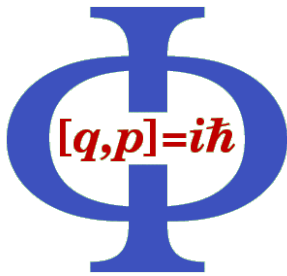




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Notes for the theory part of the lectures

Magnetism, Superconductivity and Electronic Correlations

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July 15–17, 2009

(Last modified: July 18, 2009)

PDF version of these lecture notes (with hyperlinks etc.) at

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1 Systems of identical particles

The solid-state problem is described by a Hamiltonian H of the form

$$\begin{aligned} H &= \sum_{i=1}^N \left(\frac{\hat{\mathbf{p}}_i^2}{2m} + u(\hat{\mathbf{x}}_i) \right) + \sum_{i>j} V_{i,j}(\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j) \\ &= \sum_{i=1}^N h(i) + \sum_{i>j} V(i,j) = H_0 + V. \end{aligned} \quad (1.1)$$

At this point we are thinking essentially about the motion of N electrons whose mass is given by m . One could in principle also include the motion of the nuclei (which gives rise to important phenomena such as phonons), but in these lectures we will consider them as frozen such that they just contribute to the external potentials u . This is a reasonable first approximation since the nuclei of the atoms are much heavier than the electrons. In addition, the electrons interact via a pair interaction $V_{i,j}$ (the Coulomb force between two electrons is an example for such a pairwise interaction).

The Hamiltonian (1.1) evidently is non-relativistic. While this is a reasonable approximation, also in solid-state physics there are important relativistic effects such as spin-orbit coupling. However, we will not consider them in the present lectures.

Electrons are quantum-mechanical objects such that the momentum $\hat{\mathbf{p}}_i$ and position $\hat{\mathbf{x}}_i$ of the i th electron have to be considered as operators¹.

Suppose that we know a solution of the one-particle problem for $h(i)$:

$$h(i) |\varepsilon, \nu\rangle_{(i)} = \varepsilon |\varepsilon, \nu\rangle_{(i)}. \quad (1.2)$$

Here ε is the single-particle energy and ν are additional quantum numbers including, e.g., the spin of the electron. In the case of a problem which is invariant under lattice translations, it may be useful to label the single-particle states by a lattice momentum \mathbf{k} instead of their energy ε . Usually one assumes that the eigenstates $|\varepsilon, \nu\rangle_{(i)}$ of $h(i)$ are normalized to unity.

For vanishing interaction $V = 0$, the eigenstates of the many-body Hamiltonian H can be written as a product of single-particle states:

$$|\varepsilon_1, \nu_1; \varepsilon_2, \nu_2; \dots; \varepsilon_N, \nu_N\rangle = |\varepsilon_1, \nu_1\rangle_{(1)} \otimes |\varepsilon_2, \nu_2\rangle_{(2)} \otimes \dots \otimes |\varepsilon_N, \nu_N\rangle_{(N)}. \quad (1.3)$$

The energy of such a state is given by $\sum_l \varepsilon_l$.

Unfortunately, the product state (1.3) ignores one important property, namely that the N electrons are identical and indistinguishable. We will now discuss first the consequences of indistinguishable particles in terms of symmetries of the wave function and then show how to implement these symmetries in an elegant way.

¹If there is a risk of confusion, we will denote operators by an additional hat.

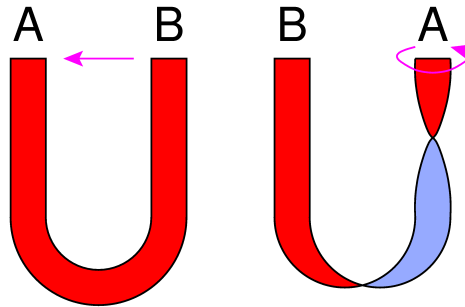


Figure 1.1: Exchange of two ends of a ribbon.

1.1 Symmetries of systems of identical particles

Now how does a wave function of identical particles behave under pair exchange? Since the particles are indistinguishable, one might assume that the wave function is the same after exchange as before, *i.e.*, that it is symmetric under exchange of two particles. However, this is not true in general, as is demonstrated by the following consideration: consider a ribbon with two ends A and B , as shown in Fig. 1.1. Now imagine that the end A is moved past B in a linear fashion, *i.e.*, without rotation. If you do this experiment, you will see that in the final state one of the ends has performed a 360° rotation with respect to the other end. However, there are no ribbons between particles in nature, so does it matter? If the angular momentum of the particles (including the internal angular momentum, called 'spin') is integer, a 360° rotation is the identity and it does not matter, *i.e.*, the wave function is symmetric. However, for half-integer angular momentum/spin, the representation of $SU(2)$ lives on a two-fold covering of three-dimensional space. In this case, a rotation by 360° is *not* an identity, only a rotation by 720° . In this case, the exchange should be different from the identity, but in such a manner that two exchanges recover the identity. The only way how we can achieve this is by having a minus sign in the pair exchange, *i.e.*, the wavefunctions of half-integer spin particles should be *antisymmetric* under pair exchange.

This heuristic consideration is the essence of the spin-statistics theorem (see, e.g., Ref. [11] for a summary of this argument and more details): identical particles with integer spin are symmetric under pair exchange and therefore called 'bosons'; identical particles with half-integer spin are antisymmetric under pair exchange and called 'fermions'. We are particularly concerned by electrons. Electrons carry a spin $1/2$ and therefore must be fermions.

In order to analyze the symmetry properties of identical particles more precisely, we define the unitary permutation operators \mathcal{P}_α with $\alpha = 1, 2, \dots, N!$ which generate

the $N!$ possible permutations of the N particles. The permutation operators \mathcal{P}_α can be written as products of pair exchange operators $P_{i,j}$. This representation is not unique, but all factorizations of a given permutation operator \mathcal{P}_α contain either an even or an odd number p_α of pair exchange operators. Accordingly, the permutation is denoted as even or odd. The many-particle states of bosons are even under an arbitrary pair exchange while they are odd for fermions. Based on the \mathcal{P}_α we define the symmetrization operator

$$\mathcal{S} = \frac{1}{N!} \sum_{\alpha=1}^{N!} \mathcal{P}_\alpha \quad (1.4)$$

and the antisymmetrization operator

$$\mathcal{A} = \frac{1}{N!} \sum_{\alpha=1}^{N!} (-1)^{p_\alpha} \mathcal{P}_\alpha, \quad (1.5)$$

where $(-1)^{p_\alpha} = 1$ for \mathcal{P}_α even and $(-1)^{p_\alpha} = -1$ for \mathcal{P}_α odd. Using that $P_{i,j}^\dagger = P_{i,j} = P_{i,j}^{-1}$, it is easy to check that $\mathcal{P}_\alpha^{-1} = \mathcal{P}_\alpha^\dagger$. This implies that \mathcal{S} and \mathcal{A} are self-adjoint operators.

We have

$$\mathcal{P}_\alpha \mathcal{S} = \frac{1}{N!} \sum_{\alpha'=1}^{N!} \mathcal{P}_\alpha \mathcal{P}_{\alpha'} = \frac{1}{N!} \sum_{\alpha''=1}^{N!} \mathcal{P}_{\alpha''} = \mathcal{S} = \mathcal{S} \mathcal{P}_\alpha \quad (1.6)$$

and

$$\mathcal{P}_\alpha \mathcal{A} = \frac{1}{N!} \sum_{\alpha'=1}^{N!} \mathcal{P}_\alpha (-1)^{p_{\alpha'}} \mathcal{P}_{\alpha'} = (-1)^{p_\alpha} \frac{1}{N!} \sum_{\alpha''=1}^{N!} (-1)^{p_{\alpha''}} \mathcal{P}_{\alpha''} = (-1)^{p_\alpha} \mathcal{A} = \mathcal{A} \mathcal{P}_\alpha. \quad (1.7)$$

Summing Eq. (1.6) over α yields

$$\mathcal{S}^2 = \mathcal{S}. \quad (1.8)$$

Likewise, multiplication of Eq. (1.7) with $(-1)^{p_\alpha}$ and summation over α leads to

$$\mathcal{A}^2 = \mathcal{A}. \quad (1.9)$$

This shows that \mathcal{S} and \mathcal{A} are projection operators. Furthermore, Eq. (1.6) implies that

$$\mathcal{A} \mathcal{S} = \frac{1}{N!} \sum_{\alpha=1}^{N!} (-1)^{p_\alpha} \mathcal{P}_\alpha \mathcal{S} = \frac{1}{N!} \sum_{\alpha=1}^{N!} (-1)^{p_\alpha} \mathcal{S} = 0 = \mathcal{S} \mathcal{A}, \quad (1.10)$$

since there are $N!/2$ even and odd permutations. We conclude that \mathcal{S} and \mathcal{A} are mutually orthogonal.

Now we can use \mathcal{A} to associate a completely antisymmetric state (as required for fermions) to Eq. (1.3). This is based on the observation that $P_{i,j}\mathcal{A} = -\mathcal{A}$ for an arbitrary pair exchange $P_{i,j}$. Up to a normalization constant C_a to be determined later, it follows that

$$\begin{aligned} |k_1, k_2, \dots, k_N\rangle_a &= C_a \mathcal{A} |k_1, k_2, \dots, k_N\rangle \\ &= \frac{C_a}{N!} \det \begin{pmatrix} |k_1\rangle_{(1)} & |k_1\rangle_{(2)} & \dots & |k_1\rangle_{(N)} \\ |k_2\rangle_{(1)} & |k_2\rangle_{(2)} & \dots & |k_2\rangle_{(N)} \\ \dots & \dots & \dots & \dots \\ |k_N\rangle_{(1)} & |k_N\rangle_{(2)} & \dots & |k_N\rangle_{(N)} \end{pmatrix}. \end{aligned} \quad (1.11)$$

Here k_l is a short-hand notation for the quantum numbers $\{\varepsilon_l, \nu_l\}$, and $|k_l\rangle_{(i)}$ denotes the state of the i th particle. The determinant in Eq. (1.11) is called ‘Slater determinant’. The resulting state satisfies $|k_1, k_2, \dots, k_N\rangle_a = -|k_2, k_1, \dots, k_N\rangle_a$ and similar relations for any other pair exchange, as required. The antisymmetry under pair exchanges ensures that each single-particle state $|k_l\rangle$ appears only once in a non-vanishing completely antisymmetric state². This is known as the ‘Pauli principle’.

The normalization constant is obtained from (note that all N quantum numbers k_l must be distinct)

$$\begin{aligned} 1 &= {}_a \langle k_1, k_2, \dots, k_N | k_1, k_2, \dots, k_N \rangle_a \\ &= |C_a|^2 \langle k_1, k_2, \dots, k_N | \mathcal{A}^\dagger \mathcal{A} | k_1, k_2, \dots, k_N \rangle \\ &= |C_a|^2 \langle k_1, k_2, \dots, k_N | \mathcal{A}^2 | k_1, k_2, \dots, k_N \rangle \\ &= |C_a|^2 \langle k_1, k_2, \dots, k_N | \mathcal{A} | k_1, k_2, \dots, k_N \rangle \\ &= \frac{|C_a|^2}{N!}, \end{aligned}$$

as $C_a = \sqrt{N!}$.

We denote the subspace of the the N -particle Hilbert space \mathcal{H} which is spanned by the completely antisymmetric states by $\mathcal{H}_a^{(N)}$. On $\mathcal{H}_a^{(N)}$ we have the completeness relation³

$$\frac{1}{N!} \sum_{k_1, k_2, \dots, k_N} |k_1, k_2, \dots, k_N\rangle_a {}_a \langle k_1, k_2, \dots, k_N | = \mathbb{1}_a. \quad (1.12)$$

²If a quantum number k_l appears more than once, the antisymmetrized state (1.11) vanishes identically, *i.e.*, there is no state in which two fermions have identical quantum numbers.

³Here we assume that the quantum numbers are discrete. Further below we will also consider the case of continuous quantum numbers.

Each state appears $N!$ times since we have written down independent sums over all the k_1, k_2, \dots, k_N . Hence, we have to divide by $N!$. Alternatively, one can express the antisymmetrized product states in terms of so-called ‘occupation numbers’: the many-body states are uniquely specified if one knows the frequency with which each quantum number appears. Because of the Pauli principle, this frequency can be only 0 or 1 for fermions. Let us order all possible k in an arbitrary but fixed sequence and denote the frequency with which the r th quantum number in this sequence appears by n_r . Now we can specify the completely antisymmetric states in the form $|\{n_r\}\rangle = |n_0, n_1, \dots, n_m, \dots\rangle$. The completeness relation (1.12) now reads

$$\sum_{\{n_r\}; \sum_r n_r = N} |\{n_r\}\rangle \langle \{n_r\}| = \mathbb{1}_a, \quad (1.13)$$

where the symbol

$$\sum_{\{n_r\}; \sum_r n_r = N}$$

stands for

$$\sum_{n_0=0,1} \sum_{n_1=0,1} \dots \sum_{n_m=0,1} \dots$$

with the constraint that $\sum_r n_r = N$.

For bosons we obtain a completely symmetric state in $\mathcal{H}_s^{(N)}$ by applying \mathcal{S} to the product state Eq. (1.3)

$$|k_1, k_2, \dots, k_N\rangle_s = C_s \mathcal{S} |k_1, k_2, \dots, k_N\rangle. \quad (1.14)$$

This state is indeed completely symmetric since $P_{i,j} \mathcal{S} = \mathcal{S}$. There is no constraint on the occupation numbers in the case of bosons. The normalization constant C_s can be shown to be

$$C_s = \sqrt{N!} \left(\prod_{r=0}^{\infty} n_r! \right)^{-1/2},$$

with $0! = 1$. Again, n_r is the frequency with which the r th quantum number appears according to a fixed ordering. The difference to fermions in the result for the normalization arises because bosons can occupy single-particle states more than once. The completeness relation on $\mathcal{H}_s^{(N)}$ reads in terms of the occupation numbers n_r :

$$\sum_{\{n_r\}; \sum_r n_r = N} |\{n_r\}\rangle \langle \{n_r\}| = \mathbb{1}_s, \quad (1.15)$$

where the sums for the individual n_r now run from 0 to N .

The ground state of a system of N non-interacting bosons is obtained by occupying the lowest single-particle state N times. Such a state is automatically completely symmetric. The ground state of a system of N non-interacting fermions is found if the lowest N levels are occupied with one particle each. In this case, the state needs to be antisymmetrized (by forming the Slater determinant). The highest occupied level is called ‘Fermi level’, the corresponding single-particle energy ‘Fermi energy’. It should be noted that the (anti-) symmetrization has physical consequences (e.g., in quantum mechanical expectation values) only if the wave functions of the considered particles overlap. If particles are sufficiently well separated from each other, it may be possible to omit (anti-) symmetrization. In a solid-state problem, however, there is typically significant overlap of at least some electronic wave functions such that proper antisymmetrization is crucial. The symmetry postulate implies that the question which single-particle level is occupied by a given particle makes no sense. It is only possible to say whether there is one particle in a given single-particle state (in the case of fermions) or how many particles are in a single-particle state (for bosons).

1.2 Second quantization

We will now present a formalism which is central to modern quantum mechanical many-body theory since it allows to formulate the symmetry postulate in the formalism in an elegant way. This formalism is known as ‘second quantization’⁴. Here we will discuss only the case of fermions (which is relevant for electrons). Please consult the literature (e.g., the book [3]) for the case of bosons.

The physical Hilbert space of a fixed number of particles N is the completely antisymmetric space $\mathcal{H}_a^{(N)}$. We will now introduce a new Hilbert space – the ‘Fock space’ \mathcal{F} – as a direct sum over all $\mathcal{H}_a^{(N)}$ with $N = 0, 1, 2, \dots$ particles:

$$\mathcal{F} = \mathcal{H}^{(0)} \oplus \mathcal{H}^{(1)} \oplus \mathcal{H}_a^{(2)} \oplus \mathcal{H}_a^{(3)} \oplus \dots \oplus \mathcal{H}_a^{(N)} \oplus \dots \quad (1.16)$$

The space $\mathcal{H}^{(0)}$ is spanned by one state $|\text{vac}\rangle = |0\rangle$ which is called ‘vacuum state’. The Fock space contains all antisymmetric states with an arbitrary number of particles. The space \mathcal{F} inherits a scalar product from the subspaces with a fixed number of particles if we define

$$0 = {}_a \langle k_1, k_2, \dots, k_{N_1} | k'_1, k'_2, \dots, k'_{N_2} \rangle_a \quad (1.17)$$

for $N_1 \neq N_2$. If the $|k\rangle$ constitute a complete orthonormal basis of $\mathcal{H}^{(1)}$, any $|\phi\rangle \in \mathcal{F}$

⁴The name is of historic origin. Evidently we are *not* performing another quantization.

can be decomposed as

$$\begin{aligned}
|\phi\rangle &= |0\rangle\langle 0|\phi\rangle + \int_{k_1} |k_1\rangle\langle k_1|\phi\rangle + \int_{k_1 < k_2} |k_1, k_2\rangle_a \langle k_1, k_2|\phi\rangle + \dots \\
&+ \int_{k_1 < k_2 < \dots < k_N} |k_1, k_2, \dots, k_N\rangle_a \langle k_1, k_2, \dots, k_N|\phi\rangle + \dots \quad (1.18)
\end{aligned}$$

Here we have generalized the notation for the case that the quantum numbers denoted by k can be both discrete or continuous. Since k is a short-hand notation for in general several quantum numbers (*i.e.*, in general not just a real number), we need to specify more precisely what we mean by $k_1 < k_2$. We choose an arbitrary but fixed sequence of the single-particle quantum numbers k , and if k_1 appears before k_2 in this sequence we say that $k_1 < k_2$.

In the next step we define operators c_k^\dagger which go from the space $\mathcal{H}_a^{(N)}$ to the space $\mathcal{H}_a^{(N+1)}$

$$\begin{aligned}
|k\rangle &= c_k^\dagger |0\rangle \\
|k, k_1\rangle_a &= c_k^\dagger |k_1\rangle \\
|k, k_1, k_2\rangle_a &= c_k^\dagger |k_1, k_2\rangle_a \\
\dots &= \dots \\
\dots &= \dots \\
|k, k_1, k_2, \dots, k_N\rangle_a &= c_k^\dagger |k_1, k_2, \dots, k_N\rangle_a \\
\dots &= \dots \quad (1.19)
\end{aligned}$$

By definition, c_k^\dagger applied to a completely antisymmetric state yields another completely antisymmetric state. This means that the ‘creation operator’ c_k^\dagger creates an antisymmetric $N + 1$ -particle state which is specified by the singly occupied single-particles states with quantum numbers k_1, k_2, \dots, k_N and the occupied single-particle states k .

We will show the existence of c_k^\dagger by constructing it:

$$\begin{aligned}
c_k^\dagger &= c_k^\dagger \mathbb{1}_{\mathcal{F}} \\
&= c_k^\dagger \left[|0\rangle\langle 0| + \int_{k_1} |k_1\rangle\langle k_1| + \int_{k_1 < k_2} |k_1, k_2\rangle_a \langle k_1, k_2| + \dots \right. \\
&\quad \left. + \int_{k_1 < k_2 < \dots < k_N} |k_1, k_2, \dots, k_N\rangle_a \langle k_1, k_2, \dots, k_N| + \dots \right]
\end{aligned}$$

$$\begin{aligned}
&= |k\rangle \langle 0| + \sum_{k_1}^{\frown} |k, k_1\rangle \langle k_1| + \sum_{k_1 < k_2}^{\frown} |k, k_1, k_2\rangle_a \langle k_1, k_2| + \dots \\
&+ \sum_{k_1 < k_2 < \dots < k_N}^{\frown} |k, k_1, k_2, \dots, k_N\rangle_a \langle k_1, k_2, \dots, k_N| + \dots
\end{aligned}$$

The antisymmetry of the states implies that

$$\begin{aligned}
c_{k'}^\dagger c_k^\dagger |k_1, k_2, \dots, k_N\rangle_a &= |k', k, k_1, k_2, \dots, k_N\rangle_a \\
&= -|k, k', k_1, k_2, \dots, k_N\rangle_a \\
&= -c_k^\dagger c_{k'}^\dagger |k_1, k_2, \dots, k_N\rangle_a,
\end{aligned}$$

and since $|k_1, k_2, \dots, k_N\rangle_a$ is arbitrary

$$\{c_k^\dagger, c_{k'}^\dagger\} = c_k^\dagger c_{k'}^\dagger + c_{k'}^\dagger c_k^\dagger = 0. \quad (1.20)$$

Here we have introduced the anticommutator

$$\{A, B\} = AB + BA \quad (1.21)$$

of two fermionic operators A and B .

Eq. (1.20) shows that the anticommutator of two creation operators disappears. In particular we have $(c_k^\dagger)^2 = 0$ which expresses the Pauli principle.

Inspection of the explicit construction of c_k^\dagger shows that its adjoint operator $c_k = (c_k^\dagger)^\dagger$ is a map from $\mathcal{H}_a^{(N)}$ to $\mathcal{H}_a^{(N-1)}$. Thus, c_k 'annihilates' a particle and is called annihilation operator. We will now compute the action of c_k on a state $|k_1, k_2, \dots, k_N\rangle_a$. Without loss of generality we assume that $k_1 < k_2 < \dots < k_N$ according to the order introduced above:

$$\begin{aligned}
c_k |k_1, k_2, \dots, k_N\rangle_a &= \sum_{N'=0}^{\infty} \sum_{k'_1 < k'_2 < \dots < k'_{N'}}^{\frown} |k'_1, k'_2, \dots, k'_{N'}\rangle_a \\
&\quad \times {}_a \langle k'_1, k'_2, \dots, k'_{N'} | c_k |k_1, k_2, \dots, k_N\rangle_a \\
&= \sum_{k'_1 < k'_2 < \dots < k'_{N-1}}^{\frown} \left\langle k_1, k_2, \dots, k_N \left| c_k^\dagger \right| k'_1, k'_2, \dots, k'_{N-1} \right\rangle_a^* |k'_1, k'_2, \dots, k'_{N-1}\rangle_a \\
&= \sum_{k'_1 < k'_2 < \dots < k'_{N-1}}^{\frown} {}_a \langle k_1, k_2, \dots, k_N | k, k'_1, k'_2, \dots, k'_{N-1} \rangle_a^* |k'_1, k'_2, \dots, k'_{N-1}\rangle_a.
\end{aligned} \quad (1.22)$$

The left and right states in the scalar product on the last line must contain the same single-particle states in order for the scalar product to be non-vanishing, Therefore,

k must be equal to one of the k_i and the k'_j must match the remaining k_i . Since both the k'_i and the k_i are sorted, we just need to insert k at the correct place among the k_i . In the case $k < k'_1$ the quantum number k is already at the correct place. In the case $k'_1 < k < k'_2$ we need to exchange k and k'_1 which yields a minus sign. For the case $k'_2 < k < k'_3$ we need to perform two swaps yield two minus signs. In general, for $k'_n < k < k'_{n+1}$ we need to perform n swaps and obtain a sign $(-1)^n$. Now we can rewrite (1.22) as

$$c_k |k_1, k_2, \dots, k_N\rangle_a = \delta(k, k_1) |k_2, \dots, k_N\rangle_a - \delta(k, k_2) |k_1, k_3, \dots, k_N\rangle_a + \delta(k, k_3) |k_1, k_2, k_4, \dots, k_N\rangle_a \mp \dots \quad (1.23)$$

Here $\delta(k, k_i)$ denotes either a Kronecker- δ or a δ -function depending on the quantum numbers appearing in k .

With the aid of the relation (1.23) we can compute the anticommutator of c_k and $c_{k'}^\dagger$. We consider

$$\begin{aligned} c_k c_{k'}^\dagger |k_1, k_2, \dots, k_N\rangle_a &= c_k |k', k_1, k_2, \dots, k_N\rangle_a \\ &= \delta(k, k') |k_1, k_2, \dots, k_N\rangle_a - \delta(k, k_1) |k', k_2, \dots, k_N\rangle_a \\ &\quad + \delta(k, k_2) |k', k_1, k_3, \dots, k_N\rangle_a \mp \dots \end{aligned}$$

and

$$\begin{aligned} c_{k'}^\dagger c_k |k_1, k_2, \dots, k_N\rangle_a &= c_{k'}^\dagger [\delta(k, k_1) |k_2, \dots, k_N\rangle_a - \delta(k, k_2) |k_1, k_3, \dots, k_N\rangle_a \\ &\quad + \delta(k, k_3) |k_1, k_2, k_4, \dots, k_N\rangle_a \mp \dots] \\ &= \delta(k, k_1) |k', k_2, \dots, k_N\rangle_a - \delta(k, k_2) |k', k_1, k_3, \dots, k_N\rangle_a \\ &\quad + \delta(k, k_3) |k', k_1, k_2, k_4, \dots, k_N\rangle_a \mp \dots \end{aligned}$$

Summation of these two equations yields

$$(c_k c_{k'}^\dagger + c_{k'}^\dagger c_k) |k_1, k_2, \dots, k_N\rangle_a = \delta(k, k') |k_1, k_2, \dots, k_N\rangle_a$$

and hence the anticommutation relations

$$\{c_k, c_{k'}^\dagger\} = c_k c_{k'}^\dagger + c_{k'}^\dagger c_k = \delta(k, k') \quad (1.24)$$

The adjoint of Eq. (1.20) yields the relation $\{c_k, c_{k'}\} = 0$. This determines all anticommutation relations of the creation and annihilation operators.

Now the basis states $|k_1, k_2, \dots, k_N\rangle_a$ can be obtained by repeated application of the creation operators to the vacuum state $|0\rangle$

$$|k_1, k_2, \dots, k_N\rangle_a = c_{k_1}^\dagger c_{k_2}^\dagger \dots c_{k_N}^\dagger |0\rangle = \left(\prod_{i=1}^N c_{k_i}^\dagger \right) |0\rangle. \quad (1.25)$$

The right-hand side of this equation specifies which single-particle states are occupied. However, the unphysical question which electron is in which particular state does not arise.

The creation and annihilation operators have been constructed in a fixed basis $\{|k\rangle\}$ of the single-particle problem. Of course, we could start from any other basis $\{|\varphi\rangle\}$ with

$$|\varphi\rangle = \sum_k |k\rangle \langle k | \varphi\rangle = \sum_k a_{k,\varphi} |k\rangle . \quad (1.26)$$

In order to see how one can go from the $c_k^{(\dagger)}$ to the $c_\varphi^{(\dagger)}$ corresponding to $\{|\varphi\rangle\}$, we first consider a special case, namely

$$c_\varphi^\dagger |0\rangle = |\varphi\rangle = \sum_k |k\rangle \langle k | \varphi\rangle = \sum_k \langle k | \varphi\rangle c_k^\dagger |0\rangle .$$

This suggests that

$$c_\varphi^\dagger = \sum_k \langle k | \varphi\rangle c_k^\dagger , \quad c_\varphi = \sum_k \langle \varphi | k\rangle c_k . \quad (1.27)$$

In order to prove these relations we consider the matrix element

$$\begin{aligned} & \left\langle \varphi_1, \varphi_2, \dots, \varphi_{N-1} \left| \left(c_\varphi - \sum_k \langle \varphi | k\rangle c_k \right) \right| k_1, k_2, \dots, k_N \right\rangle_a \\ &= {}_a \langle \varphi, \varphi_1, \varphi_2, \dots, \varphi_{N-1} | k_1, k_2, \dots, k_N \rangle_a \\ & - [\langle \varphi | k_1 \rangle {}_a \langle \varphi_1, \varphi_2, \dots, \varphi_{N-1} | k_2, k_3, \dots, k_N \rangle_a \\ & - \langle \varphi | k_2 \rangle {}_a \langle \varphi_1, \varphi_2, \dots, \varphi_{N-1} | k_1, k_3, \dots, k_N \rangle_a \\ & \pm \dots] . \end{aligned}$$

The scalar product ${}_a \langle \varphi, \varphi_1, \varphi_2, \dots, \varphi_{N-1} | k_1, k_2, \dots, k_N \rangle_a$ can be expressed as a determinant (see Eq. (1.11)). Expansion of this determinant in its first column yields exactly the expression in [...] such that the matrix element disappears. This proves the relations Eq. (1.27).

Frequently, the creation and annihilation operators are used in a single-particle basis consisting of position and spin eigenstates $\{|\mathbf{x}, \sigma\rangle\}$. In the case of continuum models, these so-called 'field operators' are written as $\psi_\sigma^{(\dagger)}(\mathbf{x})$. The field operators satisfy the anticommutation relations

$$\begin{aligned} \left\{ \psi_\sigma(\mathbf{x}), \psi_{\sigma'}^\dagger(\mathbf{x}') \right\} &= \delta_{\sigma,\sigma'} \delta(\mathbf{x} - \mathbf{x}') \\ \left\{ \psi_\sigma(\mathbf{x}), \psi_{\sigma'}(\mathbf{x}') \right\} &= 0 \\ \left\{ \psi_\sigma^\dagger(\mathbf{x}), \psi_{\sigma'}^\dagger(\mathbf{x}') \right\} &= 0 . \end{aligned} \quad (1.28)$$

1.3 Observables

We will now generalize observables of a system of N identical fermions (defined on $\mathcal{H}_a^{(N)}$) to the Fock space and express them in terms of the creation and annihilation operators. First we note that any observable O acting in $\mathcal{H}_a^{(N)}$ is symmetric under exchange of any pair of particles because these particles are indistinguishable. It follows that $[O, \mathcal{A}] = 0$ and we have for any state $|\phi\rangle \in \mathcal{H}_a^{(N)}$

$$\begin{aligned}
 O|\phi\rangle &= \frac{1}{N!} \sum_{k_1, k_2, \dots, k_N} O |k_1, k_2, \dots, k_N\rangle_a \langle k_1, k_2, \dots, k_N | \phi\rangle \\
 &= \frac{\sqrt{N!}}{N!} \sum_{k_1, k_2, \dots, k_N} OA |k_1, k_2, \dots, k_N\rangle_a \langle k_1, k_2, \dots, k_N | \phi\rangle \\
 &= \frac{1}{\sqrt{N!}} \sum_{k_1, k_2, \dots, k_N} AO |k_1, k_2, \dots, k_N\rangle_a \langle k_1, k_2, \dots, k_N | \phi\rangle . \quad (1.29)
 \end{aligned}$$

This implies that it is sufficient to know the action of the operator O on a product state $|k_1, k_2, \dots, k_N\rangle$.

Let us first consider the case that O is a single-particle operator $O = \sum_i o(i)$ such that $o(i)$ acts only on the ‘coordinates’ of the i th particle. The operator $o(i)$ satisfies

$$o(i) |k\rangle_{(i)} = \sum_{k'} |k'\rangle_{(i)} \langle k' | o | k\rangle ,$$

with $o = o(1)$. The latter is valid since all $o(i)$ have identical forms. In addition, we have dropped the particle index i in the matrix element $\langle k' | o | k\rangle$ since it does no longer play any rôle. Application of this result to a product state yields

$$\begin{aligned}
 O |k_1, k_2, \dots, k_N\rangle &= \sum_{i=1}^N o(i) |k_1, k_2, \dots, k_N\rangle \\
 &= \sum_{i=1}^N \sum_k \langle k | o | k_i\rangle |k_1, k_2, \dots, k_{i-1}, k, k_{i+1}, \dots, k_N\rangle .
 \end{aligned}$$

Insertion into Eq. (1.29) leads to

$$\begin{aligned}
O|\phi\rangle &= \frac{1}{\sqrt{N!}} \int_{k_1, k_2, \dots, k_N} \mathcal{A} O |k_1, k_2, \dots, k_N\rangle_a \langle k_1, k_2, \dots, k_N | \phi\rangle \\
&= \frac{1}{\sqrt{N!}} \int_{k_1, \dots, k_N} \sum_{i=1}^N \int_{\mathcal{J}_k} \langle k | o | k_i \rangle \mathcal{A} |k_1, \dots, k_{i-1}, k, k_{i+1}, \dots, k_N\rangle_a \langle k_1, \dots, k_N | \phi\rangle \\
&= \frac{1}{N!} \int_{k_1, \dots, k_N} \sum_{i=1}^N \int_{\mathcal{J}_k} \langle k | o | k_i \rangle |k_1, \dots, k_{i-1}, k, k_{i+1}, \dots, k_N\rangle_a \langle k_1, \dots, k_N | \phi\rangle \\
&= \frac{1}{N} \sum_{i=1}^N \int_{k, k_i} \langle k | o | k_i \rangle \frac{1}{(N-1)!} \int_{k_1, \dots, k_{i-1}, k_{i+1}, \dots, k_N} (-1)^i c_k^\dagger |k_1, \dots, k_{i-1}, k_{i+1}, \dots, k_N\rangle_a \\
&\quad \times {}_a \langle k_1, \dots, k_{i-1}, k_{i+1}, \dots, k_N | (-1)^i c_{k_i} | \phi \rangle.
\end{aligned}$$

Exploiting the completeness relation in $\mathcal{H}_a^{(N-1)}$ we find

$$O|\phi\rangle = \int_{k, k'} \langle k | o | k' \rangle c_k^\dagger c_{k'} |\phi\rangle$$

for any fixed $i = 1, 2, \dots, N$, hence

$$O = \int_{k, k'} \langle k | o | k' \rangle c_k^\dagger c_{k'} \quad (1.30)$$

for the action of O on the Fock space \mathcal{F} .

Let us consider some important examples:

a) Kinetic energy (continuum, periodic boundary conditions):

The kinetic energy is given on $\mathcal{H}_a^{(N)}$ by

$$T = \sum_{i=1}^N \frac{\hat{\mathbf{p}}_i^2}{2m}.$$

The extension to \mathcal{F} reads

$$T = \sum_{\sigma} \sum_p \frac{\mathbf{p}^2}{2m} c_{p, \sigma}^\dagger c_{p, \sigma}$$

since $\langle \mathbf{p}', \sigma' | \hat{\mathbf{p}} | \mathbf{p}'', \sigma'' \rangle = \delta_{\sigma', \sigma''} \mathbf{p}' \delta_{\mathbf{p}', \mathbf{p}''}$ if $|\mathbf{p}, \sigma\rangle$ denotes the single-particle states in the momentum-spin representation.

b) Particle density:

Starting from the particle density

$$\rho(\mathbf{x}) = \sum_{i=1}^N \delta(\mathbf{x} - \hat{\mathbf{x}}_i)$$

on $\mathcal{H}_a^{(N)}$, we find

$$\rho(\mathbf{x}) = \sum_{\sigma} \psi_{\sigma}^{\dagger}(\mathbf{x}) \psi_{\sigma}(\mathbf{x})$$

on \mathcal{F} since $\langle \mathbf{x}', \sigma' | \delta(\mathbf{x} - \hat{\mathbf{x}}) | \mathbf{x}'', \sigma'' \rangle = \delta_{\sigma', \sigma''} \delta(\mathbf{x}' - \mathbf{x}'') \delta(\mathbf{x} - \mathbf{x}')$ in the position-spin representation.

c) Single-particle part of the Hamiltonian $H_0 = \sum_i h(i)$:

The single-particle part reads on $\mathcal{H}_a^{(N)}$

$$H_0 = \sum_{i=1}^N \left(\frac{\hat{\mathbf{p}}_i^2}{2m} + u(\hat{\mathbf{x}}_i) \right) .$$

Since we have $\langle \mathbf{x}', \sigma' | \hat{\mathbf{p}} | \mathbf{x}'', \sigma'' \rangle = -i\hbar \delta_{\sigma', \sigma''} \nabla_{\mathbf{x}'} \delta(\mathbf{x}' - \mathbf{x}'')$, we find on \mathcal{F}

$$H_0 = \sum_{\sigma} \int d\mathbf{x} \psi_{\sigma}^{\dagger}(\mathbf{x}) \left(-\frac{\hbar^2}{2m} \nabla^2 + u(\mathbf{x}) \right) \psi_{\sigma}(\mathbf{x}) . \quad (1.31)$$

It is more elegant to write H_0 in the basis $\{|k\rangle\}$ of eigenstates of h (here we assume for simplicity that the k are discrete):

$$H_0 = \sum_k \varepsilon_k c_k^{\dagger} c_k = \sum_k \varepsilon_k \hat{n}_k , \quad (1.32)$$

with the particle number operator $\hat{n}_k = c_k^{\dagger} c_k$. The definition of the creation and annihilation operators implies that $\hat{n}_k |k_1, \dots, k_N\rangle_a = |k_1, \dots, k_N\rangle_a$ if the single-particle state with the quantum number k is (singly) occupied and $\hat{n}_k |k_1, \dots, k_N\rangle_a = 0$ otherwise, thus justifying the name of the operator.

The next step is to consider pair interactions on $\mathcal{H}_a^{(N)}$ of the form

$$V = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^N V(i, j) . \quad (1.33)$$

An important example for particles of charge Q is the Coulomb interaction

$$V_{\text{coul}} = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^N \frac{Q^2}{|\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j|} . \quad (1.34)$$

Using similar considerations as above, one can show that the representation of (1.33) on \mathcal{F} is

$$V = \frac{1}{2} \sum_{k_1, k_2, k_3, k_4} v_{k_1, k_2, k_3, k_4} c_{k_1}^\dagger c_{k_2}^\dagger c_{k_4} c_{k_3} \quad (1.35)$$

with $v_{k_1, k_2, k_3, k_4} = \langle k_1, k_2 | V(1, 2) | k_3, k_4 \rangle$.

This yields the following representation of (1.34)

$$V_{\text{coul}} = \frac{Q^2}{2} \sum_{\sigma_1, \sigma_2} \int d\mathbf{x}_1 \int d\mathbf{x}_2 \frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|} \psi_{\sigma_1}^\dagger(\mathbf{x}_1) \psi_{\sigma_2}^\dagger(\mathbf{x}_2) \psi_{\sigma_2}(\mathbf{x}_2) \psi_{\sigma_1}(\mathbf{x}_1)$$

in the position-spin representation.

More generally, we can combine (1.32) and (1.35) to represent the full Hamiltonian $H = H_0 + V$ given by Eq. (1.1) in a basis of eigenstates $\{|k\rangle\}$ of h (we assume again for simplicity that the quantum numbers k are discrete)

$$H = \sum_k \varepsilon_k c_k^\dagger c_k + \frac{1}{2} \sum_{k_1, k_2, k_3, k_4} v_{k_1, k_2, k_3, k_4} c_{k_1}^\dagger c_{k_2}^\dagger c_{k_4} c_{k_3} . \quad (1.36)$$

1.4 Fermi function

The computation of thermodynamic quantities is most easily performed in the *grand-canonical* ensemble. Therefore we add the particle number with a chemical potential μ to the Hamiltonian:

$$K = H - \mu \hat{N} , \quad (1.37)$$

where \hat{N} is a diagonal operator in the particle-number representation and acts as N in $\mathcal{H}_a^{(N)}$.

In complete analogy to (1.32), the non-interacting part K_0 of K can be written as

$$K_0 = \sum_k (\varepsilon_k - \mu) c_k^\dagger c_k = \sum_k (\varepsilon_k - \mu) \hat{n}_k . \quad (1.38)$$

Since the $c_k^{(\dagger)}$ with different k anticommute with each other, all particle-number operators \hat{n}_k commute. This renders it straightforward to compute the grand-canonical partition function of a non-interacting gas of electrons:

$$\begin{aligned} Z &= \text{Tr}_{\mathcal{F}} e^{-K_0/(k_B T)} = \sum_{n_0=0}^1 \sum_{n_1=0}^1 \sum_{n_2=0}^1 \dots \exp\left(-\frac{\sum_{r=0}^{\infty} n_r (\varepsilon_r - \mu)}{k_B T}\right) \\ &= \prod_{r=0}^{\infty} \left(\sum_{n_r=0}^1 \exp\left(-\frac{n_r (\varepsilon_r - \mu)}{k_B T}\right) \right) = \prod_{r=0}^{\infty} \left(1 + \exp\left(-\frac{(\varepsilon_r - \mu)}{k_B T}\right) \right) . \end{aligned} \quad (1.39)$$

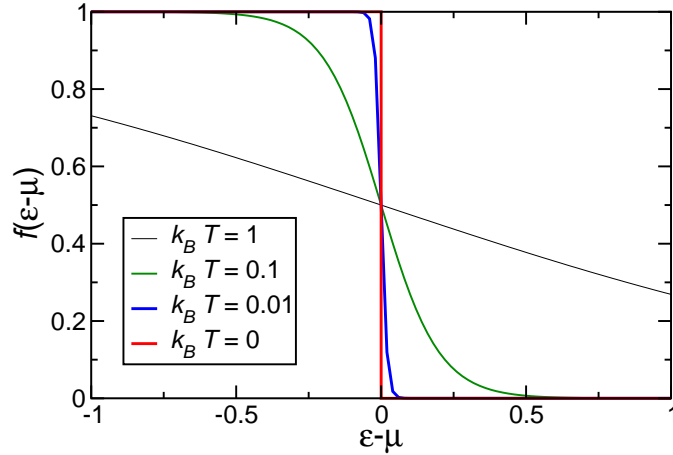


Figure 1.2: Fermi function at four different temperatures.

Here k_B is Boltzmann's constant and we have again used an enumeration of the single-particle quantum numbers k by positive integers r . Next we compute the expectation value of the occupation of the single-particle state s :

$$\begin{aligned}
 \langle \hat{n}_s \rangle &= \frac{1}{Z} \text{Tr}_{\mathcal{F}} \hat{n}_s e^{-K_0/(k_B T)} \\
 &= \frac{1}{Z} \sum_{n_0=0}^1 \sum_{n_1=0}^1 \sum_{n_2=0}^1 \cdots \sum_{n_{s-1}=0}^1 \sum_{n_{s+1}=0}^1 \cdots \\
 &\quad \times \exp \left(-\frac{\sum_{r=0}^{s-1} n_r (\varepsilon_r - \mu) + (\varepsilon_s - \mu) + \sum_{r=s+1}^{\infty} n_r (\varepsilon_r - \mu)}{k_B T} \right) \\
 &= \frac{1}{Z} \left(\prod_{r=0}^{s-1} \left(\sum_{n_r=0}^1 \exp \left(-\frac{n_r (\varepsilon_r - \mu)}{k_B T} \right) \right) \right) \exp \left(-\frac{\varepsilon_s - \mu}{k_B T} \right) \\
 &\quad \times \left(\prod_{r=s+1}^{\infty} \left(\sum_{n_r=0}^1 \exp \left(-\frac{n_r (\varepsilon_r - \mu)}{k_B T} \right) \right) \right) \\
 &= \frac{\exp \left(-\frac{\varepsilon_s - \mu}{k_B T} \right)}{1 + \exp \left(-\frac{\varepsilon_s - \mu}{k_B T} \right)} = \frac{1}{\exp \left(\frac{\varepsilon_s - \mu}{k_B T} \right) + 1} = f(\varepsilon_s - \mu). \tag{1.40}
 \end{aligned}$$

The final result is very simple because most terms of the numerator and the denominator (1.39) cancel. The result $f(\varepsilon_s - \mu)$ is called the *Fermi function*.

The Fermi function is shown in Fig. 1.2 for four different temperatures. Upon decreasing temperatures it steepens and reaches a step function for $T \rightarrow 0$. At $T = 0$, $f(\varepsilon - \mu) = 1$ for $\varepsilon < \mu$, *i.e.*, all states with $\varepsilon < \mu$ are occupied while $f(\varepsilon - \mu) = 0$ for $\varepsilon > \mu$, showing that all states with $\varepsilon > \mu$ are empty. Therefore, we can identify

the chemical potential μ with the Fermi energy. In a translationally invariant system, the momentum \mathbf{k} is a good quantum number. Thus, for $T = 0$ we can define the hypersurface in k -space separating occupied from unoccupied states by the locations where the Fermi function jumps. This surface is called the *Fermi surface*.

2 Fermi liquids

The solution of the single-electron problem (1.2) is usually comparably easy. By contrast, the solution of the interacting many-body problem (1.36) is a very difficult task. Note that in a solid-state system (Coulomb) interaction energies and kinetic energy are usually both on the scale of eV. Under certain circumstances like in transition metal compounds, the Coulomb energy can even be substantially bigger than the kinetic energy. Hence, one may wonder why it is useful to solve the problem of non-interacting electrons in the first place. We will answer this question in the present chapter by introducing the phenomenological concept of a Fermi liquid which establishes a relation between an interacting and a non-interacting electron gas. Then we will add some comments on a microscopic point of view of a Fermi liquid.

2.1 Landau-Fermi liquid

We will now introduce the concept of a Fermi liquid. The presentation will follow largely chapter 6 of the book [23] as well as chapter 8 of the lecture notes [7] (note also chapter II.2 of the lecture notes [25], as well as chapters 6.1 and 6.2 of the book [20]).

Until the 1950ies, free fermions were the only well-understood Fermi systems. At the same time, ${}^3\text{He}$ was under intensive investigation. On the one hand, ${}^3\text{He}$ is an ideal Fermi system, on the other hand there are substantial deviations from the non-interacting case. On this background Landau developed his phenomenological theory of Fermi liquids [13] (a good summary of the early developments can be found, e.g., in [2]). The basic idea is that weakly (or sometimes even strongly) interacting electrons behave in many respect as a non-interacting Fermi gas at low energies.

To be more precise, Landau's theory of normal Fermi liquids is based on the following assumptions:

1. There is a one-to-one correspondence between the low-energy excitations of the interacting system and the system without interactions. In particular, we can characterize the excitations in both systems using the same quantum numbers. For a translationally invariant system we use the momentum \mathbf{k} and spin σ .
2. The low-energy excitations are quasiparticles which can be specified by their occupation numbers $n_{\mathbf{k},\sigma}$. In particular, the energy depends only on the occupation numbers of the quasiparticle states, *i.e.*, $E = E[n_{\mathbf{k},\sigma}]$.
3. Changes in the occupation numbers are sufficiently small for low temperatures and weak external perturbations such that cubic contributions to the energy

can be neglected (this assumption allows us in particular to use linear response theory).

4. In external fields which vary slowly both in space and time, it is possible to specify a local instantaneous energy which depends only on the local instantaneous occupation numbers.

The second assumption enables us to write the energy as

$$E = E[\delta n_{\mathbf{k},\sigma}] , \quad (2.1)$$

where $\delta n_{\mathbf{k},\sigma}$ is the deviation of the occupation numbers from those of the ground state. By virtue of the third assumption we can expand the energy as follows:

$$E = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \delta n_{\mathbf{k},\sigma} + \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} f(\mathbf{k}, \mathbf{k}', \sigma, \sigma') \delta n_{\mathbf{k},\sigma} \delta n_{\mathbf{k}',\sigma'} . \quad (2.2)$$

Here we encounter a new phenomenological function f which describes the interactions. In the case of a homogeneous and isotropic system, f depends only on the combination $\mathbf{k} - \mathbf{k}'$.

The *quasiparticle energy* $\tilde{\epsilon}_{\mathbf{k},\sigma}$ is the energy which is required to increase the number of quasiparticles with the quantum numbers \mathbf{k} and σ by one. If we interpret $\delta n_{\mathbf{k},\sigma}$ as density, Eq. (2.2) implies that

$$\tilde{\epsilon}_{\mathbf{k},\sigma} = \frac{\partial E}{\partial (\delta n_{\mathbf{k},\sigma})} = \epsilon_{\mathbf{k}} + \sum_{\mathbf{k}',\sigma'} f(\mathbf{k}, \mathbf{k}', \sigma, \sigma') \delta n_{\mathbf{k}',\sigma'} . \quad (2.3)$$

In equilibrium and at $T = 0$ we have $\delta n_{\mathbf{k}',\sigma'} = 0$ and therefore

$$\tilde{\epsilon}_{\mathbf{k},\sigma} = \epsilon_{\mathbf{k}} . \quad (2.4)$$

Furthermore, if we fix the zero of energy relative to the chemical potential, the *Fermi surface* is defined by

$$\epsilon_{\mathbf{k}} = 0 . \quad (2.5)$$

For an isotropic system we have $\epsilon_{\mathbf{k}} = \epsilon_k$ with $k = |\mathbf{k}|$. In this case, we can define a Fermi momentum k_F by

$$\epsilon_{k_F} = 0 . \quad (2.6)$$

Under the assumption that the interaction does not change the order of the excited energies, we have

$$\begin{aligned} \epsilon_k &> 0 && \text{for } k > k_F, \\ \epsilon_k &< 0 && \text{for } k < k_F. \end{aligned} \quad (2.7)$$

Now the first assumption implies that the number of states with $k < k_F$ is equal to the average particle density n , i.e.,

$$n = \frac{2}{(2\pi)^3} \int d^3k \Theta(k_F - k) = \frac{k_F^3}{3\pi^2}, \quad (2.8)$$

where the factor 2 accounts for the two possible spin projections.

Furthermore, the low-energy excitations are exactly those with k close to k_F . We can therefore expand

$$\epsilon_k = \frac{k_F}{m^*} (k - k_F). \quad (2.9)$$

In this expansion we encounter a parameter m^* which is called 'effective mass'.

Next, we make a mean-field type approximation: while the occupation numbers $\delta n_{\mathbf{k},\sigma}$ are subject to thermal and quantum fluctuations, we have for low temperatures $|\delta n_{\mathbf{k},\sigma} - \langle \delta n_{\mathbf{k},\sigma} \rangle| \ll |\langle \delta n_{\mathbf{k},\sigma} \rangle|$. Thus, we can expand the functional (2.2) in fluctuations. Because of the third assumption we can neglect cubic terms as before and obtain

$$\begin{aligned} E &= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \delta n_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} f(\mathbf{k},\mathbf{k}',\sigma,\sigma') \langle \delta n_{\mathbf{k}',\sigma'} \rangle \delta n_{\mathbf{k},\sigma} \\ &\quad - \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} f(\mathbf{k},\mathbf{k}',\sigma,\sigma') \langle \delta n_{\mathbf{k},\sigma} \rangle \langle \delta n_{\mathbf{k}',\sigma'} \rangle \\ &= \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} + U_{\mathbf{k},\sigma}) \delta n_{\mathbf{k},\sigma} - \frac{1}{2} \sum_{\mathbf{k},\sigma} U_{\mathbf{k},\sigma} \langle \delta n_{\mathbf{k},\sigma} \rangle \end{aligned} \quad (2.10)$$

with a so-called molecular field

$$U_{\mathbf{k},\sigma} = \sum_{\mathbf{k}',\sigma'} f(\mathbf{k},\mathbf{k}',\sigma,\sigma') \langle \delta n_{\mathbf{k}',\sigma'} \rangle. \quad (2.11)$$

Eq. (2.10) allows us to interpret the quasi-particles as electrons with energy $\epsilon_{\mathbf{k}} + U_{\mathbf{k},\sigma}$. We can therefore copy the Fermi function (1.40) for the occupation at a finite temperature $T > 0$

$$\delta n_{\mathbf{k},\sigma} = \frac{1}{e^{\beta(\epsilon_{\mathbf{k}} + U_{\mathbf{k},\sigma})} + 1} - \Theta(k_F - k). \quad (2.12)$$

If we assume that the system is isotropic, as we have already done above, it follows that $U_{\mathbf{k},\sigma}$ is independent of the direction $\mathbf{k}/|\mathbf{k}|$, and it should not depend on the spin σ either. We conclude that $U_{\mathbf{k},\sigma} = U$ is a constant. On the other hand, particle-number conservation implies that $\sum_{\mathbf{k},\sigma} \langle \delta n_{\mathbf{k},\sigma} \rangle = 0$. If we combine this with (2.11)

and the fact that U is constant, we conclude that $U_{\mathbf{k},\sigma} = 0$. Thus, the distribution function (2.12) reads in fact

$$\delta n_{\mathbf{k},\sigma} = \frac{1}{e^{\beta \epsilon_{\mathbf{k}}} + 1} - \Theta(k_F - k). \quad (2.13)$$

This shows that the free energy of a normal Fermi liquid has the same form as that of a gas of free electrons!

Specific heat:

Let us introduce first the density of states at the Fermi surface:

$$N(0) = \frac{4\pi k^2}{(2\pi)^3} \left. \frac{dk}{dE} \right|_{k=k_F} = \frac{m^* k_F}{2\pi^2}, \quad (2.14)$$

where we have inserted dE/dk according to (2.9). Now we find the specific heat as

$$C_V = \frac{dE}{dT} = \frac{d}{dT} \frac{2}{(2\pi)^3} \int d^3k \epsilon_{\mathbf{k}} f(\epsilon_{\mathbf{k}}) = 2 N(0) \int_{-\infty}^{\infty} d\epsilon \epsilon \frac{d}{dT} \frac{1}{e^{\beta \epsilon} + 1}, \quad (2.15)$$

where we have taken the spin degeneracy into account with a factor 2. The differentiation yields

$$\frac{d}{dT} \frac{1}{e^{\beta \epsilon} + 1} = \frac{-\epsilon e^{\beta \epsilon} \frac{d}{dT} \beta}{(e^{\beta \epsilon} + 1)^2} = \frac{\frac{1}{T} \beta \epsilon}{(e^{\beta \epsilon} + 1)(e^{-\beta \epsilon} + 1)} \quad (2.16)$$

and we can evaluate (2.15):

$$\begin{aligned} C_V &= 2 N(0) \int_{-\infty}^{\infty} d\epsilon \frac{k_B (\beta \epsilon)^2}{(e^{\beta \epsilon} + 1)(e^{-\beta \epsilon} + 1)} \\ &= 2 N(0) k_B^2 T \int_{-\infty}^{\infty} dx \frac{x^2}{(e^x + 1)(e^{-x} + 1)} = \gamma T. \end{aligned} \quad (2.17)$$

Here we have substituted $x = \beta \epsilon$ under the integral. The linear behavior of the specific heat at low temperatures is one of the characteristic features of a Fermi liquid. If we further insert the value of the integral as $\pi^2/3$, we can read off the coefficient γ in (2.17) as

$$\gamma = \frac{2}{3} \pi^2 N(0) k_B^2. \quad (2.18)$$

Remember that the effective mass m^* appears in $N(0)$, see Eq. (2.14).

Effective mass:

For a translationally invariant system, the effective mass m^* depends on the phenomenological function f . In order to specify the relation more precisely, it is useful to exploit isotropy, translational invariance and $SU(2)$ -symmetry and expand the function f in Legendre polynomials P_l

$$2N(0)f(\mathbf{k}, \mathbf{k}', \sigma, \sigma') = \sum_l (F_l + Z_l \boldsymbol{\sigma} \cdot \boldsymbol{\sigma}') P_l(\cos \theta), \quad (2.19)$$

where $\mathbf{k} \cdot \mathbf{k}' = k k' \cos \theta$.

Now we consider a total system which moves with a velocity \mathbf{v} . On the one hand, the total momentum of the system is given by $\mathbf{P} = Nm\mathbf{v}$, where the total mass is given by the number of fermions N multiplied with their *free* mass m . On the other hand, the system responds to the movement with a change of the occupation numbers $\delta n_{\mathbf{k}, \sigma}$. Both points of view are related by a Galilei transformation. Here we just quote the result (derivations can be found, e.g., in chapter 8.8 of the lecture notes [7], chapter II.2.1 of the lecture notes [25] as well as in chapter 6.1(b) of the book [23]):

$$\frac{m^*}{m} = 1 + \frac{1}{3} F_1. \quad (2.20)$$

Magnetic susceptibility:

We will now discuss briefly another quantity, namely the magnetic susceptibility χ . For this end we first have to add a magnetic contribution to the energy (2.2). Using a second-quantization notation, the magnetic contribution to the Hamiltonian reads

$$H_M = \frac{1}{2} \int d^3x \psi_\sigma^\dagger(\mathbf{x}) g \boldsymbol{\sigma} \cdot \mathbf{B}(\mathbf{x}) \psi_\sigma(\mathbf{x}). \quad (2.21)$$

The magnetic susceptibility χ describes the response of the magnetization to a constant external magnetic field. We skip again a detailed derivation⁵ and just quote the result:

$$\frac{\chi}{\chi_0} = \frac{1 + \frac{1}{3} F_1}{1 + \frac{1}{4} Z_0} = \frac{m^*}{m \left(1 + \frac{1}{4} Z_0\right)}, \quad (2.22)$$

where χ_0 is the magnetic susceptibility of free fermions with mass m .

Resistivity:

Lastly, we would like to comment briefly on the electrical resistivity $\rho(T)$ which is straightforward to measure experimentally and therefore quite important. There are, however, two differences with respect to the quantities considered before. First

⁵Here we finally need the fourth assumption. Computations can be found, e.g., in chapter 6.1(d,e) of the book [23] as well as chapter II.2.2 of the lecture notes [25].

of all, the fermions now need to carry an electric charge since otherwise no charge can be transported. Secondly, the resistivity is in fact related to the dynamics of the system. This means that scattering processes need to be investigated. Electron-electron interactions give rise to a scattering rate $\tau^{-1} \propto T^2$ (see the next subsection for a qualitative discussion and, e.g., chapter 8.12.1 of the lecture notes [7] for more details). This translates into the following low-temperature asymptotics

$$\rho(T) = \rho_0 + AT^2, \quad (2.23)$$

which is characteristic of a Fermi liquid. Here, the ‘residual’ resistivity ρ_0 arises because of scattering by impurities and is therefore of extrinsic origin.

To summarize, the main feature of Landau’s theory of Fermi liquids is that the functional forms are exactly as in free electrons, however with ‘renormalized’ parameters (effective mass, etc.). Still, the interaction renders the different constants independent. For example, the magnetic susceptibility of free fermions with an effective mass m^* would be given by $\chi/\chi_0 = m^*/m$, but in a Fermi liquid the presence of the interaction parameter Z_0 allows for deviations from this relation in (2.22).

2.2 Microscopic origin of a Landau-Fermi liquid

The phenomenological picture of the preceding section can be derived in a more microscopic manner using perturbation theory for interacting electrons. Of course, a condition for such a ‘derivation’ is that perturbation theory converges. In the context of perturbation theory there is natural one-to-one correspondence between the states of the free and the interacting Fermi gas, *i.e.*, the first basic assumption comes along natural. In particular, one can view quasiparticles as electrons dressed with perturbative corrections. The formalization of this argument using perturbation theory to arbitrary order (see, e.g., chapter 6.2 of [23] and [15]) or even just the lowest orders of perturbation theory (see, e.g., chapters II.3.2 and II.3.3 of the lecture notes [25] and chapter 5.3 of the book [20]) would require Green functions which we have had no time to discuss. I will nevertheless try to give you an idea of the main ingredients.

We will now mention some essential properties of the quasiparticles. It is convenient to choose the zero of energy such that the Fermi energy is given by $\epsilon_{\mathbf{k}_F} = 0$.

Quasiparticles can be observed in the spectral function $A(\mathbf{k}, \omega)$ which describes the matrix element for the addition or removal of an electron with momentum transfer \mathbf{k} and energy transfer ω . The spectral function of a Landau-Fermi liquid is sketched in Fig. 2.1. For a free electron gas, we would have $A(\mathbf{k}, \omega) = \delta(\epsilon_{\mathbf{k}} - \omega)$. This δ -function is generally broadened by interactions such that we can describe the quasiparticle peak

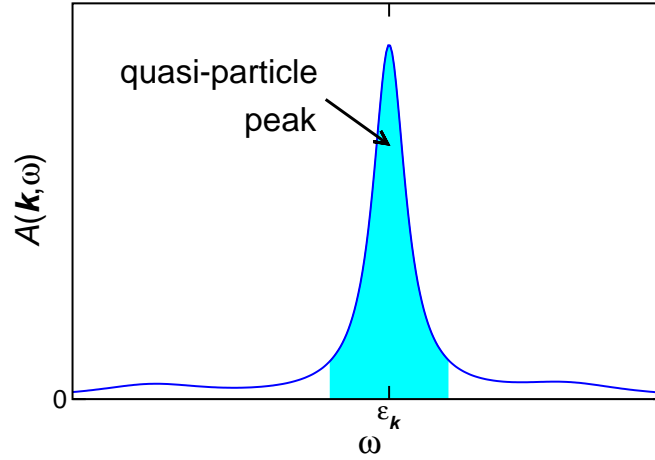


Figure 2.1: Spectral function $A(\mathbf{k}, \omega)$ with a 'quasiparticle pole' of weight Z_{k_F} .

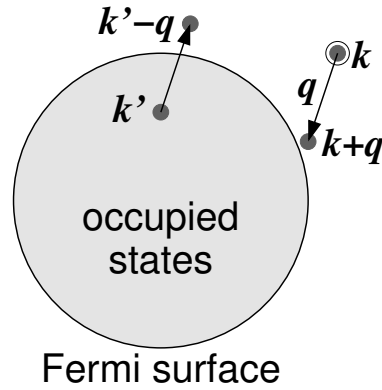


Figure 2.2: Scattering process contributing to the quasiparticle lifetime.

by a pole in the complex ω -plane with a (small) imaginary part. This broadening, or equivalently the imaginary part signifies a finite life-time τ of the quasiparticle.

A key ingredient of the Landau-Fermi liquids is that

$$\tau^{-1} \propto \epsilon_{\mathbf{k}}^2. \quad (2.24)$$

This means that the lifetime τ becomes infinite for $\epsilon_{\mathbf{k}} \rightarrow 0$, *i.e.*, very close to the Fermi surface the quasiparticles become in fact stable particles.

The reason behind (2.24) is essentially a phase-space consideration for scattering processes. This can be seen for instance if we apply Fermi's golden rule to the scattering of an occupied state $\epsilon_{\mathbf{k}}$ outside the Fermi surface while creating a particle-hole pair at the same time (compare Fig. 2.2). This yields the following contribution

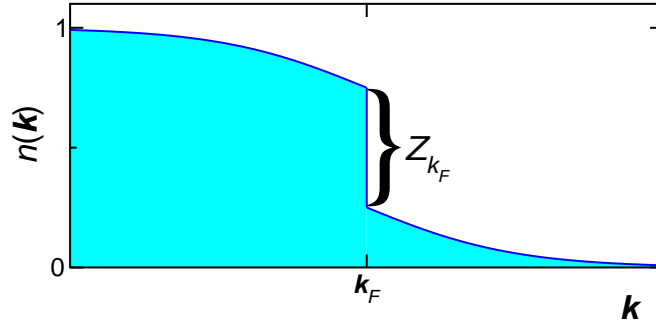


Figure 2.3: Momentum distribution for a Fermi liquid. Note the jump of height Z_{k_F} at k_F .

to the lifetime:

$$\tau^{-1} \propto \sum_{\mathbf{k}', \mathbf{q}} |V(\mathbf{q})|^2 f(\epsilon_{\mathbf{k}'}) (1 - f(\epsilon_{\mathbf{k}+\mathbf{q}})) (1 - f(\epsilon_{\mathbf{k}'-\mathbf{q}})) \times \delta(\omega - (\epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}'-\mathbf{q}} - \epsilon_{\mathbf{k}})). \quad (2.25)$$

Now $-\epsilon_{\mathbf{k}'}$, $\epsilon_{\mathbf{k}'-\mathbf{q}}$ and $\epsilon_{\mathbf{k}+\mathbf{q}}$ are all positive numbers which must add up to ω . Hence, only such states can contribute to (2.25) which satisfy $-\omega \leq \epsilon_{\mathbf{k}'} \leq 0$, $0 \leq \epsilon_{\mathbf{k}'-\mathbf{q}} \leq \omega$ and $0 \leq \epsilon_{\mathbf{k}+\mathbf{q}} \leq \omega$. Evidently, this will be less and less terms the smaller ω gets. An explicit estimate of the sum (2.25) does indeed yield $\tau^{-1} \propto \omega^2$ (see, e.g., chapter II.3.2 of [25]). After insertion of $\omega = \epsilon_{\mathbf{k}}$, we recover (2.24).

Another consequence of the interactions is the appearance of a so-called 'quasi-particle weight' Z_{k_F} . In a system of free fermions, the coefficient of the δ -function in the spectral function (or equivalently, the residue of the pole) would be equal to one. A qualitative explanation why in an interacting system this weight is in general smaller is the following: firstly, general arguments show that the spectral density must be positive. Secondly, the interactions give rise to an incoherent background in the spectral function, as sketched in Fig. 2.1. Lastly, there is a sum rule for the spectral function (essentially the total probability must be equal to one), such that the appearance of an incoherent background implies a reduction of the quasiparticle weight, i.e., $Z_{k_F} < 1$.

Finally, let us take a quick look at the momentum distribution

$$n(\mathbf{k}) = \langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \rangle. \quad (2.26)$$

At $T = 0$, there is a very useful relation (which we are not going to derive) between the momentum distribution and the spectral function: $n(\mathbf{k}) = \int_{-\infty}^0 d\omega A(\mathbf{k}, \omega)$. As

we have argued above, the lifetime of the quasiparticle becomes infinite for $\mathbf{k} \rightarrow \mathbf{k}_F$ (see (2.24)) such that $A(\mathbf{k}, \omega)$ approaches $Z_{k_F} \delta(\omega)$. If you insert this into (2.26), you find a jump in $n(\mathbf{k})$ at the Fermi surface. To be more precise, for $k < k_F$ the quasiparticle pole lies in the integration region of (2.26) whereas for $k > k_F$ it lies outside. This implies

$$\lim_{\mathbf{k} \nearrow \mathbf{k}_F} n(\mathbf{k}) - \lim_{\mathbf{k} \searrow \mathbf{k}_F} n(\mathbf{k}) = Z_{k_F}, \quad (2.27)$$

i.e., the height of the jump is exactly equal to the the quasiparticle weight Z_{k_F} ! This is sketched in Fig. 2.3. As a result of the interaction, the momentum distribution $n(\mathbf{k})$ no longer is a Fermi distribution (*i.e.*, at $T = 0$ no step function $n(\mathbf{k}) = \Theta(-\epsilon_{\mathbf{k}})$), but there is still a jump at the Fermi surface as a characteristic feature of a Fermi liquid.

3 Superconductivity

In this chapter we will present the basic ideas of a microscopic theory of superconductivity which is called ‘BCS theory’ after its inventors Bardeen, Cooper, and Schrieffer [4] (Nobel price for physics 1972).

3.1 Cooper instability

Heike Kamerlingh Onnes discovered superconductivity during the year 1911 while measuring the resistivity of mercury. This discovery led, among others, to the Nobel price for physics 1913. This phenomenon was, however, evading a microscopic understanding until Cooper was able to show in 1956 [8] that the ground state of an electron gas with an arbitrarily weak attractive interaction cannot be described by a Fermi distribution with a sharp Fermi edge. This observation was the foundation for BCS theory [4] which was the first valid microscopic theory of superconductivity.

This Cooper instability can be most easily understood with the following artificial model: consider an interaction which is constant and *attractive* in a finite energy interval above the Fermi surface and vanishes otherwise. So, we use a Hamiltonian of the form

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{q} \sigma_1 \sigma_2} \langle \mathbf{k}_1 + \mathbf{q}, \mathbf{k}_2 - \mathbf{q} | V | \mathbf{k}_1, \mathbf{k}_2 \rangle c_{\mathbf{k}_1 + \mathbf{q} \sigma_1}^{\dagger} c_{\mathbf{k}_2 - \mathbf{q} \sigma_2}^{\dagger} c_{\mathbf{k}_2 \sigma_2} c_{\mathbf{k}_1 \sigma_1} \quad (3.1)$$

with

$$\langle \mathbf{k}_1 + \mathbf{q}, \mathbf{k}_2 - \mathbf{q} | V | \mathbf{k}_2, \mathbf{k}_1 \rangle = \begin{cases} v < 0 & \text{for } \epsilon_F < \epsilon_{\mathbf{k}_1}, \dots < \epsilon_F + \hbar\omega_c \\ 0 & \text{otherwise.} \end{cases} \quad (3.2)$$

Since the Coulomb interaction between two electrons is repulsive, you may wonder how there can be an attractive interaction between electrons. The answer was in fact already known to the authors of Refs. [4,8]: electron-phonon interactions can generate an effective attraction between electrons. An intuitive picture for this is shown in Fig. 3.1: imagine that a first electron travels through a crystal, causing a lattice deformation. This lattice deformation costs elastic energy. Now, if a second electron follows along the same path, it may find the lattice deformation still in place such that it does not have to pay the elastic energy. Hence, the electron pair has to pay the elastic energy only once while two independent electrons would have to pay it twice. This amounts to an effective attraction.

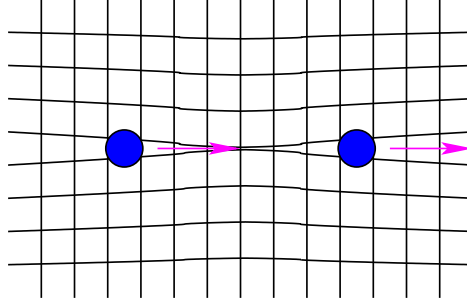


Figure 3.1: Sketch of the electron-phonon interaction: a first electron travels through a crystal and causes a lattice deformation which makes it favorable for a second electron to follow (electrons are indicated by the filled circles).

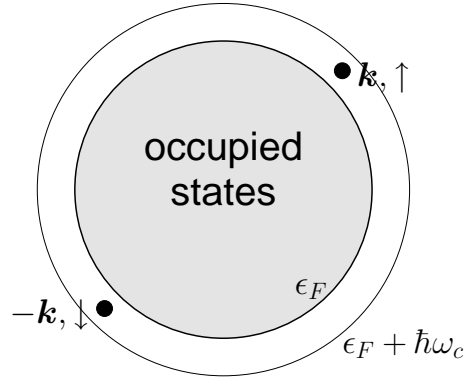


Figure 3.2: A Cooper pair consisting of two electrons with opposite spins and momenta in a shell of energy $\hbar\omega_c$ outside the Fermi surface.

The ‘ground state’⁶ of the model (3.1) is given by

$$|F\rangle = \prod_{\mathbf{k}\sigma, \epsilon_{\mathbf{k}} \leq \epsilon_F} c_{\mathbf{k}\sigma}^\dagger |0\rangle, \quad (3.3)$$

with energy

$$H|F\rangle = H_0|F\rangle = E_0|F\rangle, \quad E_0 = \sum_{\mathbf{k}\sigma, \epsilon_{\mathbf{k}} \leq \epsilon_F} \epsilon_{\mathbf{k}}. \quad (3.4)$$

Now let us add two electrons with opposite momenta and spins (compare Fig. 3.2) and define:

$$|-\mathbf{k} \downarrow, \mathbf{k} \uparrow\rangle := c_{-\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}\uparrow}^\dagger |F\rangle. \quad (3.5)$$

⁶This is indeed the ground state of the non-interacting system. We have constructed the interaction such that the ground state of the non-interacting system remains an eigenstate of the interacting system.

The action of the Hamiltonian on this state is the following

$$H|-\mathbf{k}\downarrow, \mathbf{k}\uparrow\rangle = (2\epsilon_{\mathbf{k}} + E_0)|-\mathbf{k}\downarrow, \mathbf{k}\uparrow\rangle + v \sum_{\mathbf{k}'} |-\mathbf{k}'\downarrow, \mathbf{k}'\uparrow\rangle \quad (3.6)$$

with

$$\sum_{\mathbf{k}}' = \sum_{\mathbf{k}, \epsilon_F < \epsilon_{\mathbf{k}} \leq \epsilon_F + \hbar\omega_c},$$

i.e., the interaction scatters the pair $|-\mathbf{k}\downarrow, \mathbf{k}\uparrow\rangle$ into the pair $|-\mathbf{k}'\downarrow, \mathbf{k}'\uparrow\rangle$. Therefore, the state (3.5) is no eigenstate of H . In order to find an eigenstate, we make the following ansatz

$$|\downarrow, \uparrow\rangle := \sum_{\mathbf{k}}' g(\mathbf{k}) |-\mathbf{k}\downarrow, \mathbf{k}\uparrow\rangle \quad (3.7)$$

with a function $g(\mathbf{k})$ to be determined. We are looking for a solution of $H|\downarrow, \uparrow\rangle = E|\downarrow, \uparrow\rangle$:

$$\begin{aligned} \sum_{\mathbf{k}_1}' g(\mathbf{k}_1)(2\epsilon_{\mathbf{k}_1} + E_0) |-\mathbf{k}_1\downarrow, \mathbf{k}_1\uparrow\rangle + v \sum_{\mathbf{k}_1}' g(\mathbf{k}_1) \sum_{\mathbf{k}_2}' |-\mathbf{k}_2\downarrow, \mathbf{k}_2\uparrow\rangle \\ = E \sum_{\mathbf{k}_3}' g(\mathbf{k}_3) |-\mathbf{k}_3\downarrow, \mathbf{k}_3\uparrow\rangle. \end{aligned} \quad (3.8)$$

Using orthogonality of the states $|-\mathbf{k}\downarrow, \mathbf{k}\uparrow\rangle$, we can reduce this to

$$g(\mathbf{k})(2\epsilon_{\mathbf{k}} + E_0) + v \sum_{\mathbf{k}_1}' g(\mathbf{k}_1) = E g(\mathbf{k}). \quad (3.9)$$

Since we have assumed a constant interaction v , it is straightforward to solve this integral equation. If we introduce the abbreviation

$$C = -v \sum_{\mathbf{k}_1}' g(\mathbf{k}_1), \quad (3.10)$$

we can rewrite (3.9) as

$$g(\mathbf{k}) = \frac{C}{2\epsilon_{\mathbf{k}} + E_0 - E}, \quad C = -v \sum_{\mathbf{k}}' \frac{C}{2\epsilon_{\mathbf{k}} + E_0 - E} \quad (3.11)$$

such that for $C \neq 0$ we must have

$$1 = -v \sum_{\mathbf{k}}' \frac{1}{2\epsilon_{\mathbf{k}} + E_0 - E}. \quad (3.12)$$

For discrete value of k , this eigenvalue equation has a large number of solution for E which correspond in general to slightly shifted two-particle energies. We are looking for the solution $E < E_0 + 2\epsilon_F$ which corresponds to the lowest energy for two additional particles close to the Fermi edge. It is convenient to substitute $\xi = \epsilon_{\mathbf{k}} - \epsilon_F$, $\Delta E = E - (E_0 + 2\epsilon_F)$ and replace the summation of \mathbf{k}' by an integral:

$$\begin{aligned} 1 &= -vN(\epsilon_F) \int_0^{\hbar\omega_c} d\xi \frac{1}{2\xi - \Delta E} = -vN(\epsilon_F) \frac{1}{2} \ln \left| \frac{\hbar\omega_c - \Delta E/2}{-\Delta E/2} \right| \\ &\simeq -vN(\epsilon_F) \frac{1}{2} \ln \frac{\hbar\omega_c}{|-\Delta E/2|}, \quad \hbar\omega_c \gg |\Delta E|. \end{aligned} \quad (3.13)$$

Here $N(\epsilon_F)$ is the density of states at the Fermi edge. Now we see that a solution exists only for $v < 0$. We set $\lambda = N(\epsilon_F)|v|$ and solve (3.13) for the energy gain $\Delta E < 0$:

$$\Delta E = -2\hbar\omega_c e^{-2/\lambda}, \quad E = E_0 + 2\epsilon_F - 2\hbar\omega_c e^{-2/\lambda}, \quad (3.14)$$

i.e., a pair state consisting of two electrons above the Fermi edge subject to interactions has lower energy than a state with two additional electrons at the Fermi surface without interactions. Consequently, one can lower the total energy of the electron system by bringing two electrons from directly below the Fermi surface into a pair state above the Fermi edge. This demonstrates the instability of the Fermi distribution for this model under an (arbitrarily weak) attractive interaction. However, we still do not know what will happen if several pair states are formed. This pair formation is the basis of BCS theory which assumes an attractive interaction around the Fermi surface.

The result (3.14) cannot be obtained by a perturbative treatment of the interaction since $\exp(-2/\lambda)$ is no analytic function of λ at $\lambda = 0$. This is certainly one of the reasons why it took 50 years after the discovery of superconductivity until a microscopic theory was found.

Two questions remains to be answered: 1. Why do we pair electrons with opposite momentum? 2. Why do we use opposite spins? If we pair electrons with a finite center-of-mass momentum \mathbf{q} , the energy gain by pair interaction will not be so big. However, such pair states are indeed needed to describe a state with a finite supercurrent. The answer to the second question is less obvious. At first sight, the spin orientation should play no rôle during the computation of the energy gain. That pairing with parallel spin is impossible (for the form of the interaction which we have used) is a consequence of the Pauli principle, *i.e.* the antisymmetry of the wave function of two fermions. In the above case we do indeed need a 'spin singlet'

(antiparallel spins), as we can see as follows: suppose we would have instead

$$|\uparrow, \uparrow\rangle := \sum_{\mathbf{k}} g(\mathbf{k}) |-\mathbf{k} \uparrow, \mathbf{k} \uparrow\rangle, \quad (3.15)$$

then we would have the same formula as above for the function $g(\mathbf{k})$. In particular it follows that $g(-\mathbf{k}) = g(\mathbf{k})$ for a constant interaction. On the other hand, we have $|-\mathbf{k} \uparrow, \mathbf{k} \uparrow\rangle = -|+\mathbf{k} \uparrow, -\mathbf{k} \uparrow\rangle$ by construction. Hence, the wave function (3.15) vanishes identically.

For a \mathbf{k} -dependent interaction of the form $v(\mathbf{k}, \mathbf{k}')$ with $v(-\mathbf{k}, -\mathbf{k}') = -v(\mathbf{k}, \mathbf{k}')$ one would find $g(-\mathbf{k}) = -g(\mathbf{k})$ such that pairing with parallel spin would be possible, too. This type of pairing is found in superfluid ^3He . Here, the spin degrees of freedom couple to a spin one and the antisymmetry of the wave function is ensured by a spatial part with angular momentum one. In such a case, one speaks about 'p-wave superconductivity' because of the symmetry of the spatial part of the wavefunction. In the case discussed above, the spatial part has essentially an angular momentum 0 and one refers to 's-wave superconductivity'.

3.2 Bardeen-Cooper-Schrieffer (BCS)-theory

The BCS theory of superconductivity uses a Hamiltonian of the form (3.1). Here we assume that the effective two-particle interaction is attractive for electrons close to the Fermi surface, both for states above and below the Fermi edge. Since Cooper's work [8] it is known that the Fermi distribution is unstable with respect to the formation of pair states $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$ if the interaction is attractive. Therefore we expect that matrix elements of the form $\langle N-2, G | c_{\mathbf{k}_2 \sigma_2} c_{\mathbf{k}_1 \sigma_1} | N, G \rangle$ acquire macroscopic values in the ground state $|N, G\rangle$ if $\mathbf{k}_2 = -\mathbf{k}_1$, $\sigma_2 = -\sigma_1$. The existence of such matrix elements can be seen most easily in the framework of a molecular-field approximation. It is further useful to work in the grand canonical ensemble since then it is possible to write matrix elements which do not conserve particle number as expectation values. Thus, $K = H - \mu N$ is replaced by the mean-field Hamiltonian

$$K_{\text{MF}} = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} (\Delta_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}\uparrow}^\dagger + \Delta_{\mathbf{k}}^* c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}). \quad (3.16)$$

The parameters of the mean-field Hamiltonian can be determined selfconsistently upon replacing two operators each with their expectation values in the original Hamiltonian K . If we consider only the anomalous expectation values $\langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle$ and $\langle c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger \rangle$ (the other expectation values simply yield corrections to the single-particle energies), we find the selfconsistency equation

$$\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} \mathcal{V}(\mathbf{k}, \mathbf{k}') \langle c_{\mathbf{k}'\uparrow} c_{-\mathbf{k}'\downarrow} \rangle \quad (3.17)$$

with

$$\mathcal{V}(\mathbf{k}, \mathbf{k}') = \langle -\mathbf{k}, \mathbf{k} | V | -\mathbf{k}', \mathbf{k}' \rangle \quad (3.18)$$

and

$$\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu. \quad (3.19)$$

Now we should diagonalize K_{MF} , *i.e.*, bring it into the following form:

$$K_{\text{MF}}^{\text{diag}} = \sum_{\mathbf{k}\sigma} E_{\mathbf{k}\sigma} \gamma_{\mathbf{k}\sigma}^\dagger \gamma_{\mathbf{k}\sigma}. \quad (3.20)$$

The operators $\gamma_{\mathbf{k}\sigma}$ are linear combinations of the original electronic operators $c_{\mathbf{k}\sigma}$ and must also obey the fermionic anticommutation relations which we derived in section 1.2. One way to perform this diagonalization is to use analyze the equations of motion of the operators. In the diagonal form (3.20) of K_{MF} they read

$$[K_{\text{MF}}^{\text{diag}}, \gamma_{\mathbf{k}\sigma}] = -E_{\mathbf{k}\sigma} \gamma_{\mathbf{k}\sigma}. \quad (3.21)$$

$E_{\mathbf{k}\sigma}$ can be interpreted as quasiparticle energy and $\gamma_{\mathbf{k}\sigma}^\dagger$ as creator for a quasiparticle. In the original form (3.16) of K_{MF} we find for the commutator with $c_{\mathbf{k}\uparrow}$:

$$[K_{\text{MF}}, c_{\mathbf{k}\uparrow}] = -\xi_{\mathbf{k}} c_{\mathbf{k}\uparrow} + \Delta_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger. \quad (3.22)$$

Now operators with opposite spin and momentum are mixed. In an analogous manner, we find for the commutator with $c_{-\mathbf{k}\downarrow}^\dagger$:

$$[K_{\text{MF}}, c_{-\mathbf{k}\downarrow}^\dagger] = +\xi_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger + \Delta_{\mathbf{k}}^* c_{\mathbf{k}\uparrow}. \quad (3.23)$$

This suggests the following ansatz for the quasiparticle operators

$$\gamma = x c_{\mathbf{k}\uparrow} + y c_{-\mathbf{k}\downarrow}^\dagger. \quad (3.24)$$

In the spirit of (3.21) we postulate

$$[K_{\text{MF}}, \gamma] = -\lambda \gamma. \quad (3.25)$$

With the above ansatz we find

$$\begin{aligned} [K_{\text{MF}}, \gamma] &= x(-\xi_{\mathbf{k}} c_{\mathbf{k}\uparrow} + \Delta_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger) + y(\xi_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger + \Delta_{\mathbf{k}}^* c_{\mathbf{k}\uparrow}) \\ &= -\lambda(x c_{\mathbf{k}\uparrow} + y c_{-\mathbf{k}\downarrow}^\dagger). \end{aligned} \quad (3.26)$$

Comparison of the coefficients of the electronic operators yields the following system of equations

$$(\lambda - \xi_{\mathbf{k}})x + \Delta_{\mathbf{k}}^* y = 0 \quad (3.27)$$

$$\Delta_{\mathbf{k}} x + (\lambda + \xi_{\mathbf{k}})y = 0. \quad (3.28)$$

The eigenvalues are

$$\lambda = \pm E_{\mathbf{k}}, \quad E_{\mathbf{k}} = +\sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}, \quad (3.29)$$

and the two solutions for the quasiparticle operators read:

$$1. \quad \lambda_1 = +E_{\mathbf{k}}: \quad \gamma_1 = \gamma_{\mathbf{k}\uparrow} = u_{\mathbf{k}}c_{\mathbf{k}\uparrow} - v_{\mathbf{k}}c_{-\mathbf{k}\downarrow}^\dagger \quad (3.30)$$

$$2. \quad \lambda_2 = -E_{\mathbf{k}}: \quad \gamma_2 = \gamma_{-\mathbf{k}\downarrow}^\dagger = v_{\mathbf{k}}^*c_{\mathbf{k}\uparrow} + u_{\mathbf{k}}^*c_{-\mathbf{k}\downarrow}^\dagger \quad (3.31)$$

with

$$|u_{\mathbf{k}}|^2 = \frac{1}{2} \left(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right), \quad |v_{\mathbf{k}}|^2 = \frac{1}{2} \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right), \quad u_{\mathbf{k}}v_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}. \quad (3.32)$$

According to the sign of the eigenvalues, γ_1 is an annihilation operator and γ_2 a creation operator. Notations are chose such that these two operators coincide with the electron operators far above the Fermi edge.

The absolute values of the coefficients $u_{\mathbf{k}}$, $v_{\mathbf{k}}$ are dictated by the postulate that the quasiparticle operators satisfy Fermi anticommutation rules:

$$\gamma_{\mathbf{k}\sigma}^\dagger \gamma_{\mathbf{k}'\sigma'} + \gamma_{\mathbf{k}'\sigma'}^\dagger \gamma_{\mathbf{k}\sigma} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} \quad (3.33)$$

$$\gamma_{\mathbf{k}\sigma} \gamma_{\mathbf{k}'\sigma'} + \gamma_{\mathbf{k}'\sigma'} \gamma_{\mathbf{k}\sigma} = 0. \quad (3.34)$$

This implies

$$|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1. \quad (3.35)$$

Without loss of generality, $u_{\mathbf{k}}$ can be chosen real and positive. The phase of $v_{\mathbf{k}}$ is then determined by the phase of $\Delta_{\mathbf{k}} = |\Delta_{\mathbf{k}}| \exp(i\varphi_{\mathbf{k}})$. Note that the selfconsistency equation couples the phases $\varphi_{\mathbf{k}}$ with each other. For an s-wave superconductor all phases are equal. Hence, it is possible to set this global phase equal to zero for a *single* superconductor (without external magnetic field and currents).

The transformation between electron operators and quasiparticle operators can also be written in the following compact form:

$$\gamma_{\mathbf{k}\sigma} = u_{\mathbf{k}}c_{\mathbf{k}\sigma} - v_{\mathbf{k}}\text{sign}(\sigma)c_{-\mathbf{k},-\sigma}^\dagger \quad (3.36)$$

$$c_{\mathbf{k}\sigma} = u_{\mathbf{k}}^*\gamma_{\mathbf{k}\sigma} + v_{\mathbf{k}}^*\text{sign}(\sigma)\gamma_{-\mathbf{k},-\sigma}^\dagger. \quad (3.37)$$

Then the mean-field Hamiltonian reads

$$K_{\text{MF}} = \sum_{\mathbf{k}\sigma} E_{\mathbf{k}} (\gamma_{\mathbf{k}\sigma}^\dagger \gamma_{\mathbf{k}\sigma} - 1). \quad (3.38)$$

The constant (-1) is usually omitted since it is irrelevant for the excitation spectrum. This Hamiltonian (which corresponds to $H - \mu N$) contains only positive energies $E_{\mathbf{k}}$.

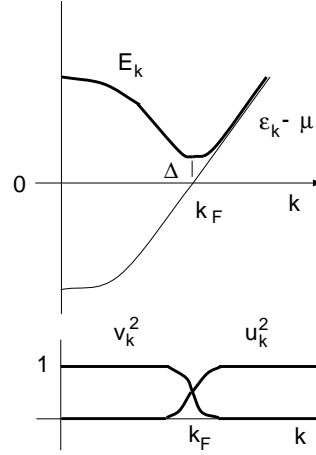


Figure 3.3: Excitation spectrum of quasi-particles and coherence factors in the superconducting state.

These are the energies of the quasiparticles (single-particle excitations). The ground state is a state without excitations, *i.e.*, without quasiparticles.

The excitation spectrum is sketched in Fig. 3.3 for constant Δ . The spectrum has a gap Δ at the Fermi surface. Fig. 3.3 also shows the so-called ‘coherence factors’ $u_{\mathbf{k}}$, $v_{\mathbf{k}}$. The excitation has particle character far above the Fermi edge while it has hole character far below the Fermi edge. Close to the Fermi surface, the excitation has a mixed particle-hole character. Note that excitations of the Fermi sea in the normal state can be characterized in the same manner. In this case $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ would be step functions.

Computation of the order parameter function $\Delta_{\mathbf{k}}$

In the present case (no magnetic fields, no magnetic impurities), the order parameter $\Delta_{\mathbf{k}}$ determines the energy gap. It is determined by the selfconsistency equation (3.17), *i.e.*, $\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} \mathcal{V}(\mathbf{k}, \mathbf{k}') \langle c_{\mathbf{k}'\uparrow} c_{-\mathbf{k}'\downarrow} \rangle$. The expectation value on the right side is computed using the mean-field Hamiltonian which is diagonal in the quasiparticle operators. So, we express the electron operators in terms of quasiparticle operators and use their Fermi statistics (1.40):

$$\begin{aligned} \langle \gamma_{\mathbf{k}\sigma}^\dagger \gamma_{\mathbf{k}'\sigma'} \rangle &= \delta_{\mathbf{k},\mathbf{k}'} \delta_{\sigma\sigma'} f(E_{\mathbf{k}}), \quad f(E_{\mathbf{k}}) = \frac{1}{e^{\beta E_{\mathbf{k}}} + 1} \\ \langle \gamma_{\mathbf{k}\sigma} \gamma_{\mathbf{k}'\sigma'} \rangle &= 0. \end{aligned} \quad (3.39)$$

We will restrict in the following to real $\Delta_{\mathbf{k}}$, $u_{\mathbf{k}}$, and $v_{\mathbf{k}}$. With the help of (3.37) and (3.39) we find that

$$\langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle = -u_{\mathbf{k}} v_{\mathbf{k}} \langle \gamma_{\mathbf{k}\uparrow} \gamma_{\mathbf{k}\uparrow}^\dagger \rangle + u_{\mathbf{k}} v_{\mathbf{k}} \langle \gamma_{-\mathbf{k}\downarrow}^\dagger \gamma_{-\mathbf{k}\downarrow} \rangle = -u_{\mathbf{k}} v_{\mathbf{k}} (1 - 2f(E_{\mathbf{k}})) \quad (3.40)$$

or

$$\langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle = -\frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}} \tanh \frac{\beta E_{\mathbf{k}}}{2}. \quad (3.41)$$

The selfconsistency condition now reads

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} \mathcal{V}(\mathbf{k}, \mathbf{k}') \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh \frac{\beta E_{\mathbf{k}'}}{2} \quad (3.42)$$

with $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$, $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$. Since $\Delta_{\mathbf{k}}$ can be interpreted as an energy gap, Eq. (3.42) is also called 'gap equation'.

There is always the trivial solution $\Delta_{\mathbf{k}} = 0$ which corresponds to the normal state. Non-trivial solutions are possible for low temperatures if the interaction $\mathcal{V}(\mathbf{k}, \mathbf{k}') < 0$ is attractive close to the Fermi edge. Depending on the form and symmetry of this interaction, one can find different pairing states (s-wave, p-wave, and d-wave pairing).

The simplest model is obtained for an interaction which is constant and attractive in a region $\pm \hbar\omega_c$ around the Fermi surface (or a bit more generally for an interaction that is factorisable in \mathbf{k}, \mathbf{k}'):

$$\mathcal{V}(\mathbf{k}, \mathbf{k}') = \begin{cases} v < 0 & \text{for } |\epsilon_{\mathbf{k}_i} - \mu| < \hbar\omega_c \\ 0 & \text{otherwise.} \end{cases} \quad (3.43)$$

$\hbar\omega_c$ corresponds to the Debye energy if the interaction is induced by phonons. For this particular interaction, the selfconsistency equation reads

$$\Delta = -v \sum_{\mathbf{k}'}^{\prime} \frac{\Delta}{2E_{\mathbf{k}'}} \tanh \frac{\beta E_{\mathbf{k}'}}{2}, \quad (3.44)$$

where the stroke denotes a termination of the sum at the cutoff energy $\hbar\omega_c$. In this energy interval Δ is independent of \mathbf{k} and outside it is zero. Evidently, a non-trivial solution is found only for $v < 0$.

Debye energies are usually much smaller than the bandwidth of the electrons. We may therefore assume that the cutoff energy is small compared to the bandwidth such that we can approximate the electronic density of states by a constant $N(\epsilon_F)$ in this energy interval. Now we can replace (3.44) by

$$1 = \lambda \int_0^{\hbar\omega_c} \frac{1}{E(\xi)} \tanh \frac{\beta E(\xi)}{2} d\xi \quad (3.45)$$

with $E(\xi) = \sqrt{\xi^2 + \Delta^2}$ and $\lambda = N(\epsilon_F)|v|$. This equation determines Δ as a function of T (see Fig. 3.4).

In the following two cases we can obtain analytic solutions:

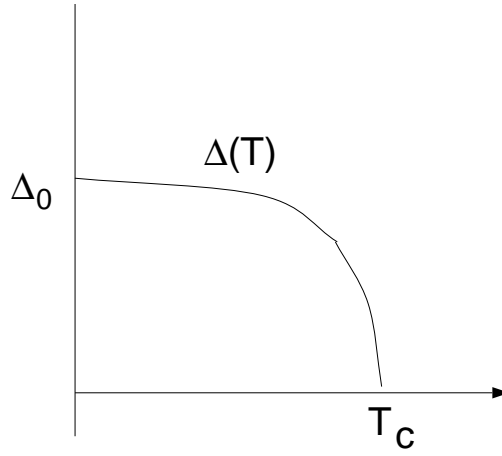


Figure 3.4: Temperature dependence of the energy gap.

a) $T = 0, \Delta(T = 0) = \Delta_0$.

In this case we have

$$1 = \lambda \int_0^{\hbar\omega_c} d\xi \frac{1}{\sqrt{\xi^2 + \Delta_0^2}} = \lambda \ln \left(\xi + \sqrt{\xi^2 + \Delta_0^2} \right) \Big|_0^{\hbar\omega_c}. \quad (3.46)$$

Usually the cutoff energy is large in comparison with Δ_0 . For $\Delta_0 \ll \hbar\omega_c$, Eq. (3.46) reduces to

$$1 = \lambda \ln \left(\frac{2\hbar\omega_c}{\Delta_0} \right), \quad (3.47)$$

which yields the value of the gap at $T = 0$:

$$\Delta_0 = 2\hbar\omega_c \exp(-1/\lambda). \quad (3.48)$$

b) $T \rightarrow T_c, \Delta \rightarrow 0$.

In this limit we have

$$1 = \lambda \int_0^{\hbar\omega_c} d\xi \frac{1}{\xi} \tanh \frac{\beta_c \xi}{2} \quad (3.49)$$

with $\beta_c = 1/(k_B T_c)$. A rough approximation for the integral is obtained if one replaces the \tanh by a constant for $\xi > k_B T_c$:

$$1 = \lambda \int_{k_B T_c}^{\hbar\omega_c} d\xi \frac{1}{\xi} = \lambda \ln \left(\frac{\hbar\omega_c}{k_B T_c} \right). \quad (3.50)$$

A more precise result is obtained as follows: we substitute $x = \beta_c \xi/2$ in the integral and set $A = \hbar\omega_c \beta_c/2$. Now we perform one partial integration and finally take the limit $A \rightarrow \infty$:

$$\begin{aligned} \int_0^A dx \frac{1}{x} \tanh x &= \ln x \tanh x \Big|_0^A - \int_0^A dx \frac{\ln x}{\cosh^2 x} \stackrel{\tanh A \rightarrow 1}{\approx} \ln A - \int_0^\infty dx \frac{\ln x}{\cosh^2 x} \\ &= \ln A - \ln \left(\frac{4}{\pi e^\gamma} \right) = \ln \left(\frac{2 e^\gamma \hbar\omega_c}{\pi k_B T_c} \right). \end{aligned} \quad (3.51)$$

Here $\gamma = 0.577\dots$ is Euler's constant. Finally, we find the value of T_c for $\hbar\omega_c \gg k_B T_c$ from Eq. (3.49):

$$k_B T_c = \frac{2 e^\gamma}{\pi} \hbar\omega_c \exp \left(-\frac{1}{\lambda} \right) = 1.134 \hbar\omega_c \exp \left(-\frac{1}{\lambda} \right). \quad (3.52)$$

Note that the ratio $2\Delta_0/(k_B T_c) = 3.527\dots$ is independent of the material's parameters in BCS theory. Δ_0 cannot be computed by perturbation theory in v since the result is non-analytic in v .

Acknowledgments

I would like to thank the DAAD for the financial support of these lectures which were given in the framework of the summer school on 'Fundamentals and Materials for Novel Sensors' which took place during July 13–24, 2009 at the Pontifícia Universidade Católica do Rio de Janeiro, Brazil.

The chapters 1 and 3 of the present lecture notes are based on the lecture notes [18]. Klaus Becker and Joachim Keller have contributed to those lecture notes in addition to Volker Meden and Thomas Pruschke. I would like to acknowledge their contributions in the present lecture notes.

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