FACULTÉ DES SCIENCES
Département de physique
de la matière condensée

Dirk van der Marel

Superconductivity

Basic notions of superfluidity and superconductivity

Lecture notes

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Contents

Chapter I:
Introduction to superfluidity and Bose-Einstein Condensation

Helium, named after Helios (who was believed by the ancient Greeks to drive his chariot of fire with a pair of horses across the sky), is the lightest of the noble gases in the periodic system. After hydrogen it is the most abundant element of the universe. *Two* stable isotopes exist: ^{4}He (~10^{-5} of the earth atmosphere) was first isolated in 1895 by Ramsey, and ^{3}He (~10^{-11} of the earth atmosphere) was first prepared in 1933 by Oliphant and collaborators. At ambient pressure ^{4}He boils at a temperature of 4.2 K. Heike Kamerlingh-Onnes was the first to prepare ^{4}He in the liquid phase. Kamerlingh-Onnes was an alumnus of the University of Groningen. He became a professor at the University of Leiden, and was awarded the Nobel Prize in 1913 for his investigations on the properties of matter at low temperatures, which, *inter alia,* led to the production of liquid helium. He did not –as is often assumed- receive the Nobel Prize for the discovery of superconductivity, although Gilles Holst and Kamerlingh-Onnes certainly made this discovery in 1911. This confusion may in part have been caused by the fact that Kamerlingh-Onnes announced their discovery of superconductivity during his Nobel-lecture.

If we cool down a liquid, it eventually will reach a temperature where it undergoes a first order phase transition to the solid phase. The transition temperature depends on the substance and on the pressure, but invariably every fluid becomes a solid if we cool it to sufficiently low temperature. Not so for helium, which, at ambient pressure remains a liquid all the way down to absolute zero! Only if a pressure of more than 25 bar is applied, ^{4}He solidifies below ~2 K, while it takes more than 30 bar to solidify the lighter ^{3}He, below ~1 K. Helium is the only liquid known which does not solidify at ambient pressure. This anomaly is a manifestation of quantum mechanics: In a solid the atoms are frozen in position because of the hard-sphere inter-atomic interactions. However, due to the uncertainty principle the atoms vibrate even at absolute zero temperature: Each lattice mode of vibration with momentum $\hbar k$ has in its lowest vibrational state still an energy $\hbar\omega_k/2$. The

amplitude of these zero-point vibrations is about $\hbar^{1/2}C^{-1/4}m^{-1/4}$, where C is the inter-atomic force constant, and m is the atomic mass. Because m is very small in helium, the zero-point fluctuations can overcome the potential barriers separating the atoms, with the result that helium remains in a liquid state even at absolute zero temperature.

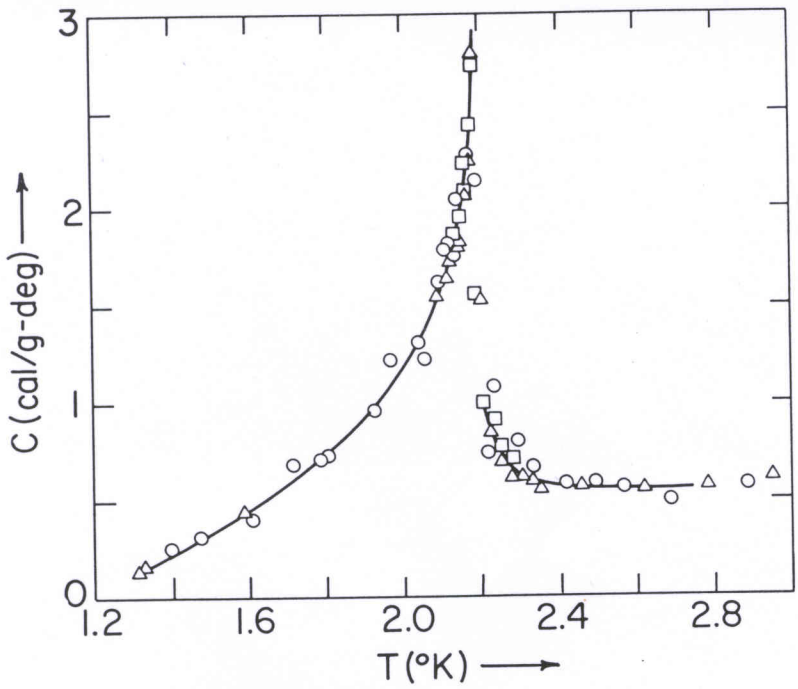


FIGURE 1.1

FIGURE 1.1. *Specific heat of liquid helium II [after Keesom and Clausius (1932)].*

Although no solid/liquid phase transition occurs at ambient pressure, in 1932 Keesom and Clausius did in fact discover a phase transition of a different kind at 2.2 K. The effect of this phase transition on the specific heat is displayed in Fig. 1.1: The C_V versus temperature curve has the shape of the character λ, and this phase transition is therefore called the "λ–transition". Clearly below 2.2 K the system has entered a different phase, but this is not the solid phase. In fact it is quite contrary to being a solid: In 1938 Kapitza, and Allen&Misener discovered that the viscosity measured in thin capillaries drops several orders of magnitude when liquid ^{4}He is cooled through the λ–transition. Further experiments have shown that below 2.2 K liquid ^{4}He is a *superfluid*, which means that the fluid can flow without any dissipation.

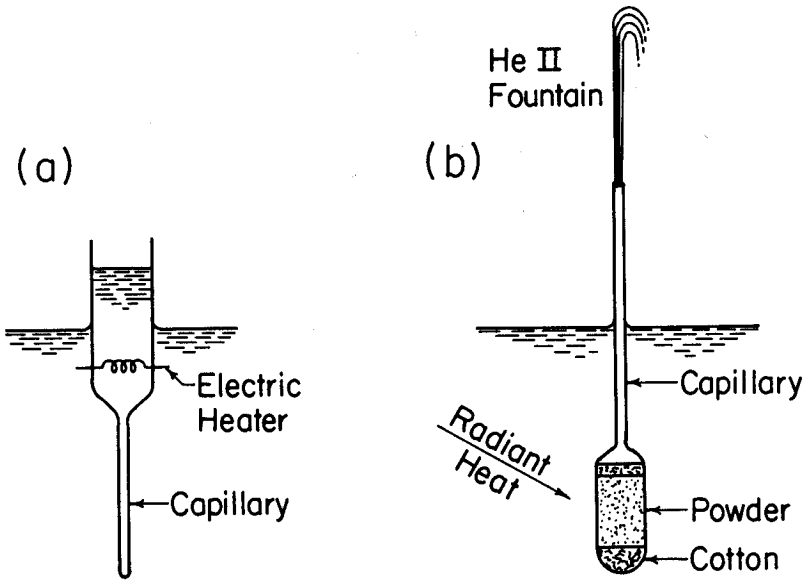


FIGURE 1.2

FIGURE 1.2. *Schematic representation of fountain effect experiments of Allen and Jones (1938) [after Atkins (1959)].*

One of the most striking effects associated with the superfluid state is the fountain effect, displayed in Fig. 1.2: Two reservoirs are connected by a thin capillary. If one supplies heat to the inner part, the level of the liquid rises considerably. If the heated helium is guided into a narrow capillary the heat imbalance even gives rise to a fountain. These effects show that transfer of matter accompanies heat transfer. These phenomena demonstrated a clash with the usual laws of hydrodynamics, and called for a fundamentally different theoretical framework when describing the physical properties of ^{4}He below the λ–transition

When a pressure of more than 25 bar is applied, ^{4}He does become solid below about 2 K. The pressure phase diagram is depicted in Fig. 1.3. Staring for a while at the phase diagram, one begins to realize that at low temperature and pressure, the solid phase of ^{4}He appears to have been replaced with the superfluid phase. This suggests that quantum effects not only inhibit solidification, but that superfluidity itself is a quantum effect.

We already saw that experimentally the history of superfluid helium began in 1932. Here we have to point out an aspect of ^{4}He which turns out to be of fundamental importance,

namely that each of these atoms consists of an even number of fermions: 2 protons, 2 neutrons, and 2 electrons. According to quantum theory composite objects consisting of an even number of fermions have boson-characteristics: Nothing prevents an arbitrary number of these composite bosons to occupy the same quantum state. (Note that for ^{3}He this situation is quite different!). On the theory front the starting shot had already been given in 1924: Satyendranath Bose studied at the University of Calcutta, then taught there in 1916, taught at the University of Dacca (1921-45), then returned to Calcutta (1945-56). He did important work in quantum theory, in particular on Planck's black body radiation law. Bose sent his work Planck's Law and the Hypothesis of Light Quanta (1924) to Einstein. He wrote a covering letter saying: "*Respected Sir, I have ventured to send you the accompanying article for your perusal and opinion. You will see that I have tried to deduce the coefficient in Planck's law independent of classical electrodynamics.*" It was enthusiastically endorsed by Einstein who saw at once that Bose had removed a major objection against light quanta. The paper was translated into German by Einstein and submitted with a strong recommendation to the Zeitschrift für Physik. Einstein extended Bose's treatment to material particles whose number is conserved and published several papers on this extension.

FIGURE 1.3

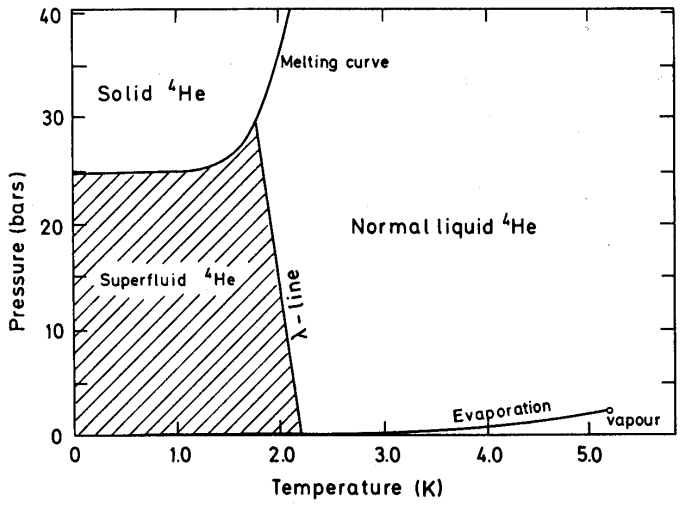


Figure 1.2 Pressure versus temperature phase diagram for ^{4}He; linear temperature scale.

In a nutshell the idea of Bose-Einstein condensation is the following: Consider a dilute gas of atoms at some finite temperature. The average kinetic energy of each of the atoms of is $3/2k_BT$, and the corresponding deBroglie wavelength is $\lambda_{dB} = \frac{h}{\sqrt{2\pi m k_B T}}$. Einstein proved that *if the atoms are bosons*, a phase transition to a fluid state takes place when the density of the gas exceeds a limiting value, *i.e.* when $n > 2.612/\lambda_{dB}^{\ 3}$. Alternatively one can keep the gas at a fixed density (by holding it in a closed container), and reduce temperature. Then condensation sets in when temperature drops below a critical value, *i.e.* when $T < T_c$, where the critical temperature is given by the expression: $T_c = \frac{3.31\hbar^2}{mk_B} n^{2/3}$.

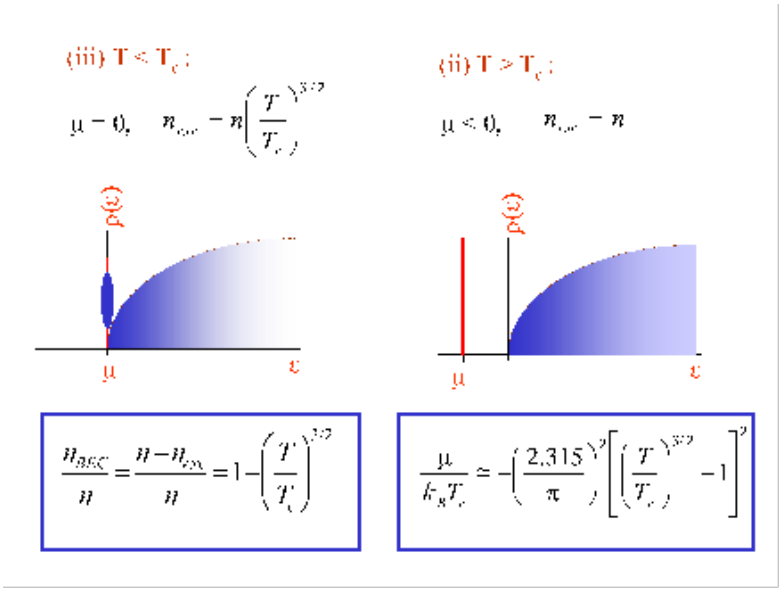


FIGURE 1.4

The bosonic character was crucial for the argument, and the mathematical proof proceeds along the following lines: We start with the assumption that the bosons behave like ideal gas particles. We therefore neglect the interactions between the particles (note that in 1925 nobody had liquid helium in mind!). The energy-momentum relation of the particles is

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m} \qquad (1.1)$$

Because ^{4}He atoms are bosons, the occupation of each energy level is controlled by Bose-Einstein statistics:

$$n_B(\varepsilon_k) = \frac{1}{e^{\beta(\varepsilon_k - \mu)} - 1} \qquad (1.2)$$

where μ is the chemical potential, which controls the total number of bosons present, and. The density of states of a 3 dimensional gas of non-interacting particles is

$$D(\varepsilon) = \eta V \sqrt{\varepsilon}$$
$$\eta \equiv 2^{-1/2} \pi^{-2} \hbar^{-3} m^{3/2} \qquad (1.3)$$

where V is the volume of the recipient containing the bosons. The total number of bosons $\beta=1/(k_BT)$ the inverse temperature. From here on we define $n=N/V$ as the density, which can not change if we alter the temperature when the volume of the box is fixed externally. On the other hand, the total number of bosons *also* follows from the Bose-Einstein occupation numbers, and the density of states:

$$N = \int_0^\infty D(\varepsilon) n_B(\varepsilon) d\varepsilon = \eta V \int_0^\infty \frac{\sqrt{\varepsilon}}{e^{(\varepsilon - \mu(T))/k_B T} - 1} d\varepsilon \qquad (1.4)$$

In order to satisfy that the external density equals the right hand side of the expression, the chemical potential has to be adjusted. In an experimental situation it is indeed so, that the chemical potential "adjusts itself" in order to satisfy the constraint on particle number expressed by Eq. 1.4. Let us look first at the possible values, which the chemical potential μ can adopt. First, we can see right away, that under all circumstances it must satisfy

$$\mu < 0 \qquad (1.5)$$

In fact, the case $\mu \to 0$ corresponds to an important limit in this context: this corresponds exactly to the Bose condensation limit. Careful mathematical analysis of this limit shows, that for μ=0 the Bose-Einstein occupation factors are provided by Eq. 1.2, except for the occupation of the state with $\varepsilon_k=0$: This state is occupied with a *macroscopic* number of bosons, N_0. The temperature where this special state sets in is easy to calculate: For $T < T_c$ we have μ=0, while $N_0=0$ above T_c. When $T=T_c$ both μ and N_0 are zero. This requires, that

$$n = \int_0^\infty \frac{\eta \sqrt{\varepsilon}}{e^{\varepsilon / k_B T_c} - 1} d\varepsilon = \eta \left(k_B T_c\right)^{3/2} \int_0^\infty \frac{x^{1/2}}{e^x - 1} dx \qquad (1.6)$$

The integral on the right hand side is a standard integral, which equals 2.31... With the help of this the expression for the critical temperature becomes

$$k_B T_c = \left(\frac{n}{2.31\ \eta} \right)^{2/3} = 3.31 \frac{\hbar^2}{m k_B} n^{2/3} \qquad (1.7)$$

Below the critical temperature, the chemical potential remains glued to the lowest energy of the bosonic band. It can't shift inside the band, because this would introduce an infinite number of particles for all states at energy below μ. The number of excited particles, i.e. those which are not the ε_k=0 state, is given by the expression

$$\frac{N_{exc}}{N} = \left(\frac{T}{T_c} \right)^{3/2} \qquad (T<T_c) \qquad (1.8)$$

The total number of particles is N =N_{exc}+N_0. This implies that at T=0 N_0=N: All bosons are condensed in the lowest-energy state. Consequently the groundstate is given by expression

$$|N_0\rangle = \left(a_0^\dagger\right)^{N_0} |0\rangle \qquad (T=0) \qquad (1.9)$$

Above the critical transition temperature the number of condensed particles, N_0=0, but now the chemical potential μ differs from zero. With some mathematical effort it can be shown, that just above the phase transition

$$\frac{\mu}{k_B T_c} \cong -\left(\frac{2.315}{\pi} \right)^2 \left[\left(\frac{T}{T_c} \right)^{3/2} - 1 \right]^2 \qquad (T>T_c) \qquad (1.10)$$

The various situations have been sketched in Fig. 1.4. In Fig. 1.5a temperature dependence of N_{exc}(T), and μ(T) is shown, obtained by solving Eq. 1.4 numerically.

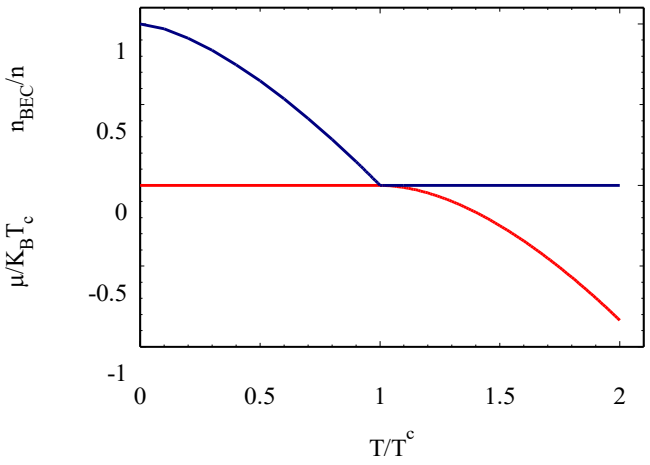


FIGURE 1.5a

The total energy of the Bose-gas is

$$E(T) = \int_0^\infty D(\varepsilon) n_B(\varepsilon) \varepsilon \, d\varepsilon = \eta V \int_0^\infty \frac{\varepsilon^{3/2}}{e^{(\varepsilon - \mu(T))/k_B T} - 1} d\varepsilon \qquad (1.11)$$

For $T<T_c$ we have $\mu(T<T_c)=0$, so that

$$E(T) = \eta V \left(k_B T\right)^{5/2} \int_0^\infty \frac{x^{3/2}}{e^x - 1} dx = 1.783 \eta V \left(k_B T\right)^{5/2} = 0.772 N k_B \frac{T^{5/2}}{T_c^{3/2}} \qquad (1.12)$$

Hence the specific heat is

$$C(T) = 1.92 N k_B \left(\frac{T}{T_c}\right)^{3/2} \qquad (T<T_c) \qquad (1.13)$$

For $T>T_c$ we have an additional term, due to the fact that $\mu(T)$ is given by Eq. (1.10). Expanding the Bose-Einstein occupation factor in Eq. (1.11) as $n(\varepsilon) + \{1 + n(\varepsilon)\} n(\varepsilon) \mu(T) / k_B T$, it is easy to prove that close to T_c

$$C(T) = 1.92 N k_B \left(\frac{T}{T_c}\right)^{3/2} - 2.46 N k_B \left(\frac{T}{T_c}\right)^{1/2} \left[\left(\frac{T}{T_c}\right)^{3/2} - 1\right] \qquad (T>T_c) \qquad (1.14)$$

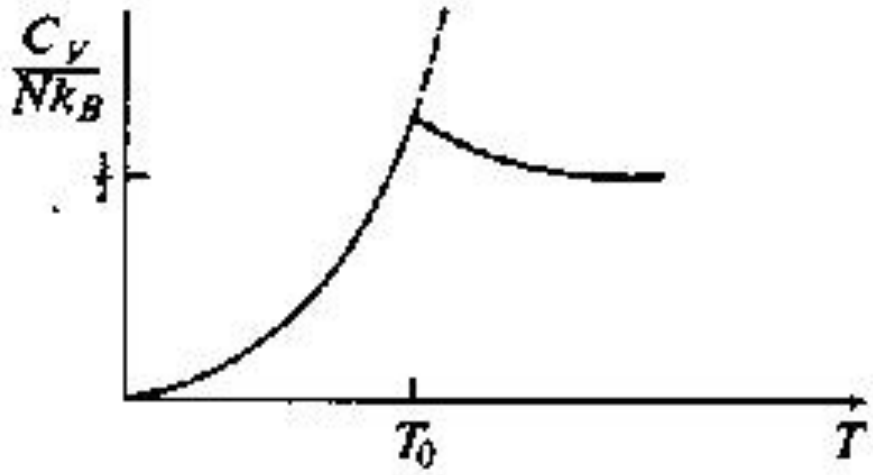


FIGURE 1.5b

In Fig. 1.5b the resulting specific heat curve is displayed.

Let us compare the theory of Bose-Einstein condensation now to the experimental facts in ^{4}He:

- First, ^{4}He atoms are bosons.

- Second, with Eq. 1.7, adopting $m=6.69 \times 10^{-24}$ *g* for the mass, and $n = 2.2 \times 10^{22}$ *(cm^{-3})* for the density of liquid ^{4}He*: the predicted phase transition is at Tc=3.14 K. Experimentally this is 2.2K.* Actually not bad considering the fact that we approximated a liquid with an ideal gas model.
- Third, the specific heat at low T was predicted to have $T^{3/2}$ behaviour. The experimentally observed temperature dependence is T^3, which is significantly different.
- In the fourth place the condensate fraction n_0 for T<<Tc approaches n_0=1 in BEC theory. Experimentally n_0=0.1 was observed (see Fig. 1.6a)
- Finally, the shape of the calculated anomaly does not at all look like a λ-transition.

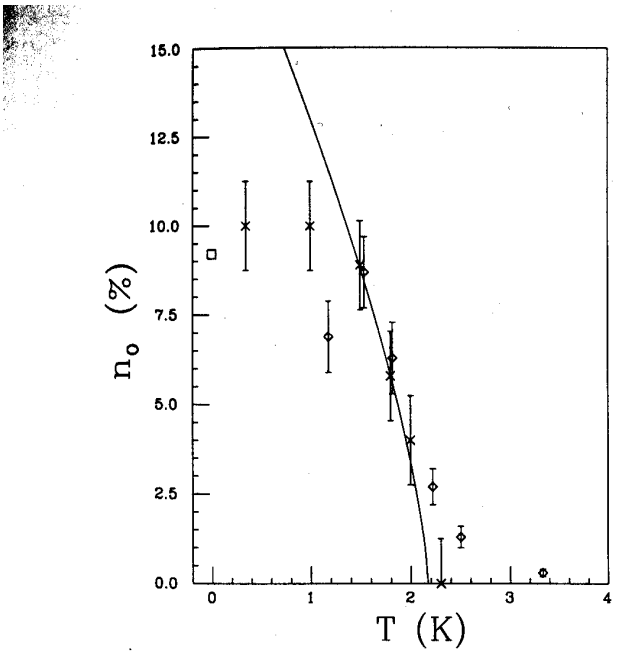


FIGURE 1.6a

Fig. 12. The value of n_0 as a function of temperature at a constant density of 0.147 g cm^{-3}, obtained from fits using the method of Snow *et al.*[50] (crosses). Also shown are the theoretical calculations of n_0 at $T = 0$ from GFMC (square) and at finite temperatures from PIMC calculations (diamonds). The solid line is a plot of the renormalization group theory prediction.

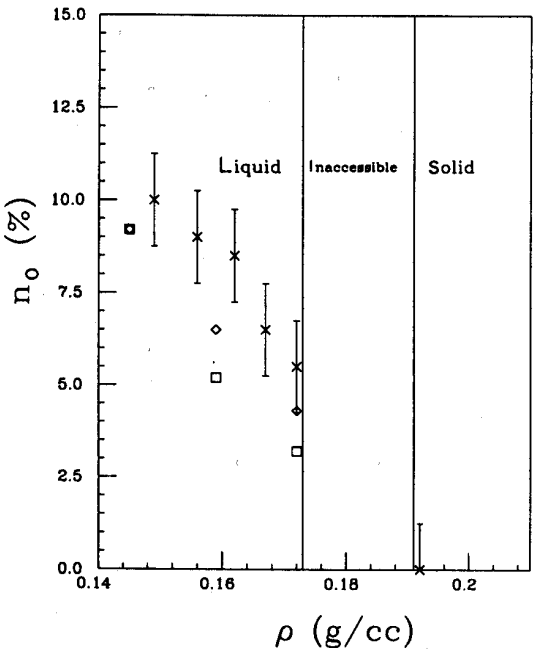


FIGURE 1.6b

Fig. 13. The value of n_0 as a function of density at 0.75 K obtained from using the method of Snow *et al.* [50] (crosses). The GFMC results for n_0 (squa and the HNC/S results (diamonds) are also shown.

A clue for the discrepancies is given by the pressure dependence of T_c. The phase diagram (Fig. 1.3) showed, that increasing the density by applying pressure, has the effect of reducing T_c, which is *opposite* to the trend expected from the Bose-Einstein formula, Eq. 1.7. A further clue is provided by the pressure dependence of the superfluid density displayed in Fig. 1.6b, where it was observed that the superfluid density *decreases* when pressure is applied.

The main reason for the disagreement between theory and experiment must be the fact that liquid ^{4}He is rather far from the realization of an ideal gas. The atoms interact strongly, on a short length scale, which has a profound effect on the excitation spectrum: Instead of the energy momentum relation of free particles expressed in Eq. (1.1), a sound like dispersion has been observed, with at high momentum a so-called 'roton-minimum' (see Fig. 1.7). This experimentally observed energy-momentum dispersion has been the subject of intense theoretical investigation during the middle of the 20th century, and legendary physicists like Boguliubov, Feynman, Landau, Nozieres, Pines, and many others have contributed to the microscopic understanding of this peculiar k-dependence, along with the low temperature physical properties.

FIGURE 1.7

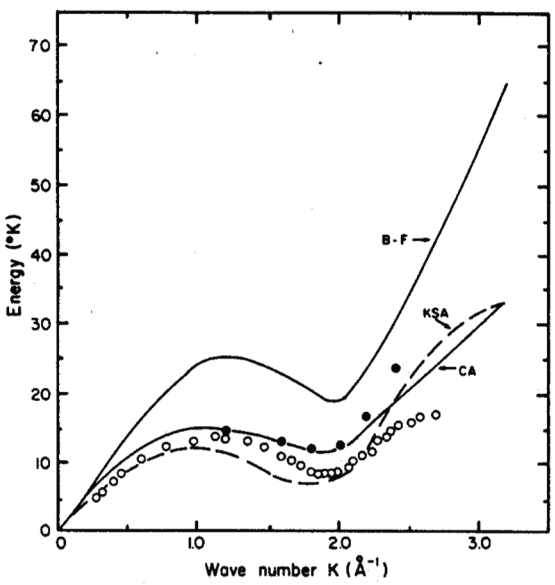


FIGURE 10.9. The excitation spectrum of liquid ^{4}He. The points are the experimental result for the superfluid. The other lines are various theories, including Bijl–Feynman (B–F) and backflow theories which use the Kirkwood superposition approximation (KSA) or convolution approximation (CA). Solid points are the Feynman–Cohen theory. *Source*: Feenberg (1969) (used with permission).

Because the long wavelength (small wave number) dispersion is now quasi-accoustical, *i.e.* the energy momentum relation of the particles is

$$\varepsilon(k) = vk \qquad (1.15)$$

Also the density of states has a different energy dependence: Instead of Eq. (1.3) the low frequency limiting behaviour of the DOS is given by the expression

$$D(\varepsilon) = \frac{\varepsilon^2}{2\pi^2} \qquad (1.16)$$

Following the same procedure as in Eq. (1.6) a different exponent is now found for $N_{exc}(T)$, and $N_0(T)$ namely

$$\frac{N_{exc}}{N} = \left(\frac{T}{T_c}\right)^3 \qquad (T<T_c) \qquad (1.17)$$

Another consequence of the interactions between the boson is, that the condensate fraction is no longer unity for T=0. This is nicely demonstrated in the momentum distribution function measured with neutron scattering below and above the phase transition, showing that the condensate fraction of ^{4}He is of the order of 10 percent.

FIGURE 1.8

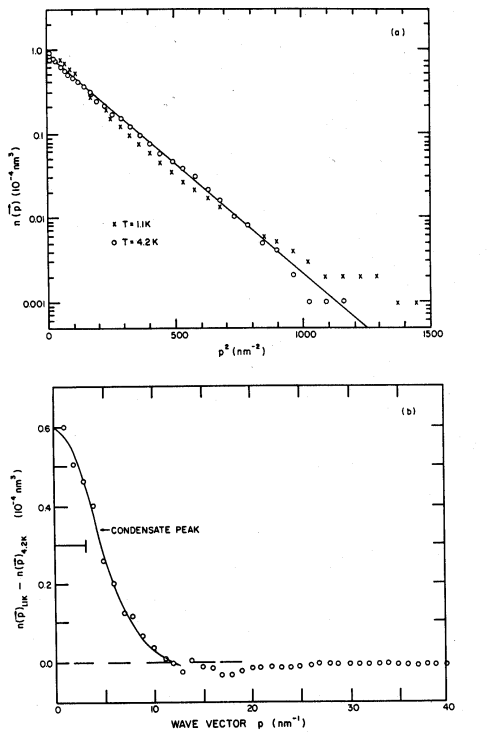


FIGURE 10.5. (a) Neutron scattering results for the momentum distribution in liquid ^{4}He at $T = 1.1$ and 4.2 K as a function of p^2. (b) The difference between the two distributions in part (a) shows a peak at small wave vector whose width equals the experimental resolution. The peak is interpreted as the condensate fraction. *Source*: Woods and Sears (1977) (used with permission).

The most important ingredient of the BEC story is, that ^{4}He is a boson. What happens if we remove one of the 4 nuclear particles? On the one hand the mass of ^{3}He is 75% of the ^{4}He mass, hence according to Eq. (1.7) one might expect the phase transition to occur at a 30% higher temperature, i.e. around 3K. However, this is not observed. In fact, no phase transition occurs below the solid/liquid transition of ^{3}He down to the mK range! Formally, we shouldn't be surprised because ^{3}He is a *fermion*: it is a composite object consisting of an odd number of fermions. It is a bit hard to imagine that removal of a nuclear particle could have any effect on the properties of a fluid, apart from reducing the mass to 75% of the ^{4}He mass. Yet, this is just one of the many strange consequences of quantum mechanics, which have now been established as experimental facts. Indeed ^{3}He is expected to form a Fermi-liquid, similar to a gas of electrons in e.g. aluminum or sodium. Given the mass of the atoms, $m=5.0\times10^{-24}$ g, and the density $n=2.3\times10^{22}$ cm^{-3} in the liquid phase, the expected Fermi temperature is

$$T_F = \frac{\hbar^2 (3\pi^2 n)^{2/3}}{2mk_B} = 6.2K \qquad (1.18)$$

That ^{3}He is a fermion, and not a boson, is nicely demonstrated by neutron scattering, showing that the distribution in momentum space indeed has the features of a Fermi-liquid., Fig. 1.9. Note also the large difference in momentum distribution with the bosonic case of ^{4}He, displayed in Fig. 1.8.

FIGURE 1.9

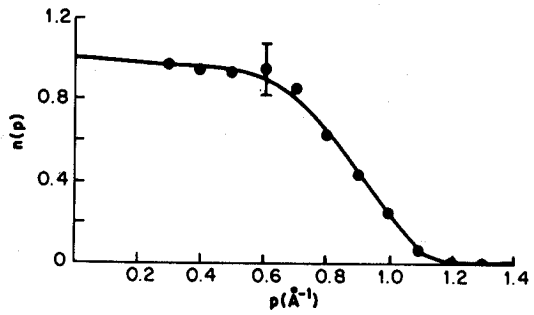


FIGURE 10.11. Momentum distribution n_p of particles in ^{3}He at $T = 0.37$ K. The solid line is a least-squares fit to the Fermi distribution with an effective temperature of $T_F = 1.8$ K. *Source*: Mook (1985) (used with permission).

In 1971 Oshereroff, Richardson and Lee *did* discover superfluidity in ^{3}He below 2.6 mK. The phase diagram (Fig. 1.10) looks rather complicated, and within the superfluid phase extra phase boundaries have been observed. In later chapters we will see, that this behaviour is more related to superconductivity, and what one really observes here is the condensations of *pairs* of ^{3}He atoms!

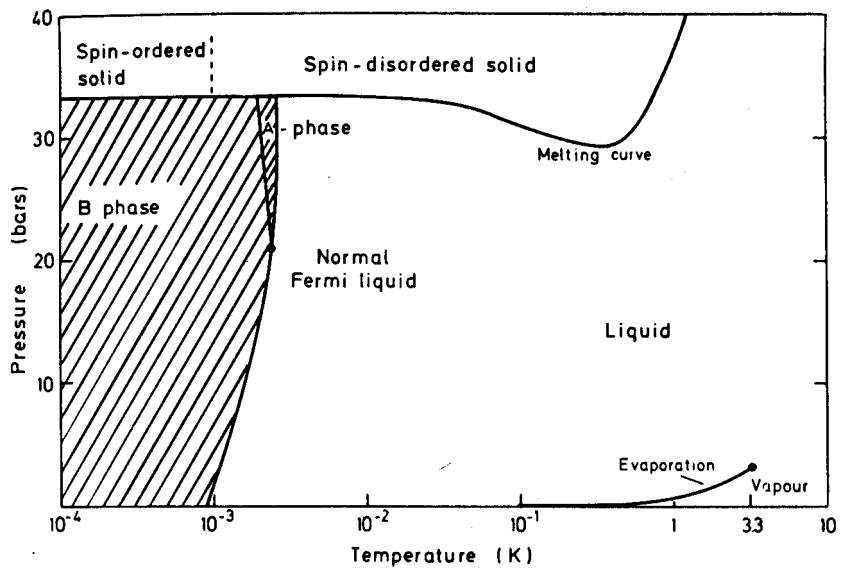


FIGURE 1.10 **Pressure versus temperature phase diagram for ^{3}He; note the logarithmic temperature scale.**

Because of the complications due to interactions between the helium atoms, causing Tc to be different from the BEC prediction, and also strongly affecting the temperature dependence of all physical properties, for a long time people have sought to perform BEC experiments under conditions closer to those of an ideal gas, i.e. for a real dilute gas of bosons. One of the consequences of working in the regime of a dilute gas, rather than a dense liquid, is that Tc will be much lower. BEC under ideal gas like conditions have been finally realized in 1995 in dilute gases of $_{11}Na^{23}$, $_{37}Rb^{85}$, and in $_3Li^7$, almost simultaneously by Ketterle, Cornell, and Hulet respectively. The densities are indeed much lower than for liquid helium: 10^{14} cm^{-3} < n < 10^{15} cm^{-3}. Because the masses of these atoms are much higher, the transition temperatures range from 0.5 μK to 2 μK. The combination of laser cooling and evaporative cooling of alkali atoms was a prerequisite for the observation of BEC in dilute atomic gases:

The following description of the experimentes was adopted from Wolfgang Ketterles web-page: “In Ketterle’s trap, the atoms start out in an oven, which is held at 350 degrees centigrade. These hot atoms are allowed to escape through a hole in the oven and shoot out in a beam traveling at about 800 meters per second (1800 miles per hour). They than aim a

laser beam in the opposite direction of the atomic beam. The laser beam hits the atoms and slows them down to about 20 meters per second (45 miles per hour) at the center of our vacuum chamber, where a magneto-optical trap (MOT) captures them. The MOT traps the atoms with six laser beams coming in from all directions. These beams push the atoms into the center of the chamber. After collecting a large number of atoms in the MOT, they turn off the lasers and turn on a large magnetic field, which confines the atoms magnetically. In the magnetic trap they cool the atoms down to very low temperatures and study them. Ground state sodium atoms can have several different spin orientations. Atoms in one of the orientations are attracted to weak magnetic fields. These are the ones which are trapped in the BEC experiment. A different spin orientation is attracted to high magnetic fields. Since the magnetic trap has a magnetic field minimum at the center, these "strong-field seeking" atoms are pushed out of the trap. The technique used by Ketterle to get extremely cold atoms is called rf-induced evaporation. To induce evaporation, radio waves are used to flip the spins of the most energetic atoms in the trap. With their spins flipped, they fly out of the trap. Since only the most energetic atoms are ejected, they take away more than their fair share of energy. When the rest of the atoms re-thermalize (by bouncing off of each other several times), the net energy per atom has dropped, and the atom cloud is cooler. It is very similar to the way evaporation works in a cup of hot coffee. A cup of coffee is made up of many molecules flying around and bumping into each other. The temperature of the coffee is just a measure of the average energy that these quickly moving molecules have. From time to time two molecules will collide in such a way that one of the two ends up with most of the energy, sometimes even gaining enough energy to fly out of the cup. Since these molecules are going relatively fast compared to the rest of the molecules, they take with them more than their fair share of energy, and the molecules which are left behind have less energy on average than they did before the fast molecules shot out. For every molecule that is kicked out, the temperature of the coffee decreases a tiny amount.

The experiment with which BEC is actually *observed*, is by turning off the trapping fields suddenly and looking at the velocity spectrum of the atoms as they flew out of the trap. This method is often referred to as a time of flight measurement, since the velocity spectrum is determined from the position of atoms in the image and the time that atoms

were allowed to expand in free flight before the image was taken. An example showing the velocity distributions, and BEC of $_{11}Na^{23}$ while it is being cooled below the BEC point is shown in Fig. 1.11 (Figure taken from Wolfgang Ketterle's webpage), clearly showing the development of the condensate at zero momentum, as temperature is lowered below Tc. It is also clear , that in this case the condensate fraction approaches 100 %, indicating that indeed the ideal gas situation envisaged in the Bose-Einstein condensation theory in 1925, has been realized here."

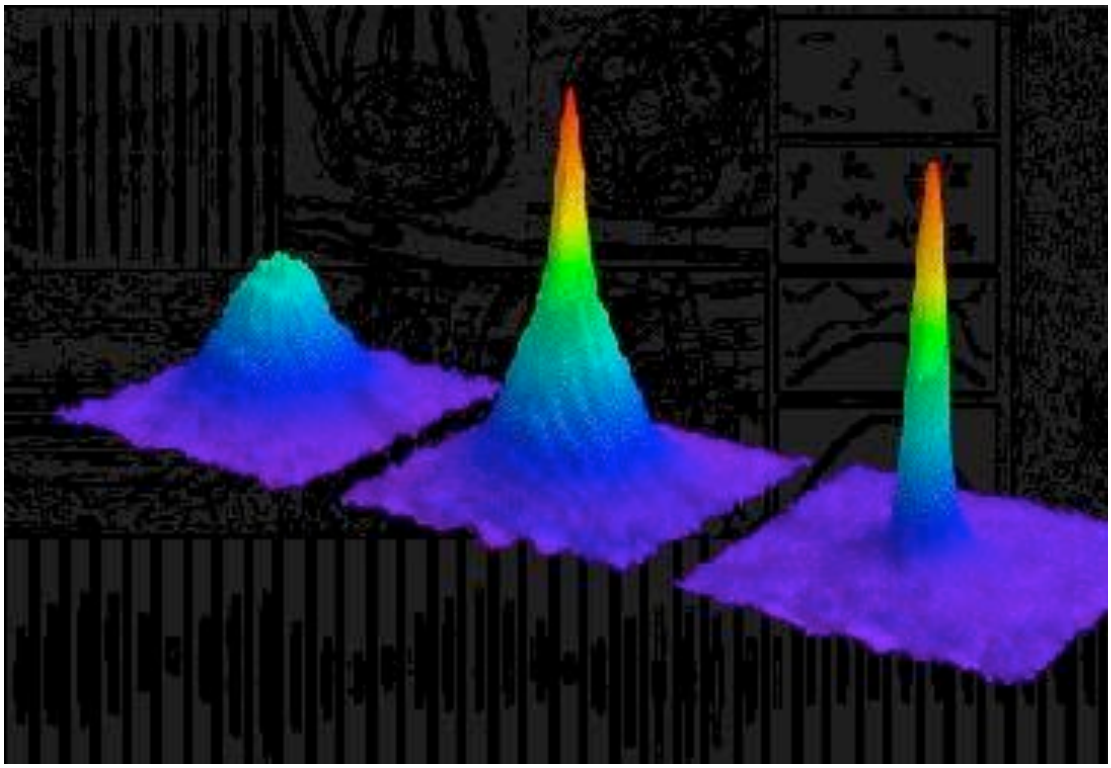


FIGURE 1.11

A final word about Bose-Einstein condensation. In fact many more phenomena are BEC, or related to BEC. Some of these will return in later chapters. We will see, for example, that superconductivity has much to do with BEC. But also the interior of nuclei and neutron stars (nn or pp pairing) have physics in common with these phenomena, but now at an entirely different energy scale. In the physics of elementary particles pairing and condensation of mesons is been studied theoretically, chiral $<q\underline{q}>$ condensates in vacuum have been proposed for the structure of elementary particles and $<t\underline{t}>$ condensates for the structure of the Higgs boson.

In principle one can also look for other bosons to do experiments like this on. The principle of a laser (photons!) has much to do with this, because it corresponds to a macroscopic occupation of the same electromagnetic state with photons. However, one can also attempt to do condensation experiments of elementary excitations in solids, such as excitons, bi-excitons, or magnons.

Problems

1. Calculate Tc of $_{11}Na^{23}$, $_{37}Rb^{85}$, and in $_{3}Li^{7}$, if the density is 10^{14} cm^{-3}.

2. Calculate Tc of a mixture of 10 % ^{4}He and 90% ^{3}He, if the density is $2.3x10^{22}$ cm^{-3}.

3. Calculate Tc of a ferro-magnet containing a fixed number of magnons, with a density of 10^{22} cm^{-3}., and adopting the dispersion relation $\hbar\omega(k) = Ja^2k^2$, where $J = 200\ K$ is the exchange constant, and $a = 0.3\ nm$ is a cell parameter.

Chapter II:

The main characteristics of superconductivity

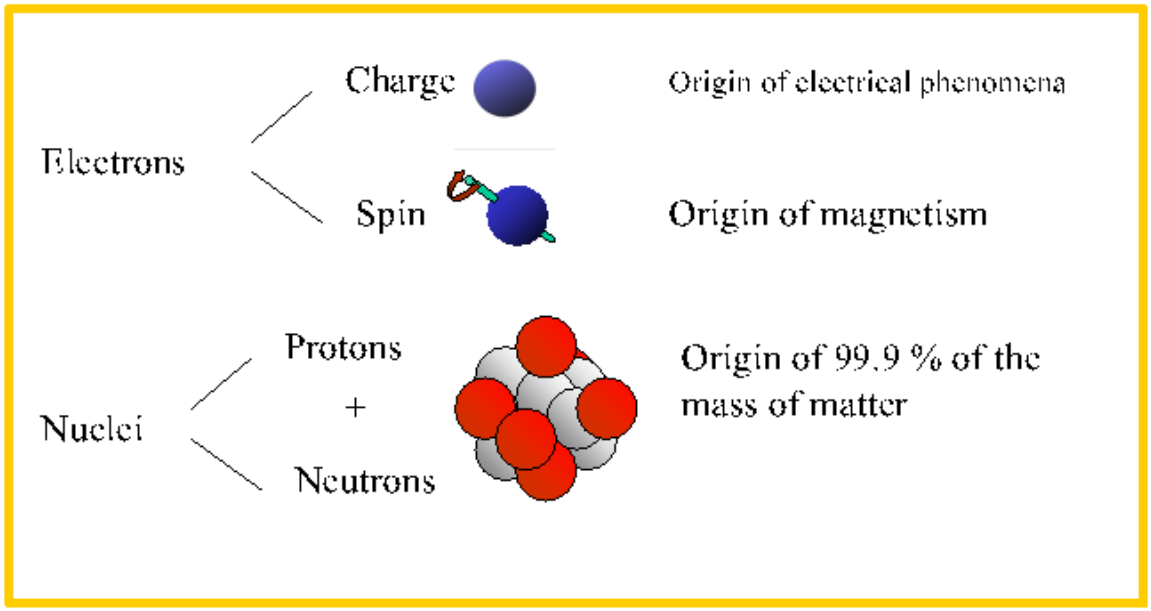


FIGURE 2.1

Electrons and nuclei (protons and neutrons) are the particles from which solids are formed. Electrons couple to the electromagnetic field in two different ways: First of all as a result of their electrical charge, second due to their spin.

- The charge of electrons is at the heart of all 'electrical' phenomena, i.e. metallic conductivity and superconductivity and optical properties, and it is responsible for part of the magnetic phenomena, in particular the diamagnetic properties of superconductors, but also orbital magnetism of rare earth elements.
- The spin of the electrons causes magnetism in typical ferromagnets such as iron. It is also a crucial element in many quantum mechanical phenomena (the Einstein Podolsky Rosen paradox is probably one of the most well known). We will see later, that the spin

quantum number plays a crucial role in the concept of the pairing phenomenon in superconductors.

- The nuclei enter the game in more than one way. First, they provide the electrically positive background, which acts as a container for the negatively charged electrons, which would otherwise disperse. Moreover, the dynamical vibration spectrum of the atoms depends strongly on the mass of the nuclei. We have already seen that in the exceptional case of helium at ambient pressure, the zero-point fluctuations prevent the formation of a solid. We also know, that lattice vibrations, when coupled to the electronic motion, have a strong influence on the transport properties of the electrons. Important in the context of superconductivity is, that electron-phonon coupling can play the role of a 'glue', causing pair-formation and superconductivity.

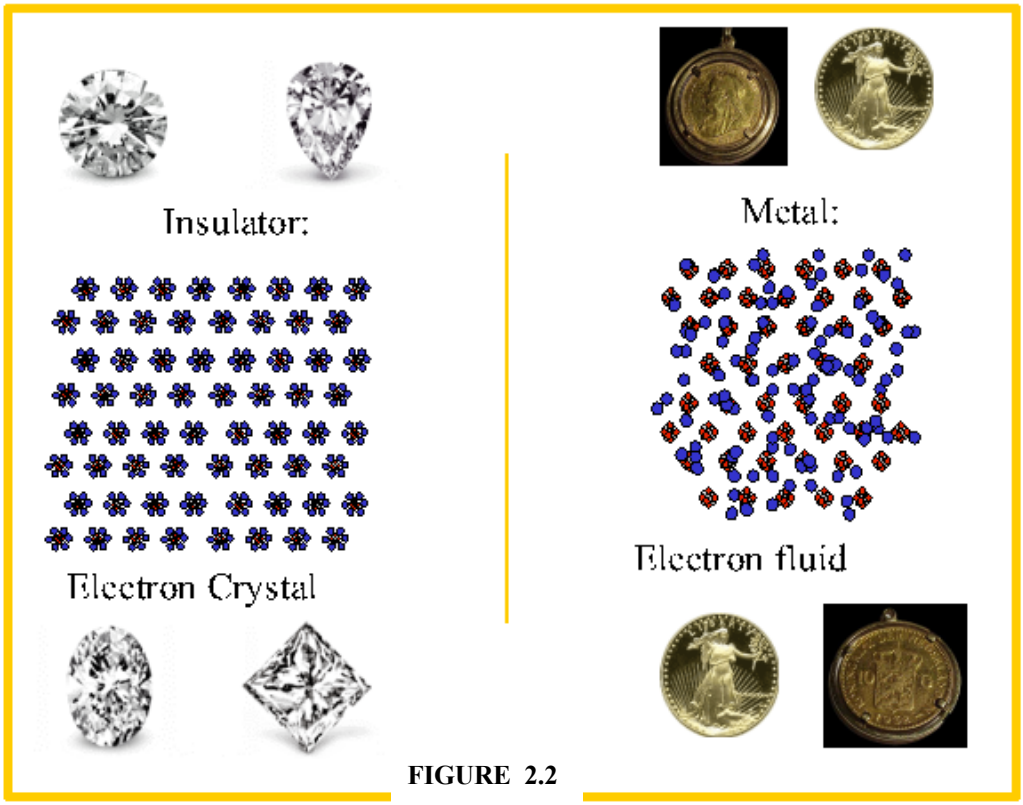


FIGURE 2.2

The reason that typical insulators such as diamond don't conduct electricity is a quantum mechanical effect. Four ingredients are needed:

(i) The Pauli-principle, forbidding two electrons of the same spin to occupy the same state.

(ii) The formation of bands due to the periodic potential produced by the lattice

(iii) Complete filling of the valence band

(iv) The valence band should be separated from the conduction band by an energy gap

When all four conditions are fulfilled, the sub-system of the electrons forms a crystal, and the material is an insulator. If condition (iii) or (iv) is not fulfilled, the electron subsystem is a fluid. Now the electrons can migrate through the crystal and the material is metallic.

When metals are cooled to low temperature, usually the resistivity decreases as a result of a reduction of the inelastic scattering by phonons. The temperature dependence of a classical metal is: $\rho(T) = \rho_0 + cT^5$, where is ρ_0 the residual resistivity, which is proportional to the density of impurities in the crystal. If no impurities are present, one might therefor expect that the metal would become a perfect conductor only at T=0. Kamerlingh-Onnes was interested in exactly this question, and put his assistent Gilles Holst (who later became the director of Philips Research Laboratories in Eindhoven) on the job of measuring the resistivity of a very pure metal as a function of temperature. They selected mercury (liquid at room temperature, but solid below 234 K) because it can be purified rather easily using destillation techniques, resulting in a metal with practically zero residual resisitivity. To their surprise, the resistivity signal disappeared when the temperature dropped below 4.2 K. It took Holst quite some time and effort to convince his supervisor that he had *not* made a trivial experimental mistake. It also took many decades before the scientific community started to pay attention to the important role of Gilles Holst in the discovery of superconductivity.

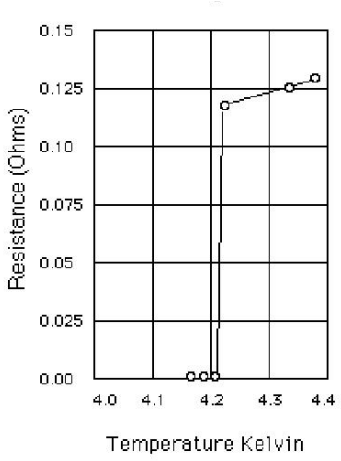


FIGURE 2.3
The discovery of supercondcuctivity by Holst and Kamerlingh-Onnes in 1911

Superconductivity has been observed in about 25 elements. Some examples are:

Element	T_c
Tl	2.4 K
In	3.4 K
Hg	4.1 K
Ta	4.5 K
V	5.4 K
Pb	7.2 K
Nb	9.5 K
La	11.93 K*

*at a pressuare of 149 bar

It is of interest to remark, that

- the alkali-halides are not superconductors
- ferro- and anti-ferromagnetic elements are not superconductors
- the higher T_c's are usually observed in metals with a *low* electrical conductivity.

Innumerable compounds exist, which exhibit the phenomenon of superconductivity. Many of those are intermetallic materials, but also a large class of organic superconductors exist, the record holder is electron-doped Cs_3C_{60} under applied pressure, with a transition temperature of 38 K.

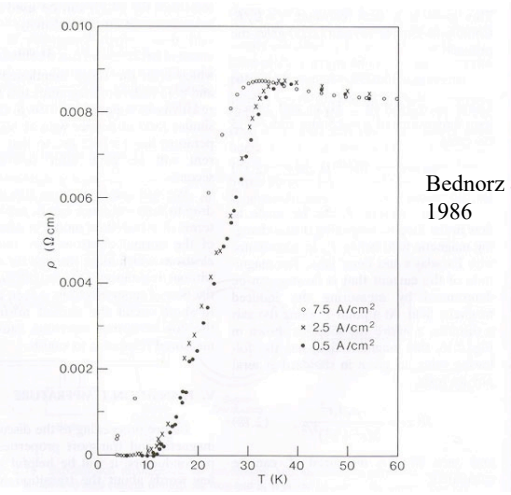


FIGURE 2. 4

Bednorz & Muller
1986

Until 1985 the highest Tc known was 23 K, in the compound Nb_3Ge. However, the field of superconductivity obtained an enormous boost when, in 1986, Bednorz and Muller published a paper in Zeitschrift fuer Physik, announcing superconductivity below 30 K in a *ceramic* compound containing the elements La, Ba, Cu and O. This led to the discovery of a whole class of superconductors, all of them containing Cu and O as the main ingredient, with ever rising transition temperatures. The record holder is Hg2Sr2Ca2Cu3O10, with a Tc of 136 K, under pressure even 164K.

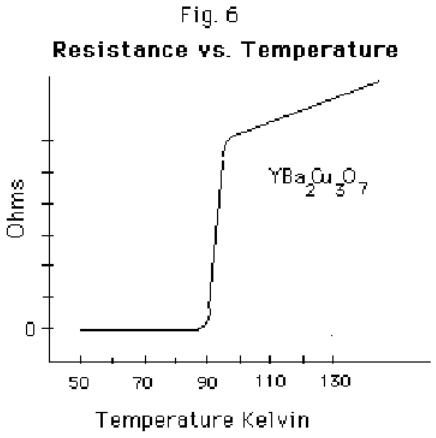


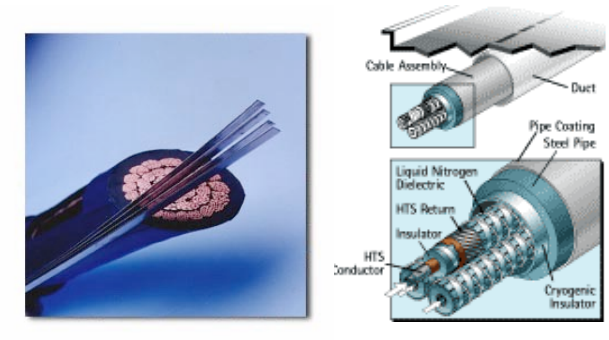
FIGURE 2..5

Paul Chu
1987

One of the most widely used cuprate superconductors is YBa2Cu3O7, with a Tc of 92 K. This transition temperature is well above the temperature of boiling nitrogen (77K), which makes this compound very popular as a classroom demonstration tool. YBCO was discovered ain 1987 by Paul Chu, who realized that replacing La3+ with the smaller Y3+ ion would have the same effect on the crystal structure as applying pressure. It was already known at that time that the effect of applying pressure on LaBaCuO was, to increase Tc. Indeed Chu's trick worked wonderfully, and YBa2Cu3O3 was born. It is a stable compound, which easily survives exposure to air and even moisture. It therefor is widely

applied in superconducting electronics applications, such as SQUID detectors, stripline filters, and Josephson-logic.

FIGURE 2.6



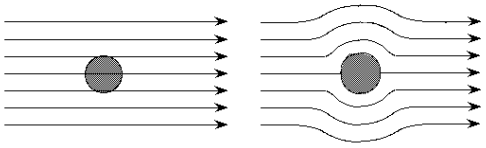
Among the many applications of superconducors, superconducting wires are probably the most important. For many years already superconducting wire finds wide-spread applications in high field magnets. The most spectacular form is for high power applications in the commercial electrical power networks around the world. Although superconducting power cable is still an order of magnitude more expensive than conventional copper wire, commercial niches exist in situations where the capacity needs to be increased without disrupting the existing infrastructure of underground tubes, in which the cables have to be fitted. One can imagine that for a city like Tokyo it is a lot cheeper to replace the existing coppercables with 10 times more expensive superconducting cable, than to break down Tokyo, replace the underground tubes with thicker ones, put in new copper cables, and finally rebuild the city.

Although the property of zero resistance is often regarded as the defining property of a superconductor, this is not really true. Superconductors have an additional property. The two properties are:

(i) The electrical resistance of a superconductor is exactly zero: $\rho=0$

(ii) Magnetic fields can not enter a superconductor. Deep inside the bulk of a superconductor: $B=0$ (Meissner-Ochsenfeld effect).

FIGURE 2.8



Apparently in the presence of an external field $B_{ext} = H$, surface currents set up a net magnetization M (NB: $4\pi M = B - H$), such that $H = 4\pi M$ or $\chi = -1/4\pi$. The superconducting state is said to be *perfectly diamagnetic.*

Another aspect of the fundamental importance of the Meissner-Ochselnfeld effect is, that it shows, that the transition from the normal to the superconducting state is reversible in the thermodynamic sense. To see this, consider the following two experiments:

(a) A specimen is first cooled below Tc, and then an external magnetic field is applied.

(b) A specimen is brought in a magnetic field at T > Tc, and then cooled to Tc.

FIGURE 2.9

According to Meissner-Ochsenfeld, *B=0* in both final states, *i.e. B=0* independent of the history. To appreciate the fundamental importance of this discovery one should realize, that the MO effect *goes beyond* what one would expect from a "perfect conductor" and Maxwell's equations. In fact, from the classical relation

$$\vec{E} = \frac{m}{ne^2}\left[\frac{\vec{j}}{\tau} + \frac{d\vec{j}}{dt}\right]$$

where $1/\tau$ is the rate of momentum transfer, E is the electric field and j the current density, it follows that for a perfect conductor $(1/\tau=0)$

$$\vec{E} = \frac{m}{ne^2}\frac{d\vec{j}}{dt}$$

Consequently

$$\nabla \times \vec{E} = \frac{m}{ne^2}\frac{d[\nabla \times \vec{j}]}{dt} \quad .$$

and from Faraday's law $\left(\frac{1}{c}\frac{d\vec{B}}{dt} = \nabla \times \vec{E}\right)$ one expects

$$\frac{1}{c}\frac{d\vec{B}}{dt} = \frac{m}{ne^2}\frac{d[\nabla \times \vec{j}]}{dt} \quad .$$

We substitute for j the expression for the current density from Ampère's law $\left(\vec{j} = \frac{c}{4\pi}\vec{\nabla} \times \vec{B}\right)$, and obtain

$$\nabla^2 \frac{\partial \vec{B}}{\partial t} = \frac{4\pi ne^2}{mc^2}\frac{\partial \vec{B}}{\partial t}.$$

The solution is that the time-derivative of the magnetic flux density decays expentially away from the sample surface,

$$\frac{\partial \vec{B}(x,t)}{\partial t} = \frac{\partial \vec{B}(0,t)}{\partial t}\mathrm{e}^{-x/\lambda} \quad \text{with} \quad \lambda = \sqrt{\frac{mc^2}{4\pi ne^2}}.$$

Deep inside the sample one therefore has

$dB/dt=0.$

While having *B=0* is a sufficient condition for this, *B* can in fact have an arbitrary finite value as long as it is stationary. *Hence the property that B=0 goes beyond the expected behaviour of a 'perfect conductor'.*

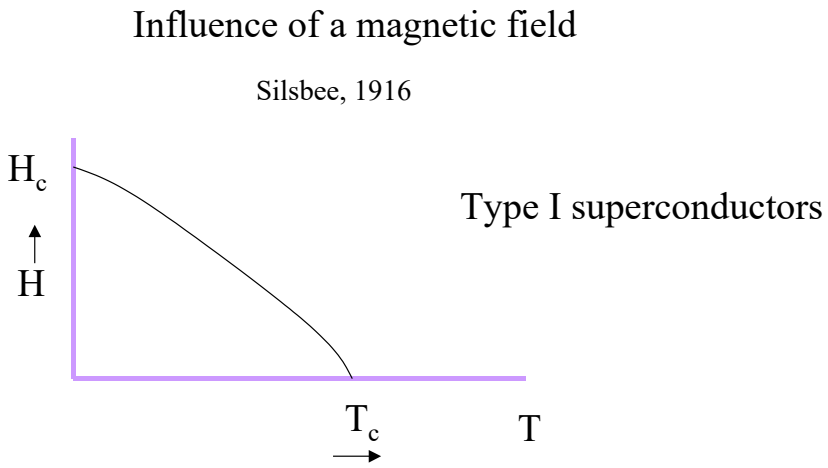


FIGURE 2.12

$$H_c(T) \cong H_c(0)\left[1-\left(\frac{T}{T_c}\right)^2\right] \quad \text{with} \quad H_c(0) \cong \{80 \pm 20\} T_c^{1.3}$$

In the Meissner state $M(B_{ext})$ is fully reversible, *i.e.* $M(B_{ext})$ does not depend on the history of field, magnetization, or temperature of the sample. Superconductors exhibiting this behaviour are so-called type-I superconductors. However, most superconducting materials are *not* type-I: When the external field is lower than the the lower critical field B_{c1}, they still have fully reversible $M(B_{ext})$ behaviour *and* a complete flux expulsion. For higher external fields, the material remains superconducting, but inside the superconductor $B \neq 0$: The actual value of *M* and *B* now depend strongly on the history of field, magnetization and temperature. For fields in the interval $B_{c1} < B_{ext} < B_{c2}$ the superconductor is in the "mixed state". For $B_{c2} < B_{ext}$ the material returns to the normal state. The *B*-*T* phase-diagram of a type-I and a type II superconductor is indicated in Figs. 2.12 and Fig. 2.13 respectively.

Type-II behaviour in superconductors is caused by the fact, that for magnetic flux partially penetrates the superconducting specimen in the form of tiny microscopic filaments, called vortices. Each vortex carriers a magnetic flux $\Phi_0 = \frac{h}{2e} = 2.067 \cdot 10^{-15}$ Weber.

B.S. Deaver, W. M. Fairbank,
Phys. Rev. Lett. ***15****, 43 (1961)*
Flux quantization in superconducting cylinders

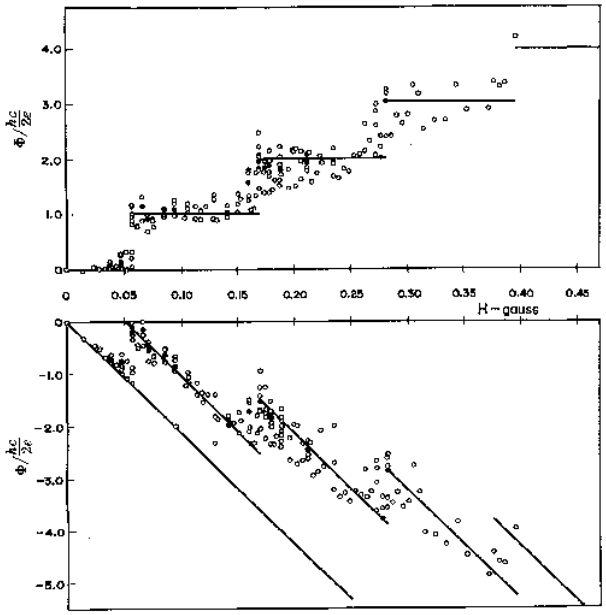


FIG. 1. (Upper) Trapped flux in cylinder No. 1 as a function of magnetic field in which the cylinder was cooled below the superconducting transition temperature. The open circles are individual data points. The solid circles represent the average value of all data points at a particular value of applied field including all the points plotted and additional data which could not be plotted due to severe overlapping of points. Approximately two hundred data points are represented. The lines are drawn at multiples of $hc/2e$. (Lower) Net flux in cylinder No. 1 before turning off the applied field in which it was cooled as a function of the applied field. Open and solid circles have the same significance as above. The lower line is the diamagnetic calibration to which all runs have been normalized. The other lines are translated vertically by successive steps of $hc/2e$.

FIGURE 2.13

A related magnetic flux quantization phenomenon was discovered by Deaver and Fairbank, by measuring the amount of flux trapped in a hollow superconducting cylinder (see Fig. 2.14). When they cooled a cylinder machined out of a superconducting material below the phase transition in a magnetic field, and measured the total magnetic flux trapped inside the cylinder using a magnetometer, they observed that the amount of flux increases in steps as a function of the external magnetic field in which the sample was placed. The height of each step was close to *hc/2e*, and later experiments have confirmed, that magnetic flux is indeed quantized in exact amounts of this 'elementary flux quantum' $\Phi_0 = hc/2e$. The importance of

this discovery is, that the size of the elementary flux quantum depends on the Planck constant h. In a 'classical world', where the Planck constant would be zero, no flux quantization would exist. This is the clearest demonstration, that superconductivity is an inherently quantum mechanical effect. It also suggests, that an intimate connection may exist between superconductivity, and Bose-Einstein condensation, because BEC is also a manifestation of quantum coherence on a macroscopic scale (remember, that in the theory of BEC the transition temperature is proportional to $\hbar^2$). We will come back to this intimate relationship later, and we shall see that indeed superconductivity, superfluidity and BEC belong to a single class of macroscopic quantum phenomena.

Important properties of superconductors:

- Zero resistance state
- Meissner effect (B=0)
- Perfect diamagnetism (M=-4π H)
- Macroscopic quantum state:
  - -Flux quantisation
  - -Josephson effects
- Electrons form pairs.

Chapter III: Superconducting pairing mechanisms

III.1 The Hamiltonian of interacting electrons

The energy-momentum dispersion relation of electrons relative to the chemical potential μ is $\xi_k = \varepsilon_k - \mu$. The Hamiltonian describing the energy levels of an arbitrary number of conduction electrons is

$$\hat{K} = \sum_{k,\sigma} \xi_k c^\dagger_{k,\sigma} c_{k,\sigma} \tag{3.1}$$

When considering the interaction potential between two electrons in vacuum, we know that the two equal charges cause a repulsive Coulomb interaction of the form

$$V(r_1 - r_2) = \frac{e^2}{|r_1 - r_2|} \tag{3.2}$$

The Hamiltionian describing the Coulomb interaction in quantum many-body physics is

$$\hat{H}^C = \sum_{\sigma,\sigma'} \int d^3\vec{r}_1 \int d^3\vec{r}_2 V(r_1 - r_2) \psi^\dagger_\sigma(\vec{r}_1) \psi_\sigma(\vec{r}_1) \psi^\dagger_{\sigma'}(\vec{r}_2) \psi_{\sigma'}(\vec{r}_2)$$

where $\psi^\dagger_\sigma(\vec{r}_1)$, and $\psi_\sigma(\vec{r}_1)$ are the field-operators and σ denotes the spin. These field-operators create or anihilite a partice in a state which is localized on a particular space coordinate. Such a localized state is usually not an eigen-state of the system. Since in a translationally invariant space the eigenstates are plane waves, it is usually more convenient to express the interaction using operators which create or annihilate a plane wave. These are defined as $c^\dagger_{k\sigma} = \frac{1}{V} \int e^{ikr} \psi^\dagger_\sigma(\vec{r}\,) d^3r$ where V is the system volume. We can substitute the inverse Fourier transform, $\psi^\dagger_\sigma(\vec{r}\,) = \sum_k e^{-ikr} c^\dagger_{k\sigma}$ in the expression for the interaction. For each of the four field operators we choose an independend summation variable.

$$\hat{H}^C = \sum_{\sigma,\sigma'} \sum_{l,l',p,p'} \int d^3\vec{r}_1 \int d^3\vec{r}_2 e^{-ik'r_1} e^{ikr_1} e^{-ip'r_2} e^{pr_2} V(r_1 - r_2) c^\dagger_{k'\sigma} c_{k\sigma} c^\dagger_{p'\sigma'} c_{p\sigma'}$$

To simplify the expression we decompose the coordinates r_1 and r_2 in the relative ($\rho = r_1 - r_2$) and the center-of-mass coordinate ($R = \frac{1}{2}\{ r_1 + r_2 \}$)

$$\hat{H}^C = \sum_{\sigma,\sigma'} \sum_{l,l',p,p'} \int d^3\vec{\rho} \int d^3\vec{R} e^{i(k-k')(R+\rho/2)} e^{i(p-p')(R-\rho/2)} V(\rho) c^\dagger_{k'\sigma} c_{k\sigma} c^\dagger_{p'\sigma'} c_{p\sigma'}$$

One way to read the interaction Hamiltonian, is that each one of the two annihilation operators devours a particle with spin σ' and σ respectively, whereas the two creation operators expectorate two particles, having also spin σ' and σ.

The integrals over the center of mass coordinate give the Kronecker delta-function describing the conservation of momentum in a particle-particle collision

$$\int e^{i(k-k'+p-p')R} d^3\vec{R} = \delta_{k-k',p'-p}$$

A momentum q=p'−p is transferred from the electron which had initially momentum p, to the electron which had initially momentum k. In the Coulomb interaction this momentum is transported by the virtual photon which carries the interaction between the two electrons. We use the Fourier transform of 1/r

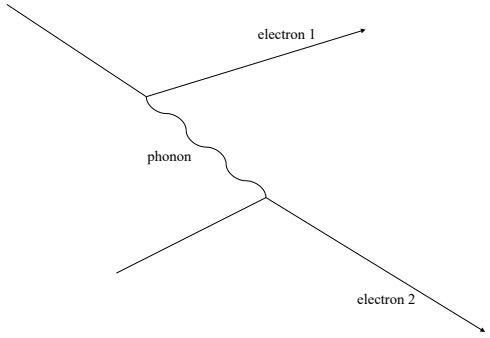
$$\int e^{i\vec{q}\cdot\vec{\rho}} \frac{1}{\rho} d^3\vec{\rho} = \frac{4\pi}{|\vec{q}|^2} \tag{3.3}$$

to finally arrive at the expression for the Coulomb interaction

$$\hat{H}^C = \sum_{\sigma,\sigma' k,p,q} \sum \frac{4\pi e^2}{|\vec{q}|^2} c^{\dagger}_{k-q\sigma} c_{k\sigma} c^{\dagger}_{p+q\sigma'} c_{p\sigma'} \tag{3.4}$$

III.2 The Hamiltonian of two fermions coupled via a bosonic field

In this chapter we consider the processes in a solid whereby two electrons are scattered from each other. Initially electron 1 is in a quantum state $|k\rangle$, and electron 2 in a quantum state $|p\rangle$. In a solid their interaction is not just the bare Coulomb repulsion, but the much weaker screened interaction, which is supposed to vanish for $\xi_k \rightarrow 0$.



Interactions between electrons are generally caused by the virtual exchange of bosons. Such a process is represented by the above Feynmann diagram. This is also true for the Coulomb repulsion between electrons, in which case the exchanged bosons are photons. However,

the Coulomb repulsion is somewhat special, and its treatment requires the full machinery of quantum electrodynamics, which is the subject of another course. Here we will consider the Coulomb repulsion as an effectively instantaneous interaction.

In addition to the Coulomb repulsion, another interaction of great importance in the theory of nuclear forces is the "Yukawa force", between nucleons coupled through mesons. The mechanism of electron-electron attraction mediated by phonons in a solid is very similar to the Yukawa interaction. For this reason we discuss it here in some detail. We call b_q the annihilation operator of a boson of momentum $\hbar q$ and energy $\hbar\omega_q$. We assume that the bosons have an energy-momentum relation

$$\omega_q^2 = v^2\left(q^2 + k_0^2\right) \tag{3.5}$$

where the bosonic mass is introduced by the constant k_0. The interaction Hamiltonion of fermions interacting with this boson field is

$$H_{fb}^i = -\sum_{k,q,\sigma} ig\left(2\hbar\omega_q\right)^{-1/2} c_{k+q\sigma}^\dagger c_{k\sigma} b_q + H.C. \tag{3.6}$$

Consider the case that an electron is present at position r. The expectation value of the operator product $c_{k+q\sigma}^\dagger c_{k\sigma}$ is then $\left\langle r\left|c_{k+q\sigma}^\dagger c_{k\sigma}\right|r\right\rangle = e^{-i(k+q)r}e^{ikr} = e^{-iqr}$. We now consider a state with two electrons at positions r_1 and r_2. Repeating the previous argument we obtain $\left\langle r_1, r_2\left|c_{k+q\sigma}^\dagger c_{k\sigma}\right|r_2, r_1\right\rangle = e^{-iqr_1} + e^{-iqr_2}$, and the corresponding perturbation of the boson field is

$$H_b^i = -\sum_{j=1}^{2}\sum_q ig\left(2\hbar\omega_q\right)^{-1/2}\left(e^{-iqr_1} + e^{-iqr_2}\right)b_q^t + H.C. \tag{3.7}$$

Where the matrix element is calculated over the Fermion coordinates, while the boson-coordinates are still operators at this stage. To calculate the correction on the energy of the two electrons due to coupling to the boson field we use second order perturbation theory

$$\Delta E = \sum_q \frac{\left|\langle 0|H_b^i|q\rangle\right|^2}{E(0) - E(q)} = \sum_q \frac{g^2\left(2\hbar\omega_q\right)^{-1}\left|e^{-iqr_1} + e^{-iqr_2}\right|^2}{-\hbar\omega_q} = -\sum_k \frac{g^2}{\hbar^2\omega_q^2}\left(1 + \cos\vec{q}\cdot\vec{\rho}\right)$$

where $\rho = r_1 - r_2$ is the relative coordinate of the two electrons. The force acting between the two fermions corresponds to the gradient of the above potential energy. We can therefore replace $(1+\cos q\rho)$ with $\cos q\rho$, since this only adds a distance independent constant to the interaction. The q-space integral is easily performed. For the boson energies we substitute the dispersion relation (3.5) with the result

$$\Delta E = \frac{-g^2}{(2\pi)^3}\int \frac{\cos(\vec{q}\cdot\vec{\rho})}{v^2\hbar^2\left(k^2+k_0^2\right)}d^3q = \frac{-g^2}{(2\pi)^3\hbar^2v^2}\int_0^\infty \frac{\sin(q\rho)}{q^2+k_0^2}\frac{4\pi q^2}{q\rho}dq = \frac{-g^2}{2\pi^2\hbar^2v^2\rho}\int_0^\infty \frac{x\sin x}{x^2+(k_0\rho)^2}dx$$

with the help of which we arrive at the famous expression for the Yukawa interaction

$$V^Y(\rho) = -\frac{g^2}{4\pi\hbar^2v^2}\frac{e^{-k_0\rho}}{\rho} \tag{3.8}$$

Thus the interaction between two fernions mediated by bosons is attractive. At short distances it decays as *1/ρ*, like the Coulomb interaction (except for the sign!) while at distances larger than k_0, it decays exponentially.

To obtain the Hamiltionian corresponding to the effective interaction of Eq. 3.8 we have to proceede in the same way as we used to obtain from Eq. 3.4 from Eq. 3.2: we multiply $V^Y(\rho)$ with the product of field operators $\psi_\sigma^\dagger(\vec{r}_2+\vec{\rho})\psi_\sigma(\vec{r}_2+\vec{\rho})\psi_{\sigma'}^\dagger(\vec{r}_2)\psi_{\sigma'}(\vec{r}_2)$, and express these in terms of the creation and annihilation operators $c_{k\sigma}^\dagger, c_{p\sigma'}$. The resulting expression

$$\hat{H}^Y = -\frac{g^2}{v^2\hbar^2}\sum_{\sigma,\sigma'}\sum_{k,p,q}\frac{1}{q^2+k_0^2}c_{k-q\sigma}^\dagger c_{k\sigma}c_{p+q\sigma'}^\dagger c_{p\sigma'} \tag{3.9}$$

Has a structure similar to the Coulomb interaction, Eq. 3.4, of the previous chapter, except that the sign of the interaction is opposite, and the denominator on the right hand side contains an additional term k_0^2. However, this expression contains a deficiency in that it was derived using second order perturbation theory taking a *static* configuration of two fermions at positions r_1 and r_2 as the starting point. Effectively this means that the derived effective Hamiltonion applies to the case where the energies of the outgoing particles, and the incoming particles are the same, i.e. $\varepsilon_{k-q}-\varepsilon_k=0$, and $\varepsilon_{p+q}-\varepsilon_p=0$. These *on-energy shell* processes are relevant for scattering processes whereby the electrons remain in free propagating incoming and outgoing states, i.e. no bound pair-states are formed. More generally we should consider the coupling between 2-particle states having different energies. A more complete treatment of the Yukawa interaction reveals that for $(\varepsilon_{k-q}-\varepsilon_k)^2>>\hbar^2\omega_q^2$ the interaction $V^Y(\rho)\approx 0$. We will take a closer look at this dynamical aspect of the effective interaction in the following section.

III.3 Quasiparticles

In a metal the interacting fermions responsible for superconductivity are the so-called quasiparticles. These are *not* the electrons. Instead they are fermionic fundamental exitations of the solid with the following properties:

(i)Their collection of momentum values at zero energy spans a surface in momentum space, which is *by definition* the Fermi surface.

(ii) Their interactions vanish in the limit of energy going to zero relative to the Fermi surface.

The principle of forming quasiparticles out of the original electron is exemplified by the process of screening of the Coulomb interation. Taking the original electron as the starting point, they repel each other by the Coulomb interaction. However, we are not interested in the bare electrons, but in the fundamental excitations of the solid, which are as close an approximation as possible to the eigenstates of the material. Consider a metal in its ground state. We are interested to describe a fundamental excitation with charge e and spin ½. Imagine that we try to realize such an excitation by adding one extra electron to the metal, which we add in a state with momentum $\hbar k$ and energy E_k. This extra electron will interact with all other electrons present via the Coulomb interaction, the average electron-density will shift a bit such as to screen the extra charge on the length scale of the Thomas Fermi screening length. The resulting eigen-state with momentum $\hbar k$, extra charge e and spin ½ is our quasiparticle. Its energy relative to the Fermi energy is ξ_k, is no longer the bare E_k, in fact ξ_k is renormalized by the interaction with the screening cloud. This corresponds to an electron and a screening cloud surrounding it! The exact calculation of the quasiparticle energy dispersion ξ_k is a major scientific challenge. Only approximate solutions exist to this problem.

III.4 The screened Coulomb interaction

Since quasiparticles are "renormalized" electrons, interactions between the quasiparticles are necessarily different from those between bare electrons. In general some approximation scheme needs to be employed to obtain the renormalized interaction between quasiparticles. One such approximation scheme treats the effective interactions using the model of screening, which is based on the so-called random phase approximation. It is not particularly good approximation, but since it is simple to understand and it illustrates some interesting and important physics, we will explain it here.

The Coulomb interaction is a non-retarded interaction. Suppose that at position r_1 a charge e pops up at time t_1 and disappears immediately afterwards, and the same happens at position r_2 and time t_2. If $t_1 \neq t_2$ there is no interaction energy at all, since the two charges do not coexist at the same time. The expression for the interaction energy is apparently

$$V(r_1, r_2; t_1, t_2) = \frac{e^2}{|r_1 - r_2|}\delta(t_1 - t_2). \tag{3.10}$$

In solids this is different: A quasiparticle moving through the solid leaves behind a trace of perturbations of all electrons and ions with which is has been interacting. It takes a certain amount of time for this trace to heal, after which the system has returned to the ground state. Another quasiparticle feels the influence of this trace for the time that it exists, in other words, the interaction with the earlier electron should be integrated over all time from the distant past until the actual time. The resulting interaction is the Fourier transform of the Coulomb potential devided by the dielectric constant. Since the dielectric function is generally momentum dependend, the potential $V(r_1,r_2;t_1,t_2)$ is the Fourier transform in frequency and momentum space of the screened interaction in frequency-momentum space

$$V(r_1, t_1; r_2, t_2) = \int d\Omega e^{i\Omega(t_1 - t_2)} \int d^3q e^{iq(r_1 - r_2)} \frac{4\pi e^2}{|q|^2} \frac{1}{\varepsilon(q,\Omega)} \tag{3.11}$$

When the two particles are still far away from each other, their states are described by Bloch waves, i.e. particle 1 is in a quantum state $|k\rangle$, while particle 2 is in a quantum state $|p\rangle$. After the scattering, as the particles are moving away from each other at a long distance, they are again in states described by a Blochwave. Moreover, due to kinematic constrants the center of mass momentum is conserved throughout the process.

Consequently, if particle 1 scatters from state $|k\rangle$ to $|k-q\rangle$, than particle 2 has to scatter from $|p\rangle$ to $|p+q\rangle$.

During the time that the collision process is taking place, each of the two particles is in an intermediate state, which in principle can be quite complicated. Here we consider only scattering processes in the limit of weak interaction, and therefore assume that only leading orders in perturbation theory need be considered. Consequently the intermediate state of each particle is a linear superposition of the initial and final state

$$\left.\begin{aligned}\psi(r_1,t) &= e^{i\varepsilon_k t/\hbar}\psi_k(r_1) + e^{i\varepsilon_{k-q}t/\hbar}\psi_{k-q}(r_1)\\ \psi'(r_2,t) &= e^{i\varepsilon_p t/\hbar}\psi_p(r_2) + e^{i\varepsilon_{p+q}t/\hbar}\psi_{p+q}(r_2)\end{aligned}\right\} \tag{3.12}$$

The corresponding amplitudes are

$$\left.\begin{aligned}&|\psi(r_1,t)|^2 = |\psi_k(r_1)|^2 + |\psi_{k-q}(r_1)|^2 + 2\,\mathrm{Re}\{\psi_k(r_1)\psi^*_{k-q}(r_1)\}\cos(\omega t) - 2\,\mathrm{Im}\{\psi_k(r_1)\psi^*_{k-q}(r_1)\}\sin(\omega t)\\ &|\psi'(r_2,t)|^2 = |\psi_p(r_2)|^2 + |\psi_{p+q}(r_2)|^2 + 2\,\mathrm{Re}\{\psi_p(r_2)\psi^*_{p+q}(r_2)\}\cos(\omega' t) - 2\,\mathrm{Im}\{\psi_p(r_2)\psi^*_{p+q}(r_2)\}\sin(\omega' t)\\ &\text{where } \omega = \hbar^{-1}(\varepsilon_k - \varepsilon_{k-q}) \text{ and } \omega' = \hbar^{-1}(\varepsilon_p - \varepsilon_{p+q})\end{aligned}\right\}$$

from which we see, that in perturbation theory the two particle amplitudes oscillate harmonically as a function of time, the oscillation frequency given by the energy difference in their respective initial and final states. Due to negative interference, all frequency components of the interaction average to zero, except the components having $\hbar\omega = \varepsilon_k - \varepsilon_{k-q}$. Hence the (only) frequencies relevant for the screening of the interaction are the energy differences of the intital and final states of each of the two particles. If in addition the center of mass motion of the incoming and scattered states is zero, we have $p+k=0$. Consequently $\hbar\omega = \varepsilon_k - \varepsilon_{k-q}$ and $\hbar\omega' = \varepsilon_p - \varepsilon_{p+q} = \varepsilon_{-k} - \varepsilon_{q-k}$, and $\omega=\omega'$.

In summary, a scattering event by the screened Coulomb interaction corresponds to the following process:

1) The quasiparticle with momentum $\hbar k$ and energy ξ_k emits a boson with momentum $\hbar q$ after which it continues with momentum $\hbar(k-q)$ and energy ξ_{k-q}.
2) The boson is captured by the other quasiparticle having momentum $\hbar p$ and energy ξ_p, which thereafter continues its journey with momentum $\hbar(p+q)$ and energy ξ_{p+q}.

Attention: The final state energies are not necesserily *on-energy shell.* This means that in the final state the quasiparticles have momentum $\hbar(k-q)$ and $\hbar(p+q)$, with energies ξ_{k-q} and ξ_{p+q} *irrespective of the energy* $\hbar\omega_q$ of the intermediate boson.

If the center of mass motion of the incoming and scattered quasiparticles is zero (implying $k=p$) the resulting interaction between the two quasiparticles involves an intermediate state which oscillates at the frequency $\hbar\omega = \varepsilon_k - \varepsilon_{k-q} = \varepsilon_p - \varepsilon_{p+q}$.

The interaction is then described by the Hamiltonion

$$\hat{H}^i = \sum_{k,p,q}\sum_{\sigma,\sigma'}\frac{4\pi e^2}{q^2\varepsilon(q,\omega)}c^\dagger_{k-q\sigma}c_{k\sigma}c^\dagger_{p+q\sigma'}c_{p\sigma'} \tag{3.13}$$

The choice of sign of ω makes no difference in the expression for H^i, because $\varepsilon(q,\omega)$ is an even function of frequency. The ω-dependence implies that the interaction is retarded, *i.e.* the time-evolution of a collision process is described by a memory function.

In a metal, the electronic contribution to the dielectric function is to a good approximation given by the expression for the Thomas-Fermi screening

$$\varepsilon(q,\omega) = 1 + \frac{k_o^{\ 2}}{|\vec{q}|^2} \tag{3.14}$$

where k_0 is the Thomas-Fermi screening wavevector

$$(k_o a_0)^2 = 4\cdot\left(\frac{3}{\pi}\right)^{1/3} a_0 n^{1/3} \tag{3.15}$$

Where $a_0=\hbar^2/(me^2)$ is the Bohr radius and n is the electron density. The resulting screened electron-electron interaction takes the form

$$\hat{H}^i = \sum_{k,p,K}\sum_{\sigma,\sigma'}\frac{4\pi e^2}{q^2+k_0^2}c^\dagger_{k+q\sigma}c_{k\sigma}c^\dagger_{p-q\sigma'}c_{p\sigma'} \tag{3.16}$$

In real space, the screening term k_0^2 in the denominator reduces the Coulomb interaction by an exponential factor

$$V(r) = \sum_q e^{-i\vec{q}\cdot\vec{r}}\,\frac{4\pi e^2}{|\vec{q}|^2+k_0^2} = \frac{e^2}{r}e^{-k_0 r} \tag{3.17}$$

We point out that the above screened Coulmb interaction still represents a repulsive interaction regardless of the distance between the electrons. Apparently Thomas-Fermi

screening does not *over*screen the repulsive Coulomb force. However, the Thomas-Fermi model is an approximation; the actual screening has a more complex q-dependence, resulting in weak overscreening in certain parts of direct and momentum-space. While interesting as a matter of principle, this type of attractive interaction is too weak to be of importance in realistic superconducting materials.

However, overscreening becomes very important when, in addition to the free charge carriers, the presence of the nuclear particles is considered. The dielectric function describes now a two-component plasma with one light component (the electrons) and one heavy component (the nuclei). In view of their much higher mass, the nuclear particles can be treated in the classical limit, hence they contribute to the dielectric function a term $-\Omega_p^2/\omega^2$, where $\Omega_p^2 = 4\pi nQ^2/M$, n is the density, and M is the mass of the nuclei and Q their charge. The longitudinal dielectric function of such a system is

$$\varepsilon(q,\omega) = 1 + \frac{k_0^2}{q^2} - \frac{\Omega_p^2}{\omega^2} \tag{3.18}$$

The dielectric function is the constant of proportionality between the electric field E inside a medium and the field D due to the external sources

$$De^{i(qr-\omega t)} = \varepsilon(q,\omega)Ee^{i(qr-\omega t)} \tag{3.19}$$

A particular case is presented when $\varepsilon(q,\omega)=0$: In this case the above egality has a non trivial solution for E in the absence of an externally applied field, i.e. while $D=0$. Consequenly an oscillating electric field with these precise frequency and wavenumber can propogate without an external source. The collective modes of the two-component plasma following from the condition $\varepsilon(q,\omega)=0$, are combined (and out-of-phase) oscillations of the positive nuclear charge screened by the electronic charge. In fact, these are just the sound-modes of the solid. Hence the sound-dispersion is given by the relation

$$0 = 1 + \frac{k_0^2}{q^2} - \frac{\Omega_p^2}{\omega^2} \tag{3.20}$$

Which can be solved easily with the result

$$\omega_q = \frac{v_s\, q}{\sqrt{1 + k_0^{-2} q^2}} \tag{3.21}$$

Where $v_s = k_0^{-1}\Omega_p$ is the sound-velocity in the hydrodynamic limit (q→0). The screened Coulomb interaction in the presence of sound-waves and electronic screening is:

$$\hat{H}^i = -\sum_{k,p,q}\sum_{\sigma,\sigma'}\frac{4\pi e^2}{q^2+k_0^2}\frac{\omega^2}{\omega_q^2-\omega^2}c^\dagger_{k-q\sigma}c_{k\sigma}c^\dagger_{p+q\sigma'}c_{p\sigma'} \tag{3.22}$$

The most important implication of this expression is, that the sign of this interaction is *negative* for frequencies smaller than ω_q. We see, that the combination of sound-waves and electronic screening *does* result in overscreening of the Coulomb interaction, resulting in a net effective interaction for frequencies $\omega<\omega_D$ where ω_D is the "typical" frequency of soundwaves in a solid, i.e the Debye frequency. With a bit of re-shuffling of the operators

$$\hat{H}^i = -\sum_{k,p,q}\sum_{\sigma,\sigma'}\frac{4\pi e^2}{q^2+k_0^2}\frac{\omega^2}{\omega_q^2-\omega^2}c^\dagger_{k-q\sigma}c^\dagger_{p+q\sigma'}c_{p\sigma'}c_{k\sigma} \tag{3.23}$$

We will soon see, that the only terms of importance in BCS theory are those which have center of mass momentum $p+k=0$, resulting in the so-called *reduced* interaction Hamiltonian

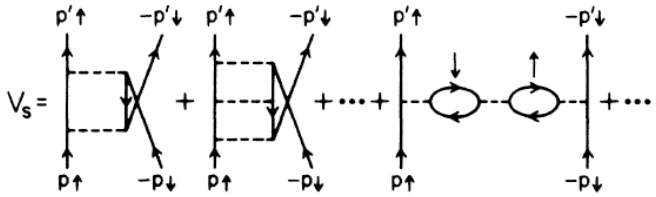
$$\hat{H}^i_{red} = -\sum_{k,l,\sigma,\sigma'}\frac{4\pi e^2}{\left|\vec{k}-\vec{l}\right|^2+k_0^2}\frac{\left(\varepsilon_k-\varepsilon_l\right)^2}{\hbar^2\omega_{k-l}^2-\left(\varepsilon_k-\varepsilon_l\right)^2}c^\dagger_{l\sigma}c^\dagger_{-l\sigma'}c_{-k\sigma'}c_{k\sigma} \tag{3.24}$$

In the following chapters we will sometimes use the following shorthand notation for the interaction:

$$\begin{aligned}\hat{H}^i_{red} &= \sum_{k,l,\sigma,\sigma'}V_{k,l}c^\dagger_{l\sigma}c^\dagger_{-l\sigma'}c_{-k\sigma'}c_{k\sigma}\\ V_{k,l} &= -\frac{4\pi e^2}{\left|\vec{k}-\vec{l}\right|^2+k_0^2}\frac{\left(\varepsilon_k-\varepsilon_l\right)^2}{\hbar^2\omega_{k-l}^2-\left(\varepsilon_k-\varepsilon_l\right)^2}\end{aligned} \tag{3.25}$$

III.5 Magnetic fluctuations, and their interaction with electrons

The magnetic susceptibility of a substance describes the amount of magnetization induced by a magnetic field, $M(q,\omega) = \chi(q,\omega)H(q,\omega)$. Spontaneous magnetic order requires that $M \neq 0$ while $H = 0$ for a certain momentum value q. This will happen when $\chi(0,q) = \infty$. We consider an example of the susceptibility of a metal close to a spontaneous antiferromagnetic instability. The most important feature is, that this susceptibility is large for a 'soft' wavevector $Q = (\pi,\pi)$. An effective interaction between electrons is then induced through so-called paramagnon exchange processes, represented by the following Feynmann diagrams:



"Possible Antiferromagnetic Paramagnon Pairing Mechanism"
D.J. Scalapino, MRS Symp. Proc. Vol EA-11,35 (1987)

A qualitative description of these diagrams is as follows: When we introduce an electron at coordinate *r=0* for an infitely short amount of time at *t=0*, its spin σ (=±1) introduces a δ-function shaped magnetization pulse, which by virtue of the effective on-site electron-electron interaction *U*, induces a local exchange potential

$$\bar{U}\sigma\delta(r)\delta(\mathrm{t}) = \bar{U}\sigma\sum_{q,\omega} \mathrm{e}^{i(qr+\omega t)} \tag{3.29}$$

The magnetic susceptibility of the material induces a magnetization that oscillates as a function of distance *r* and decays algebraically at large distances. This magnetization interacts with the magnetic moment of the other electrons through the local interaction *U*. The resulting interaction energy between two electrons at a distance *r* rom each other is

$$V(r,t) = -\bar{U}^2\sigma\sigma'\sum_{q,\omega} \mathrm{e}^{i(qr+\omega t)}\chi(q,\omega) \tag{3.31}$$

As in the previous section, the frequency ω represents the energy difference of the two

interacting particles. The detailed calculation of the Feynmann diagrams shows that the righthand side of Eq. 3.31 must be multiplied with a factor 3/2. This way we obtain the reduced interaction in the BCS model

$$H^i = \sum_{k,l} V_{kl} c^t_{k\sigma} c^t_{-k\sigma'} c_{-l\sigma'} c_{l\sigma}$$
$$V_{kl} = -\sigma\sigma' \frac{3}{2} \bar{U}^2 \chi(k-l, \xi_k - \xi_l) \qquad (3.32)$$

If the material is close to a spin-density-wave instability with momentum Q, without actually being in antiferromagnetic state, the susceptibility is very large (but does not diverge) for a particular momentum k-l=Q. Note, that our sign convention is such, that a positive sign of V_{kl} indicates a repulsive interaction. In the present case the interaction between electrons of opposite spin ($\sigma\sigma' = -1$) is repulsive, but strongly dependent on k-l, and it becomes very large for $k-l=Q$. Such a momentum-dependend interaction can also provide a mechanism for pairing, and is believed to constitute a mechanism for pairing in the high Tc superconductors.

Chapter IV: Microscopic theory of superconductivity

IV.1 Macroscopic wavefunction of a Bose-Einstein condensate

The electrodynamical behaviour of a superconductor has strong similarities to the properties of the quantum mechanical wavefunction of a single charged particle. *If* the charge carriers would be bosons with charge e^* and mass m^*, a BEC of the charge carriers would indeed behave as a single quantummechanical particle. The reason is, that all particles in a BEC occupy the same quantum state:

The quantum state with m bosons occupying the same state φ_0 is

$$|m\rangle = (a_0^\dagger)^m|0\rangle. \tag{4.1}$$

We anticipate, based on the similarities between the properties of ^{3}He, and of superconductors, that a superconductor behaves like a BEC of pairs of electrons, where center-of-mass coordinates of the pairs are Bose-Einstein condensed in a macroscopic zero-momentum plane wave-function with K=0. Let us first consider a single pair of electrons. In second quanization notation a pair of fermions at position r_1 and r_2 is described by

$$\left|\mathbf{r}\alpha,\mathbf{r}'\beta\right\rangle = c^\dagger_{r\alpha}c^\dagger_{r'\beta}\left|0\right\rangle. \tag{4.2}$$

where α and β are the spin coordinates.

We assume that there exists an effective attractive interaction between the fermions, so that they can form bound states. The Hamiltonion of two interacting particles

$$H = -\frac{\hbar^2}{2m}\nabla_r\cdot\nabla_r - \frac{\hbar^2}{2m}\nabla_{r'}\cdot\nabla_{r'} + V\left(r-r'\right). \tag{4.3}$$

can be split in two separate Schrodinger equations for the center of mass coordinate $\boldsymbol{R}=(\boldsymbol{r}+\boldsymbol{r}')/2$ and for the relative coordinate $\rho = \boldsymbol{r} - \boldsymbol{r}'$ giving

$$H = -\frac{\hbar^2}{2M}\nabla_R\cdot\nabla_R - \frac{\hbar^2}{2\mu}\nabla_\rho\cdot\nabla_\rho + V\left(\rho\right). \tag{4.4}$$

with M=2m and μ=m/2. The total wavefunction of such a pair can be factorized in a product of two wavefunctions, one describing the motion of the center of mass and the other the motion of the paired electrons relative to each other

$$\Psi\left(r,r'\right) = \psi(R)w\left(\rho\right). \tag{4.3}$$

If the superconductor has translational invariance, the wavefunction is a plane-wave

$$\psi_K(R) = \frac{1}{\sqrt{\Omega}} e^{iK\cdot R}.$$

whereas the relative motion will be a bound wave-function for sufficiently attractive interaction V(ρ). In a state where there is no net flow of current, the center-of-mass momentum will be K=0 giving $\psi_0(R)=\Omega^{-1/2}$, a constant value which can be absorbed in the definition of $w(\rho)$. Consequently the stationary (non current-carrying) two-electron eigenstates are

$$|1\rangle = \int \left\{ \int w(\rho) c^{\dagger}_{R+\rho/2,\alpha} c^{\dagger}_{R-\rho/2,\beta} d^3\rho \right\} d^3R |0\rangle \tag{4.4}$$

where |1> indicates that this state contains 1 pair of electrons. A more compact expression is obtained by Fourier transforming the creation operators in momentum space, $c^{\dagger}_{p\alpha}$ and $c^{\dagger}_{q\beta}$

$$\begin{aligned} c^{\dagger}_{R+\rho/2,\alpha} &= \sum_k e^{-ip(R+\rho/2)} c^{\dagger}_{p\alpha} \\ c^{\dagger}_{R-\rho/2,\beta} &= \sum_{k'} e^{-iq(R-\rho/2)} c^{\dagger}_{q\beta} \end{aligned} \tag{4.5}$$

The precise form of the relative coordinate wavefunction $w(\rho)$ depends on the type of attractive interaction, as well as on the collective effect of the background of condensed pairs on each other. We will determine this wavefunction by searching for the form which has the minimal energy of the interacting particle system. The function $w(\rho)$ is therefor a variational wavefunction describing the "shape" of a pair of electrons. We define its Fourier-expansion

$$w(\rho) = \sum_k e^{ik\rho} w_k \tag{4.6}$$

and insert Eqs. 4.5 and 4.6 into Eq. 4.4. After some re-arranging of the terms we obtain

$$|1\rangle = \sum_{k,p,q} \left\{ \int e^{-i(p+q)R} d^3R \int e^{i(k-p/2+q/2)\rho} d^3\rho \right\} w_k c^{\dagger}_{p\alpha} c^{\dagger}_{q\beta} |0\rangle$$

We can subsitute the identities familiar from the theory of Fourier expansions

$$\begin{aligned} \Omega^{-1} \int e^{-i(p+q)R} d^3R &= \delta_{0,p+q} \\ \Omega^{-1} \int e^{i(k-p/2+q/2)\rho} d^3\rho &= \delta_{2k,p-q} \end{aligned}$$

So that

$$|1\rangle = \sum_k w_k c^\dagger_{k,\alpha} c^\dagger_{-k,\beta} |0\rangle$$

The sum over pairs of creation-operators creates a pair of electrons with center-of-mass momentum K=0 and spin $\alpha+\beta$. Since the latter is necessarily an integer number (i.e. m_s= -1, 0 or 1) we identify this as the creation operator of a K=0 boson

$$a_0^\dagger = \sum_k w_k c^\dagger_{k,\alpha} c^\dagger_{-k,\beta} \tag{4.7}$$

Suppose that the superconducting state is indeed a BEC of such pairs. Similar to Eq. 4.1 we expect the ground state wavefunction of *m pairs* in the state with center-of-mass *K=0*

$$\boxed{|m\rangle = \left(a_0^\dagger\right)^m |0\rangle = \left(\sum_q w_k c^\dagger_{k\alpha} c^\dagger_{-k\beta}\right)^m |0\rangle} \tag{4.8}$$

Eq. 4.8 is the ground-state wavefunction of a superconductor with *m* pairs of electrons. Usually the BCS formalism is applied to clean systems, and concentrates more on the electronic structure having to do with the relative coordinate ρ of the electrons forming the Cooper-pairs. For a description of the microscopic properties, it is easier to consider an ideal situation, *i.e.* a homogeneous superconductor that is in equilibrium.

Note that the real-space representation of this wavefunction (Eq. 4.4) is a plane wave with *K=0*, and therefore has no dependence on the center of mass coordinate *R* of the pairs. In other words: the 'macroscopic wavefunction' corresponding to the “clean” conditions considered in the BCS theory, is a constant and has no dependence on the center-of-mass coordinate *R*. However, the presence of boundaries, fields, impurities, etcetera, distorts the wavefunction in the groundstate and introduces some finite *R*-dependence. The GL equations discussed in a later chapter deal with the macroscopic properties described by the *R-dependence,* related with the motion of the condensate of Cooper-pairs in its entirety such as currents, vortices, etc.

You may wonder at this point how accurate Eq. 4.8 can be, even for a homogeneous superconductor without magnetic fields applied. A serious source of concern is for example that pairs are not 'real' bosons. Pairs of electrons, for example, *don't* satisfy the same type of commutation relations as ordinary bosons. You may wonder how the BEC picture can work in the case of ^{4}He, which after all is also a composite boson with two electrons and 4 nuclear fermionic particles? If one works out the commutation relations for composite

bosons, it turns out that as long as the charge clouds don't overlap, composite bosons do satisfy the usual commutation relations. In the case of ^{4}He the charge clouds of the He-atoms don't overlap very strongly. In superconductors it turns out, that the wavefunction $w(\rho)$ of the relative coordinates extends over a distance of order ξ, the coherence length, which we will discuss later on in the context of the Ginzburg-Landau model. The length scale ξ can vary from a few nm upto a few hundred nm in superconductors. On the other hand, the average distance between the electrons is about one lattice spacing, which is less than a nm. Hence, in superconductors the charge clouds of overlap with housands of other pairs, so that Bose-Einstein commutation relations don't hold at all. Yet, the *wavefunction* of a BCS superconductor is of the BEC form presented in Eq. 4.8. The pairs in Eq. 4.8 are the so-called Cooper-pairs. The most important property of a Cooper-pair is, that its center-of-mass momentum quantum number is zero. Therefore the two electrons inside a pair must individually have a momentum of exactly the same value, but of opposite sign.

IV.2 The BCS wave-function

In spite of its simplicity, Eq. 4.8 is not the most convenient representation for the purpose of calculating physical properties. Bardeen, Cooper and Schrieffer proposed the following related, but different, variational wavefunction

$$\boxed{\begin{array}{c} |\Psi_0\rangle = \prod_k \left\{ u_k + v_k c^\dagger_{k\alpha} c^\dagger_{-k\beta} \right\} |0\rangle \\ |u_k|^2 + |v_k|^2 = 1 \end{array}} \qquad (4.9)$$

In later section we will come back to the relation to BEC, and we will see that the parameters describing the wavefunction of a pair, w_k (Eq. 4.7) is related to the variational parameters u_k and v_k by the relation

$$w_k = \frac{v_k}{u_k}$$

The BCS wavefunction corresponds in fact to the superposition of a huge number states corresponding to Bose-condensates with different numbers of condensed bosons. The main idea of BCS was, that, since a fluctuation in the number of bosons costs zero energy, the energy of such a superposition is the same as that of a state with a specific number of condensed bosons.

The most important thing to note here, is that Eq. 4.9 has in common with a Fermi-gas state that it is product of operators. Each term is in itself a superposition of two states, one with amplitude v_k where a pair of electrons occupies the states with opposite momentum {k,-k}, and the other one with amplitude u_k where these two states are empty. It is precisely this factorization in a product of terms, which makes the calculation of expectation values of the many-particle hamiltionian a relatively easy task, with a result, which can be expressed in analytically closed form. We begin by analyzing the energy at *T=0*. The free energy of the electrons is just the expectation value of the total Hamiltonian

$$\boxed{\begin{aligned}&\Omega = \left\langle \Psi_0 \middle| \hat{K} + \hat{H}^i \middle| \Psi_0 \right\rangle \\ &\text{where} \\ &\hat{K} = \sum_{k,\sigma} \xi_k c^\dagger_{k,\sigma} c_{k,\sigma} \\ &\hat{H}^i = \frac{1}{2} \sum_{k,l,\sigma,\sigma'} V_{k,l} c^\dagger_{l\sigma} c^\dagger_{-l\sigma'} c_{-k\sigma'} c_{k\sigma}\end{aligned}} \qquad (4.10)$$

It is important to remember that the energies ξ_k are defined as the band energies relative to the chemical potential. The chemical potential has to be substracted since particle number fluctuations necessarily imply transfer of electrons to a reservoir. Hence the equilibrium energy in the reservoir, μ, needs to be accounted for, and this is achieved by subtracting μ from the energy of the electrons. Consequently the free energy to be minimized is the Landau potential *Ω*.

Following the BCS approach, we will assume that the ground-state wavefunction is of the form given by Eq. 4.9. As said before, the representation given in Eq. 4.9 is the most convenient one for calculating physical quantitites. Two types of averages are needed to evaluate Ω:

$$\begin{aligned}&\left\langle \Psi_0 \middle| c^\dagger_{k,\sigma} c_{k,\sigma} \middle| \Psi_0 \right\rangle = v_k v^*_k \\ &\left\langle \Psi_0 \middle| c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} \middle| \Psi_0 \right\rangle = \prod_{k''} \prod_{k'} \left\langle 0 \middle| \left\{ u^*_{k''} + v^*_{k''} c_{-k''\downarrow} c_{k''\uparrow} \right\} c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} \left\{ u_{k'} + v_{k'} c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow} \right\} \middle| 0 \right\rangle = \\ &\qquad = \left\langle 0 \middle| \left\{ v^*_k c_{-k\downarrow} c_{k\uparrow} \right\} c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} \left\{ u_k \right\} \middle| 0 \right\rangle = v^*_k u_k\end{aligned} \qquad (4.11)$$

With the help of these averages it is straightforward to show, that

$$\begin{aligned}K &= \left\langle \Psi_0 \middle| \hat{K} \middle| \Psi_0 \right\rangle = 2 \sum_k v_k v^*_k \xi_k \\ H^i &= \left\langle \Psi_0 \middle| \hat{H}^i \middle| \Psi_0 \right\rangle = \sum_{kl} u_k v^*_k V_{kl} u^*_l v_l\end{aligned} \qquad (4.12)$$

The average number of electrons in the ground state is

$$N = -\frac{\partial \Omega}{\partial \mu} = -\frac{\partial K}{\partial \mu} = 2\sum_k v_k v_k^* \tag{4.13}$$

The expression of the free energy then becomes

$$\boxed{\Omega = 2\sum_k v_k v_k^* \xi_k + \sum_{kl} u_k v_k^* V_{kl} u_l^* v_l} \tag{4.14}$$

We are searching for the solution with the minimum free energy. The variation of the free energy is

$$\delta\Omega = \sum_p \left\{ \left(2v_p^* \xi_p + u_p^* \sum_k u_k v_k^* V_{kp} \right) \delta v_p + \left(2v_p \xi_p + u_p \sum_l V_{pl} u_l^* v_l \right) \delta v_p^* + \left(v_p^* \sum_l V_{pl} u_l^* v_l \right) \delta u_p + \left(v_p \sum_k u_k v_k^* V_{kp} \right) \delta u_p^* \right\}$$

Since at the free energy minimum $\delta\Omega=0$, and the parameters for different momentum values are independent, all terms on the righthand side of the above expression have to be individually equal to zero for each momentum index *p*. We furthermore note, that that due to the fact that $v_p v_p^* + u_p u_p^* = 1$, the variations of v_p, v^*_p, u_p and u^*_p are not independent i.e. $v_p^* \delta v_p + u_p \delta u_p^* + v_p \delta v_p^* + u_p^* \delta u_p = 0$. Secondly we notice in the wavefunction Eq. 4.9, that each of the terms in the product can be multiplied with an arbitrary k-dependent phase factor, while the wavefunction remains the same. Since the phase factors can be absorbed in the definition of u_k and v_k we see, that without loss of generality we are allowed to apply one more constraint on the parameters v_p, v^*_p, u_p and u^*_p which fixes the overall phase of each term $(u_p + v_p c_{p\alpha}^\dagger c_{-p\beta}^\dagger)$ but does not affect the relative phase between v_p and u_p. There are various ways to do this, all of which ultimately lead to the same expressions for the ground state. Most frequently one sets $v_p^* \delta v_p + u_p \delta u_p^* = 0$ which, by taking the complex conjugate implies $v_p \delta v_p^* + u_p^* \delta u_p = 0$. Taken together still corresponds to the substitutions

$$\delta v_p = -\frac{u_p}{v_p^*} \delta u_p^* \qquad ; \qquad \delta v_p^* = -\frac{u_p^*}{v_p} \delta u_p$$

We furthermore introduce the shorthand notation for the summations over V_{kp}

$$\Delta_p = -\sum_k u_k v_k^* V_{kp} \tag{4.15a}$$

and its conjugate

$$\Delta_p^* = -\sum_l V_{pl} u_l^* v_l \tag{4.15b}$$

The result is the condition

$$0 = \left\{ -\frac{u_p}{v_p^*}\left(2v_p^*\xi_p - u_p^*\Delta_p\right) - v_p\Delta_p \right\}\delta u_p + \left\{ -\frac{u_p^*}{v_p}\left(2v_p\xi_p - u_p\Delta_p^*\right) - v_p^*\Delta_p^* \right\}\delta u_p^*$$

Since the variations δu_p and δu^*_p are independend from each other, each of the terms in curly brackets is zero separately. However, since these expressions are complex conjugates of each other it is sufficient to solve just one of them. We take the first one and rearrange the terms as

$$\Delta_p \equiv \frac{2u_p v_p^*}{u_p u_p^* - v_p v_p^*}\xi_p \tag{4.16}$$

Later we will identify Δ_p as the order parameter. Using elementary arithmetics we express u_p and v_p in terms of Δ_p

$$\boxed{\begin{aligned} 2u_p v_p^* &= \frac{\Delta_p}{\sqrt{\xi_p^2 + \left|\Delta_p^2\right|}} \quad ; \quad 2u_p^* v_p = \frac{\Delta_p^*}{\sqrt{\xi_p^2 + \left|\Delta_p^2\right|}} \\ 2u_p u_p^* &= 1 + \frac{\xi_p}{\sqrt{\xi_p^2 + \left|\Delta_p\right|^2}} \quad ; \quad 2v_p v_p^* = 1 - \frac{\xi_p}{\sqrt{\xi_p^2 + \left|\Delta_p\right|^2}} \end{aligned}} \tag{4.17}$$

Combining Eqs. (4.15), (4.16) and (4.17) we obtain the self-consistent expression for Δ_p

$$\boxed{\Delta_p = -\sum_k \frac{\Delta_k V_{kp}}{2\sqrt{\xi_k^2 + \left|\Delta_k\right|^2}}} \tag{4.18a}$$

Where Δ_p is now the complex order parameter, the phase of which can have finite k-dependence.In the remainder of this section we will assume that the interaction dependes on the energies ξ_k, ξ_{-k}, ξ_p, and ξ_{-p} of the electrons forming the Cooper-pairs, but that there is no dependence on the direction in momentum space. The summation over *k* can then be replaced with an integral over the energy, and Eq. 4.18 becomes an integral equation

$$\Delta(\xi) = \int_{-\infty}^{\infty} V_{\xi,\omega} \frac{\Delta(\omega)}{2\sqrt{\omega^2 + \left|\Delta(\omega)\right|^2}} N(\omega) d\omega \tag{4.18b}$$

where $N(\omega)d\omega$ is the number of states in the energy interval $d\omega$, in other words $N(\omega)$ is the density of states. In the previous section we have seen that that the interaction between

quasiparticles is attractive in a shell $\hbar\omega_D$ around the Fermi surface, where ω_D is the typical phonon frequency (the Debye frequency). It is common practice to replace the full expression for the interaction with a toy model of the interaction potential, which captures the essential aspects:

$$V(\xi,\omega) = -V \quad \text{for} \quad \sqrt{\omega^2 + |\Delta(\omega)|^2} < \omega_D \tag{4.19}$$

$$V(\xi,\omega) = 0 \qquad \text{otherwise}$$

Another reasonable assumption is, that the density of states, *N(ω)*, doesn't vary appreciably within this narrow shell around ξ_F. Hence we may set *N(ω)=N(0)* in the region where the interaction is finite. One then often replaces the dimensionless product *N(0)V* with the parameter λ, which is called the electron-phonon coupling constant, and which is proportional to the effective attractive interaction between the electrons. This implies, that also $\Delta(\xi)=0$ for $\sqrt{\omega^2 + |\Delta(\omega)|^2} > \omega_D$, and moreover $\Delta(\omega)$=constant=Δ for $\sqrt{\omega^2 + |\Delta(\omega)|^2} < \omega_D$. We can than make a transformation of variables $x = \sqrt{1 + \xi^2/\Delta^2}$, with the help of which Eq. 4.18b, becomes

$$\frac{1}{\lambda} = \int_1^{\omega_D/\Delta} \frac{1}{\sqrt{x^2-1}}\,dx$$

The solution of the above integral equation is

$$\frac{1}{\lambda} = \int_1^{\omega_D/\Delta} \frac{1}{\sqrt{x^2-1}}\,dx = \left[-\coth^{-1}(x)\right]_1^{\omega_D/\Delta} = -\coth^{-1}(\omega_D/\Delta) + 0$$

Inversion of this equation gives $D/\Delta = \coth(-1/\lambda) = \left(e^{-1/\lambda} + e^{1/\lambda}\right)/2$, hence

$$\Delta = 2\omega_D e^{-1/\lambda}\left(1 + e^{-2/\lambda}\right)^{-1} \tag{4.20}$$

Which for weak coupling ($\lambda << 1$) corresponds to the famous BCS expression for the order parameter at zero temperature

$$\boxed{\Delta \approx 2\omega_D e^{-1/\lambda}} \tag{4.21}$$

We still have to check, that this extremum actually corresponds to a stable minimum, and that it is not a maximum of the function $\Omega(\Delta)$. We can do this by resubstituting the solution for Δ in the expression for the free energy, Eq. 4.14. With a little algebra we obtain

$$
\begin{aligned}
K &= N(0)\int_{-\omega_D}^{\omega_D} d\xi \left(|\xi| - E + \frac{\Delta^2}{E} \right) \\
H^i &= -\lambda N(0) \int_{-\omega_D}^{\omega_D} d\xi \int_{-\omega_D}^{\omega_D} d\xi' \frac{\Delta^2}{4EE'}
\end{aligned}
\tag{4.22}
$$

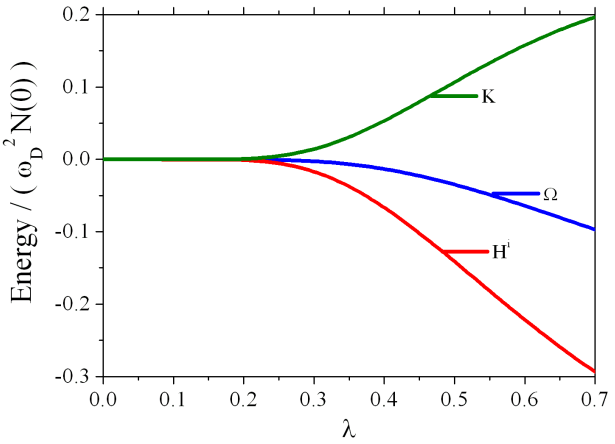
From the above expression we see that automatically *K* is positive definite, and *in*creases as a function of increasing *Δ*. On the other hand, the sign of H^i depends on the sign of the coupling constant, λ. From this we can already see, that for a repulsive net interaction *Δ=0.* As this implies that in the BCS wavefunction v_k=0 for $\varepsilon_k > \varepsilon_F$, ($v_k$=1 for $\varepsilon_k < \varepsilon_F$) the groundstate wavefunction for V<0 corresponds to the usual metallic state, with no pairing, and no superconductivity. The integrals can be solved, with the result for λ<<1

$$
\begin{aligned}
K &= N(0)\Delta^2 \ln\left(\frac{2\omega_D}{\Delta}\right) - N(0)\frac{\Delta^2}{2} \\
H^i &= -\lambda N(0)\Delta^2 \left[\ln\left(\frac{2\omega_D}{\Delta}\right)\right]^2 \\
\Omega &= K + H^i
\end{aligned}
$$

For a superconducting solution to occur, having *Δ≠0*, it is necessary that the interaction is attractive, i.e. λ>0. At the free energy minimum:

$$
\begin{aligned}
\frac{\partial \Omega}{\partial \Delta} &= 0 \Rightarrow \Delta = 2\omega_D e^{-1/\lambda} \\
&\Downarrow \\
K &= N(0)\omega_D^2 e^{-2/\lambda}\,(1/\lambda - 1/2) \\
H^i &= -N(0)\omega_D^2 e^{-2/\lambda}/\lambda \\
\Omega &= -\frac{1}{2}N(0)\omega_D^2 e^{-2/\lambda}
\end{aligned}
\tag{4.23}
$$

Pay attention that these expressions are only valid in the limit of weak coupling, *λ << 1.*



Above we plot the three energies, K, H^i, and Ω as a function of the coupling constant $\lambda=N(0)V$. It is clear from this, that the effect of superconducting order is to *increase* the kinetic energy in the superconducting state, and to *decrease* the interaction energy H^i. For the latter to occur it is necessary that the quasiparticles have a net attractive interaction. If the interation is repulsive, both K>0 and H^i>0 for any value of Δ, and the only stable minimum is found when Δ=0. Hence, in the model of Eq. 4.10 the superconducting order is strictly limited to the situation where the interaction is attractive.

IV.3 Relation between the BCS wave-function and a Bose-Einstein condensate of Cooper-pairs

The energy of each pairs in a BEC is given by μ=0, where μ is the chemical potential. Therefore the thermodynamical potential of a superconductor does not depend on whether it is occupied with N_p, N_p-1, N_p+1... Cooper-pairs. A famous theorem of quantum mechanics says, that a linear superposition of different quantummechanical states, all having the same energy, is again an eigenstate. Consequently a linear superposition of states containing N_p, N_p-1, N_p+1 *etc.* Cooper-pairs is also an eigenstate. A particularly useful example of this property is constituted by the "coherent state"

$$|\phi\rangle = C'\exp\left\{e^{i\phi}a_0^{\dagger}\right\}|0\rangle \qquad (4.24)$$

where C' is a normalization constant, which can be expressed as a Tayler-series expansion of states with *m* condensed pairs

$$|\phi\rangle = C' \sum_m \frac{1}{m!} e^{im\phi} \left(a_0^\dagger\right)^m |0\rangle = C' \sum_m \frac{1}{m!} e^{im\phi} \left(\sum_q w_k c_{k\alpha}^\dagger c_{-k\beta}^\dagger \right)^m |0\rangle$$

This state is now characterized by the *phase* quantum number ϕ, instead of the number of particles in the system. To keep the notation compact we combine the phase factor exp{iϕ} and w_k by the definition

$$\omega_k = e^{i\phi} w_k$$

We now apply to Eq. 4.24 the following property of a set of *commuting* operators *{a,b,c,..}: exp{a+b+c…}=$e^a e^b e^c$….*

$$|\phi\rangle = C' \prod_k \exp\left\{\omega_k c_{k\alpha}^\dagger c_{-k\beta}^\dagger\right\} |0\rangle$$

The next step is, to make a Taylor-series expansion of each of the exponential factors

$$\exp\left\{\omega_k c_{k\alpha}^\dagger c_{-k\beta}^\dagger\right\} = 1 + \omega_k c_{k\alpha}^\dagger c_{-k\beta}^\dagger + \frac{1}{2!}\left(\omega_k c_{k\alpha}^\dagger c_{-k\beta}^\dagger\right)^2 + \ldots$$

Here we can employ the fact, that the due to the Pauli-principle, terms like $\left(\omega_k c_{k\alpha}^\dagger c_{-k\beta}^\dagger\right)^n |\Psi\rangle$ = 0 for *any* state |Ψ⟩, *unless* n=0, or n=1. Hence

$$|\varphi\rangle = C' \prod_k \left\{1 + e^{i\phi} w_k c_{k\alpha}^\dagger c_{-k\beta}^\dagger\right\} |0\rangle$$

Normalization is obtained with $C' = \prod_q \left(1 + |w_q|^2\right)^{-1/2}$. One then defines

$$u_k = \frac{1}{\sqrt{1+|w_k|^2}} \qquad v_k = \frac{w_k}{\sqrt{1+|w_k|^2}}$$

together satisfying the normalization condition $|u_k|^2 + |v_k|^2 = 1$. We thus see, that the BCS wavefunction (Eq. 4.9)

$$|\Psi_0(\phi)\rangle = \prod_k \left\{u_k + e^{i\phi} v_k c_{k\alpha}^\dagger c_{-k\beta}^\dagger\right\} |0\rangle$$

is a coherent sum of Bose-condensates for the particular phase-value, $\phi=0$. Vice versa, a BEC with a fixed number of pairs N is obtained by taking a superposition of BCS-wavefunctions with different phases (exercice !)

$$\left(a_0^\dagger\right)^N |0\rangle = \frac{1}{2\pi} \int_0^{2\pi} d\phi e^{i\phi N} |\Psi_0(\phi)\rangle \qquad (4.25)$$

Chapter V: Superconducting properties at finite temperature

V.1 The Bogoliubov-Valatin transformation

To explore the physical properties at finite temperature, it is important to know the exact nature of the excitations of the superconductor. Due to the presence of an interaction, in principle an excitation reached by adding a single electron with momentum p and spin ↑ to the system, $c^{\dagger}_{p\uparrow}|\Psi_0\rangle$, is in fact a wavepackage of several true eigenstates of the system with different energies. $c^{\dagger}_{p\uparrow}|\Psi_0\rangle$ is *not* an eigenstate! Due to Galilean invariance non-relativistic interactions between particles usually have the following structure in k-space representation

$$\hat{H}^i = \sum_q \sum_{k,l,\sigma,\sigma'} V_{kl} c^{\dagger}_{k+q,\sigma} c^{\dagger}_{-k+q,\sigma'} c_{-l+q,\sigma'} c_{l+q,\sigma} \tag{5.1}$$

independent of their microscopic origine. In chapter III we have already seen, that the only terms in the interaction which matter for the groundstate are those for which q=0. This is because in $|\Psi_0\rangle$ the electron creation operators only occur in the combination $c^{\dagger}_{p\uparrow}c^{\dagger}_{-p\downarrow}$. In the BCS model it is assumed, that the excitations do not carry the superconductor far from the groundstate, so that also for the excited states the only relevant terms in the interaction Hamiltonian are those for which q=0.

For the calculation of the excitation spectrum the first approximation is to consider only those interactions which scatter a (-k↑,k↓) pair with total momentum equal to zero, to a similar state (-p↑,p↓)

$$\hat{H}^i_{red} = \sum_{k,p} V_{kp} c^{\dagger}_{p,\uparrow} c^{\dagger}_{-p,\downarrow} c_{-k,\downarrow} c_{k,\uparrow} \tag{5.2}$$

We have already seen, that this hamiltonian will lead to a ground state where pairs of Bloch states (p↑,-p↓) are in a mixed state of being empty (with amplitude u_p) and occupied (with amplitude v_p). Because of coherence, operators such as $c^{\dagger}_{p\uparrow}c^{\dagger}_{-p\downarrow}$ can have nonzero expectation values $\left\langle c^{\dagger}_{p,\uparrow} c^{\dagger}_{-p,\downarrow} \right\rangle$ in such a state, rather than averaging to zero as in a normal metal. In the previous section (Eq. 4.11), we have already seen that $\left\langle c^{\dagger}_{p,\uparrow} c^{\dagger}_{-p,\downarrow} \right\rangle = u_p v^*_p$,

where the expectation value is taken for the groundstate at T=0. However, in the remaining sections we are interested in the statistically weighted average at finite temperature

$$\left\langle c^{\dagger}_{p,\uparrow} c^{\dagger}_{-p,\downarrow} \right\rangle_T = u_p v^*_p \tag{5.3}$$

Moreover, because of the large numbers of particles involved, the fluctuations about these expectation values, defined as

$$\phi^{\dagger}_p = c^{\dagger}_{p,\uparrow} c^{\dagger}_{-p,\downarrow} - \left\langle c^{\dagger}_{p,\uparrow} c^{\dagger}_{-p,\downarrow} \right\rangle_T \tag{5.4}$$

should be small. This suggests that it will be useful to express such a product of operators formally as

$$c^{\dagger}_{p\uparrow} c^{\dagger}_{-p\downarrow} = u_p v^*_p + \varphi^{\dagger}_p \tag{5.5}$$

With this definition terms quartic in the creation and annihilation operators become

$$c^{\dagger}_{p,\uparrow} c^{\dagger}_{-p,\downarrow} c_{-k,\downarrow} c_{k,\uparrow} = c^{\dagger}_{p,\uparrow} c^{\dagger}_{-p,\downarrow} \left\langle c_{-k,\downarrow} c_{k,\uparrow} \right\rangle + \left\langle c^{\dagger}_{p,\uparrow} c^{\dagger}_{-p,\downarrow} \right\rangle c_{-k,\downarrow} c_{k,\uparrow} - \left\langle c^{\dagger}_{p,\uparrow} c^{\dagger}_{-p,\downarrow} \right\rangle \left\langle c_{-k,\downarrow} c_{k,\uparrow} \right\rangle + \varphi^{\dagger}_p \varphi_k$$

The central approximation consists of neglecting the 4th term in the above expression, because it is the product of two fluctuation operators, each of which has a small expectation value, and the product in mean-field theory averages to zero. If we follow this procedure with our pairing Hamiltonian, we obtain

$$H = \sum_{k,\sigma} \xi_k c^{\dagger}_{k,\sigma} c_{k,\sigma} + \sum_{k,p} V_{kp} u^*_k v_k c^{\dagger}_{p,\uparrow} c^{\dagger}_{-p,\downarrow} + \sum_{k,p} V_{kp} u_p v^*_p c_{-k,\downarrow} c_{k,\uparrow} - \sum_{k,p} V_{kp} u_p v^*_p u^*_k v_k \tag{5.6}$$

Similar to what we did in Eq. 4.15, the summations over $V_{kp}\, u_p v^*_p$ can be substituted with a the variational parameter

$$\Delta_p = -\sum_k u_k v^*_k V_{kp} \tag{5.7}$$

With the help of this, we obtain the central Hamiltonian of BCS theory

$$\boxed{H = \sum_{k,\sigma} \xi_k c^{\dagger}_{k,\sigma} c_{k,\sigma} - \sum_p \Delta^*_k c^{\dagger}_{p,\uparrow} c^{\dagger}_{-p,\downarrow} - \sum_k \Delta_k c_{-k,\downarrow} c_{k,\uparrow} + \sum_k \Delta_k u^*_k v_k} \tag{5.8}$$

which is now bi-linear in the creation and annihilation operators. The energies of a state with one electron removed, or one electron added relative to the ground-state energy, is $-\xi_k$ and ξ_k respectively. Note, that, due to the fact that the terms proportional to Φ_k mix one-electron removal with one-electron addition states in this Hamiltonian, the number of electrons is not a good quantum number. Consequently the eigenstates should have the form

$$\left|\Psi_{k,\downarrow}\right\rangle = \left\{u_k c_{k,\downarrow} + v_k c^{\dagger}_{-k,\uparrow}\right\}\left|\Psi_0\right\rangle \tag{5.9}$$

As was shown by Bogoliubov and by Valatin, we can diagonalize the Hamiltonian in second quantized form by introducing a new set of creation and annihilation operators

$$\begin{array}{ll} \gamma_{k\uparrow} = u_k c_{k\uparrow} - v_k c^{+}_{-k\downarrow} & \gamma^{+}_{k\uparrow} = u^{*}_k c^{+}_{k\uparrow} - v^{*}_k c_{-k\downarrow} \\ \gamma_{-k\uparrow} = u_{-k} c_{-k\uparrow} - v_{-k} c^{+}_{k\downarrow} & \gamma^{+}_{-k\uparrow} = u^{*}_{-k} c^{+}_{-k\uparrow} - v^{*}_{-k} c_{k\downarrow} \\ \gamma_{-k\downarrow} = u_k c_{-k\downarrow} + v_k c^{+}_{k\uparrow} & \gamma^{+}_{-k\downarrow} = u^{*}_k c^{+}_{-k\downarrow} + v^{*}_k c_{k\uparrow} \\ \gamma_{k\downarrow} = u_{-k} c_{k\downarrow} + v_{-k} c^{+}_{-k\uparrow} & \gamma^{+}_{k\downarrow} = u^{*}_{-k} c^{+}_{k\downarrow} + v^{*}_{-k} c_{-k\uparrow} \end{array} \tag{5.10}$$

The inversion of this transformation is

$$\begin{array}{ll} c_{k\uparrow} = u^{*}_k \gamma_{k\uparrow} + v_k \gamma^{+}_{-k\downarrow} & c^{+}_{k\uparrow} = u_k \gamma^{+}_{k\uparrow} + v^{*}_k \gamma_{-k\downarrow} \\ c_{-k\uparrow} = u^{*}_{-k} \gamma_{-k\uparrow} + v_{-k} \gamma^{+}_{k\downarrow} & c^{+}_{-k\uparrow} = u_{-k} \gamma^{+}_{-k\uparrow} + v^{*}_{-k} \gamma_{k\downarrow} \\ c_{-k\downarrow} = -v_k \gamma^{+}_{k\uparrow} + u^{*}_k \gamma_{-k\downarrow} & c^{+}_{-k\downarrow} = -v^{*}_k \gamma_{k\uparrow} + u_k \gamma^{+}_{-k\downarrow} \\ c_{k\downarrow} = -v_{-k} \gamma^{+}_{-k\uparrow} + u^{*}_{-k} \gamma_{k\downarrow} & c^{+}_{k\downarrow} = -v^{*}_{-k} \gamma_{-k\uparrow} + u_{-k} \gamma^{+}_{k\downarrow} \end{array} \tag{5.11}$$

We substitute the new operators $\gamma_{k\sigma}$ for the creation and annihiliation operators in Eq. 5.8. With the help of some straightforward algebra we can verify that, when we take the following values for the coefficients u_k and v_k

$$\begin{array}{l} \mathrm{u_k} = \dfrac{1}{\sqrt{2}}\sqrt{1+\xi_k / E_k} \\ \mathrm{v_k} = \dfrac{1}{\sqrt{2}}\sqrt{1-\xi_k / E_k} \\ \text{where } E_k \equiv \sqrt{\xi_k{}^2 + |\Delta_k|^2} \end{array}, \tag{5.12}$$

the Hamiltonian of Eq. 5.8 takes the simple bilinear form

$$H = \sum_{k,\sigma} E_k \gamma^{\dagger}_{k,\sigma} \gamma_{k,\sigma} + \sum_k \left(\Delta_k u^{*}_k v_k + \xi_k - E_k\right) \tag{5.13}$$

where Δ_k must be obtained by solving this equation self-consistently for each temperature. We will perform that task in the following section. The first term corresponds to excitations where we *add* a particle of energy $\mathrm{E_k} = \sqrt{\xi_k^2 + |\Delta_k|^2}$ to the system, and has the usual form of an energy-momentum dispersion of *non-interacting* particles. In the previous section Δ emerged as an energy scale which characterizes the superconducting order. Its exact physical meaning remained unclear. We have now discovered that Δ_k has the physical meaning of a gap in the single particle excitation-spectrum. From the expression for the

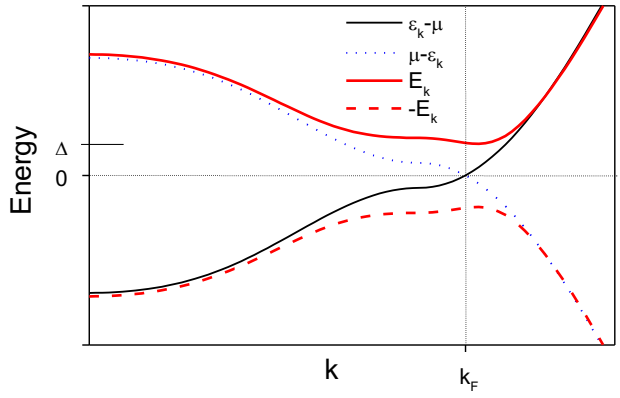
eigen-energies, and from the dispersion relations shown in Fig. IV.1, we see that terns mixing particle and hole character create a gap at the Fermi energy in the single particle excitaton spectrum.

Let us now investigate the nature of the particles described by the creation operators $\gamma^{\dagger}_{k\sigma}$. A table of their most important properties is given below:

Property	**Value**
Energy	$E_k = \sqrt{\xi_k^{\,2} + \lvert \Delta_k^* \rvert^2}$ is always positive
Mininum value of the energy	$E_k > \lvert\Delta\rvert$
Statistical properties	Fermionic
Anti-commutation relations	$\gamma_{k\alpha}\,\gamma^{\dagger}_{k\beta} + \gamma^{\dagger}_{k\beta}\,\gamma_{k\alpha} = \delta_{k,q}\delta_{\alpha,\beta}$, etc.
Momentum	$\hbar k$
Spin	S=1/2
Charge is not a good quantum number	$q_k = -\lvert e \rvert \xi_k / E_k$
Charge at minimal energy, $E_k = \lvert\Delta\rvert$	$q_k = 0$
Charge for $\lvert k\rvert >> k_F$	$q_k = -\lvert e\rvert$
Charge for $\lvert k\rvert << k_F$	$q_k = +\lvert e\rvert$

The particles generated by $\gamma^{\dagger}_{k\sigma}$ are called "Bogoliubov quasiparticles". Although they are in many ways equivalent to electrons or holes, they differ in one essential respect: The charge of these particles is not a good quantum number! The Bogoliubov quasiparticles are quantum-superpositions of an electron-excitation and a hole-excitation. This should not be confused with an electron-hole pair! An excitated state containing a single Bogoliubov quasiparticle is of the form $\left\{u_k c_{k,\downarrow} + v_k c^{\dagger}_{-k,\uparrow}\right\}\left|\Psi_0\right\rangle$, and describes a linear superposition of two states containing one electron or one hole, and each being a singe fermionic excitation. An e-h pair consists of two excited fermions and is described by the *product* of an electron

creation and an electron annihilation operator $c_{k,\sigma}c^{\dagger}_{q,\sigma'}|\Psi_0\rangle$. Since composite particles consisting of an even number of bosons, an electron-hole pair has bosonic character.



V.2 The critical temperature of a BCS superconductor

Sofar we have evaluated Δ only at T=0, which was obtained from the selfconsistancy expression, Eq. 5.7, $\Delta_p = -\sum_k u_k v_k^* V_{kp}$. The product $u_k v^*_k$ is obtained from the thermally averaged quantity

$$\langle c_{-k,\downarrow}c_{k,\uparrow}\rangle_T \equiv \sum_\lambda e^{-\beta(E_\lambda-\mu N_\lambda-\Omega)}\langle\Psi_\lambda|c_{-k,\downarrow}c_{k,\uparrow}|\Psi_\lambda\rangle$$
$$\text{where } e^{-\beta\Omega} \equiv \sum_\lambda e^{-\beta(E_\lambda-\mu N_\lambda)} \qquad (5.14)$$

The result is

$$\langle c_{-k,\downarrow}c_{k,\uparrow}\rangle_T = u_k v_k^* \qquad (5.15)$$

and the selfconsistency condition at finite temperatures is

$$\Delta_p(T) = -\sum_p V_{kp}\langle c_{-k,\downarrow}c_{k,\uparrow}\rangle_T \qquad (5.16)$$

In the superconducting state the Bogoliubov quasiparticles behave like ordinary fermions, and their occupation factors are described by the Fermi-Dirac distribution. We therefor express the *c*-creation operators in the γ-creation and annihilation operators with the help of the transformation of Eq. 5.11. Aforementioned self-consistancy condition then becomes

$$\Delta_p = -\sum_k V_{kp}\langle\{-v_k\gamma^+_{k\uparrow}+u^*_k\gamma_{-k\downarrow}\}\{u^*_k\gamma_{k\uparrow}+v_k\gamma^+_{-k\downarrow}\}\rangle_T =$$
$$= -\sum_k V_{kp}\{u^*_k v_k\langle\gamma_{-k,\downarrow}\gamma^\dagger_{-k,\downarrow}-\gamma^\dagger_{k,\uparrow}\gamma_{k,\uparrow}\rangle_T + v_k v_k\langle\gamma^\dagger_{k,\uparrow}\gamma^\dagger_{-k,\downarrow}\rangle_T - u^*_k u^*_k\langle\gamma_{-k,\downarrow}\gamma_{k,\uparrow}\rangle_T\} \qquad (5.17)$$

The last two terms $\left\langle \gamma^{\dagger}_{k,\uparrow}\gamma^{\dagger}_{-k,\downarrow}\right\rangle$ and $\left\langle \gamma_{-k,\downarrow}\gamma_{k,\uparrow}\right\rangle$ are zero, because the Bogoliubov quasiparticles are Fermions with the usual properties of creation and annihilation of particles. The product $u^{*}_{k}v_{k}$ of the first term can be evaluated with the help of Eq. 5.12. Finally, because the quasiparticles are Fermions the thermal averages in the first term of the equation above are given by the Fermi-Dirac distribution:

$$\begin{aligned}\left\langle \gamma^{\dagger}_{k,\uparrow}\gamma_{k,\uparrow}\right\rangle_{T} &= f(E_k) = \frac{1}{1+\exp\{E_k/k_BT\}} \\ \left\langle \gamma_{-k,\downarrow}\gamma^{\dagger}_{-k,\downarrow}\right\rangle_{T} &= 1-f(E_k) = \frac{1}{1+\exp\{-E_k/k_BT\}}\end{aligned} \tag{5.18}$$

Combining all this, we obtain the following self-consistent expression for the gap-function

$$\boxed{\Delta_p = -\sum_{l}\frac{V_{kp}\Delta_k}{2E_k}\tanh\left(\frac{E_k}{2k_BT}\right)} \tag{5.19}$$

The gap equation (5.19) determines the temperature dependence of Δ(T) in the Bogoliuov quasiparticle spectrum. Making the usual transformation from summation in k-space to energy integral, the equation reads

$$\frac{1}{\lambda} = \int_{\Delta}^{\hbar\omega_D}\frac{1}{\sqrt{E^2-\Delta^2}}\tanh\left(\frac{\beta E}{2}\right)dE \tag{5.20}$$

Substituting $x=\beta E$:

$$\frac{1}{\lambda} = \int_{\beta\Delta}^{\beta\hbar\omega_D}\frac{\tanh(x/2)}{\sqrt{x^2-\beta^2\Delta^2}}dx \tag{5.21}$$

The transition temperature can be easily calculated, by realizing that just at T_c the gap should vanish. Hence setting Δ=0 with we obtain the expression for Tc

$$\boxed{\frac{1}{\lambda} = \int_{0}^{\hbar\omega_D/k_BT_c}\frac{\tanh(x/2)}{x}dx} \tag{5.22}$$

Integration in parts yields

$$\begin{aligned}\frac{1}{\lambda} &= \ln\left(\frac{\hbar\omega_D}{k_BT_c}\right)\tanh\left(\frac{\hbar\omega_D}{2k_BT_c}\right) - \int_{0}^{\hbar\omega_D/k_BT_c}\ln(x)\frac{\partial}{\partial x}\tanh\left(\frac{x}{2}\right)dx \approx \\ &\approx \ln\left(\frac{\hbar\omega_D}{k_BT_c}\right) - \int_{0}^{\infty}\ln(x)\frac{\partial}{\partial x}\tanh\left(\frac{x}{2}\right)dx\end{aligned} \tag{5.23}$$

The second integral $\int_0^\infty \ln(x)\frac{\partial}{\partial x}\tanh\left(\frac{x}{2}\right)dx = -0.122$. Consequently

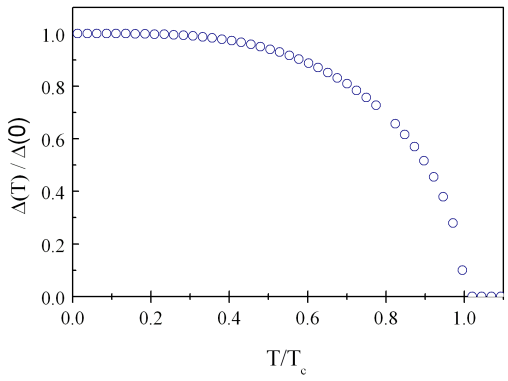
$$\boxed{k_B T_c = 1.13\hbar\omega_D e^{-1/\lambda}} \tag{5.24}$$

In the previous subsection we have already seen, that $\Delta \approx 2\hbar\omega_D e^{-1/\lambda}$, hence the gap-over-Tc ratio satisfies the wellknown BCS-relation

$$\boxed{\frac{2\Delta(0)}{k_B T_c} = 3.53} \tag{5.25}$$

V.3 Temperature dependence of the gapfunction

The temperature dependence of the gap, Δ(T), is obtained by solving Eq. 5.21. The general solution is only possible by numerical means. The numerical solution is shown in the following graph



Close to T_c the solution by series expansion is

$$\frac{\Delta(T)}{k_B T_c} = 3.1\sqrt{1-\frac{T}{T_c}} \qquad (\Delta << k_B T_c) \tag{5.26}$$

V.4 Thermodynamics of a BCS superconductor

The presence of a gap in the Bogoliubov quasiparticle density of states of a superconductor has strong consequences for the thermodynamical properties. The primary thermodynamic functions of interest for this chapter are summarized in the following table:

Statistical probability of many - body state $\left\|\Psi_\lambda\right\rangle$:	$w_\lambda = e^{\beta(E_\lambda - \mu N_\lambda)}/Q$
"Grand" partition function (with fixed μ) :	$Q = \sum_\lambda e^{\beta(E_\lambda - \mu N_\lambda)}$
Entropy :	$S = -k_B \sum_\lambda w_\lambda \ln w_\lambda$
Specific heat with μ fixed :	$C_V = T\left.\frac{\partial S}{\partial T}\right\|_V$
Internal energy with μ fixed :	$U' = E - \mu N = U_0^{'} + \int_0^T C_V(T')dT'$
Landau free energy :	$\Omega = U' - TS$

where $\beta=1/(k_BT)$. We begin by calculating the entropy. The partial entropy associated with the bogoliubov quasiparticle of wavevector k and spin σ is

$$\boxed{S_k = -k_B \sum_{n=0}^{1} w_n \ln w_n} \tag{5.27}$$

Where *n*, the number of bogoliobons with the same quantum number is necessary restricted to zero or one, since Bogoliubov quasiparticles are fermions. The probabilites w_n are therefore given by the Fermi-Dirac distribution:

$$\begin{aligned} w_1 &= f_k = \frac{1}{1+e^{\beta E_k}} \\ w_0 &= 1 - f_k \\ &\text{where } E_k = \sqrt{\xi_k{}^2 + \left|\Delta_k\right|^2} \end{aligned} \tag{5.28}$$

and consequently the total entropy is given by the general relation for fermions:

$$\boxed{S(T) = -k_B \sum_{k,\sigma} \left\{ f_k \ln f_k + (1-f_k)\ln(1-f_k) \right\}} \tag{5.29}$$

One obtains the specific heat from the relation $C_V = T\frac{\partial S}{\partial T}\Big|_V = -\beta\frac{\partial S}{\partial \beta}\Big|_V$. In taking the derivative with respect to temperature, we should take into account the fact that Δ(T) is a function of temperature. We furthermore employ the fact that temperature and energy occur exclusively in the combination βE_k in the Fermi functions. Consequently

$$\frac{\partial f_k}{\partial \beta} = \frac{\partial f_k}{\partial(\beta E_k)}\frac{\partial(\beta E_k)}{\partial \beta} = \frac{1}{\beta}\frac{\partial f_k}{\partial E_k}\left(E_k + \beta\frac{\partial E_k}{\partial \Delta}\frac{\partial \Delta}{\partial \beta}\right) = \frac{1}{\beta}\frac{\partial f_k}{\partial E_k}\left(E_k + \beta\frac{\Delta}{E_k}\frac{\partial \Delta}{\partial \beta}\right) \qquad (5.30)$$

Applying now the chain rule

$$C_V = -\beta\frac{\partial S}{\partial \beta} = k_B\beta\sum_{k,\sigma}\left\{\frac{f_k}{f_k} + \ln f_k - \frac{1-f_k}{1-f_k} - \ln(1-f_k)\right\}\frac{\partial f_k}{\partial \beta} \qquad (5.31)$$

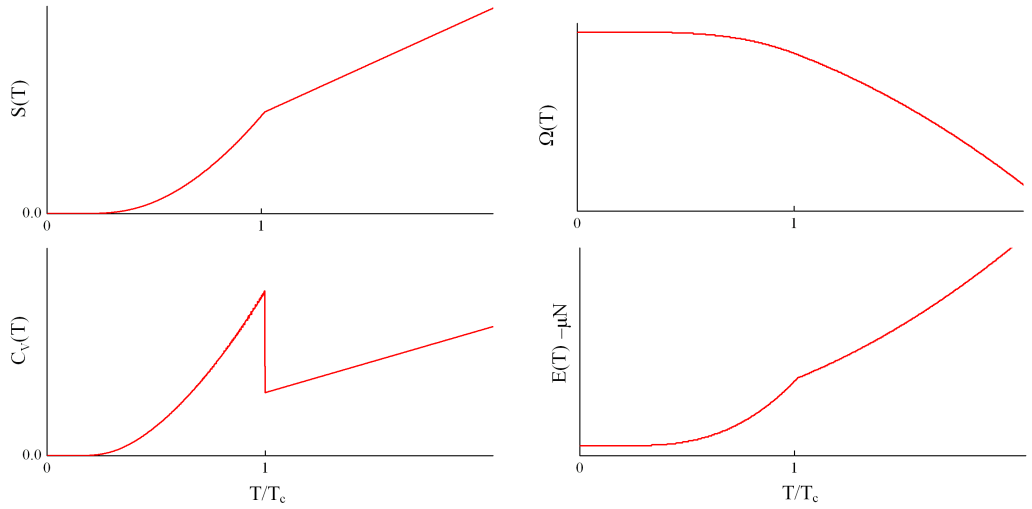
We use the fact that $\ln(f_k/(1-f_k)) = -\beta E_k$

$$C_V = k_B\beta\sum_{k,\sigma}(-\beta E_k)\frac{1}{\beta}\left(E_k + \beta\frac{\Delta_k}{E_k}\frac{\partial \Delta_k}{\partial \beta}\right)\frac{\partial f_k}{\partial E_k} = -\frac{1}{T}\sum_{k,\sigma}\left(E_k^{\,2} - \frac{T}{2}\frac{\partial \Delta_k^{\,2}}{\partial T}\right)\frac{\partial f_k}{\partial E_k} \qquad (5.32)$$

Making the usual replacement of the k-space sum with an integral, we obtain

$$\boxed{C_V = \int_{-\infty}^{\infty}\left(\frac{\partial \Delta^2}{\partial T} - \frac{2E^2}{T}\right)\frac{\partial f}{\partial E}N(\xi)\partial\xi} \qquad (5.33)$$

The specific heat at general temperatures, as well as the other thermodynamic functions such as entropy, free energy, etcetera, can be obtained by solving the above integrals numerically. We summarize below the numerical solution of the main thermodynamic quantities as a function of temperature



Of particular interest is the behaviour of the specific heat at T_c. In an ordinary metal the specific heat is known to have a term proportional to temperature, $C_V = \gamma T$, which can be observed at low enough temperature where the phonon-contribution (proportional to T^3) becomes negligeable. The coefficient γ is proportional to the density of states at the Fermi energy. However, in a superconductor the Bogoliubov quasiparticle spectrum is gapped. Consequently we expect that below Tc the specific heat is suppressed! Indeed, this can be easily calculated. We have already seen in the previous subsection, that the temperature derivative of $\Delta^2(T)$ is discontinuous at T_c:

$$\frac{\partial \Delta^2}{\partial T} = 0 \qquad (T = T_c + 0^+)$$
$$\frac{\partial \Delta^2}{\partial T} = -\left(3.1 k_B\right)^2 \mathrm{T_c} \qquad (T = T_c - 0^+)$$

Consequently

$$C_V = -\frac{2}{T_c} N(0) \int_{-\infty}^{\infty} \xi^2 \frac{\partial f}{\partial \xi} \partial \xi \qquad (T = T_c + 0^+)$$
$$C_V = -\frac{2}{T_c} N(0) \int_{-\infty}^{\infty} \xi^2 \frac{\partial f}{\partial \xi} \partial \xi - \left(3.1 k_B\right)^2 T_c N(0) \int_{-\infty}^{\infty} \frac{\partial f}{\partial \xi} \partial \xi \qquad (T = T_c - 0^+)$$

The first integral gives the familiar result for the normal state:

$$\int_{-\infty}^{\infty} \xi^2 \frac{\partial f}{\partial \xi} \partial \xi = -k_B^2 T^2 \int_{-\infty}^{\infty} \frac{x^2}{e^x + e^{-x} + 2} dx = -k_B^2 T^2 \frac{\pi^2}{3}.$$

The integral of the second term on the right hand side gives

$$\int_{-\infty}^{\infty} \frac{\partial f}{\partial \xi} \partial \xi = -1.$$

Together:

$$C_V = \frac{2\pi^2}{3} N(0) k_B^2 T_c \qquad (T = T_c + 0^+)$$
$$C_V = \frac{2\pi^2}{3} N(0) k_B^2 T_c + \left(3.1 k_B\right)^2 N(0) T_c \qquad (T = T_c - 0^+) \qquad (5.34)$$

Hence, we see that the specific heat has a jump at Tc with the universal ratio

$$\boxed{\frac{C_{V,S} - C_{V,N}}{C_{V,N}} = \frac{3}{2} \cdot \left(\frac{3.1}{\pi}\right)^2 = 1.43} \qquad (5.35)$$

V.5 Tunneling spectra and infrared-conductivity spectra.

In the previous section we have seen, that as a result of the pair-correlations, the single-particle excitations in a superconductor are no longer electrons or holes, as in an ordinary metal, but quasiparticle excitations which have a gap Δ at the Fermi energy. Because the single particle states which originally had an energy ξ_k relative to μ, have been shifted away from μ up to an energy $(\xi_k^2 + \Delta^2)^{1/2}$, density of states has been moved from the region below Δ, to the region just above Δ. Let N(k) be the number of states with momentum quantum number smaller than k. The density of states of the new quasiparticles is $dN(k)/dE_k = (dN/d\xi)*(d\xi_k/dE_k)$. The first term is the density of states in the normal state: $dN/d\xi=\rho_F$. The second term is

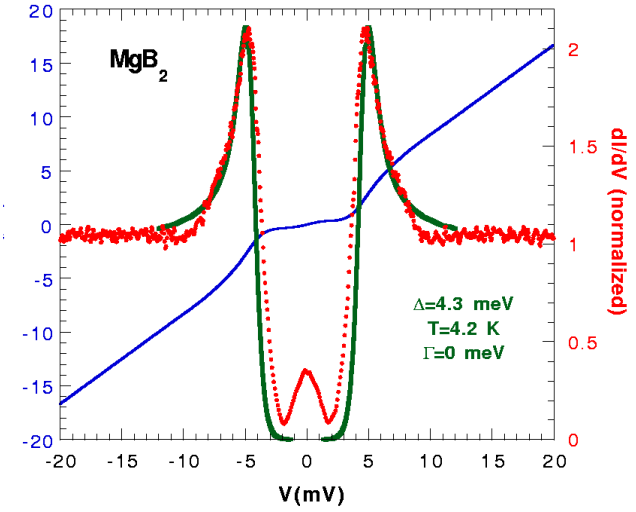
$$\rho(E) = \frac{d\xi}{dE} = \begin{cases} E/(E^2 - \Delta^2)^{1/2} & (E > \Delta) \\ 0 & (E < \Delta) \end{cases} \qquad (5.36)$$

A standard method for determining the gap is by measuring the tunneling current, I, through a metal-insulator-superconductor sandwich structure, as a function of the voltage V across the insulating barrier. The barrier has to be sufficiently thin, that to allow quantum-mechanical tunneling of electrons through the barrier. In such a device Ω's law is not satisfied, and dI/dV depends strongly on the applied voltage. It can be shown, that $dI/dV \sim C\,\rho(eV)$, where eV is the potential energy difference of an electron between both sides of the tunneling barrier, and $\rho(eV)$ is the density of states of Eq. 5.36. The tunneling data of MgB2 is given in the figure below

Figure

Tunneling spectroscopy of MgB2 (Tc = 39 K)

H.Schmidt et al (2001)

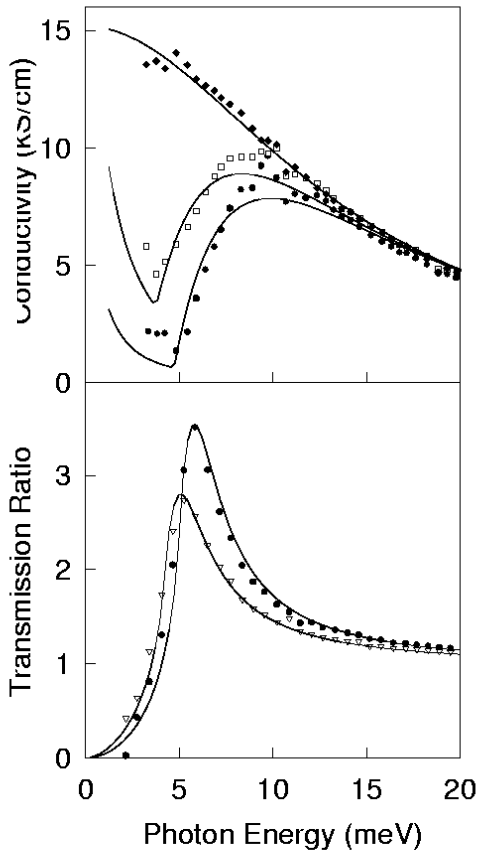


The presence of a region of zero density of states for $E<\Delta$, implies that the material absorbs no photons of energy $\hbar\omega<2\Delta$, because the absorption of lightquanta involves the excitation of *two* quasiparticles with total spinquantum number. For a material with T_c=16 K, the gap is thus $2\Delta=3.5k_BT_c\sim5$meV, which is in the far infrared range of the optical spectrum. The superconducting gap can for example be detected by measuring the transmittivity through a thin film (see, Figure below for an example of the latter procedure).

Figure

Infrared Conductivity and transmission of NbN (Tc= 16 K)

H.S. Somal et al., Phys. Rev. Letters 76 (1996)



Chapter VII:

Ginzburg - Landau theory

VII.1 The free energy as a function of $\psi(r)$

Until now we have not yet found the explanation of the two main properties of a superconductor: zero resistance and Meissner effect. *We will address these important issues in the present chapter, in particular in the discussion following Eq. 7.14.* In our discussion of the condensate wavefunction in Chapter IV we pointed out that the total wavefunction of a pair can be factorized in a product of two wavefunctions, one describing the motion of the center of mass, r, and the other the motion of the relative coordinate, ρ, within a pair

$$\Psi\left(r+\rho/2, r-\rho/2\right) = \psi(r) w\left(\rho\right).$$

In the simplest case of a clean translationally invariant superconductor with no fields applied and no current flowing, the function $\psi(r)$ becomes a constant independent of position r, which can be absorbed in the definition of the wavefunction w(ρ) of the relative coordinate. While the previous chapters on the microscopic theory of pairing concentrated on such a simple situation, the physics of the center-of-mass motion is also very interesting, and pertains to such interesting phenomena as vortices, Josephson effect, type I and type II superconductors, and several other aspects of the phase diagram as well as the transport properties of superconductors.

Although in principle the thermodynamical, and electrodynamical properties of a superconductor can be derived starting from microscopic considerations, such as the BCS model, the model proposed in 1950 by Vitaly Ginzburg and Lev Landau provides an elegant and direct way to calculate the macroscopic properties of superconductors, which bypasses the aspects of the pairing mechanism and summarizes a large range of properties in a group of three (temperature dependent) model parameters. The key assumpti is, that the superconductor is described by a single macroscopic wavefunction $\psi(\mathbf{r})$. which is nothing else than to the center-of-mass wavefunction of the pairs. The Ginzburg-Landau theory provides a simple method to calculate $\psi(\mathbf{r})$ in the presence of electromagnetic fields, sample boundaries, currents, etcetera. So we see, that while in previous sections we have

concentrated on w(ρ) under the condition that $\psi(\boldsymbol{r})$=*constant,* in the present chapter we will concentrate on the variations of $\psi(\boldsymbol{r})$ on length scales larger than the size of a Cooper pair. Since the Cooper pair wavefunction is described by w(ρ) we assume that w(ρ) effectively represents a point-particle and need not bother about the details of this function in the context of this chapter.

The basic postulate of GL theory is, that the amplitude $|\psi(\boldsymbol{r})|$ is small. Due to this restriction GL-theory can be expected to be quantitatively correct close to T_c. GL furthermore next write the free energy in form of a Taylor series expension of $\psi(\boldsymbol{r})$, and magnetic field $\boldsymbol{h}(\boldsymbol{r})$. Due to the smallness of $|\psi(\boldsymbol{r})|$, it is assumed that terms of order $|\psi(\boldsymbol{r})|^6$ and higher can be neglected. Based on these and other considerations they postulated that Helmholtz free energy has the following dependence on the phase and amplitude of $\psi(\boldsymbol{r})$

$$F_s = F_n + \int \left\{ \alpha |\psi(r)|^2 + \frac{\beta}{2} |\psi(r)|^4 + \frac{1}{2m} \left| \left(-i\hbar \nabla - \frac{2e}{c} \boldsymbol{A}(r) \right) \psi(r) \right|^2 + \frac{|\mathbf{h}(r)|^2}{8\pi} \right\} d^3 r \qquad (7.1)$$

where $\boldsymbol{h}(\boldsymbol{r}) = \nabla \times \boldsymbol{A}(\boldsymbol{r})$ is the microscopic magnetic field. The parameters α and β are model parameters, and they may vary as a function of temperature. In GL-theory the following temperature dependence is assumed:

$$\alpha(T) = -\alpha'(1 - T/T_c)$$

$$\beta(T) = \beta$$

$$(\alpha'>0;\ \beta>0) \qquad (7.2)$$

The basic idea of this free energy density is, that at every temperature the free energy must be minimal with respect to the fields $\psi(\boldsymbol{r})$ and $\boldsymbol{A}(\boldsymbol{r})$. This way the GL free energy has four adjustable parameters: α', T_c , β, and m.

VII.2 Temperature dependence of Ψ

If no fields and gradients are present, the last two terms of 4.1 are zero and $\psi(\boldsymbol{r}) = \psi_0$. In Fig. 7.1 a sketch is given of the free energy for $T>T_c$ and for $T<T_c$. Clearly a nontrivial equilibrium value of ψ_0 is only obtained for $T<T_c$. We can minize the free energy with respect to ψ_0 and obtain the so-called *superfluid density*

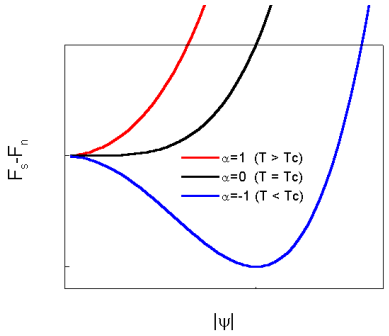
$$n_0 = |\psi_0|^2 = -\alpha/\beta = (\alpha'/\beta)(1 - T/T_c) \qquad (7.3)$$

The value of the free energy at temperature $T<T_c$ of a sample with volume V is then

$$F_s - F = -V\frac{\alpha'^2\left(1-T/T_c\right)^2}{2\beta} \qquad (7.4)$$

If an external magnetic field is applied, in first instance no field penetrates the bulk of the superconductor: The expulsion of the flux lines means that due to the presence of the superconducting sampe some extra work has to be done by the current generator when the field is switched on (or when the superconductor is cooled through the phase transition).

FIGURE 7.1



This amount of work is exactly $W = -V\int_0^H \mathbf{M(H')}\cdot\mathbf{dH'}$. Because in a type I superconductor $4\pi\mathbf{M}=-\mathbf{H}$, the extra energy stored in the magnetic field due to the presence of the superconductor is exactly $W = VH^2/8\pi$, where **H** is the external field. Hence the total free energy is

$$F_s = F_n - V\frac{\alpha'^2\left(1-T/T_c\right)^2}{2\beta} + V\frac{H^2}{8\pi} \qquad (7.5)$$

If the field H exceeds the critical value

$$H_c = -2\alpha\sqrt{\frac{\pi}{\beta}} = 2\alpha'\sqrt{\frac{\pi}{\beta}}\left(1-\frac{T}{T_c}\right) \qquad (T<T_c) \qquad (7.6)$$

it becomes energetically favourable to switch to the normal state: The energy advantage of the second term in Eq. 7.5 will be lost, but since the field can now penetrate the sample, the third term also disappears, offering a net energy saving for $H > H_c$. The field H_c is called the *thermodynamical* critical field. With this definition Eq. 7.5 can also be written as

$$F_s = F_n + V\frac{H^2 - H_c(T)^2}{8\pi} \qquad (7.7)$$

The specific heat is calculated from the free energy using $S(T) = -\partial F / \partial T$, and $c(T) = V^{-1} T dS / dT$, so that

$$c(T) = c_n(T) + \frac{\alpha'^2}{\beta}\frac{T}{T_c^{\,2}} \qquad (T<T_c)$$

$$c(T) = c_n(T) \qquad (T>T_c) \qquad (7.8)$$

The GL-model predicts, that the specific heat has a discontinuous jump at the phase transition, in good agreement with experimental observations on superconductors, and with the fact that the transition into the superconducting state is a *second* order phase transition.

VII.3 The Ginzburg-Landau equations

The GL-equations are obtained by minimizing the GL free energy, Eq. 7.1, with respect to the fields $\psi^*(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$:

$$\frac{\delta F_s}{\delta \psi^*(r)} = 0 \quad ; \quad \frac{\delta F_s}{\delta \mathbf{A}(r)} = 0$$

Here it is important that the functional derivatives with involve also the variation of derivatives of the fields. Since the free energy dependes on $\psi(\mathbf{r})$ as well as its gradient, we will need the following general property of functional derivatives:

$$\frac{\delta F_s}{\delta \psi(r)} = \frac{\partial F_s}{\partial \psi(r)} - \nabla \cdot \frac{\partial F_s}{\partial \nabla \psi(r)}$$

And the same for its complex conjugate. To make it easier to recognize the gradient of $\psi(\mathbf{r})$ in the free energy expressions, we use

$$\boldsymbol{\theta}(r) \equiv \nabla \psi(r)$$

With this definition the Ginzburg-Landau free energy reads

$$F_s = F_n + \int \left\{ \alpha \psi^*(r')\psi(r') + \frac{\beta}{2}\psi^*(r')^2 \psi(r')^2 \right\} d^3 r' +$$

$$+ \int \left\{ \frac{1}{2m}\left(-i\hbar\boldsymbol{\theta}(r') - \frac{2e}{c}\mathbf{A}(r')\psi(r') \right)\left(i\hbar\boldsymbol{\theta}^*(r') - \frac{2e}{c}\mathbf{A}(r')\psi^*(r') \right) + \frac{\mathbf{h}(r')\cdot\mathbf{h}(r')}{8\pi} \right\} d^3 r'$$

For the first Landau equation we begin by calculating the functional derivative

$$\frac{\delta F_s}{\delta \psi^*(r)} = \frac{\partial F_s}{\partial \psi^*(r)} - \nabla \cdot \frac{\partial F_s}{\partial \boldsymbol{\theta}^*(r)}$$

We obtain for the first and second term by straightforward differentiation

$$\frac{\partial F_s}{\partial \psi^*(r)} = \alpha\psi(r) + \beta\psi(r)^2\psi^*(r) + \frac{1}{2m}\left(-i\hbar\boldsymbol{\theta}(r) - \frac{2e}{c}\mathbf{A}(r')\psi r'\right)\left(-\frac{2e}{c}\mathbf{A}(r)\right)$$

$$\frac{\partial F_s}{\partial \boldsymbol{\theta}^*(r)} = \frac{1}{2m}\left(-i\hbar\boldsymbol{\theta}(r) - \frac{2e}{c}\mathbf{A}(r)\,\psi(r)\right)(i\hbar)$$

We combine these in expression for the functional derivitage and obtain by some re-arranging of terms

$$\frac{\delta F_s}{\delta \psi^*(r)} = \left\{\alpha + \beta|\psi(r)|^2\right\}\psi(r) + \frac{e}{mc}\mathbf{A}(r)\cdot\left(i\hbar\boldsymbol{\theta}(r) + \frac{2e}{c}\mathbf{A}(r)\,\psi(r)\right) - \frac{i\hbar}{2m}\nabla\cdot\left(-i\hbar\boldsymbol{\theta}(r) - \frac{2e}{c}\mathbf{A}(r)\,\psi(r)\right) =$$

$$= \left\{\alpha + \beta|\psi(r)|^2\right\}\psi(r) + \frac{1}{2m}\left\{-\frac{\hbar^2}{m}\nabla\cdot\nabla\psi(r) + \frac{4e^2}{c^2}|\mathbf{A}(r)|^2\psi(r) + i\frac{4e\hbar}{c}\mathbf{A}(r)\cdot\nabla\psi(r) + i\frac{2e\hbar}{c}\psi(r)\nabla\cdot\mathbf{A}(r)\right\} =$$

$$= \left\{\alpha + \beta|\psi(r)|^2 + \frac{1}{2m}\left[-i\hbar\nabla - \frac{2e}{c}\vec{A}(r)\right]\cdot\left[-i\hbar\nabla - \frac{2e}{c}\mathbf{A}(r)\right]\right\}\psi(r)$$

The condition $\delta F_s / \delta\psi^*(r) = 0$ then implies the first Ginzburg Landau equation:

$$\left\{\alpha + \beta|\psi(r)|^2 + \frac{1}{2m}\left[-i\hbar\nabla - \frac{2e}{c}\mathbf{A}(r)\right]^2\right\}\psi(r) = 0$$

The free energy depends both on **A**(r) and $\mathbf{h}(r) = \nabla\times\mathbf{A}(r)$. For the second Landau equation we therefore need the following property of functional derivatives:

$$\frac{\delta F_s}{\delta\mathbf{A}(r)} = \frac{\partial F_s}{\partial\mathbf{A}(r)} + \nabla\times\frac{\partial F_s}{\partial\nabla\times\mathbf{A}(r)}$$

We combine these terms in a single expression and obtain

$$\frac{\delta F_s}{\delta\mathbf{A}(r)} = \frac{1}{2m}\left(-\frac{2e}{c}\psi(r)\right)\left(i\hbar\boldsymbol{\theta}^*(r) - \frac{2e}{c}\mathbf{A}(r)\psi^*(r)\right) + \frac{1}{2m}\left(-i\hbar\boldsymbol{\theta}(r) - \frac{2e}{c}\mathbf{A}(r)\psi(r)\right)\left(-\frac{2e}{c}\psi^*(r)\right) + \frac{\nabla\times\mathbf{h}(r)}{4\pi}$$

On the righthand side of the second expression we can use Ampère's law. Since we consider here a steady state situation, there are no time-varying electric fields, hence $c\nabla\times\mathbf{h}(r) = 4\pi\,\mathbf{J}(r)$. After some re-arranging of terms

$$\frac{\delta F_s}{\delta\mathbf{A}(r)} = -\frac{ie\hbar}{mc}\psi(r)\nabla\psi^*(r) + \frac{2e^2}{mc^2}\mathbf{A}(r)|\psi(r)|^2 + \frac{ie\hbar}{mc}\psi^*(r)\nabla\psi(r) + \frac{2e^2}{mc^2}\mathbf{A}(r)|\psi(r)|^2 + \frac{1}{c}\mathbf{J}(r) =$$

$$= \frac{e}{mc}\psi^*(r)\left[i\hbar\nabla + \frac{2e}{c}\mathbf{A}(r)\right]\psi(r) + c.c. + \frac{1}{c}\mathbf{J}(r)$$

The condition $\delta F_s / \delta\mathbf{A}(r) = 0$ then implies the second Ginzburg Landau equation:

$$\frac{e}{m}\psi^*(r)\left[i\hbar\nabla+\frac{2e}{c}\mathbf{A}(r)\right]\psi(r)+c.c.+\mathbf{J}(r)=0$$

Thus we have obtained the first and second Ginzburg-Landau equations

$$\boxed{\begin{aligned}&\left\{\alpha+\beta|\psi(r)|^2+\frac{1}{2m}\left[\frac{\hbar}{i}\nabla-\frac{2e}{c}\mathbf{A}(r)\right]^2\right\}\psi(r)=0 \qquad \text{(a)}\\ &\mathbf{J}(r)\equiv(2e)|\psi(r)|^2\mathbf{v_s}(r)=\frac{e}{m}\psi^*(r)\left[\frac{\hbar}{i}\nabla-\frac{2e}{c}\mathbf{A}(r)\right]\psi(r)+c.c. \qquad \text{(b)}\end{aligned}} \qquad (7.9)$$

in the second equation we recognize the result for the microsopic model of a charged quantum fluid, which becomes the London equation (A16 of Appendox A) in the Meisner state of a superconductor.

VII.4 Relevant length-scales in GL-theory

Before we attack the coupled equations 7.9 for the fields **A*(r)*** and ***Ψ(r)***, we will first carry out an analysis of the relevant length scales of the problem. Using the definition of the superfluid density $n_0=|\psi_0|^2$ (Eq. 7.3) and combining 7.6 and 7.3

$$\boxed{\begin{aligned}\alpha&=-\frac{H_c^2}{4\pi n_0}\\ \beta&=\frac{H_c^2}{4\pi n_0^2}\end{aligned}} \qquad (7.10)$$

We devide left and righthand side of Eq. 7.9a by α, and substitute for α and β the expressions 4.10, with the result

$$\boxed{\left\{1-\frac{|\psi|^2}{n_0}-\frac{2\pi n_0\hbar^2}{mH_c^2}\left(-i\nabla-\frac{2e}{c\hbar}\boldsymbol{A}\right)^2\right\}\psi=0}$$

Since the operator ∇^2 has dimensions of inverse length squared, the factor multiplying it must have the dimension of length squared. This is one of the two important characteristic length scales, which we define as

$$\xi\equiv\sqrt{\frac{2\pi n_0\hbar^2}{mH_c^2}}$$

The so-called *coherence length, ξ,* is in principle a temperature dependent quantity, which diverges when the temperature approaches T_c, and $\xi=\infty$ in the normal state. A general rule of thumb is, that ξ is small, the higher the T_c of the material is.

A different combination of parameters provides the London penetration depth

$$\lambda^2 = \frac{mc^2}{4\pi n_0 (2e)^2}$$

discussed in chapter III. It represents the length scale on which magnetic fields decay inside the superconductor.

The dimensionless Ginzburg-Landau parameter

$$\boxed{\kappa = \frac{\lambda}{\xi}}$$

(7.11)

characterizes the superconductor by the ratio of the two relevant length scales. We will see in a later section, that for type II superconductors $\kappa > 0.7$, while for $\kappa < 0.7$ we expect a type I superconductor. We also observe, that close to the phase transition κ has no important temperature dependence, because β does not depend on temperature in the GL model.

It is easy to verify the following useful relation between λ, ξ, and H_c

$$\boxed{\sqrt{2}\xi\lambda H_c = \frac{\Phi_0}{2\pi}} \qquad (7.12)$$

stating that the product of two length scales and H_c is temperature independent, and in fact proportional to the f*lux quantum*

$$\boxed{\Phi_0 = \frac{hc}{2e}} = 2.0678\cdot 10^{-15} \text{ Weber} . \qquad (7.13)$$

The first and second Ginzburg-Landau equations are with these definitions

$$\boxed{\begin{aligned} &\left[1 - \frac{|\psi|^2}{n_0} + \xi^2 \left(\boldsymbol{\nabla} - i\frac{2\pi}{\Phi_0}\boldsymbol{A}\right)^2\right]\psi = 0 \qquad \text{(a)} \\ &\mathbf{J} = -\frac{c}{8\pi\, n_0 \lambda^2}\left\{\psi^*\left(\boldsymbol{A} + i\frac{\Phi_0}{2\pi}\boldsymbol{\nabla}\right)\psi + c.c.\right\} \qquad \text{(b)} \end{aligned}} \qquad (7.14)$$

The coherence length ξ characterizes the minimal length scale over which the superconducting order can vary. To verify this, we consider the situation that the vector-

potential is zero, and we take the limit where the order parameter variations are small compared to the average value: $\psi(\mathbf{r})= \psi_0\cdot(1+g(\mathbf{r}))$, and $|g(r)| << 1$. We can then expand the GL equations in $|g(r)|$. Keeping only the leading terms in the first GL equation, we obtain

$$2g(\boldsymbol{r}) = \xi^2 \Delta g(\boldsymbol{r})$$

with the solution in 1 dimension

$$g(\mathbf{x}) = g(0)\exp\left\{-\sqrt{2}\mathbf{x}/\xi(T)\right\}$$

We see, that the $2^{-1/2}\xi$ represents the exponential decay length of the superconducting order parameter.

As to the interpretation of the second length scale, λ, we apply a small magnetic field and assume that we can neglect the variations of ψ. The second GL equation, 7.14b, gives

$$\boxed{\mathbf{J} = -\frac{c}{4\pi\lambda^2}\mathbf{A}} \qquad (7.14c)$$

In a usual metal the current is proportional to the electric field E. Eq. 7.14c expresses the essence of superconductivity: Having current proportional to the vector potential implies that a static electrical current can flow with no physical field (E or B) acting on the electrons. A detailed discussion of the differences and correspondances between ordinary metals and superconductors is given in Appendix A.

With the help of Maxwell equation $\nabla\times\mathbf{h} = 4\pi c^{-1}\mathbf{J}$ (Eq. A3 of appendix A), the definition $\mathbf{h} = \nabla\times\mathbf{A}$, and the property $\nabla\times\nabla\times\mathbf{A} = -(\nabla\cdot\nabla)\mathbf{A}$ our expression relating **J** and **A** takes the simple form

$$(\nabla\cdot\nabla)\mathbf{A} = \frac{1}{\lambda^2}\mathbf{A}$$

The solution of this differential equation is an exponentially decaying field with decay length λ:

$$\mathbf{A} = \mathbf{A}_0 e^{-x/\lambda}$$

VII.5 Upper critical field

Let us now consider the situation where a magnetic field is applied. The effect is to suppress the order parameter ψ, until a field value is reached where ψ becomes suppressed altogether. Close to this critical field $|\psi/\psi_0|<<1$. Under those conditions we can expand the first GL equation in leading orders of ψ, and retain only the linear terms. So when ψ is small, Eq. 4.14a can be approximated in the following way

$$\left[1+\xi^2\left(\nabla - i\frac{2\pi}{\Phi_0}\boldsymbol{A}\right)^2\right]\psi = 0$$

In the limit of a uniform magnetic field along *z*, $A_x=Hy$, we obtain the wave equation

$$\left[1+\left(\xi\frac{\partial}{\partial x} - i\frac{2\pi\,\xi\,H}{\Phi_0}y\right)^2 + \xi^2\frac{\partial^2}{\partial y^2} + \xi^2\frac{\partial^2}{\partial z^2}\right]\psi = 0$$

Introducing dimensionless coordinates $u=x/\xi$, $v=y/\xi$, $w=z/\xi$ and substituting a shorthand notation for the term multiplying *y*: $\varphi \equiv \frac{2\pi\,\xi^2 H}{\Phi_0}$ we obtain

$$\left[1-\varphi^2\left(v+\frac{i}{\varphi}\frac{\partial}{\partial u}\right)^2 + \frac{\partial^2}{\partial v^2} + \frac{\partial^2}{\partial w^2}\right]\psi = 0 \qquad (7.15)$$

The fact that the operator multiplying ψ depends on the coordinate *v*, but not on *u* and *w*, suggest a solution which is a propagating wave of the *u* and *w* coordinate. Consequently we may anticipate that in general the solutions have the form

$$\psi(u,v,w) = V(v)e^{i\xi(k_x u + k_z w)}$$

Inserting in Eq. 4.15 provides

$$\left[1-\varphi^2\left(v-\frac{\xi k_x}{\varphi}\right)^2 + \frac{\partial^2}{\partial v^2} - k_z^2\xi^2\right]V(v) = 0$$

To simplify further we can make the following change of variables

$$s = \phi^{1/2}(v - v_0)$$

where $v_0 \equiv \frac{\xi k_x}{\varphi}$

Substituting this in the wave equation we obtain

$$\left[1-\varphi\left\{\left(\frac{\partial}{\partial s}+s\right)\left(\frac{\partial}{\partial s}-s\right)+1\right\} - k_z^2\xi^2\right]V(v) = 0$$

The operators in round brackets are hermitian conjugated and satisfy commutation relations

$$\sqrt{2}a^+ \equiv \frac{\partial}{\partial s} + s \quad ; \quad \sqrt{2}a \equiv \frac{\partial}{\partial s} - s \quad ; \quad aa^+ - a^+a = 1$$

Consequently a^+ and *a* are respectively raising- and lowering-operators. The wave equation becomes with this notation

$$\left[1-\varphi\left\{2a^+a+1\right\} - k_z^2\xi^2\right]V(v) = 0$$

Since a^+a is the number operator, and resubstiting the definition of φ, the eigenvalues of the wave-equation have to satisfy

$$\frac{2\pi\xi^2 H}{\Phi_0}(1+2n)+k_z^2\xi^2=1$$

Now the z-momentum can take any value, hence

$$k_z^2\xi^2 \in \{0,\infty\}$$

Consequently the magnetic field has an upper limit, given by

$$H < \frac{\Phi_0}{2\pi\xi^2(1+2n)}$$

The lowest eigenvalue has *n=0*, for which we write this condition as

$$\boxed{\begin{array}{l} H < H_{c2} \\ \text{where} \\ H_{c2} \equiv \dfrac{\Phi_0}{2\pi\xi^2} \end{array}} \qquad (7.16)$$

H_{c2} is called the 'upper critical field' of a type II superconductor. It corresponds to the lowest field which can penetrate the superconducting material uninhibited. Since for fields higher than H_{c2} there is no flux expulsion, the material has lost its superconducting properties for those fields. For $H > H_{c2}$ the material is therefore in the normal (as opposed to superconducting) state. Any field value lower than H_{c2} will be expelled, in part at least, by the superconductor.

Let us compare the upper critical field to the *thermodynamical* critical field. With the help of Eqs. 7.11, 7.12 and 7.16

$$\boxed{H_{c2} = \sqrt{2}\kappa H_c} \qquad (7.17)$$

We can now distinguish two types of superconductors:

(I) $H_{c2} < H_c$, equivalent to $\kappa < 1/\sqrt{2}$

(II) $H_{c2} > H_c$, equivalent to $\kappa > 1/\sqrt{2}$

VII.6 Type I superconductivity

Ad I: Consider a type I superconductor. Let us assume, that we are below T_c and that we have applied an external field H which is larger than H_c. Let us now gradually reduce the external field. When H drops below H_c all flux will be expelled from the superconductor. From now on, if we keep decreasing the external field, $\boldsymbol{h}$ will be zero in the interior of the

superconductor, and the criterion of Eq. 7.16 will never be reached. In fact is has been 'skipped' due to the fact that the external field is removed at once as soon as H drops below H_c. Hence H_{c2} is of no practical importance in a type I superconductor.

VII.7 Type II superconductivity

We begin with an external field H which is larger than H_{c2}. According to the criterion of Eq. 4.16 there is no superconductivity for $H>H_{c2}$. However, when the field becomes equal to H_{c2}, the criterion of Eq. 7.16 is satisfied, and the macroscopic wavefunction has a solution with a finite amplitude, corresponding to the cyclotronic motion of the paired charge carriers in the field $H=H_{c2}$. The cyclotron radius of a boson of charge e^* is $l_c=\Phi_0/2\pi H$, so that the condition that $H=H_{c2}$ corresponds exactly to the condition, that the coherence length matches exactly the cyclotron radius $l_c=\xi$. Since Eq. 7.15 is a linear differential equation, the amplitude of the cyclotronic wavefunction is arbitrary, implying that Ψ, which is zero for $H>H_{c2}$, could increase without bound as soon as H becomes smaller than H_{c2}. However, the actual GL equation is non-linear, causing $|\Psi|$ to increase continuously as a function of H for $H < H_{c2}$.

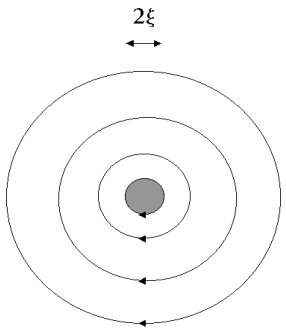


Figure 7.2

What happens when we apply an external field just below H_{c2} *?* The magnetic field is still almost homogenous and passing through the superconductor, but as the field is reduced below H_{c2} Cooper-pairs are progressively beginning to condense in a cyclotron

wavefunction $\psi(\boldsymbol{r})$ described by Eq. 7.15. The magnetic field distribution becomes progressively corrugated as the field is lowered, until at a certain moment regions of B=0 form. Eventually the situation becomes reversed, and most of the material has B=0, with "islands" of finite (but quantized) flux density. Ultimately, the last of these vortices disappears when the field passes below the lower critical field, H_{c1}.

We have seen above that, type-II behaviour in superconductors is characterized by the fact, that for fields H larger than H_{c1} magnetic flux partially penetrates the superconducting specimen in the form of tiny microscopic filaments, called vortices. Each vortex carries a magnetic flux $\Phi_0 = \frac{hc}{2e} = 2.067 \cdot 10^{-15}$ Weber. The magnetic induction inside the superconductor is directly related to n, the number of vortices per unit area, $B = n\Phi_0$.

Let us now explore some of the properties of a vortex. In Fig. 7.2 a sketch is given of a top view on a vortex line. Physically a vortex corresponds to a whirlwind of supercurrents, circling around a region which is in the normal state (even though the temperature is below T_c). This phenomenon is somewhat analogous to a tornado or a hurricane, and to whirls, which occur under certain conditions in fast flowing water. An important difference is, that, of course, hurricanes and waterwhirls are not quantized, they are classical phenomena. The central part of the vortex, which is in the normal state, is called the 'vortex core'. The diameter of this region is usually small (2-5 nm in high T_c superconductors, a micrometer in very clean low T_c superconductors).

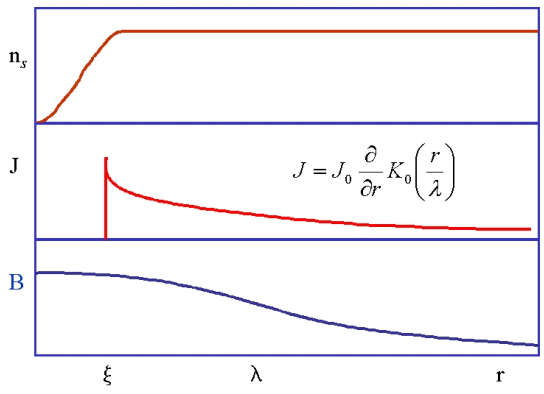


Figure 7.3

In Fig. 7.3 we also indicate the current, field, and superfluid density distribution as a function of distance with respect to the center of the vortex. In the sketch it is shown, that the scale on which the superfluid density is recovered is the so-called 'coherence length', ξ. The current density approaches zero at large distances, and increases as a function of decreasing distance from the vortex core. At the boundary of the vortex core, the current density has reached the critical value. The magnetic field has its maximal value in the center of the vortex core. Both J and B decay on a lengthscale larger than the coherence length, called the London penetration depth, λ.

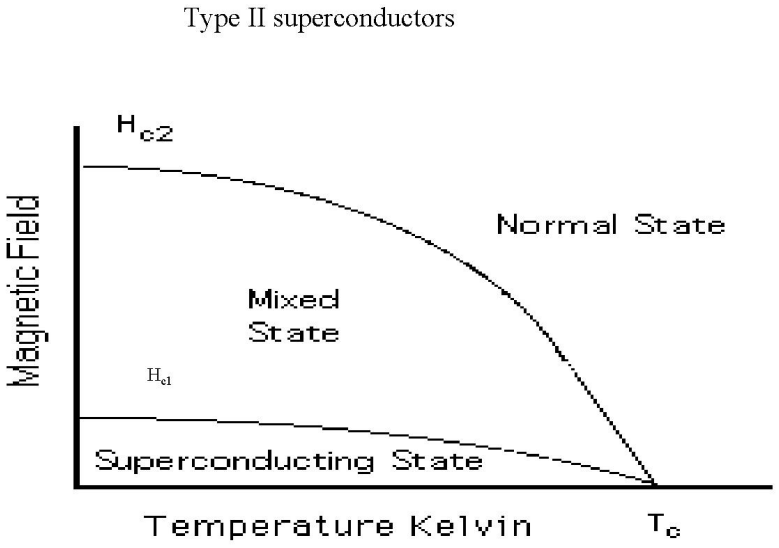


Figure 7.4

For a sufficiently low external field type II superconductors exhibit the Meisner effect, just like in type I superconductor. The corresponding phase diagram is sketched in Fig. 7.4 This happens for an external field smaller than the *lower critical field,* H_{c1}: If we cool down below T_c, and subsequently increase the external field, H_{c1} corresponds to the external field value where the first isolated vortex forms. A crude estimate of H_{c1} can be made as follows (see fig. 7.5) : From general principles the condensation energy is $E_{cond} = -\int M(H)dH$ (in a type I superconductor, because $M=-H/4\pi$, this quantity is $H_c^2/8\pi$). In a type II superconductor $M=-H/4\pi$ for fields upto H_{c1} only, after which the magnetization decays

until it reaches $M(H_{c2})=0$ at the upper critical field. The area under the magnetization curve in the mixed state ($H_{c1}<H<H_{c2}$) is crudely speaking a triangle. The integral over the magnetization triangle of the mixed state region is therefor approximately $\{-H_{c1}/4\pi\}*\{H_{c2}-H_{c1}\}*0.5$. For an extreme type II superconductor $H_{c1}<<H_{c2}$, hence, $-\int M(H)dH \sim H_{c2}H_{c1}/8\pi$. Hence we see, that based on a crude estimation of the magnetization curve we expect that in an extreme type II superconductor $H_c^2 \sim H_{c2}H_{c1}$. Hence, together with properties, Eq. 7.12 and 7.17, we expect that $H_{c1} \sim \Phi_0 / (4\pi\lambda^2)$.

Les paramètres nécessaires sont manquants ou erronés.

Figure 7.5: Magnetization curve of type II superconductor. The linearized behaviour for $H_{c1} < H < H_{c2}$ is an idealization of the true (non-linear) field dependence.

A more precise estimate of H_{c1} can be made using the GL equations, from which the GL free-energy of a vortex can be calculated. This is a lenghty calculation. For a more detailed discussion, we refer to "Introduction to superconductivity" by Tinkham. The calculation is done along the following steps: When the density of vortices, n, is low, the interaction energy between vortices can be neglected, and the energy of formation is nLu_v, where Lu_v is the energy of forming an isolated vortex, and L is the length of the vortex. As each vortex carries a magnetic flux Φ_0, the macroscopic (average) magnetic flux density, B, inside the superconductor is $B=n\Phi_0$. When the external field H is held constant (rather than the fluxdensity B), we should subtract the work done by the generator of the external field from the Helmholtz free energy. This is called the Gibbs free energy

$$G = E_{core} + E_{kin} + \frac{1}{8\pi}\int |h(r)|^2 d^3r - \int Hh(r)d^3r$$

This thermodynamical quantity should be minimized under equilibrium conditions. The first two terms are kinetic energy of the circulation currents, and the condensation energy of the core region. From the previous discussion, we already know that the microscopic flux density around a vortex decreased exponentially where λ is the *1/e* length.. Because the integrated flux density correspond to the flux quantum, Φ_0, the detailed dependence on space coordinate must be $h(r)=\Phi_0 e^{-r/\lambda}/(2\pi\lambda^2)$. To calculate the kinetic energy we also need to know the dependence on space coordinate of $J(r)$. Here we can use Ampere's law

$(4\pi/c)J(r)=\nabla\times h(r)$, we obtain immediately, that $(4\pi/c)|J(r)| = |h(r)|/\lambda$. For the details of this calculation I refer to the book of Tinkham. For the free energy difference between mixed and Meissner state one obtains then

$$G_{mixed} - G_{Meissner} = nL\left(\frac{\Phi_0}{4\pi\lambda}\right)^2 \ln\kappa - nLH\Phi_0$$

The factor $\ln\kappa$ in the first term is a result of including the energy of the core region. The lower critical field is the value of H for which $G_{mixed} < G_{Meissner}$.This requires, that $H > H_{c1}$, where

$$H_{c1} = \frac{\Phi_0}{4\pi\lambda^2}\ln\kappa$$

We can combine this with the expression relating H_c and H_{c2} (Eq. 7.17), and obtain

$$\boxed{\frac{H_{c1}H_{c2}}{H_c^{\,2}} = \ln\kappa}$$

Typically κ~10-1000 in a type II superconductor, hence $\ln\kappa$~3-7. We see, that having a high upper critical field, implies that the lower critical field is small.

Chapter VIII: Capita selecta of advanced subjects in superconductivity

VIII.1: The gap equation of unconventional superconductivity:

Let us take a look at the gap equation.

$$\Delta_k = -\sum_{k'} \frac{V_{k,l}\Delta_l}{2E_l} \tanh\left(\frac{E_l}{2k_BT}\right) \tag{8.1}$$

If Δ_k is independend of k, and $V_{k,l} > 0$, this equation has no solution other than the trivial one (i.e. $\Delta=0$). Things change Δ_k depends on k. We may expect this to happen when the interaction potential V_{kl} varies strongly as a function of momentum. We have encountered this when we discussed the pairing interaction mediated by paramagnetic fluctuations in section III.5. The interaction which we discussed in that section was strongly peaked around $k-l=(\pi, \pi)$. Note that in this example we have in mind a 2-dimensional strongly interacting electron system such as the high T_c cuprates. We approximate V_{kl} resulting from the magnetic susceptibility as a frequency independent potential within a shell of width J around the Fermi energy

$$\begin{aligned} V_{k,l} &= U - 2V_0 \cdot \cos(k_x - l_x) \cdot \cos(k_y - l_y) \qquad (\xi_k^2 < J^2; \xi_l^2 < J^2) \\ V_{k,l} &= U \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{(otherwise)} \end{aligned} \tag{8.2}$$

Note that for $k-l=(\pi,\pi)$ the interaction has its maximum valule: $V_{kl}=U+2V_0$. We write the k-dependent term as a sum over 4 terms in "separable" form

$$\begin{aligned} V_{kl} &= U - V_0\left(\cos k_x + \cos k_y\right)\left(\cos l_x + \cos l_y\right) \\ &- V_0\left(\cos k_x - \cos k_y\right)\left(\cos l_x - \cos l_y\right) \\ &- 2V_0 \sin k_x \sin l_x - 2V_0 \sin k_y \sin l_y \end{aligned} \tag{8.3}$$

For an interaction of the form

$$V_{k,l} = -V_0 g_k g_l \tag{8.4}$$

the BCS gap equation is

$$\Delta_k = V_0 g_k \sum_l \frac{g_l \Delta_l}{2\sqrt{\xi_l^{\,2} + g_l^{\,2}\Delta_0^{\,2}}} \tanh\left(\frac{\sqrt{\xi_l^{\,2} + \Delta_l^{\,2}}}{2k_BT}\right) \tag{8.5}$$

Since the summation on the righthand side of the expression is independend of k, we see that the momentum dependence of the gap function is entirely given by g_k:

$$\Delta_k = \Delta_0 g_k \tag{8.6}$$

where the constant Δ_0 is solved selfconsistently by inserting Eq. (8.6) in (8.5)

$$\Delta_0 \equiv V_0 \sum_l \frac{g_l \Delta_l}{2El} \tanh\left(\frac{\sqrt{\xi_l^{\,2} + \Delta_l^{\,2}}}{2k_B T} \right) \tag{8.7}$$

This way we arrive at the self-consistent expression for Δ_0

$$1 = V_0 \sum_l \frac{g_l^{\,2}}{2\sqrt{\xi_l^{\,2} + g_l^{\,2}\Delta_0^{\,2}}} \tanh\left(\frac{\sqrt{\xi_l^{\,2} + g_l^{\,2}\Delta_0^{\,2}}}{2k_B T} \right) \tag{8.8}$$

Usually one has to solve this equation numerically. The trick is to calculate T_c for each of the pairing channels constituted by the separable interaction terms of Eq. (8.3). One of the T_c's will have the value, and since all order parameters are zero at this temperature, the gap-equation is indeed of the form (8.7) with g_k representing to the "dominant" pairing channel (i.e. the pairing-symmetry with the highest T_c). For lower temperatures additional gaps may open, and the problem of coupled gap-equations needs to be addressed, a problem which we will not treat here.

The most important conclusion is, that a non-trivial solution of the gap-equation can be found, even resulting from a repulsive interaction such as the spin-fluctuation mediated pairing in the singlet channel. For the high T_c cuprates the dominant pairing channel turns out to be the third term of Eq. (8.3)

$$V_{kk'} = -V_0 \left(\cos k_x - \cos k_y\right)\left(\cos l_x - \cos l_y\right)$$

The resulting gapfunction has the form

$$\Delta_k = \Delta_0 \left(\cos k_x - \cos k_y\right)$$

which has regions of opposite sign around the Fermi surface, separated by nodes for the directions $k_x = \pm k_y$. The fact that nodes are present in the gap-function implies that also the wavefunction describing the relative motion of quasiparticles forming a Cooper pair have wavefunctions with nodes. In the example above, this would imply that the orbital momentum of the Cooperpairs is L=2. This is called "d-wave pairing".

Spin and orbital quantum numbers of Cooper pairs

In case that spin-orbit interaction is zero, the quasiparticle energies obey the following symmetry: $\xi_{k\uparrow} = \xi_{-k\uparrow} = \xi_{-k\downarrow} = \xi_{k\downarrow}$. If the orbital momentum of the Cooperpairs is either L=0, or L=2, the wavefunction has even symmetry for its orbital part, while the spin-part must be odd. Odd symmetry of the spin coordinates implies S=0. For the gap-function this implies that it obeys the symmetry relation $\Delta_k = \Delta_{-k}$. Examples:

Pb, Al, Nb, MgB_2: **L=0, S=0**

$La_{2-x}Ba_xCuO_4$, $YBa_2Cu_3O_7$: **L=2, S=0** *(J.R.Kirtley, C. Tsuei, Nature 373, 225 (1995))*

$CeCoIn_5$: L=2, S=0 *(W. K. Park et al, Phys. Rev. Lett. 100, 177001 (2008))*

In the previous discussion we arrived at the conclusion that spin-fluctuation mediated paring leads to d-wave (L=2, S=0) pairing. This was obtained for a spin-susceptibility which is characteristic of a metal close to an anti-ferromagnetic instability. If the metal is close to a Ferro-magnetic instability, similar arguments can be used to show that p-wave (L=1, S=1) pairing is favored. If the orbital momentum of the Cooperpairs is L=1, or L=3, etc, the wavefunction has odd symmetry for its orbital part, while the spin-part must be even. Even symmetry of the spin coordinates implies S=1. For the gap-function this implies that it obeys the symmetry relation $\Delta_k = -\Delta_{-k}$. These properties can be easily verified from the gap equation and the Cooperpair wavefunction (Eq. 4.8 or 4.9). Experiments to test for orbital and spin quantum numbers are difficult, and often several experimental techniques need to be combined in order to obtain conclusive evidence.

Some famous examples where such tests have been carried out are:

Superfluid ^3He: **L=1, S=1**

(A. J. Leggett, Rev. Mod. Phys. 47, 331-414 (1975))

Sr_2RuO_4: **L=1, S=1**

(D.F. Agterberg, T.M. Rice and M. Sigrist, Phys. Rev. Lett. 78, 3374 (1997))

VIII.2 The Anderson-Higgs mechanism

Previously we have pointed out, that the only terms that matter for the groundstate in

$$H^i = \sum_q \sum_{k,l,\sigma,\sigma'} V_{kl} c^\dagger_{k+q,\sigma} c^\dagger_{-k+q,\sigma'} c_{-l+q,\sigma'} c_{l+q,\sigma} \qquad (8.9)$$

are those for which q=0. This is because in $|\Psi_0\rangle$ the electron creation operators only occur in the combination $c^\dagger_{p\uparrow} c^\dagger_{-p\downarrow}$. In the BCS model it is assumed, that the excitations do not carry the superconductor far from the groundstate, so that also for the excited states the only relevant terms are those for which q=0.

A few years after the BCS theory was published, P.W. Anderson explored the consequences of the full interaction hamiltonian, which resulted in the prediction of novel collective excitations with a mass gap. This model was later applied in elementary particle physics to predict the existance of a novel elementary particle, the Higgs boson, with a finite mass, and to explain the fact, that the $W^{+/-}$ and Z bosons have a finite mass.

However, usually in elementary treatments of superconductivity phase-fluctuations, and coupling of phase-fluctuations to the EM-field are ignored. For many practical purposes this is OK. For example, the tunneling spectra and specific heat can usually be calculated reliably using the so-called reduced Hamiltonion (q=0 in the equation above), at least for most superconductors with a low T_c.

Theory of Superconductivity	**Theory of weak nuclear interactions**
Spontaneous symmetry breaking of the pairing-amplitude field	Spontaneous symmetry breaking of the Higgs field
Gap amplitude $\|\Delta\|^2$ is proportional to the density of Cooper-pairs	Finite amplitude of the Higgs field corresponds to the mass of the Higgs-boson
Macroscopic phase fluctuations: $\phi(r,t)$	Fluctuations of the phase of the Higgs-field
Coupling of macroscopic phase, $\phi(r,t)$, to the EM-field: $\phi(r,t) + \frac{2e}{\hbar c}\int_0^r A(r',t)dr'$	Coupling of the phase of the Higgs-field to the $W^{+/-}$ and Z gauge fields
Coupling of $\phi(r,t)$ to the EM-field causes a gap in the photon-dispersion relation of photons travelling inside a superconductor.	This coupling causes a gap in the $W^{+/-}$ and Z excitations, which corresponds to the finite mass of the $W^{+/-}$ and Z bosons.

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Shaker Publishing, Oktober 2000, ISBN 90-423-0128-7

Appendix A: Electrodynamics of superconductors in the quasi-static limit

In this section we will show, that the characteristic properties of superconductors can not be explained from classical electrodynamics of solids. For this purpose we will need Maxwell's equations in solids, summarized in Boxes I and II.

The starting points are the following:

- We will assume that the electric and magnetic fields are quasi-stationary, *i.e.*, that the external electromagnetic fields are either constant, or vary only linearly as a function of time: $\mathbf{D}(t) = \mathbf{D}_0 + \dot{\mathbf{D}} * (t - t_0)$, ***etc***. As a result

  $\partial^2 \mathbf{D} / \partial t^2 = 0$, $\partial^2 \mathbf{h} / \partial t^2 = 0$, etc. for a quasi-stationary field (A1)

- $\mathbf{b} = \mathbf{h}$ (absence of magnetization **m** in microscopic description of SC) (A2)

- $\nabla \times \mathbf{h} - \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t} = \frac{4\pi}{c}\mathbf{J}$ (Ampere's law) (A3)

- $\nabla \times \mathbf{E} + \frac{1}{c}\frac{\partial \mathbf{h}}{\partial t} = 0$ (Faraday's law) (A4)

- $\nabla \bullet \mathbf{h} = 0$ (A5)

- The current density in a solid is the product of the charge, the density, and the (drift) velocity of the charge carriers: **J** = -e n **v**. (A6)

- $\vec{\nabla} \times \left(\vec{\nabla} \times \mathbf{G}\right) = -\left(\vec{\nabla} \bullet \vec{\nabla}\right)\mathbf{G} + \vec{\nabla}\left(\vec{\nabla} \bullet \mathbf{G}\right)$ (A7)

Let us consider an ideal conductor, with no dissipation. If we apply an electric field, each of the electrons in the conductor will be accelerated according to Newton's law:

$$\frac{d}{dt}\mathbf{v} = -\frac{e}{m}\mathbf{E} \Rightarrow \boxed{\frac{\partial}{\partial t}\mathbf{J} = \frac{ne^2}{m}\mathbf{E}} \quad \text{(A8)}$$

As we are going to use Ampere's law to substitue **J** with the fields **h** and **D**, and Faraday's law to substitute **E** with **h**, we first have to take the curl of both sides of the expression:

$$\nabla \times \frac{\partial}{\partial t}\mathbf{J} = \frac{ne^2}{m}\nabla \times \mathbf{E} \quad \text{(A9)}$$

This, after substitution with Amperes and Faradays law becomes:

$$\nabla \times \left(\nabla \times \frac{\partial}{\partial t}\mathbf{h} - \frac{1}{c}\frac{\partial^2}{\partial t^2}\mathbf{D} \right) = -\frac{4\pi ne^2}{mc^2}\frac{\partial}{\partial t}\mathbf{h} \quad \text{(A10)}$$

Because we are only considering quasi-stationary fields here, $d^2\boldsymbol{D} / dt^2 = 0$ in this case. Using further the properties of vector operators, and the fact that no magnetic monopoles

are present, we obtain as a final result a differential equation for the magnetic field distribution of a superconductor

$$(\nabla \bullet \nabla)\frac{\partial}{\partial t}\mathbf{h} = \frac{4\pi n e^2}{mc^2}\frac{\partial}{\partial t}\mathbf{h} \qquad \text{(Field in a perfect conductor)} \qquad \text{(A11)}$$

If we place a sample with a flat surface perpendicular to a uniform external field parallel to the z-axis, and we ramp up the field linearly as a function of time, eq. A11 tells us that outside the superconductor (z<0), where *n=0*, dh_z/dt is independent of the position *z*. Inside the superconductor (z>0) , the field drops exponentially to zero on a length scale λ_L , the so-called *London penetration depth*:

$$\begin{aligned} &\frac{\partial}{\partial t}h_z = \frac{\partial}{\partial t}H_{ext,z} && (z<0) \\ &\frac{\partial}{\partial t}h_z = \frac{\partial}{\partial t}H_{ext,z}e^{-z/\lambda_L} && (z>0) \\ &\lambda_L{}^2 = \frac{mc^2}{4\pi n e^2} \end{aligned} \qquad \text{(A12)}$$

This implies, that deep inside the superconductor ($z>>\lambda_L$) $d\boldsymbol{h}/dt = 0$. On the other hand, the Meissner effect requires that deep inside the superconductor $\boldsymbol{h}=0$. This condition would be satisfied satisfied if

$$\boxed{(\nabla \bullet \nabla)\mathbf{h} = \frac{4\pi n e^2}{mc^2}\mathbf{h}} \qquad \text{(Field inside a superconductor)} \qquad \text{(A13)}$$

Apparently, the Meissner effect requires a different ingredient, not already contained in the classical description of electromagnetic fields coupled to a dissipationless charged fluid. The fact that flux quantisation is observed in quanta which require Planck's constant suggests, that the additional ingredient required for the description of superconductivity and the Meissner-effect, is quantum-mechanics. To make this more explicit requires that we return to Maxwell's equations. We can substitute Faraday's law (Eq. A4) in Eq. A9, and obtain for the quasi-stationary field in a perfect conductor

$$\boxed{\frac{\partial}{\partial t}\mathbf{h} = -\frac{mc}{ne^2}\nabla \times \frac{\partial}{\partial t}\mathbf{J}} \qquad \text{(Maxwell)} \qquad \text{(A14)}$$

For a superconductor it is required, that the same expression holds for stationary field in a superconductor. This was postulated by the London-brothers:

$$\boxed{\mathbf{h} = -\frac{mc}{ne^2}\nabla \times \mathbf{J}} \qquad \text{(London-equation)} \qquad \text{(A15)}$$

Using the fact, that the magnetic field is the curl of the vector potential, $h = \nabla \times A$, we can write the London equation in the form

$$\boxed{\mathbf{J} = -\frac{ne^2}{mc}\mathbf{A}} \qquad \text{(London-equation)} \qquad \text{(A16)}$$

Usually the vector potential A is determined apart from choice of gauge: Adding an arbitrary term of the form $\vec{\nabla} g$ to A does not influence the field ***h***, because $\vec{\nabla} \times \vec{\nabla} g = \vec{0}$. Since also the current on the left hand side of A16 is gauge-independent, Eq. A16 represents a particular choice of gauge for the vector potential A, the so-called "London gauge". In a steady-state situation the charge distribution is constant as a function of time. The condition of continuity ($\partial\rho / \partial t + \nabla \cdot J = 0$) then implies that $\nabla \cdot J = 0$. Consequently $\nabla \cdot A = 0$ in the London gauge, and the normal component of A at a sample surface vanishes. Eq. A16 is reminiscent of Ohm's law

$$\boxed{\mathbf{J} = \sigma \quad \mathbf{E}} \qquad \text{(Ohm's law)} \qquad \text{(A17)}$$

with the difference that Ohm's law expresses a dissipative current response to a Coulomb potential, while the linear relation between current and vector potential expresses a dispersive electrical response to a vector potential. Up to this point, the London equation emerges 'out of the blue'. Although it can be regarded as a very economical way to describe the phenomenology of the electromagnetic properties of quasi-stationary fields and static fields in superconductors, we would like to understand a little better the microscopic foundation. In fact, we are already rather close to a microscopic description. Let us take a closer look at Eq. A16. This expresion appears to tell us, that the electrons behave collectively like a single electron in a vector potential. Quantum mechanics tells that the effect of applying a vector potential ***A***, while the magnetic field $B = \nabla \times A = 0$, to a particle of charge 2e is equivalent to making a transformation (Appendix D)

$$\boxed{\begin{array}{l}\nabla \to \nabla - \dfrac{i2e}{\hbar c}\mathbf{A}(\mathrm{r},\mathrm{t}) \\ \text{and} \\ \psi(\mathrm{r},t) \to e^{i\eta(\mathrm{r},t)}\psi(\mathrm{r},t) \\ \text{where} \\ \eta(\mathrm{r},t) = \dfrac{2e}{\hbar c}\int_0^{\mathrm{r}} \mathbf{A}(\mathrm{r}',t)\cdot \mathrm{d}\mathbf{r}'\end{array}} \qquad \text{(A18)}$$

and to substitute the transformed ψ and ∇ quantities in the Schrödinger equation. The integral corresponds to **B**=0 along the trajectories: Differentiating both sides of the last equation of A18 we have $q\mathbf{A} = \hbar c\nabla\eta$, hence $q\mathbf{B} = \hbar c\nabla\times\nabla\eta$, which implies that **B**=0. Another way to understand this, is to consider a strip without holes. The integral along two different paths, labeled 1 and 2, is

$$\int_1 \mathbf{A}(\mathbf{r}',t)\bullet \mathrm{d}\mathbf{r}' - \int_2 \mathbf{A}(\mathbf{r}',t)\bullet \mathrm{d}\mathbf{r}' = \oint \mathbf{A}(\mathbf{r}',t)\bullet \mathrm{d}\mathbf{r}' = \int_S \nabla\times\mathbf{A}(\mathbf{r}',t)\bullet d\mathbf{S} = \Phi \qquad \text{(A19)}$$

Thus only if B=0 in this strip will the phase factor η be independent of the choice of path in the line integral. Such an independence is required, in order to ascertain that the wave function is single-valued.

We will see later, that in a superconductor the current is carried by *pairs* of electrons, with charge *2e,* mass *2m*, and with a density *n/2*. The ∇ operator corresponds to the momentum of a particle, which is proportional to the velocity. When applied to a *pair* of electrons, Eq. A18 corresponds to the velocity transformation

$$\mathbf{v} \to \mathbf{v} + \frac{(2e)}{(2m)c}\mathbf{A}$$

Consider a superconductor in equilibrium, with no vector potential present. In this situation, the drift velocity of the charge carriers is zero. If we now switch on the vector potential **A**, the velocity of the charged fluid becomes *(e/mc)***A**, and the current density becomes

$$\mathbf{J} = -\frac{(n/2)(2e)^2}{(2m)c}\mathbf{A} = -\frac{ne^2}{mc}\mathbf{A}$$

in the presence of the vector potential. This is just the London equation, so we see that the London equation expresses the fact that the electrons form a quantum fluid on a macroscopic scale.

Appendix B

Maxwell's equations in solids

The best book on this subject is *Classical Electrodynamics* by J. D. Jackson (Wiley, 1962, 1975).

Maxwell's equations are

$$\nabla \bullet D = 4\pi\rho \qquad \textit{Coulomb} \qquad (1)$$

$$\nabla \times H - \frac{1}{c}\frac{\partial D}{\partial t} = \frac{4\pi}{c} J \qquad \textit{Ampere} \qquad (2)$$

$$\nabla \times E + \frac{1}{c}\frac{\partial B}{\partial t} = 0 \qquad \textit{Faraday} \qquad (3)$$

$$\nabla \bullet B = 0 \qquad \textit{no monopoles} \qquad (4)$$

where **E** and **B** are the avaraged **E** and **B** of the microscopic, or vacuum, Maxwell equations. The quantities **D** and **H**, usually called the electric displacement and magnetic field (**B** is called the magnetic induction), have components given by

$$D_\alpha = E_\alpha + 4\pi\left(P_\alpha + ...\right) \qquad (5)$$

$$H_\alpha = B_\alpha - 4\pi\left(M_\alpha + ...\right) \qquad (6)$$

The quantities ***P***, ***M***, and similar higher order objects represent the macroscopically averaged electric dipole, magnetic dipole, and higher moment densities of the material in the presence of applied fields. Similarly the charge and current densities $\rho=\rho_{ext}+\rho_i$ and $J=J_{ext}+J_i$ are macroscopic averages of the external and internal charges and currents, and the charges and currents and densities in the medium. Bound charges and currents appear in the equations via ***P*** and ***M***. (However, the distinction between bound and free charge and current in a solid is somewhat arbitrary, allowing different and equally correct definitions of the fields ***D*** and ***H***, see **Appendix C**). The electromagnetic force on a charged particle moving in a dielectric and diamagnetic medium are controlled by ***E*** and ***B***

$$\boldsymbol{F=q(E+c^{-1}v\times B)}$$

Together, Eqs. 1 and 2 imply that ***D*** and ***H*** are controlled by the free charges and currents. So if no free charges and currents are present in the solid, ***D*** and ***H*** correspond exactly to the electric and magnetic field set up by the external charge and current sources, e.g. the fields produced by a lightsource and/or an external electromagnet.

Appendix C
Gauge transformations in electromagnetism

There exists a freedom of definition in this set of equations allowing us to inteprete a net magnetization as a surface current. This becomes clear, when we insert Eq. (6) in Eq. (2) of Box I. The current consists of an external contribution, i.e. a current source placed somewhere outside the sample, and currents inside the sample or at the sample surface. In the following discussion it is useful to make this distinction explicit by writing $J = J_{ext} + J_i$. We then obtain Ampere's law in a slightly modified form:

$$\nabla \times B - \frac{1}{c}\frac{\partial D}{\partial t} = \frac{4\pi}{c}\left(J_{ext} + J_i + c\nabla \times M\right)$$

We see, that Ampere's law is invariant under the transformation of the internal quantities

$$J_i = \tilde{J}_i - c\nabla \times M'$$
$$M = \tilde{M} + M'$$

Hence, a space-varying magnetic field can be represented by an electrical current. In particular a current flowing at the surface of the sample can be represented by a net magnetization inside the material. In the special case of a superconductor, the Meissner effect is represented in two different ways.

(i) When describing the superconductor on a *macroscopic* scale, the absence of magnetic field deep inside the superconductor is ascribed to a net macroscopic magnetization $\mathbf{M} = -\mathbf{H}/4\pi$, causing the total macroscopic field, $\mathbf{B} = \mathbf{H}+4\pi\mathbf{M}$ to vanish. This corresponds to assuming that the surface currents are described completely by $\boldsymbol{J}_i = -c\,\nabla\times\boldsymbol{M}$, and that $\tilde{J}_i = 0$. With this choice of gauge

$$\nabla \times B - \frac{1}{c}\frac{\partial D}{\partial t} = \frac{4\pi}{c}\left(J_{ext} + c\nabla \times \tilde{M}\right)$$

(ii) When describing the superconductor on a *microscopic* scale, one realizes that microscopically no magnetic moments are involved (the situation is quite different in ferromagnet, where a magnetic polarization is generated by the gyromagnetic moments of the electron-spins): The net magnetization in a superconductor is entirely due to the surface currents. In this case one writes $\tilde{M} = 0$, so that $J_i = \tilde{J}_i$ in the transformation. With this choice of gauge

$$\nabla \times B - \frac{1}{c}\frac{\partial D}{\partial t} = \frac{4\pi}{c}\left(J_{ext} + \tilde{J}_i\right)$$

The magnetic flux density has a strong dependence on spacial coordinates. In textbooks on superconductivity the lowercase symbol **h** is reserved to describe the magnetic fluxdensity on a microscopic scale *i.e.* to describe the field variations in and around vortices, surface layers, etcetera.. Hence **h** satisfies the relation $\nabla\bullet\boldsymbol{h} = 0$, and **h** is described by a the vector potential **A**: $\mathbf{h}=\nabla\times\mathrm{A}$. The macroscopic flux

density ***B*** is the average value of **h** over a suitably chosen length scale (typically the penetration depth). Deep inside the superconductor **h = B** = **0.** Near the surface boundary $\mathbf{J}_i = c\nabla\times\mathbf{h}/4\pi$. The relevant electromagnetic equations for a superconductor are

No distinction between **b** and **h** on a microscopic scale		(1)
$\nabla\times\mathbf{h}-\frac{1}{c}\frac{\partial\mathbf{D}}{\partial t}=\frac{4\pi}{c}\mathbf{J}$	**(Ampere)**	(2)
$\nabla\times\mathbf{E}+\frac{1}{c}\frac{\partial\mathbf{h}}{\partial t}=0$	**(Faraday)**	(3)
$\nabla\bullet\mathbf{h}=0$	**(no monopoles)**	(4)

Appendix D
Charged quantum particle in an electromagnetic field

We want to verify, that

$$-\frac{\hbar^2}{2m}\widetilde{\nabla}\cdot\widetilde{\nabla}\,\widetilde{\psi}(\mathrm{r},t)+V(r)\widetilde{\psi}(\mathrm{r},t)=E\widetilde{\psi}(\mathrm{r},t)$$

where

$$\widetilde{\nabla}=\nabla-\frac{i2e}{\hbar c}\mathbf{A}(r,t),\ \ \widetilde{\psi}(\mathrm{r},t)=e^{i\eta(\mathrm{r},t)}\psi(\mathrm{r},t),$$

and

$$\eta(\mathrm{r},t)=\frac{2e}{\hbar c}\int_0^{\mathrm{r}}\mathbf{A}(\mathrm{r}',t)\bullet\mathrm{d}\mathbf{r}'.$$

By differentiating in parts we can show that

$$\widetilde{\nabla}\,\widetilde{\psi}(\mathrm{r},t)=e^{i\eta}\nabla\psi(\mathrm{r},t),$$

and subsequently that

$$\widetilde{\nabla}\cdot\widetilde{\nabla}\,\widetilde{\psi}(\mathrm{r},t)=e^{i\eta}\nabla\cdot\nabla\psi(\mathrm{r},t).$$

The transformed Schrodinger equation

$$-\frac{\hbar^2}{2m}\widetilde{\nabla}\cdot\widetilde{\nabla}\,\widetilde{\psi}+V(r)\widetilde{\psi}=E\widetilde{\psi}$$

then reduces to

$$-\frac{\hbar^2}{2m}e^{i\eta}\nabla\cdot\nabla\psi+V(r)e^{i\eta}\psi=Ee^{i\eta}\psi.$$

Since the phase factor $e^{i\eta}$ is a scalar, it can be devided out from both sides of the expression, from which results the original –untransformed- Schrodinger equation. This concludes the proof that the transformed states $e^{i\eta}\psi$ are solutions of the Schrodinger equation with the transformation $\nabla\rightarrow\nabla-\frac{i2e}{\hbar c}\mathbf{A}$.