Lecture 10 Fermi liquid continued, and the BCS theory of superconductivity

Literature for Fermi liquid: T. Giamarchi, Quantum Physics in One Dimension, Oxford Science Publications, Chapter 1.1., G.D. Mahan, Many-Particle Physics, Kluwer, Chapter 11.2.1, E.M. Lifshitz and L.P. Pitaevskii, Landau and Lifshitz Course of Theoretical Physics, Statistical Physics Part 2, Chapters 1 and 2 *Literature for the BCS theory:* A.L. Fetter and J.D. Walecka, Quantum theory of many-particle systems, Dover, Chapters 36-37; P.G. De Gennes, Superconductivity of metals and alloys, Westview Press, Chapters 4-5

Learning goals

- To learn the concept of a quasi-particle, to understand why there can be well-defined quasiparticles close to the Fermi level.
- *•* To learn what is a Fermi liquid.
- *•* To know what is Cooper instability.
- *•* To understand how the mean-field approximation is done in the BCS theory of superconductivity.
- To be able to diagonalize the BCS Hamiltonian using the Bogoliubov transformation: to understand the character of the obtained quasiparticles and the energy gap.

19 Scattering close to the Fermi level and the quasiparticle lifetime

We are now convinced that entities like quasiparticles might exist. Let us say they have an energy $E(k)$; at the moment we do not know its value. Close to the Fermi surface, one can linearize this dispersion in powers of $k - k_F$ (here we use the notation $|\mathbf{k} - \mathbf{k}_F| \equiv k - k_F$

$$
E(k) \simeq E(k_F) + \frac{\hbar^2 k_F}{m^*} (k - k_F). \tag{19.1}
$$

This is how the effective mass m^* of the quasiparticle is defined. One can also immediately check that for the non-interacting system this becomes (note that $E(k)$ includes the chemical potential, that is, $E(k_F) = \hbar^2 k_F^2 / 2m - \mu = 0$

$$
E(k) \simeq \frac{\hbar^2 k_F}{m} (k - k_F). \tag{19.2}
$$

As we already learned, the quasiparticles must have a finite life-time τ , due to the interactions. The wavefunction of the quasiparticle with energy $E(k)$ and lifetime τ would evolve according to

$$
e^{-iE(k)t/\hbar}e^{-t/\tau}.\tag{19.3}
$$

Such a time-dependence corresponds to a Lorentzian lineshape for the spectral function $A(k,\omega)$. In case the lifetime τ was a constant, the system would become overdamped when approaching the Fermi level, i.e. the damping time τ would be smaller than the period $\hbar/E(k)$ since $E(k)$ approaches zero close to the Fermi level. However, τ in general is not a constant but depends on the interactions, that is, on the scatterings between the particles. Well above the Fermi surface, the particles can is equivalent to saying that there exists a Fermi surface. For an interacting system in a Fermi liquid state, there are still well defined, long-lived quasiparticle excitations close to the Fermi surface: therefore one sees a sharp drop in the momentum distribution. However, the drop is smaller than in the non-interacting case: the smoothening of the Fermi surface is due to the fact that not all of the liquid can be described as quasiparticles, only the area close to the Fermi energy. The proportion of the "sharp drop" compared to the size of the drop in the non-interacting case (which is one, obviously) is called the quasiparticle weight and often denoted *Z*. It tells how big proportion of the liquid can actually thought to be described as free quasiparticles.

QUIZ

20 Interactions between the quasiparticles

Now we go to the truly non-trivial part of the Fermi liquid theory, namely the residual interactions between the quasiparticles. First, let us assume that in the ground state the quasiparticles follow, approximately and at least close to the Fermi level, the standard Fermi distribution given by

$$
n_k^0 = n_F(E_k - \mu) = \frac{1}{e^{\beta(E_k - \mu)} + 1}.
$$
\n(20.1)

The corresponding ground state energy would be

$$
E_g = E_0 + \sum_{k\sigma} E_k n_k^0.
$$
 (20.2)

Here E_0 is the energy when all quasiparticles would be at $k = 0$, and σ is the spin index. Again, this is only approximately valid, since quasiparticles are not real particles. However, this does not matter much since what we are interested here is how the distribution is changed when there are excitations in the system. In that case, we have some other distribution n_k . Now, what we will actually consider is just the difference between n_k and n_k^0 , namely $\delta n_k = n_k - n_k^0$. One can show that the free energy becomes (Exercise Set 10)

$$
F = E - \mu N = E_g - \mu N_0 + \sum_{k\sigma} (E_k - \mu) \delta n_k \equiv F_0 + \sum_{k\sigma} (E_k - \mu) \delta n_k.
$$
 (20.3)

Here N is the total number of particles and N_0 the number of particles in the ground state. In this form, no interactions between the quasiparticles were included. It is assumed that the interactions are described by some functional $F(\delta n_k)$, and it is sufficient to expand the functional for small δn_k and include terms of the second order in it. The free energy becomes (here *V* is the volume)

$$
F = F_0 + \sum_{k\sigma} (E_k - \mu)\delta n_k + \frac{1}{2V} \sum_{kk'\sigma\sigma'} f_{k\sigma k'\sigma'} \delta n_{k\sigma} \delta n_{k'\sigma'}.
$$
 (20.4)

scatter freely. But close to the Fermi level, the phase space for scattering is limited since the states below the Fermi level are already occupied. Landau has shown that in three dimensions, the lifetime diverges as $\tau \sim 1/E(k)^2$. Since the period of the wavefunction oscillation diverges only as $\sim 1/E(k)$, the growth of the lifetime is always stronger, and the quasiparticles at the Fermi level become very long-lived compared to the inverse of their energy. In other words, the quasiparticles close to the Fermi level are indeed well-defined quasiparticles. This non-availability of phase space for scattering in a Fermi system is basically the reason why the simple Fermi liquid theory with quasiparticles is often a reasonably good description of the complex system. Actually, the lifetimes close to the Fermi surface are so long that the damping is often neglected and quasiparticle spectral functions are approximated by delta-functions. The free electron model that you may have learned previously is hopefully more intuitive now!

This discussion has also a further implication: the concept of a quasiparticle is *not* good when one is too far away from the Fermi level. Temperature has the effect of broadening the Fermi level: the particles are located in energy in a region around the Fermi surface that is characterized by $k_B T$. The phase space argument of scattering, based on Pauli blocking, is partly removed from this area. Thus for the quasiparticles to be well-defined (long-lived), one should have the temperature smaller than the Fermi energy. For metals, the Fermi energy is about 10 000 K, so one can be sure that that quasiparticles at room temperature (of the order 100 K) are well defined. The Fermi liquid theory sometimes works also when the temperature difference is not so huge.

The spectral functions of the non-interacting (left) and the interacting (right) system are shown in the figure below. While in the former the spectral functions are delta-functions, in the latter the width of the spectral function is finite but approaches zero when going closer to the Fermi energy.

Also the momentum distributions $n(k)$ are shown in the above figure. For a noninteracting system, the momentum states are filled up to the Fermi level. Then there is a sharp drop in the momentum distribution. The existence of such a drop

Here the interaction coefficient $f_{k\sigma k'\sigma'}$ is the second order expansion coefficient of $F(\delta n_k)$. The interaction coefficient can be divided into spin symmetric (s) and antisymmetric (a) contributions, and those can be expanded in terms of Legendre polynomials as

$$
f_{kk'}^{s,a} = \frac{1}{N_F} \sum_{l=0}^{\infty} F_l^{s,a} P_l(\cos \theta),
$$
 (20.5)

where $N_F = m^* k_F / \pi^2 \hbar^3$ is the density of states at the Fermi level (for the noninteracting case, N_{F0} is the same, just with the mass m).

The coefficients $F_l^{s,a}$ are important: they are so-called Landau parameters. They can be estimated, or measured, for specific physical systems. From the free energy one can calculate various quantities, and it turns out that they are in simple ways given by the Landau parameters. The low lying excitations that can be obtained from the Fermi liquid theory are 1) particle-hole excitations which are excitations of single quasiparticles: a quasiparticle is created above the Fermi level and a hole is left below it, 2) density oscillations which are the plasmons for a charged electron gas and sound waves for a neutral Fermi liquid, 3) damped spin waves, called paramagnons. Here 1) are single quasiparticle excitations, and 2) and 3) can be viewed as collective excitations of interacting quasiparticles. The Landau parameters determine the quantities of interest: for instance, the specific heat, compressibility, sound velocity and the spin susceptibility are given in the following way.

Specific heat

Non-interacting (free particles)

$$
C_{V0} = \frac{\pi^2}{3} k_B^2 T N_{F0}
$$
\n(20.6)

Fermi liquid theory

$$
\frac{C_V}{C_{V0}} = \frac{m^*}{m} = 1 + \frac{1}{3}F_1^s \tag{20.7}
$$

Compressibility

Non-interacting (free particles)

$$
\frac{1}{K_f} = \frac{n_0^2}{N_{F0}}\tag{20.8}
$$

Fermi liquid theory

$$
\frac{K}{K_f} = \frac{1 + F_0^s}{1 + F_1^s/3} \tag{20.9}
$$

Sound velocity

Non-interacting (free particles)

$$
c_0^2 = \frac{n_0}{mN_{F0}} = \frac{v_F^2}{3}
$$
\n(20.10)

Fermi liquid theory

$$
\left(\frac{c}{c_0}\right)^2 = \frac{K}{K_f} \tag{20.11}
$$

Spin susceptibility

Non-interacting (free particles)

$$
\chi_0 = \mu_0^2 N_{F0} \tag{20.12}
$$

Fermi liquid theory

$$
\frac{\chi}{\chi_0} = \frac{1 + F_1^a / 3}{1 + F_0^a} \tag{20.13}
$$

21 Concluding remarks

After all the vagueness of the derivation in this lecture, it is perhaps difficult to imagine that the Fermi liquid theory is able to describe anything. But it actually is: it gives a good description for instance of the He quantum liquid, as well as predicts many basic features of metals. However, there are important states of fermionic matter that cannot be described by the Fermi liquid theory. For instance superconductivity/superfluidity that will be discussed in the following cannot be explained using the Fermi liquid theory. The concept of a quasiparticle will be used also there, but its meaning is different from the Fermi liquid context. Furthermore, in one-dimensional systems the Fermi liquid theory always fails. There, a somewhat analogous description is given by the Luttinger liquid theory. Fermi liquid theory can be considered as the "default", basic description that one should try to apply for an interacting fermion system to start with. Often it applies pretty well; if not, one probably has a highly interesting and non-trivial many-body system at hand.

QUIZ

The BCS theory of superconductivity

22 Fermi sea and the possibility of condensation for fermions

Now we will learn the basic description of superconductivity/superfluidity of Fermionic interacting particles. Due to the Pauli exclusion principle, identical fermions occupy the energy levels of the system until the Fermi level. In Lecture 9 we discussed the concepts of Fermi level μ , Fermi energy E_F , Fermi wave vector k_F (E_F and k_F are given by the non-interacting, $T = 0$ case), and Fermi sphere. Note also the relation between the density $n = N/V$ and Fermi wave vector k_F for spin 1/2 particles, where N is the number of particles and V is the volume:

$$
n = \frac{N}{V} = 2\frac{4\pi k_F^3}{3} \frac{1}{(2\pi)^3} = \frac{k_F^3}{3\pi^2}.
$$
 (22.1)

Fermi sea refers to the particles (for instance electrons) that are below the Fermi level. The concept is used often when we wish to remind that the presense of many other particles in different energy states affects the behaviour of what happens

to one particle, or to two particles in a scattering process. The existence of the Fermi sea turned out to be essential in explaining the phenomenon of superconductivity, as we will learn in this lecture.

Condensation is by definition a phenomenon where one single quantum state (e.g. the ground state) becomes occupied by a macroscopic number of particles: it cannot happen for noninteracting fermions due to the Pauli exclusion principle.

However, if there is a system with two different types of (non-identical, distinguishable) Fermions, they can via interactions form effective bosons which may then form a Bose-Einstein condensate (BEC). This is essentially what happens, e.g., in superconductivity in metals and in superfluidity in ultracold Fermi gases.

In metals, the electrons have repulsive interactions due to the Coulomb force. However, the electrons interact also with the lattice and this can cause effective attractive interactions between the electrons. Consequently, a spin up and a spin down electron can form a so-called Cooper pair which is effectively a boson. Superconductivity is the condensation of these Cooper pairs. In ultracold Fermi gases, the interactions between atoms can be attractive as such, and Cooper pairs of atoms in different hyperfine states may form and condense.

23 Cooper instability

L.N. Cooper presented the following calculation: Consider

- the scattering of two particles

- which have an attractive interaction

- in the presence of a Fermi sea (restricting the possible momenta where the particles can scatter).

Based on this, he showed that even for arbitrarily small interactions, pairs (later named as Cooper pairs) will be formed in the system. This is referred to as instability of the Fermi sea: pair formation happens for any non-zero, attractive interaction. Thus it is enough to consider only two-particle scattering (i.e. not many-body physics), added with the constraint of the Fermi sea (which is a many-body effect), to predict that there will be pairing. It is interesting to note that also here the simple existence of the Fermi sea and its ability to restrict the phase space for scattering is crucial; remember above where the restriction of the phase space for scattering was essential to the existence of well-defined (long-lived) quasiparticles in the Fermi liquid.

Condensation and superfluidity are essentially many-body effects, and to predict and describe them one needs a many-body description. We will learn below the BCS (Bardeen-Cooper-Schrieffer) mean-field description of superconductivity/superfluidity.

24 The BCS theory

Let us consider a system of two types of Fermions. We label them spin up and spin down as in metals, however, in ultracold gases this labeling could mean just atoms in two different hyperfine states. The Hamiltonian, using field operators, is

$$
H = \int d\mathbf{r} \sum_{\sigma = \uparrow, \downarrow} \psi_{\sigma}^{\dagger}(\mathbf{r}) \left(-\frac{\hbar^2 \nabla^2}{2m_{\sigma}} - \mu_{\sigma} \right) \psi_{\sigma}(\mathbf{r}) +
$$

$$
+\frac{1}{2}\sum_{\alpha,\beta=\uparrow,\downarrow,\alpha\neq\beta}\int d\mathbf{r}\int d\mathbf{r}'V_{\uparrow\downarrow}(\mathbf{r},\mathbf{r}')\,\psi_{\alpha}^{\dagger}(\mathbf{r})\,\psi_{\beta}^{\dagger}(\mathbf{r}')\,\psi_{\alpha}(\mathbf{r})\,. \tag{24.1}
$$

We set here

$$
\mu_{\uparrow} = \mu_{\downarrow}, \quad m_{\uparrow} = m_{\downarrow}.
$$
\n(24.2)

To simplify the description, let us assume that the interaction is a contact interaction (in ultracold gases, this is often also a good approximation):

$$
V_{\uparrow\downarrow}(\mathbf{r}, \mathbf{r}') = V_0 \delta(\mathbf{r} - \mathbf{r}'). \tag{24.3}
$$

The Hamiltonian becomes

$$
H = \int d\mathbf{r} \sum_{\sigma = \uparrow, \downarrow} \psi_{\sigma}^{\dagger}(\mathbf{r}) \left(-\frac{\hbar^2 \nabla^2}{2m} - \mu \right) \psi_{\sigma}(\mathbf{r}) +
$$

+
$$
V_0 \int d\mathbf{r} \psi_{\uparrow}^{\dagger}(\mathbf{r}) \psi_{\downarrow}^{\dagger}(\mathbf{r}) \psi_{\downarrow}(\mathbf{r}) \psi_{\uparrow}(\mathbf{r}). \qquad (24.4)
$$

24.1 The mean-field approximation

It is usually extremely difficult or practically impossible to solve exactly a quantum many-body system with a large number of particles. One of the most used approximations to make the problems tractable is the mean-field approximation. This means basically that we replace some of the operators in the Hamiltonian by their mean values (which are just complex numbers, not operators), assuming that the deviations from the mean values are small.

Let us consider the example of operators *A* and *B* and their product *AB*. Let us write the operators *A* and *B* as their mean values and the deviation from the mean value (no approximation made at this point, just rewriting), and then calculate *AB*:

$$
A = \langle A \rangle + \delta A \tag{24.5}
$$

$$
B = \langle B \rangle + \delta B \tag{24.6}
$$

 \Rightarrow

$$
AB = \langle A \rangle \langle B \rangle + \langle A \rangle \delta B + \langle B \rangle \delta A + \delta A \delta B. \tag{24.7}
$$

Assuming that the fluctuations around the mean values are small, one can neglect the last term which is quadratic in the fluctuations, i.e.

 \Rightarrow

$$
\delta A \delta B \approx 0 \tag{24.8}
$$

Then insert $\delta A = A - \langle A \rangle$, $\delta B = B - \langle B \rangle$ in (24.7)

$$
AB = \langle A \rangle B + \langle B \rangle A - \langle A \rangle \langle B \rangle.
$$
 (24.9)

One can generalize this kind of consideration for products of more than two operators (Wick's theorem).

Now we do the BCS mean-field approximation to the interaction term of the Hamiltonian, leading to Hartree-fields and pairing-fields (Fock-fields are zero in the BCS theory). Let us denote $\psi_{\sigma}(\mathbf{r}) \equiv \psi_{\sigma}$. Terms of the form $\langle \rangle$ $\langle \rangle$ are neglected here (they are just numbers, not operators, and thus will cause only a constant shift in the energy; note, however, that they can be important sometimes, for instance if one is interested in the absolute energy of the state e.g. compared to some other state).

Note that here we organize the operators in *pairs* and then take the expectation values, unlike in the example above where we had expectation values of single operators A and B. This is done because in a Fermi system which is expected to show pairing correlations, this is a good choice: expectation values of single fermion operators are zero in this case. In general, when doing a mean-field approximation, some pre-knowledge or an educated guess/argument about the relevant non-zero expectation values and correlations are needed. When organizing the fermion operators in pairs, one has to sometimes move them with respect to each other. This may give minus signs due to the Fermi statistics, and one has to keep track on them. To understand these things more deeply, you may search more information on the topic "Wick's theorem".

$$
\psi_{\uparrow}^{\dagger}\psi_{\downarrow}^{\dagger}\psi_{\downarrow}\psi_{\uparrow} = \langle\psi_{\downarrow}\psi_{\uparrow}\rangle\psi_{\uparrow}^{\dagger}\psi_{\downarrow}^{\dagger} + \langle\psi_{\uparrow}^{\dagger}\psi_{\downarrow}^{\dagger}\rangle\psi_{\downarrow}\psi_{\uparrow} + \langle\psi_{\uparrow}^{\dagger}\psi_{\uparrow}\rangle\psi_{\downarrow}^{\dagger}\psi_{\downarrow} + \langle\psi_{\downarrow}^{\dagger}\psi_{\downarrow}\rangle\psi_{\uparrow}^{\dagger}\psi_{\uparrow} -\left(\langle\psi_{\uparrow}^{\dagger}\psi_{\downarrow}\rangle\psi_{\downarrow}^{\dagger}\psi_{\uparrow} + \langle\psi_{\downarrow}^{\dagger}\psi_{\uparrow}\rangle\psi_{\uparrow}^{\dagger}\psi_{\downarrow}\right)
$$
(24.10)

 $\textbf{Pairing fields } \braket{\psi_{\downarrow}\psi_{\uparrow}}{\psi_{\uparrow}^{\dagger}\psi_{\downarrow}^{\dagger}}, \left\langle \psi_{\uparrow}^{\dagger}\psi_{\downarrow}^{\dagger} \right\rangle$ $\Big\} \psi_{\downarrow}\psi_{\uparrow}$ ${\bf Hartree~ fields} \left\langle \psi^\dagger_\dagger \psi_\dagger \right\rangle \psi^\dagger_\downarrow \psi_\downarrow , \left\langle \psi^\dagger_\downarrow \psi_\downarrow \right\rangle \psi^\dagger_\uparrow \psi_\uparrow$

 ${\rm The\; Fock\; fields}\left<\psi^\dagger_\uparrow\psi_\downarrow\right>=\left<\psi^\dagger_\downarrow\psi_\uparrow\right>=0\ {\rm here},\ {\rm so\; the\; corresponding\; terms\; in\; (24.10)}$ are zero.

Note that $\langle \psi_{\perp} \psi_{\uparrow} \rangle \neq 0$, c.f. $\langle a \rangle \neq 0$ for BEC.

The order parameter of the BCS theory turns out to be given by the pairing fields in the following way:

$$
\Delta(\mathbf{r}) = V_0 \langle \psi_{\downarrow}(\mathbf{r}) \psi_{\uparrow}(\mathbf{r}) \rangle. \tag{24.11}
$$

This quantity will also be the energy gap in the excitation spectrum of the BCS theory, as we will see later. One can also assume that it does not depend on the spatial coordinate, this is a good assumption for a homogeneous system within the usual BCS theory:

$$
\Delta \left(\mathbf{r} \right) = \Delta = \Delta^*.
$$
\n(24.12)

We also insert the Hartree fields within redefined chemical potentials. Denoting $\langle \psi_{\sigma}^{\dagger} \psi_{\sigma} \rangle = n_{\sigma}$, we get

$$
-\mu \psi_{\uparrow}^{\dagger} \psi_{\uparrow} + V_0 n_{\downarrow} \psi_{\uparrow}^{\dagger} \psi_{\uparrow} = -\tilde{\mu} \psi_{\uparrow}^{\dagger} \psi_{\uparrow}
$$
 (24.13)

$$
\tilde{\mu} = \mu - V_0 n_{\downarrow}.\tag{24.14}
$$

The Hamiltonian becomes now (terms of the form $\langle \rangle$ $\langle \rangle$ are neglected here)

$$
H = \int d\mathbf{r} \sum_{\sigma = \uparrow, \downarrow} \psi_{\sigma}^{\dagger}(\mathbf{r}) \left(-\frac{\hbar^2 \nabla^2}{2m} - \tilde{\mu} \right) \psi_{\sigma}(\mathbf{r}) + + \int d\mathbf{r} \left(\Delta \psi_{\uparrow}^{\dagger}(\mathbf{r}) \psi_{\downarrow}^{\dagger}(\mathbf{r}) + \Delta \psi_{\downarrow}(\mathbf{r}) \psi_{\uparrow}(\mathbf{r}) \right).
$$
 (24.15)

Now, let us expand the field operators using the annihilation operators for momentum states

$$
\psi_{\sigma}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} c_{\mathbf{k}\sigma}.
$$
\n(24.16)

The Hamiltonian is then (calculated in Exercise Set 10):

$$
H = \sum_{\mathbf{k}} \xi_{\mathbf{k}} c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} + \xi_{\mathbf{k}} c_{\mathbf{k}\downarrow}^{\dagger} c_{\mathbf{k}\downarrow} + \Delta c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} + \Delta c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}, \tag{24.17}
$$

where

QUIZ

24.2 Diagonalizing the Hamiltonian: the Bogoliubov transformation

When describing a quantum system, the first thing to do is find the eigenvalues and eigenfunctions of the Hamiltonian. Since we have done the mean-field approximation, the Hamiltonian has transformed into the above simple quadratic form which in fact can be written in matrix form and diagonalized, leading to results that give a α lot of insight into the system. The Hamiltonian in the matrix form is (the coefficient *A* is calculated in Exercise Set 10):

$$
H = A + \sum_{\mathbf{k}} \left(c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow} \right) \left(\begin{array}{cc} \xi_{\mathbf{k}} & \Delta \\ \Delta & -\xi_{\mathbf{k}} \end{array} \right) \left(c_{-\mathbf{k}\downarrow}^{\dagger} \right). \tag{24.19}
$$

The Hamiltonian is hermitian, so there exists a unitary transformation that diagonalizes it:

$$
H = A + \sum_{\mathbf{k}} \left(c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow} \right) U U^{\dagger} \left(\begin{array}{cc} \xi_{\mathbf{k}} & \Delta \\ \Delta & -\xi_{\mathbf{k}} \end{array} \right) U U^{\dagger} \left(\begin{array}{c} c_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow}^{\dagger} \end{array} \right) = (24.20)
$$

$$
= A + \sum_{\mathbf{k}} \left(\begin{array}{cc} \gamma_{\mathbf{k}\uparrow}^{\dagger} & \gamma_{-\mathbf{k}\downarrow} \end{array} \right) \left(\begin{array}{cc} E_{\uparrow\mathbf{k}} & 0 \\ 0 & -E_{\downarrow\mathbf{k}} \end{array} \right) \left(\begin{array}{cc} \gamma_{\mathbf{k}\uparrow} \\ \gamma_{-\mathbf{k}\downarrow}^{\dagger} \end{array} \right). \tag{24.21}
$$

The minus sign in the second eigenvalue is chosen for convenience. The eigenvalues and the eigenvectors (elements of the unitary transformation) can be calculated from the eigenvalue equation

 \Rightarrow

 \Rightarrow

 \Rightarrow

$$
\begin{pmatrix} \xi_{\mathbf{k}} & \Delta \\ \Delta & -\xi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} u_{j\mathbf{k}} \\ v_{j\mathbf{k}} \end{pmatrix} = \lambda_{j\mathbf{k}} \begin{pmatrix} u_{j\mathbf{k}} \\ v_{j\mathbf{k}} \end{pmatrix}
$$
 (24.22)

$$
\begin{pmatrix} \xi_{\mathbf{k}} - \lambda_{j\mathbf{k}} & \Delta \\ \Delta & -\xi_{\mathbf{k}} - \lambda_{j\mathbf{k}} \end{pmatrix} \begin{pmatrix} u_{j\mathbf{k}} \\ v_{j\mathbf{k}} \end{pmatrix} = 0
$$
 (24.23)

$$
\det\left(\begin{array}{cc} \xi_{\mathbf{k}} - \lambda_{j\mathbf{k}} & \Delta \\ \Delta & -\xi_{\mathbf{k}} - \lambda_{j\mathbf{k}} \end{array}\right) = 0
$$
 (24.24)

$$
E_{\uparrow \mathbf{k}} = \lambda_{\uparrow \mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}
$$
 (24.25)

$$
E_{\downarrow \mathbf{k}} = -\lambda_{\downarrow \mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}.
$$
 (24.26)

Eigenvectors:

$$
\xi_{\mathbf{k}} u_{j\mathbf{k}}^2 + \Delta u_{j\mathbf{k}} v_{j\mathbf{k}} = \lambda_{j\mathbf{k}} u_{j\mathbf{k}}^2 \tag{24.27}
$$

$$
-\xi_{\mathbf{k}}v_{j\mathbf{k}}^2 + \Delta u_{j\mathbf{k}}v_{j\mathbf{k}} = \lambda_{j\mathbf{k}}v_{j\mathbf{k}}^2
$$
 (24.28)

and $u_{j\mathbf{k}}^2 + v_{j\mathbf{k}}^2 = 1$ from unitarity

$$
u_{\mathbf{k}} = u_{\uparrow \mathbf{k}} = v_{\downarrow \mathbf{k}} = \sqrt{\frac{1}{2} \left(1 + \frac{\xi_{\mathbf{k}}}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}} \right)}
$$
(24.29)

$$
v_{\mathbf{k}} = v_{\uparrow \mathbf{k}} = -u_{\downarrow \mathbf{k}} = \sqrt{\frac{1}{2} \left(1 - \frac{\xi_{\mathbf{k}}}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}} \right)}
$$
(24.30)

$$
u_{\mathbf{k}}v_{\mathbf{k}} = \frac{1}{2} \frac{\Delta}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}}.
$$
\n(24.31)

The unitary transformation above is called the Bogoliubov transformation. It defines the relations between the original annihilation operators and the operators corresponding to the diagonalized Hamiltonian:

$$
U\left(\begin{array}{c}\gamma_{\mathbf{k}\uparrow}\\ \gamma_{-\mathbf{k}\downarrow}^{\dagger}\end{array}\right) = \left(\begin{array}{c}c_{\mathbf{k}\uparrow}\\ c_{-\mathbf{k}\downarrow}^{\dagger}\end{array}\right). \tag{24.32}
$$

$$
\begin{pmatrix} c_{\mathbf{k}\uparrow}^{\dagger} & c_{-\mathbf{k}\downarrow} \end{pmatrix} = \begin{pmatrix} \gamma_{\mathbf{k}\uparrow}^{\dagger} & \gamma_{-\mathbf{k}\downarrow} \end{pmatrix} U^{\dagger}
$$
 (24.33)

Thus

$$
c_{\mathbf{k}\uparrow} = u_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow} - v_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow}^{\dagger} \tag{24.34}
$$

$$
c_{-\mathbf{k}\downarrow}^{\dagger} = v_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow} + u_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow}^{\dagger} \tag{24.35}
$$

and

$$
\gamma_{\mathbf{k}\uparrow} = u_{\mathbf{k}} c_{\mathbf{k}\uparrow} + v_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^{\dagger} \tag{24.36}
$$

$$
\gamma_{-\mathbf{k}\downarrow}^{\dagger} = v_{\mathbf{k}} c_{\mathbf{k}\uparrow} - u_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^{\dagger}.
$$
 (24.37)

The γ 's are called **quasiparticle** annihilation (creation) operators. They fulfill the same fermionic anticommutation relations than the original operators, thus they are well-defined fermionic quasiparticles. A quasiparticle is, in general, an excitation of an interacting system, characterized e.g. by its energy, effective mass, life time, etc. Compare to Lecture 9 where the concept of a quasiparticle was introduced:

In the BCS theory, the quasiparticles are linear combinations of annihilation and creation operators of opposite spins, so it is not easy to make an intuitive picture about them. They are superpositions of a particle, and a hole of opposite spin and momentum. In the Fermi liquid, the quasiparticles could be understood, roughly, as the original particles "dressed" by the presence of and interactions with the other

particles. Here the quasiparticles are somewhat different, they are superpositions of particles and holes and thus describe the pairing correlations present in the BCS state.

The nature of the quasiparticles is described in the below picture. In the BCS state, one either has, with some probability, both k and $-k$ states occupied, or both empty. An excitation means that one of these states can be occupied while the other one is empty. As the picture shows, there are two routes for forming such an excitation: to destroy one particle, or to create another. The quasiparticle is a superposition of these possibilities.

At zero temperature, there are no quasiparticles in the BCS description. This is easy to see: the Hamiltonian is diagonal when expressed with the quasiparticle operators. This means that the quasiparticles are non-interacting (remember that in the Fermi liquid theory, the residual interactions between the quasiparticles were essential), and we can directly apply the statistical physics of non-interacting fermionic particles. For instance, the occupation number of the quasiparticles is simply given by the Fermi distribution:

$$
\left\langle \gamma_{\mathbf{k}\sigma}^{\dagger} \gamma_{\mathbf{k}\sigma} \right\rangle = \frac{1}{e^{\frac{E_{\sigma}}{kT}} + 1} \equiv f(E_{\sigma}, T). \qquad \sigma = \uparrow, \downarrow \qquad (24.38)
$$

Note also that

$$
\left\langle \gamma_{\mathbf{k}\uparrow}^{\dagger} \gamma_{\mathbf{k}\downarrow} \right\rangle = \left\langle \gamma_{\mathbf{k}\uparrow}^{\dagger} \gamma_{\mathbf{k}\downarrow}^{\dagger} \right\rangle = 0. \tag{24.39}
$$

The eigenvalues are always positive, thus in the limit $T = 0$ the occupation numbers go to zero. Therefore, in the ground state there are no quasiparticles. By giving energy to the system, one may create excitations, that is, quasiparticles. Breaking a Cooper pair is equivalent to creating two quasiparticles. To create two quasiparticles, the energy of $2E_k$ is needed:

$$
E_{\uparrow \mathbf{k}} + E_{\downarrow \mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2} + \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}.
$$
 (24.40)

The minimum of $\xi_{\mathbf{k}}^2 = \left(\frac{\hbar^2 \mathbf{k}^2}{2m} - \tilde{\mu}\right)^2$ is zero, thus

$$
[E_{\uparrow \mathbf{k}} + E_{\downarrow \mathbf{k}}]_{\text{min}} = 2\Delta. \tag{24.41}
$$

This means that the order parameter defines the energy gap for creating excitations. The existence of an energy gap is behind many important properties: one

cannot make single particle excitations to the system if one tries to give or take an amount of energy that is less than the value of the energy gap. In other words, dissipation is restricted. This is basically why supercurrents can flow without resistance. However, to really prove the existence of supercurrents and superflows one has to describe the dynamics of the system in a way that goes beyond this lecture. To describe collective modes of the superfluid, one has to introduce interactions between the quasiparticles (this can be conveniently done, e.g. with the so-called generalized random phase approximation (GRPA)), just like in the case of the Fermi liquid. However, in case of the BCS theory, one can predict many important phenomena, such as the existence of an energy gap, even without considering quasiparticle interactions.

QUIZ QUIZ QUIZ

24.3 The gap equation

Now, let us see how does one actually calculate the value of the order parameter. Using the Bogoliubov transformation, the order parameter becomes (shown in Exercise Set 10):

$$
\Delta = -\frac{V_0}{V} \sum_{\mathbf{k}} \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle = -\frac{V_0}{V} \sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} \left(1 - \left\langle \gamma_{\mathbf{k}\uparrow}^{\dagger} \gamma_{\mathbf{k}\uparrow} \right\rangle - \left\langle \gamma_{-\mathbf{k}\downarrow}^{\dagger} \gamma_{-\mathbf{k}\downarrow} \right\rangle \right) \tag{24.42}
$$

$$
1 = -\frac{V_0}{V} \sum_{\mathbf{k}} \frac{1 - f(E_{\uparrow \mathbf{k}}, T) - f(E_{\downarrow \mathbf{k}}, T)}{2\sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}}.
$$
 (24.43)

This is the so-called gap equation. Because we assumed a contact interaction, this equation is actually divergent. This unphysical divergence can be avoided by renormalization, for instance, by simply removing the diverging part

$$
\frac{1}{V_0} \to \frac{1}{T^{2B}} - \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2\epsilon_{\mathbf{k}}},\tag{24.44}
$$

where $\epsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m}$, and the two-body T-matrix $T^{2B} = \frac{4\pi a_s \hbar^2}{m}$ describes the scattering for two particles.

Usually the gap equation is written in the continuum

$$
\frac{1}{V} \sum_{\mathbf{k}} \rightarrow \left(\frac{1}{2\pi}\right)^3 \int d^3 \mathbf{k} \tag{24.45}
$$

$$
\Rightarrow
$$

$$
1 = -\frac{T^{2B}}{2\pi^2} \int_0^\infty k^2 dk \left(\frac{1 - f(E_{\uparrow \mathbf{k}}, T) - f(E_{\downarrow \mathbf{k}}, T)}{2\sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}} - \frac{1}{2\epsilon_{\mathbf{k}}} \right). \tag{24.46}
$$

From this form, the order parameter Δ can be solved numerically, at a given temperature *T* and for a given interaction strength and a chemical potential. If the order parameter Δ has a finite value, one generally has a superconducting/superfluid ground state (i.e. a condensate of Cooper pairs). If it is zero, the ground state is simply a normal state. Thus one can obtain the critical temperature where the condensation happens by setting $\Delta = 0$ in the gap equation and then solving the temperature *T* from the equation. This can be done analytically (with some approximations) and leads to

$$
T_c = \frac{8E_F}{k_B \pi} e^{\gamma - 2} \exp\left(-\frac{\pi}{2k_F |a_s|}\right),\tag{24.47}
$$

where γ is Euler's constant.

One can see from the above that the critical temperature cannot be developed into a Taylor series with respect to the scattering length (interaction strength) *aS*. This means that one cannot predict superconductivity from the ideal gas $(a_S = 0)$ by perturbation theory!