extending it by addition of the chemical potential, the BCS-Hamiltonian becomes

$$\begin{aligned} H_{BCS} &\rightarrow H_{BCS} - \mu \hat{N} \\ &\simeq \sum_k \left[\epsilon \left(\boldsymbol{k} \right) - \mu \right] f_k^\dagger f_k \\ &\quad + \frac{1}{2} \sum_{k,k'} W_{kk'} \left(f_k^\dagger f_{-k}^\dagger \, \psi_{k'} + \psi_k^* \, f_{-k'} f_{k'} - \psi_k^* \psi_{k'} \right) \, . \end{aligned} \tag{6.67}$$

With such an approximation (*mean-field approximation*), the originally interacting system is approximated by non-interacting fermions under the influence of a field that has to be determined self-consistently. On the other hand, since now the Hamiltonian is bilinear in the fermionic operators, it is possible to diagonalize it by means of a *Bogoliubov-transformation*, where new operators are introduced as follows

$$\begin{aligned} f_k &= u_k \, \gamma_k + v_k \, \gamma_{-k}^\dagger \\ f_{-k}^\dagger &= -v_k \, \gamma_k + u_k \, \gamma_{-k}^\dagger \, , \end{aligned} \tag{6.68}$$

with the properties of the coefficients

$$u_k = u_{-k} \, , \quad v_k = -v_{-k} \, , \quad u_k^2 + v_k^2 = 1 \, , \tag{6.69}$$

such that the new operators obey canonical anticommutation relations for fermions,

$$\left\{\gamma_k, \gamma_{k'}^\dagger\right\} = \delta_{kk'} \ , \quad \left\{\gamma_k, \gamma_{k'}\right\} = \left\{\gamma_k^\dagger, \gamma_{k'}^\dagger\right\} = 0 \ , \tag{6.70}$$

and hence, we have a canonical transformation. This leads to the different products

$$\begin{aligned} f_k^\dagger f_k &= \left(-v_{-k}\,\gamma_{-k} + u_{-k}\,\gamma_k^\dagger\right)\left(u_k\,\gamma_k + v_k\,\gamma_{-k}^\dagger\right) \\ &= u_{-k}u_k\gamma_k^\dagger\gamma_k + v_{-k}v_k\gamma_{-k}^\dagger\gamma_{-k} \\ &\quad -v_{-k}u_k\gamma_{-k}\gamma_k + u_{-k}v_k\gamma_k^\dagger\gamma_{-k}^\dagger - v_{-k}v_k \qquad (6.71) \\ f_k^\dagger f_{-k}^\dagger &= \left(-v_{-k}\,\gamma_{-k} + u_{-k}\,\gamma_k^\dagger\right)\left(-v_k\,\gamma_k + u_k\,\gamma_{-k}^\dagger\right) \\ &= v_{-k}u_k\gamma_{-k}^\dagger\gamma_{-k} - u_{-k}v_k\gamma_k^\dagger\gamma_k \\ &\quad +v_{-k}v_k\gamma_{-k}\gamma_k + u_{-k}u_k\gamma_k^\dagger\gamma_{-k}^\dagger - v_{-k}u_k \ . \qquad (6.72) \end{aligned}$$

Inserting these products into (6.67), we have

$$\begin{aligned} (6.67) \;=\; & \sum_k \left\{\left[\epsilon\left(\boldsymbol{k}\right) - \mu\right]\left(u_k^2 - v_k^2\right) - 2\sum_{k'} W_{kk'}\,\psi_{k'}\,u_k v_k\right\}\gamma_k^\dagger\gamma_k \\ & + \sum_k \left\{\left[\epsilon\left(\boldsymbol{k}\right) - \mu\right]u_k v_k + \frac{1}{2}\sum_{k'} W_{kk'}\,\psi_{k'}\left(u_k^2 - v_k^2\right)\right\} \\ & \qquad \times\left(\gamma_k^\dagger\gamma_{-k}^\dagger + \gamma_{-k}\gamma_k\right) \ . \qquad (6.73) \end{aligned}$$

We can get rid of the non-diagonal terms by requiring

$$2\left[\epsilon\left(\boldsymbol{k}\right) - \mu\right]u_k v_k \;=\; -\left(u_k^2 - v_k^2\right)\sum_{k'} W_{kk'}\,\psi_{k'} \equiv \left(u_k^2 - v_k^2\right)\Delta_k \ , \tag{6.74}$$

where we defined

$$\Delta_k = -\sum_{k'} W_{kk'}\,\psi_{k'} \ . \tag{6.75}$$

The minus sign was taken into account due to the fact that $W_{kk'} < 0$, as stated in (6.63). Equation (6.74) together with the condition $u_k^2 + v_k^2 = 1$ constitute the equations that determine the coefficients u_k and v_k of the canonical transformation. The solution is easily found by setting

$$u_k = \cos\phi_k \qquad v_k = sin\phi_k \ , \tag{6.76}$$

such that (6.74) goes over into

$$\left[\epsilon\left(\boldsymbol{k}\right) - \mu\right]\sin 2\phi_k = \Delta_k \cos 2\phi_k \quad \Longrightarrow \quad \tan 2\phi_k = \frac{\Delta_k}{\epsilon\left(\boldsymbol{k}\right) - \mu} \ . \tag{6.77}$$

Using the relations

$$1 + \tan^2 x = \frac{1}{\cos^2 x} \ , \quad 1 + \frac{1}{\tan^2 x} = \frac{1}{\sin^2 x} \ , \tag{6.78}$$

we have

$$\cos 2\phi_k = u_k^2 - v_k^2 = \pm \frac{\epsilon(\boldsymbol{k}) - \mu}{E_k} \tag{6.79}$$

$$\sin 2\phi_k = \pm \frac{\Delta_k}{E_k} , \tag{6.80}$$

where we defined

$$E_k \equiv \sqrt{[\epsilon(\boldsymbol{k}) - \mu]^2 + \Delta_k^2} . \tag{6.81}$$

Replacing the results above into (6.73), we have the Hamiltonian $\tilde{H}$ after the canonical transformation

$$\tilde{H} = \sum_k E_k \gamma_k^\dagger \gamma_k , \tag{6.82}$$

where we have taken the positive root, since a meaningfull Hamiltonian should have a ground state. This shows that the spectrum of the quasiparticles has now a gap given by Δ_k. The ground-state of the system is given by the vacuum for the new operators

$$\gamma_k \mid 0 >= 0 , \quad < 0 \mid \gamma_k^\dagger = 0 , \tag{6.83}$$

such that in the ground-state,

$$\psi_k = < f_{-k} f_k >= u_k v_k = \frac{\Delta_k}{2E_k} , \tag{6.84}$$

according to (6.72) and (6.80). With this result relating the order parameter to energy gap, we finally obtain the *gap-equation*, by recalling the definition (6.75)

$$\Delta_k = -\frac{1}{2} \sum_{k'} W_{kk'} \frac{\Delta_{k'}}{E_{k'}} . \tag{6.85}$$

Since this is a homogeneous equation, the trivial case $\Delta_k = 0$ is allways a solution.

6.3.1 Solution of the gap-equation

In the following we consider the solution of the gap-equation for the case where $W_{kk'} = -W$, is a constant in the shell given by δ in (6.63). Then, we have

$$\Delta_k = \frac{W}{2} \sum_{k'} \frac{\Delta_{k'}}{E_{k'}} , \tag{6.86}$$

showing that Δ should also be momentum indenpendent. Then, the gap-equation reduces to

$$1 = \frac{W}{2} \sum_{k'} \frac{1}{\sqrt{[\epsilon(\boldsymbol{k}) - \mu]^2 + \Delta^2}} . \tag{6.87}$$

At this point, it can be clearly seen that we can have a non-trivial solution only when $W > 0$, i.e. when an attractive interaction among electrons is present. Repulsive interactions can only lead to superconductivity, when the order parameter has a non-trivial momentum dependence. This is the case e.g., in high temperature superconductors, where the experimentally measured properties of the order parameter are consistent with a so-called *d-wave* symmetry, with

$$\Delta_k \sim \cos k_x a - \cos k_y a \ , \tag{6.88}$$

a being the lattice constant. In the following we will concentrate us on the simple case that is generally found in ordinary superconductors, where the gap, and isotope effect result in a natural form from the BCS-theory.

As we have already stated at the begining of Sec. 6.3, the attractive interaction is present for $\mid \epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{q}} \mid < \hbar\omega_D$, where ω_D is the Debye frequency. We can therefore write

$$W_{kk'} \ = \ -\frac{\lambda}{V}\,\theta\left(\hbar\omega_D - \mid \xi_k \mid\right)\theta\left(\hbar\omega_D - \mid \xi_{k'} \mid\right) \ , \tag{6.89}$$

where we introduced the short notation

$$\xi_k \equiv \epsilon\left(\boldsymbol{k}\right) - \mu \ . \tag{6.90}$$

Introducing this into the gap-equation (6.85), we have

$$\Delta_k \ = \ \frac{\lambda}{2V}\sum_{k'}\theta\left(\hbar\omega_D - \mid \xi_k \mid\right)\theta\left(\hbar\omega_D - \mid \xi_{k'} \mid\right)\frac{\Delta_{k'}}{E_{k'}} \ , \tag{6.91}$$

with a solution $\Delta_k = \Delta\,\theta\left(\hbar\omega_D - \mid \xi_k \mid\right)$ that leads to the equation

$$1 = \frac{\lambda}{2V}\sum_{k}\frac{\theta\left(\hbar\omega_D - \mid \xi_k \mid\right)}{\sqrt{\Delta^2 + \xi_k^2}} \ . \tag{6.92}$$

It is convenient to go from a summation over momenta over to an integral over energies introducing thus the density of states, as already done in Sec. 4.3.3:

$$\frac{1}{V}\sum_{\boldsymbol{k}} \ \rightarrow \ \int N(\xi)\,\mathrm{d}\xi \simeq N(0)\int \mathrm{d}\xi \ , \tag{6.93}$$

where we have assumed that $\hbar\omega_D \ll E_F$. Then, we have for (6.92),

$$\begin{aligned} 1 \ &= \ \frac{\lambda N(0)}{2}\int_{-\hbar\omega_D}^{\hbar\omega_D}\frac{\mathrm{d}\xi}{\sqrt{\Delta^2+\xi^2}} = \lambda N(0)\int_0^{\hbar\omega_D}\frac{\mathrm{d}\xi}{\sqrt{\Delta^2+\xi^2}} \\ \hookrightarrow 1 \ &= \ \lambda N(0)\ln\left[\frac{\hbar\omega_D + \sqrt{\left(\hbar\omega_D\right)^2+\Delta^2}}{\Delta}\right] \\ &\simeq \ \lambda N(0)\ln\frac{2\hbar\omega_D}{\Delta} \ , \end{aligned} \tag{6.94}$$

leading finally to

$$\Delta = 2\hbar\omega_D \exp\left[-\frac{1}{\lambda N(0)}\right] , \tag{6.95}$$

where the gap depends in a non-analytic fashion on the coupling constant, showing that such a result cannot be obtained in the frame of a perturbation theory.

Once we obtained the gap, we can go back to the coefficients u_k and v_k. Using the condition $u_k^2 + v_k^2 = 1$, and (6.79), we have

$$u_k^2 = \frac{1}{2}\left[1 + \frac{\xi_k}{\sqrt{\Delta^2 + \xi_k^2}}\right] , \tag{6.96}$$

$$v_k^2 = \frac{1}{2}\left[1 - \frac{\xi_k}{\sqrt{\Delta^2 + \xi_k^2}}\right] . \tag{6.97}$$

Apart from having the full solution, we notice that if we take the ground-state expectation value of (6.71), we have

$$< f_k^\dagger f_k >= v_k^2 , \tag{6.98}$$

i.e. we have the occupation number of the original fermions in the new ground state. In fact, if $\Delta = 0$, then we have

$$v_k^2 = \frac{1}{2}\left[1 - \frac{\xi_k}{\mid \xi_k \mid}\right] = \theta\left[\epsilon\left(\boldsymbol{k}\right) - \mu\right] , \tag{6.99}$$

as expected for free fermions.

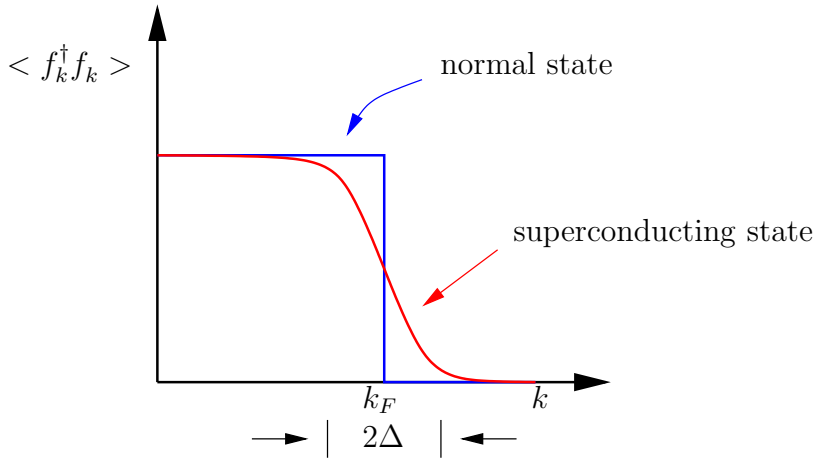

Figure 6.13: Momentum distribution function for the normal (blue line) and superconducting state (red line) with a gap Δ, both at $T = 0$.

For the superconducting state with $\Delta \neq 0$, a gap opens destroying the Fermi surface, such that the momentum distribution function shows a smooth decrease across the Fermi energy.

In order to find the critical temperature, we should perform an analogous calculation at finite temperatures. Without going through the calculation, we know that the temperature scale should be essentially given by the value of the gap at $T = 0$. In fact, the result is

$$T_c \simeq 1.14\,\hbar\omega_D \exp\left[-\frac{1}{\lambda N(0)}\right] , \tag{6.100}$$

showing that $T_c \sim \omega_D \sim M^{-1/2}$, explaining thus, the isotope effect. The exponent of the mass can vary from system to system, since the strength of the Coulomb interaction, that was not accounted for in this treatment may vary. A whole theoretical development was devoted, after the BCS-theory appeared, to describe the behavior of superconductors beyond the limitations of the BCS-theory and they can be seen in elective lectures. We close by noticing that the success of the BCS-theory is not only limited to ordinary superconductors, but it was also applied to understand the pairing states in ^{3}He, and nuclear matter.