12 BCS Theory at Zero Temperature

This chapter deals with the microscopic theory of superconductivity, which was worked out by Bardeen, Cooper, and Schrieffer in 1957. To this end one considers the pairing Hamiltonian (11.127), which was derived throughout the preceding chapter by perturbatively eliminating the phonon operators from a linearized electron-phonon interaction. On the one hand, the pairing Hamiltonian (11.127) contains the kinetic energy of the electrons forming a Cooper pair. On the other hand, the interaction term describes the scattering of one Cooper pair in state $\vec{k}$ to another one in state $\vec{k}'$. And such a scattering process emerges from virtually exchanging a phonon between the Cooper pairs characterized by wave vector $\vec{k}$ and $\vec{k}'$. In this chapter we determine approximately the ground state of the pairing Hamiltonian (11.127).

12.1 BCS ground state:

The underlying many-body problem of superconductivity is so complicated that it cannot be solved exactly. Therefore, one needs an appropriate approximation scheme. In similar complicated situations in molecular physics it turned out to be useful to choose a finite set of wave functions and to determine then with the help of the Ritz variational procedure a corresponding minimal energy eigenvalue. In analogy to this procedure in molecular physics we make here a plausible ansatz for the ground-state wave function of a superconductor at zero temperature and determine the still free parameters by minimizing the energy, thus obtaining a reasonable approximation for the ground-state energy. This approach is justified provided that we find an approximative ground-state energy for the superconductor, which is smaller than the ground-state energy of the normal conductor.

In the following we invoke the BCS ansatz for the ground-state wave function. It is based on the fundamental assumption that the superconducting state is essen-

tially based on Cooper pairs. Although the previous three chapters have already collected theoretical arguments, which support this assumption, the main justification stems from the experiment. As described in Chapter 4 the measurement of the flux quantum unambiguously showed that the elementary charge involved is $2e$.

12.1.1 First Ansatz:

In molecular physics one models the H_2 molecule for the case that both H atoms are far apart from each other by writing the whole electron wave function as a product of the wave functions of the individual electrons. Correspondingly, the N-particle wave function is written here as a product of $\frac{N}{2}$ Cooper pairs

$$\Psi_N^{(1)}(\vec{r}_1,\dots,\vec{r}_N) = \underbrace{\{\psi(\vec{r}_1-\vec{r}_2)(1\uparrow)(2\downarrow)\}}_{1\text{st Cooper pair}}\cdots\underbrace{\{\psi(\vec{r}_{N-1}-\vec{r}_N)(N-1\uparrow)(N\downarrow)\}}_{\frac{N}{2}\text{th Cooper pair}} \quad (12.1)$$

Here $\psi(\vec{r}_1-\vec{r}_2)$ denotes the spatial wave function with $\vec{r}_1, \vec{r}_2$ representing the coordinates of both electrons and $(1\uparrow), (2\downarrow)$ stand for the corresponding spin wave functions, respectively. According to Cooper the former spatial wave function of a Cooper pair can be decomposed into plane waves

$$\psi(\vec{r}_1-\vec{r}_2) = \sum_{\vec{k}_1} g(\vec{k}_1)\, e^{i\vec{k}_1(\vec{r}_1-\vec{r}_2)} \quad (12.2)$$

Inserting (12.2) into (12.1) we get

$$\Psi_N^{(1)}(\vec{r}_1,\dots,\vec{r}_N) = \sum_{\vec{k}_1}\cdots\sum_{\vec{k}_{N/2}} g(\vec{k}_1)\cdot\ldots\cdot g(\vec{k}_{N/2})\, e^{i\vec{k}_1(\vec{r}_1-\vec{r}_2)}$$
$$\cdot\ldots\cdot e^{i\vec{k}_{N/2}(\vec{r}_{N-1}-\vec{r}_N)}(1\uparrow)(2\downarrow)\cdot\ldots(N-1\uparrow)(N\downarrow) \quad (12.3)$$

12.1.2 Second Ansatz:

According to the Pauli principle an electronic wave function must be antisymmetric. Therefore, the first ansatz $\Psi_N^{(1)}$ must be multiplied with the antisymmetrization operator $\hat{A}$:

$$\Psi_N^{(2)} = \hat{A}\,\Psi_N^{(1)} \quad (12.4)$$

This second ansatz $\Psi_N^{(2)}$ is then most efficiently formulated with the Slater determinant. For two functions we have, for instance,

$$\hat{A}\,\varphi_1(\vec{r}_1)\varphi_2(\vec{r}_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \varphi_1(\vec{r}_1) & \varphi_1(\vec{r}_2) \\ \varphi_2(\vec{r}_1) & \varphi_2(\vec{r}_2) \end{vmatrix} \qquad (12.5)$$

In one row we have the same one-particle wave function with different particle numbers. And, conversely, in one column we have the same particle number but different one-particle wave functions. Extending (12.5) to two Cooper pairs we get

$$\Psi_2^{(2)} = \frac{1}{\sqrt{2}} \sum_{\vec{k}_1} \sum_{\vec{k}_2} \begin{vmatrix} g(\vec{k}_1) e^{i\vec{k}_1(\vec{r}_1-\vec{r}_2)} (1\uparrow)(2\downarrow) & g(\vec{k}_1) e^{i\vec{k}_1(\vec{r}_3-\vec{r}_4)} (3\uparrow)(4\downarrow) \\ g(\vec{k}_2) e^{i\vec{k}_2(\vec{r}_1-\vec{r}_2)} (1\uparrow)(2\downarrow) & g(\vec{k}_2) e^{i\vec{k}_2(\vec{r}_3-\vec{r}_4)} (3\uparrow)(4\downarrow) \end{vmatrix} \qquad (12.6)$$

The N-particle wave function $\Psi_N^{(2)}$ follows correspondingly.

12.1.3 Third Ansatz:

In second quantization one does not need any Slater determinant as the antisymmetrization of the wave function is already guaranteed by the anticommutation relations of the electron operators. In the notation of second quantization the electron wave function built up by Cooper pairs reads

$$|\Psi_N^{(3)}\rangle = \prod_{\vec{k}=1}^{N/2} g(\vec{k}) \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow} |0\rangle \qquad (12.7)$$

Now we have to determine the total number of all states, i.e. the number of terms in the antisymmetrized wave function $\Psi_N^{(2)}$. Here N denotes the number of electrons and M the number of possible states, which are characterized by different wave vectors $\vec{k}$. This corresponds to the combinatorial problem, where $N/2$ balls have to be distributed at M sites. As the ordering is arbitrary, we obtain

$$\binom{M}{N/2} = \frac{M!}{(M-N/2)!\,(N/2!)} \approx 10^{10^{20}} \qquad (12.8)$$

Here $M!$ denotes the number of all places, $(M-N/2)!$ the number of free places and $(N/2)!$ the number of occupied places, i.e. the number of Cooper pairs. As the number of states (12.8) is so huge, we can not expect to resolve the problem exactly. Therefore, we have to resolve to an approximative scheme, which we now describe.

12.1.4 BCS Ansatz:

In BCS theory one starts with the following wave function:

$$|\Psi_{BCS}\rangle = \prod_{\vec{k}=\vec{k}_1,\dots,\vec{k}_M} (u_{\vec{k}} + v_{\vec{k}}\, \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow})|0\rangle \qquad (12.9)$$

Here $|0\rangle$ denotes the vacuum state, $\hat{a}^+_{\vec{k}\uparrow}\hat{a}^+_{-\vec{k}\downarrow}$ creates a Cooper pair, and $u_{\vec{k}}, v_{\vec{k}}$ stand for respective weight factors. Furthermore, the product allows for all possible wave vectors $\vec{k}$. Multiplying out the product explicitly yields terms with a different number of Cooper pairs. For instance, the following terms appear:

1) $\left(\prod_{\vec{k}=\vec{k}_1,\dots,\vec{k}_M} u_{\vec{k}}\right)|0\rangle$: All M terms are unoccupied with Cooper pairs.

2) $\left(\prod_{\vec{k}=\vec{k}_1,\dots,\vec{k}_M} v_{\vec{k}}\, \hat{a}^+_{\vec{k}\uparrow}\hat{a}^+_{-\vec{k}\downarrow}\right)|0\rangle$: All M terms are occupied with Cooper pairs.

This means that the BCS ground-state wave function contains states with different particle numbers corresponding to the present weight factors $u_{\vec{k}}, v_{\vec{k}}$:

$$|\Psi_{BCS}\rangle = \sum_{N=0}^{M} \lambda_N |\Psi_N^{(3)}\rangle \qquad (12.10)$$

Thus, we have for instance

$$\lambda_0 = \prod_{\vec{k}=\vec{k}_1,\dots,\vec{k}_M} u_{\vec{k}} \qquad (12.11)$$

$$\lambda_N = \prod_{\vec{k}=\vec{k}_N,\dots,\vec{k}_M} v_{\vec{k}} \qquad (12.12)$$

Going over from the wave function $|\Psi_N^{(3)}\rangle$ with fixed particle number N to the wave function $|\Psi_{BCS}\rangle$ with a variable particle number corresponds to the transition from a microcanonical to a grand-canonical ensemble in statistical physics. Like in statistical physics one expects that the distribution λ_N in (12.10) yields a sharp maximum for large particle numbers N, so that the performed error is negligibly small. Thus, the self-consistency of the BCS ansatz amounts to the condition

$$\frac{\sqrt{\langle(\hat{N}-\bar{N})^2\rangle}}{\bar{N}} \to 0 \quad \text{for } \bar{N}\to\infty \qquad (12.13)$$

12.1.5 Normalisation Condition:

The coefficients $u_{\vec{k}}, v_{\vec{k}}$ in (12.9) must be chosen such that the BCS wave function is normalised:

$$\langle \Psi_{BCS} | \Psi_{BCS} \rangle = 1 \tag{12.14}$$

Inserting (12.9) in (12.14) yields at first

$$\langle 0 | \prod_{\vec{k}} \left(u^*_{\vec{k}} + v^*_{\vec{k}} \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} \right) \prod_{\vec{k}'} \left(u_{\vec{k}'} + v_{\vec{k}'} \hat{a}^+_{\vec{k}'\uparrow} \hat{a}^+_{-\vec{k}'\downarrow} \right) | 0 \rangle = 1 \tag{12.15}$$

As the Fermi operators appear here always pairwise, forming bosonic operators for creating or annihilating a Cooper pair, we conclude that Cooper pair operators with different wave vectors commute:

$$\left[\hat{a}_{\vec{k}_1\uparrow} \hat{a}_{-\vec{k}_1\downarrow}, \hat{a}_{\vec{k}_2\uparrow} \hat{a}_{-\vec{k}_2\downarrow} \right]_- = \left[\hat{a}^+_{\vec{k}_1\uparrow} \hat{a}^+_{-\vec{k}_1\downarrow}, \hat{a}^+_{\vec{k}_2\uparrow} \hat{a}^+_{-\vec{k}_2\downarrow} \right]_-$$

$$= \left[\hat{a}_{\vec{k}_1\uparrow} \hat{a}_{-\vec{k}_1\downarrow}, \hat{a}^+_{\vec{k}_2\uparrow} \hat{a}^+_{-\vec{k}_2\downarrow} \right]_- = 0 \quad \text{for } \vec{k}_1 \neq \vec{k}_2 \tag{12.16}$$

Therefore, (12.15) reduces to

$$\langle 0 | \prod_{\vec{k}} \left(u^*_{\vec{k}} + v^*_{\vec{k}} \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} \right) \left(u_{\vec{k}} + v_{\vec{k}} \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow} \right) | 0 \rangle = 1 \tag{12.17}$$

Multiplying out the brackets and applying the fermionic anti-commutation relations (11.91) yields

$$\langle 0 | \prod_{\vec{k}} \Big\{ |u_{\vec{k}}|^2 + u_{\vec{k}} v^*_{\vec{k}} \hat{a}_{-\vec{k}} \hat{a}_{\vec{k}\uparrow} + u^*_{\vec{k}} v_{\vec{k}} \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow}$$

$$+ |v_{\vec{k}}|^2 \hat{a}_{-\vec{k}\downarrow} \left(1 - \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} \right) \hat{a}^+_{-\vec{k}\downarrow} \Big\} | 0 \rangle = 1 \tag{12.18}$$

These terms vanish as indicated because an annihilation operator acting to the right or a creation operator acting to the left annihilates the vacuum state. Another application of the fermionic anti-commutation relations (11.91) gives

$$\langle 0 | \prod_{\vec{k}} \Big\{ |u_{\vec{k}}|^2 + |v_{\vec{k}}|^2 \left(1 - \hat{a}^+_{-\vec{k}\downarrow} \hat{a}_{-\vec{k}\downarrow} \right) \Big\} | 0 \rangle = 1 \tag{12.19}$$

As the vacuum state is normalised

$$\langle 0 | 0 \rangle = 1 \tag{12.20}$$

we conclude that a sufficient but not necessary condition to satisfy (12.19) reads

$$|u_{\vec{k}}|^2 + |v_{\vec{k}}|^2 = 1 \tag{12.21}$$

Note that we simplify the following calculations by as-

suming that the Bogoliubov amplitudes are real. With an explicit calculation it can be shown that this simplifying assumption has no consequences for the physical results of the BCS theory.

12.1.6 Particle Number Average:

Once we accept (12.9) as a candidate for the ground-state wave function of a superconductor at zero temperature, we can calculate observables as expectation values of operators:

$$\langle \cdot \rangle = \langle \Psi_{BCS} | \cdot | \Psi_{BCS} \rangle \tag{12.22}$$

However, the final result for such expectation values (12.22) depends on the concrete results for the weight factors $u_{\vec{k}}$, $v_{\vec{k}}$ in (12.9), which are not yet determined.

As a first example, let us calculate the expectation value of the particle number operator for a single electron:

$$\langle \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} \rangle \overset{(12.22)}{=} \langle \Psi_{BCS} | \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} | \Psi_{BCS} \rangle \tag{12.23}$$

Inserting (12.9) in (12.23) we obtain at first

$$= \langle 0 | \prod_{\vec{k}'} (u_{\vec{k}'} + v_{\vec{k}'} \hat{a}_{-\vec{k}'\downarrow} \hat{a}_{\vec{k}'\uparrow}) \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} \prod_{\vec{k}''} (u_{\vec{k}''} + v_{\vec{k}''} \hat{a}^+_{\vec{k}''\uparrow} \hat{a}^+_{-\vec{k}''\downarrow}) | 0 \rangle \tag{12.24}$$

Decomposing both products according to

$$\prod_{\vec{k}'} = \prod_{\vec{k}' \neq \vec{k}} \cdot \prod_{\vec{k}} \tag{12.25}$$

and taking into account (12.16) then yields

$$= \langle \Psi_{\vec{k}} | (u_{\vec{k}} + v_{\vec{k}} \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow}) \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} (u_{\vec{k}} + v_{\vec{k}} \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow}) | \Psi_{\vec{k}} \rangle \tag{12.26}$$

where we have introduced as an abbreviation

$$|\Psi_{\vec{k}}\rangle = \prod_{\vec{k}' \neq \vec{k}} (u_{\vec{k}'} + v_{\vec{k}'} \hat{a}^+_{\vec{k}'\uparrow} \hat{a}^+_{-\vec{k}'\downarrow}) | 0 \rangle \tag{12.27}$$

Multiplying out the brackets in (12.26) we get

$$= \langle \Psi_{\vec{k}} | u_{\vec{k}} \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} + u_{\vec{k}} v_{\vec{k}} (\hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\downarrow} \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} + \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow}) + v^2_{\vec{k}} \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow} | \Psi_{\vec{k}} \rangle$$

$$\overset{(11.91)}{=} 1 - \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} \qquad \overset{(11.91)}{=} 1 - \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} \tag{12.28}$$

Thus, (12.28) reduces to

$$= v_{\vec{k}}^2 \langle \psi_{\vec{k}} | \hat{a}_{-\vec{k}\downarrow} \hat{a}^+_{-\vec{k}\downarrow} | \psi_{\vec{k}} \rangle \overset{(11.91)}{=\!=} v_{\vec{k}}^2 \langle \psi_{\vec{k}} | \psi_{\vec{k}} \rangle = v_{\vec{k}}^2 \quad (12.29)$$

With this we conclude

$$\langle \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} \rangle = v_{\vec{k}}^2 \quad (12.30)$$

which turns out to be independent of the spin, so we also have

$$\langle \hat{a}^+_{\vec{k}\downarrow} \hat{a}_{\vec{k}\downarrow} \rangle = v_{\vec{k}}^2 \quad (12.31)$$

This means that the weight factor $v_{\vec{k}}^2$ corresponds to the probability to find an electron with wave vector $\vec{k}$. Due to the normalisation condition (12.24) this also says that $u_{\vec{k}}^2$ represents the probability of not finding an electron at wave vector $\vec{k}$. Furthermore, we read off from (12.30), (12.31) how to determine the particle number expectation value from the weight factor $v_{\vec{k}}$:

$$\overline{N} = \langle \hat{N} \rangle = \sum_{\vec{k}} \sum_{\sigma} \langle \hat{a}^+_{\vec{k}\sigma} \hat{a}_{\vec{k}\sigma} \rangle = 2 \sum_{\vec{k}} v_{\vec{k}}^2 \quad (12.32)$$

12.1.7 Anomalous Expectation Value:

In the same way we can also determine the anomalous expectation value

$$\langle \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} \rangle \overset{(12.22)}{=\!=} \langle \psi_{BCS} | \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} | \psi_{BCS} \rangle \quad (12.33)$$

Inserting (12.9) in (12.33) and taking into account (12.16), (12.25), (12.27) leads to

$$= \langle \psi_{\vec{k}} | (u_{\vec{k}} + v_{\vec{k}} \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow}) \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} (u_{\vec{k}} + v_{\vec{k}} \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow}) | \psi_{\vec{k}} \rangle \quad (12.34)$$

Multiplying out the brackets reduces (12.34) to

$$= \langle \psi_{\vec{k}} | u_{\vec{k}}^2 \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} + u_{\vec{k}} v_{\vec{k}} \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} + u_{\vec{k}} v_{\vec{k}}$$

$$\cdot \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow} + v_{\vec{k}}^2 \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow} | \psi_{\vec{k}} \rangle$$

$\hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow} = 1 - \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} \hat{a}_{-\vec{k}\downarrow} \hat{a}^+_{-\vec{k}\downarrow}$

$= 1 - \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} - \hat{a}^+_{-\vec{k}\downarrow} \hat{a}_{-\vec{k}\downarrow}$

$\hat{a}_{\vec{k}\uparrow} \hat{a}_{-\vec{k}\downarrow} \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow} = 1 - \hat{a}^+_{-\vec{k}\downarrow} \hat{a}_{-\vec{k}\downarrow} \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow}$

$= 1 - \hat{a}^+_{-\vec{k}\downarrow} \hat{a}_{-\vec{k}\downarrow} - \hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow}$

$\equiv 0 \quad (12.35)$

Thus we obtain for the anomalous expectation value

$$\langle \hat{a}_{-\vec{k}\downarrow} \hat{a}_{\vec{k}\uparrow} \rangle = u_{\vec{k}} v_{\vec{k}} \quad (12.36)$$

12.2 Energy Gap:

Now we come back to the pairing Hamiltonian (11.127) and use the wave function of the BCS-theory (12.9) in order to approximately determine the ground state of a superconductor. To this end we consider the yet unknown weight factors $u_{\vec{k}}$, $v_{\vec{k}}$ for each wave vector $\vec{k}$ as variational parameters, which have to be determined according to a certain extremization procedure.

12.2.1 Variational Procedure:

The underlying variational procedure of the BCS theory is based on the following considerations. The main condition consists of minimizing the expectation value of the pairing Hamiltonian (11.127) with respect to the BCS wave function (12.9):

$$\langle \Psi_{BCS} | \hat{H}_P | \Psi_{BCS} \rangle \Rightarrow \text{minimal} \tag{12.37}$$

But this minimization has to respect two constraints:

1) The first constraint demands that the BCS wave function (12.9) is normalized. According to section 12.1.5 this means that the weight factors $u_{\vec{k}}$, $v_{\vec{k}}$ are not independent but are related via (12.21).
2) As discussed in section 12.1 the BCS wave function (12.9) describes states with different particle numbers. Therefore, following the basic idea of a grand canonical ensemble in statistical mechanics, the second constraint demands that the expectation value of the particle number operator $\hat{N}$ with respect to the BCS wave function (12.9) is given by a fixed particle number:

$$\langle \Psi_{BCS} | \hat{N} | \Psi_{BCS} \rangle = \overline{N} = \text{fixed} \tag{12.38}$$

12.2.2 Incorporation of Constraints:

The two constraints represent certain conditions for the weight factors $u_{\vec{k}}$, $v_{\vec{k}}$ of the BCS wave function, which have to be taken into account during the minimization of the expectation value of the pairing Hamiltonian (12.37):

1) The normalization (12.21) allows to express, e.g., $u_{\vec{k}}$ via $v_{\vec{k}}$ according to

$$u_{\vec{k}} = \sqrt{1 - v_{\vec{k}}^2} \tag{12.39}$$

Thus, for each wave vector $\vec{k}$, one has not to vary two parameters $u_{\vec{k}}, v_{\vec{k}}$ but only the single parameter $v_{\vec{k}}$.

2) Both the main condition (12.37) and the second constraint (12.38) can be combined due to the method of Lagrange multipliers:

$$\langle \Psi_{BCS} | \hat{H}_p | \Psi_{BCS} \rangle \Rightarrow \text{minimal} \tag{12.40}$$

where we have introduced the grand-canonical pairing Hamiltonian

$$\hat{H}'_p = \hat{H}_p - \mu \hat{N} \tag{12.41}$$

where the chemical potential μ represents the corresponding Lagrange multiplier.

12.2.3 Preparations:

Inserting the pairing Hamiltonian (11.127) and the particle-number operator $\hat{N}$ defined already in (12.32) into the grand-canonical Hamiltonian (12.41) yields

$$\langle \hat{H}'_p \rangle = \langle \Psi_{BCS} | \sum_{\vec{k}} \xi_{\vec{k}} \sum_{\sigma} \hat{a}^+_{\vec{k}\sigma} \hat{a}_{\vec{k}\sigma} + \sum_{\vec{k},\vec{k}'} V_{\vec{k}\vec{k}'} \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow} \hat{a}_{-\vec{k}'\downarrow} \hat{a}_{\vec{k}'\uparrow} | \Psi_{BCS} \rangle \tag{12.42}$$

where we have introduced the abbreviation

$$\xi_{\vec{k}} = \varepsilon(\vec{k}) - \mu \tag{12.43}$$

as the deviation of the free dispersion $\varepsilon(\vec{k})$ from the Lagrange multiplier μ. The expectation values from the particle numbers follow from (12.32). Furthermore, as the interaction Hamiltonian in (12.42) only consists of terms with $\vec{k} \neq \vec{k}'$, its expectation value factorizes into independent contributions for $\vec{k}$ and $\vec{k}'$, which are each given by (12.36). Thus, (12.42) reduces to

$$\langle \hat{H}'_p \rangle = \sum_{\vec{k}} \xi_{\vec{k}} 2 v_{\vec{k}}^2 + \sum_{\vec{k} \neq \vec{k}'} V_{\vec{k},\vec{k}'} u_{\vec{k}} v_{\vec{k}} u_{\vec{k}'} v_{\vec{k}'} \tag{12.44}$$

This represents a physically intuitive expression for the expectation value of the grand-canonical Hamiltonian. For both terms we sum the respective energy independent of the wave vector multiplied with

the probability of its occurrence over all wave vectors. Inserting (12.39) in (12.44) yields the final expression, which has to be extremized

$$\langle \hat{H}'_P \rangle = \sum_{\vec{k}} 2\zeta_{\vec{k}} v_{\vec{k}}^2 + \sum_{\vec{k}\neq\vec{k}'} V_{\vec{k},\vec{k}'} v_{\vec{k}} \sqrt{1-v_{\vec{k}}^2}\, v_{\vec{k}'} \sqrt{1-v_{\vec{k}'}^2} \quad (12.45)$$

12.2.4 Extremization:

Finally, we are in the position to extremize the expectation value of the grand-canonical Hamiltonian (12.45) with respect to the weight factor $v_{\vec{k}}$ for all wave vectors $\vec{k}$:

$$\frac{\partial \langle \hat{H}'_P \rangle}{\partial v_{\vec{k}}} = 0 \quad (12.46)$$

Inserting (12.45) into (12.46) we obtain

$$4\zeta_{\vec{k}} v_{\vec{k}} + 2 \sum_{\vec{k}'\neq\vec{k}} V_{\vec{k},\vec{k}'} \left\{ \sqrt{1-v_{\vec{k}}^2} + v_{\vec{k}} \frac{-v_{\vec{k}}}{\sqrt{1-v_{\vec{k}}^2}} \right\} v_{\vec{k}'} \sqrt{1-v_{\vec{k}'}^2} = 0 \quad (12.47)$$

Note that the prefactor 2 in front of the second term takes into account the symmetry of the interaction in (12.45) with respect to $\vec{k}$ and $\vec{k}'$. It is now suitable to introduce as a new abbreviation the gap parameter

$$\Delta_{\vec{k}} = -\sum_{\vec{k}'\neq\vec{k}} V_{\vec{k},\vec{k}'} v_{\vec{k}'} \sqrt{1-v_{\vec{k}'}^2} \quad (12.48)$$

where we have $\Delta_{\vec{k}} > 0$ due to the attractive interaction $V_{\vec{k},\vec{k}'} < 0$. Taking into account (12.48) reduces (12.47) to

$$2\zeta_{\vec{k}} = \Delta_{\vec{k}} \cdot \frac{1-2v_{\vec{k}}^2}{v_{\vec{k}}\sqrt{1-v_{\vec{k}}^2}} \quad (12.49)$$

Thus, solving (12.49) for $v_{\vec{k}}^2$ just represents a pure algebraic problem, which leads to a quadratic equation:

$$4\frac{\zeta_{\vec{k}}^2}{\Delta_{\vec{k}}^2} = \frac{1-4v_{\vec{k}}^2+4v_{\vec{k}}^4}{v_{\vec{k}}^2(1-v_{\vec{k}}^2)}$$

$$4v_{\vec{k}}^4 - 4v_{\vec{k}}^2 + 1 = 4\frac{\zeta_{\vec{k}}^2}{\Delta_{\vec{k}}^2} v_{\vec{k}}^2 - 4\frac{\zeta_{\vec{k}}^2}{\Delta_{\vec{k}}^2} v_{\vec{k}}^4$$

$$4\left(1+\frac{\zeta_{\vec{k}}^2}{\Delta_{\vec{k}}^2}\right) v_{\vec{k}}^4 - 4\left(1+\frac{\zeta_{\vec{k}}^2}{\Delta_{\vec{k}}^2}\right) v_{\vec{k}}^2 + 1 = 0 \quad (12.50)$$

This quadratic equation in $v_{\vec{k}}^2$ has two solutions:

$$v_{\vec{k}}^2 = \frac{4\left(1+\frac{\zeta_{\vec{k}}^2}{\Delta_{\vec{k}}^2}\right) \pm 4\sqrt{\left(1+\frac{\zeta_{\vec{k}}^2}{\Delta_{\vec{k}}^2}\right)^2 - \left(1+\frac{\zeta_{\vec{k}}^2}{\Delta_{\vec{k}}^2}\right)}}{8\left(1+\frac{\zeta_{\vec{k}}^2}{\Delta_{\vec{k}}^2}\right)}$$

$$= \frac{1}{2}\left\{1 \pm \sqrt{1 - \frac{\Delta_{\vec{k}}^2}{\Delta_{\vec{k}}^2 + \xi_{\vec{k}}^2}}\right\} = \frac{1}{2}\left\{1 \pm \frac{\xi_{\vec{k}}}{\sqrt{\xi_{\vec{k}}^2 + \Delta_{\vec{k}}^2}}\right\} \qquad (12.51)$$

Inserting (12.51) into (12.39) yields correspondingly

$$u_{\vec{k}}^2 = \frac{1}{2}\left\{1 \mp \frac{\xi_{\vec{k}}}{\sqrt{\xi_{\vec{k}}^2 + \Delta_{\vec{k}}^2}}\right\} \qquad (12.52)$$

But, due to physical reasons, the solutions for $u_{\vec{k}}^2$ and $v_{\vec{k}}^2$ have to be unique. To this end we demand that in the limit of a vanishing gap, i.e. $\Delta_{\vec{k}} \to 0$, we have to recover for the expectation value of the particle number at wave vector $\vec{k}$, which coincides due to (12.30) with $v_{\vec{k}}^2$, the Fermi-Dirac distribution at $T = 0\,K$:

$$\lim_{\Delta_{\vec{k}} \to 0} v_{\vec{k}}^2 = f_{\vec{k}} = \begin{cases} 1 ; & \varepsilon(\vec{k}) < E_F \\ 0 ; & \varepsilon(\vec{k}) > E_F \end{cases} \qquad (12.53)$$

The condition (12.53) has now two immediate consequences:

1) From the two signs in (12.51) only the lower one is correct. Thus we conclude

$$v_{\vec{k}}^2 = \frac{1}{2}\left\{1 - \frac{\xi_{\vec{k}}}{\sqrt{\xi_{\vec{k}}^2 + \Delta_{\vec{k}}^2}}\right\} \xrightarrow{(12.39)} u_{\vec{k}}^2 = \frac{1}{2}\left\{1 + \frac{\xi_{\vec{k}}}{\sqrt{\xi_{\vec{k}}^2 + \Delta_{\vec{k}}^2}}\right\} \qquad (12.54)$$

2) The Lagrange multiplier μ has to be identified with the Fermi energy E_F:

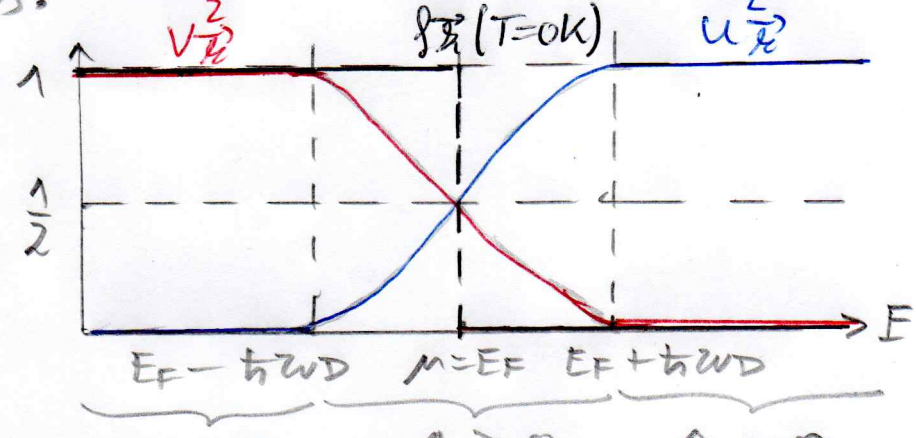
$$\mu = E_F \qquad (12.55)$$

12.2.5 Interpretation:

Although we describe a superconductor at zero temperature, its particle number distribution $v_{\vec{k}}^2$ deviates from a Fermi-Dirac distribution due to the emergence of Cooper pairs:

$u_{\vec{k}}^2$: probability of not having a Cooper pair

$v_{\vec{k}}^2$: probability of having a Cooper pair



The softening of the Fermi-Dirac distribution due to the emergence of Cooper pairs is accompanied with

a redistribution of energies. Some electrons are shuffled from energies below the Fermi energy to energies above the Fermi energy, which amounts to an increase of kinetic energy. But this energy increase is compensated by a reduction of the potential energy, as the virtual exchange of phonons, which accompanies the emergence of Cooper pairs, leads to a reduction of potential energy.

12.2.6 Gap Equation:

During the extremization procedure we introduced the gap parameter $\Delta_{\vec{k}}$ in (12.48), which allows the following interpretation:

$$\Delta_{\vec{k}} = -\sum_{\vec{k}' \neq \vec{k}} V_{\vec{k},\vec{k}'}\, u_{\vec{k}'} v_{\vec{k}'} \qquad (12.56)$$

summation over all possible $\vec{k}'$ — energy for scattering a Cooper pair from $-\vec{k}'$ to $\vec{k}$ — probability for the occurrence of a Cooper pair at $\vec{k}'$

Thus, the gap parameter $\Delta_{\vec{k}}$ represents the average energy for scattering a Cooper pair from some state $\vec{k}'$ into the state $\vec{k}$. In other words, it describes within a mean-field description the interaction of one Cooper pair at $\vec{k}$ with all possible other Cooper pairs at some $\vec{k}'$. Inserting the solution (12.54) of the extremization procedure into (12.56) leads to the gap equation:

$$\Delta_{\vec{k}} = -\sum_{\vec{k}' \neq \vec{k}} V_{\vec{k},\vec{k}'}\, \frac{1}{2}\left(1 - \frac{\xi_{\vec{k}'}}{\sqrt{\xi^2_{\vec{k}'} + \Delta^2_{\vec{k}'}}}\right)\left(1 + \frac{\xi_{\vec{k}'}}{\sqrt{\xi^2_{\vec{k}'} + \Delta^2_{\vec{k}'}}}\right)$$

$$= -\frac{1}{2}\sum_{\vec{k}' \neq \vec{k}} V_{\vec{k},\vec{k}'}\, \frac{\Delta_{\vec{k}'}}{\sqrt{\xi^2_{\vec{k}'} + \Delta^2_{\vec{k}'}}} \qquad (12.57)$$

This gap equation is analogous to the equation of the energy gain due to the emergence of a Cooper pair as worked out in Chapter 9 within the Cooper problem.

12.2.7 Gap Parameter:

In close analogy to the Cooper problem we also assume within the BCS theory that the matrix elements $V_{\vec{k},\vec{k}'}$ are

1) homogeneous and isotropic, i.e. that they are constant

2) attractive within a thin shell of the thickness of the Debye energy around the Fermi sphere.

Both assumptions can be summarised by

$$V_{\vec{k},\vec{k}'} = \begin{cases} -g/V & ; |\xi_{\vec{k}}|, |\xi_{\vec{k}'}| < \hbar\omega_D \\ 0 & ; \text{otherwise} \end{cases} \tag{12.58}$$

Due to the gap equation (12.57) the ansatz (12.58) for the matrix element $V_{\vec{k},\vec{k}'}$ has the following consequence for the gap parameter:

$$\Delta_{\vec{k}} = \begin{cases} \Delta & ; |\xi_{\vec{k}}| < \hbar\omega_D \\ 0 & ; \text{otherwise} \end{cases} \tag{12.59}$$

Inserting (12.58) and (12.59) into (12.57) then yields for $|\xi_{\vec{k}}| < \hbar\omega_D$

$$\Delta = \frac{g}{2V} \sum_{|\xi_{\vec{k}'}| < \hbar\omega_D} \frac{\Delta}{\sqrt{\xi_{\vec{k}'}^2 + \Delta^2}} \quad \Rightarrow \quad \frac{2}{g} = \frac{1}{V} \sum_{|\xi_{\vec{k}'}| < \hbar\omega_D} \frac{1}{\sqrt{\xi_{\vec{k}'}^2 + \Delta^2}} \tag{12.60}$$

In the thermodynamic limit the discrete sum over the wave vectors $\vec{k}'$ converts into an integral according to (9.49), (9.50):

$$\sum_{|\xi_{\vec{k}}| < \hbar\omega_D} \bullet = \frac{V}{(2\pi)^3} \int_{|\xi_{\vec{k}}| < \hbar\omega_D} d^3k \, \bullet \tag{12.61}$$

Due to (12.43) and (12.60) we have an isotropic integrand, so we get

$$\frac{2}{g} = \int_{-\hbar\omega_D}^{+\hbar\omega_D} d\xi \, N(\xi) \cdot \frac{1}{\sqrt{\xi^2 + \Delta^2}} \tag{12.62}$$

Here $N(\xi)$ represents the density of states around the Fermi edge. As in section 9.2.7 we can now use the fact that the density of states $N(\xi) \sim \sqrt{E_F + \xi}$ varies within the integration interval $\xi \in [0, \hbar\omega_D]$ due to $\hbar\omega_D \ll E_F$ only slightly. Therefore we can approximately take out the density of states at the Fermi edge of the integral

$$\frac{2}{g} = N(E_F) \int_{-\hbar\omega_D}^{+\hbar\omega_D} d\xi \, \frac{1}{\sqrt{\xi^2 + \Delta^2}} \tag{12.63}$$

As the integrand in (12.63) is even, the integral reduces to

$$\frac{1}{g} = N(E_F) \int_0^{\hbar\omega_D} d\xi \, \frac{1}{\sqrt{\xi^2 + \Delta^2}} \tag{12.64}$$

The remaining integral is elementary and can be

immediately evaluated:

$$\frac{1}{N(E_F)g} = \left[\operatorname{arsinh}\frac{\xi}{\Delta}\right]_0^{\hbar\omega_D} = \operatorname{arsinh}\frac{\hbar\omega_D}{\Delta}$$

$$\Rightarrow \quad \Delta = \hbar\omega_D \cdot \frac{1}{\sinh\frac{1}{gN(E_F)}} \tag{12.65}$$

Here we consider the following special cases:

1) In case of a strong coupling $gN(E_F) \gg 1$ we get from (12.65) the perturbative result that the energy gap Δ is proportional to the coupling:

$$\Delta = \hbar\omega_D \cdot gN(E_F) \tag{12.66}$$

2) In case of a weak coupling $gN(E_F) \ll 1$ we get from (12.65) instead the non-perturbative result

$$\Delta = 2\hbar\omega_D \cdot e^{-\frac{1}{gN(E_F)}} \tag{12.67}$$

Note that in comparison of (12.67) with the Cooper result (9.60) the factor 2 in the exponent is missing. This is due to the assumption of the BCS theory to consider an energy shell $\hbar\omega_D$ both within and outside of the Fermi sphere. In contrast to that the Cooper problem considered the energy shell $\hbar\omega_D$ only outside of the Fermi sphere.

12.2.8 High Tc-Superconductors:

Finally, we remark that the BCS theory, as worked out here, is not applicable for high Tc superconductors. Similar to the Cooper problem the following approximations are not valid there:

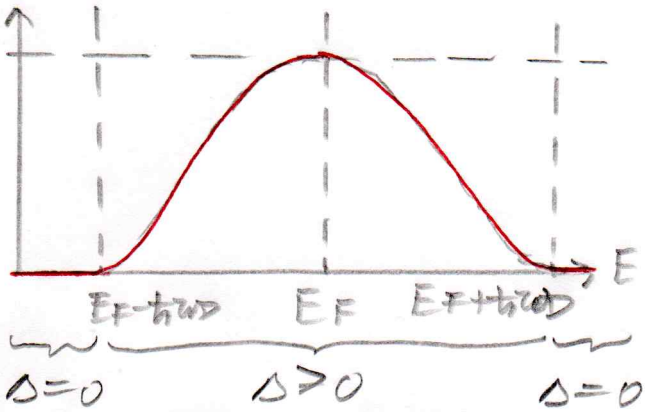
1) High Tc-superconductors are extremely anisotropic.
2) They have quite large Debye energies and, thus, large phonon frequencies in comparison with the Fermi energy.
3) As a consequence, the density of states at the Fermi edge can not be approximated by a constant.

12.2.9 Remark:

The weight factors $u_{\vec{k}}, v_{\vec{k}}$ represent the probability amplitudes to not find and to find a Cooper pair. This pro-

duct determines the anomalous expectation value (12.36) and, thus, quantifies how strong the creation and annihilation of a Cooper pair is:

$$u_{\vec{k}} \cdot v_{\vec{k}} \overset{(12.54)}{=\!=} \frac{1}{2} \cdot \frac{\Delta_{\vec{k}}}{\sqrt{\xi_{\vec{k}}^2 + \Delta_{\vec{k}}^2}} \qquad (12.68)$$



12.2.10 Summary:

Due to the ansatz for the BCS wave function (12.9) it is assumed that at zero temperature all electrons exist in form of Cooper pairs. Thus, in conclusion, unpaired electrons, which would be normal conducting, do not exist in the BCS theory at zero temperature.

The virtual exchange of phonons and, thus, the scattering of Cooper pairs does only exist within a thin shell around the Fermi edge. Only in this region of Fourier space the expectation value of the creation and annihilation of Cooper pairs is largest. Thus, there the largest fluctuations occur. In the next section we show that they ultimately lead to a reduction of the energy of the superconducting state in comparison to the normal conducting state.

12.3 Condensation Energy:

The discussion of the thermodynamic properties of a superconductor in Chapter 3 led to the conclusion that the superconducting state is energetically lower than the normal conducting state due to the expulsion of flux quanta. This so-called condensation energy turned out to be given by the critical magnetic field. Generalising the former finding (3.25) to zero temperature yields the concrete relation

$$E_s - E_n = -\frac{\mu_0}{2} V H_c^2 \qquad (12.69)$$

Here H_c denotes the critical magnetic field at zero temperature, i.e. $H_c = H_c(T = 0\,K)$.

From the point of view of the microscopic BCS theory

the question arises whether also here the superconducting state is energetically lower than the normal conducting state. If this would be the case, then equating the microscopic expression for the condensation energy with the corresponding thermodynamic one (12.69) should determine how the critical magnetic field H_c depends on the microscopic parameters of the BCS theory.

12.3.1 Derivation:

The expectation value of the grand-canonical Hamiltonian (12.42) defines the total energy. Inserting therein the definition of the gap parameter (12.48) leads to

$$\langle \hat{H}'_p \rangle = 2 \sum_{\vec{k}} \xi_{\vec{k}} v_{\vec{k}}^2 - \sum_{\vec{k}} \Delta_{\vec{k}} u_{\vec{k}} v_{\vec{k}} \qquad (12.70)$$

This total energy can now be specialized to both the superconducting and the normal conducting state, respectively, as follows. To this end we summarize our previous findings in form of a well-arranged table:

superconducting state	normal conducting state
$\Delta_{\vec{k}} \begin{cases} > 0 \; ; \; \lvert \xi_{\vec{k}} \rvert < \hbar\omega_D \\ = 0 \; ; \; \text{otherwise} \end{cases}$	$\Delta_{\vec{k}} = 0$ for all $\vec{k}$
$u_{\vec{k}}^2 = \begin{cases} 0 \\ \frac{1}{2}\left\{1 + \frac{\xi_{\vec{k}}}{\sqrt{\xi_{\vec{k}}^2 + \Delta_{\vec{k}}^2}}\right\} \\ 1 \end{cases} \begin{matrix} ; \; \xi_{\vec{k}} < -\hbar\omega_D \\ ; \; \lvert \xi_{\vec{k}} \rvert < \hbar\omega_D \\ ; \; \xi_{\vec{k}} > \hbar\omega_D \end{matrix}$	$u_{\vec{k}}^2 = \begin{cases} 0 \; ; \; \xi_{\vec{k}} < 0 \\ 1 \; ; \; \xi_{\vec{k}} > 0 \end{cases}$
$v_{\vec{k}}^2 = \begin{cases} 1 \\ \frac{1}{2}\left\{1 - \frac{\xi_{\vec{k}}}{\sqrt{\xi_{\vec{k}}^2 + \Delta_{\vec{k}}^2}}\right\} \\ 0 \end{cases} \begin{matrix} ; \; \xi_{\vec{k}} < -\hbar\omega_D \\ ; \; \lvert \xi_{\vec{k}} \rvert < \hbar\omega_D \\ ; \; \xi_{\vec{k}} > \hbar\omega_D \end{matrix}$	$v_{\vec{k}}^2 = \begin{cases} 1 \; ; \; \xi_{\vec{k}} < 0 \\ 0 \; ; \; \xi_{\vec{k}} > 0 \end{cases}$

With these values for $\Delta_{\vec{k}}$, $u_{\vec{k}}$, $v_{\vec{k}}$ the condensation energy of the BCS theory follows from (12.70):

$$E_s - E_n = \sum_{\vec{k}} \left\{ 2 \xi_{\vec{k}} u_{\vec{k}} v_{\vec{k}} - \Delta_{\vec{k}} u_{\vec{k}} v_{\vec{k}} \right\} - 2 \sum_{\xi_{\vec{k}} < 0} \xi_{\vec{k}} \qquad (12.71)$$

This result for the condensation energy can be decomposed according to

$$E_s - E_n = E_{\text{kin}} + E_{\text{pot}} \qquad (12.72)$$

into the kinetic contribution

$$E_{kin} = 2 \sum_{\xi_{\vec{k}}<0} \xi_{\vec{k}} \left(V_{\vec{k}}^2 - 1\right) + 2 \sum_{\xi_{\vec{k}}>0} \xi_{\vec{k}} V_{\vec{k}}^2 \qquad (12.73)$$

and the potential contribution

$$E_{pot} = -\sum_{\vec{k}} \Delta_{\vec{k}} U_{\vec{k}} V_{\vec{k}} \qquad (12.74)$$

12.3.2 Kinetic Energy:

Due to the normalization condition (12.21) the kinetic energy (12.73) reduces to

$$E_{kin} = -2 \sum_{\xi_{\vec{k}}<0} \xi_{\vec{k}} U_{\vec{k}}^2 + 2 \sum_{\xi_{\vec{k}}>0} \xi_{\vec{k}} V_{\vec{k}}^2 \qquad (12.75)$$

Inserting (12.54) then yields

$$E_{kin} = -2 \sum_{-\hbar\omega_D \le \xi_{\vec{k}} \le 0} \xi_{\vec{k}} \frac{1}{2}\left\{1 + \frac{\xi_{\vec{k}}}{\sqrt{\xi_{\vec{k}}^2 + \Delta_{\vec{k}}^2}}\right\} + 2 \sum_{0 \le \xi_{\vec{k}} \le \hbar\omega_D} \xi_{\vec{k}} \frac{1}{2}\left\{1 - \frac{\xi_{\vec{k}}}{\sqrt{\xi_{\vec{k}}^2 + \Delta_{\vec{k}}^2}}\right\} \qquad (12.76)$$

Performing the thermodynamic limit (12.61) allows to convert the sums over the discrete wave vectors $\vec{k}$ into corresponding integrals. Furthermore, we can take into account that $\Delta_{\vec{k}} = \Delta$ holds within the integration boundary:

$$\frac{E_{kin}}{V} = -\int_{-\hbar\omega_D}^{0} d\xi\, N(\xi)\,\xi\left(1 + \frac{\xi}{\sqrt{\xi^2+\Delta^2}}\right) + \int_{0}^{\hbar\omega_D} d\xi\, N(\xi)\,\xi\left(1 - \frac{\xi}{\sqrt{\xi^2+\Delta^2}}\right) \qquad (12.77)$$

Here we can use again that the density of states is constant within the integration boundary. Furthermore, we perform the substitution $\xi \to -\xi$ in the first integral:

$$\frac{E_{kin}}{V} = -N(E_F)\int_{0}^{\hbar\omega_D} d\xi\,(-\xi)\left(1 + \frac{-\xi}{\sqrt{\xi^2+\Delta^2}}\right) + N(E_F)\int_{0}^{\hbar\omega_D} d\xi\,\xi\left(1 - \frac{\xi}{\sqrt{\xi^2+\Delta^2}}\right) \qquad (12.78)$$

Thus, we recognise that both integrals are equal:

$$\frac{E_{kin}}{V} = 2N(E_F)\int_{0}^{\hbar\omega_D} d\xi\,\xi\left(1 - \frac{\xi}{\sqrt{\xi^2+\Delta^2}}\right) \qquad (12.79)$$

The integral is calculated by performing at first a partial integration:

$$\frac{E_{kin}}{V} = 2N(E_F)\left\{\left[\frac{1}{2}\xi^2 - \xi\sqrt{\xi^2+\Delta^2}\right]_0^{\hbar\omega_D} + \int_0^{\hbar\omega_D} d\xi\,\sqrt{\xi^2+\Delta^2}\right\}$$

$$= 2N(E_F)\left[\frac{1}{2}\xi^2 - \frac{1}{2}\xi\sqrt{\xi^2+\Delta^2} + \frac{1}{2}\xi\sqrt{\xi^2+\Delta^2} + \frac{\Delta^2}{2}\operatorname{arsinh}\frac{\xi}{\Delta}\right]_0^{\hbar\omega_D}$$

$$= N(E_F)(\hbar\omega_D)^2\left\{1 - \sqrt{1 + \frac{\Delta^2}{(\hbar\omega_D)^2}}\right\} + N(E_F)\Delta^2 \operatorname{arsinh}\frac{\hbar\omega_D}{\Delta} \qquad (12.80)$$

Inserting for the last term in (12.80) the expression (12.65) for the gap parameter Δ yields, finally:

$$E_{kin} = V\left\{\frac{\Delta^2}{g} + N(E_F)(\hbar\omega_D)^2\left[1-\sqrt{1+\left(\frac{\Delta}{\hbar\omega_D}\right)^2}\right]\right\} \quad (12.81)$$

12.3.3 Potential Energy:

Inserting (12.54) into the potential energy (12.74) leads to

$$E_{Pot} = -\sum_{|\xi_{\vec{k}}|<\hbar\omega_D} \Delta \frac{1}{2}\frac{\Delta}{\sqrt{\xi_{\vec{k}}^2+\Delta^2}} \quad (12.82)$$

The thermodynamic limit (12.61) converts the sum (12.82) into an integral which is evaluated as follows:

$$\frac{E_{Pot}}{V} = -\frac{\Delta^2}{2}\int_{-\hbar\omega_D}^{\hbar\omega_D} d\xi N(\xi)\frac{1}{\sqrt{\xi^2+\Delta^2}} = -\Delta^2 N(E_F)\int_0^{\hbar\omega_D} d\xi \frac{1}{\sqrt{\xi^2+\Delta^2}}$$

$$= -\Delta^2 N(E_F)\left[\operatorname{arsinh}\frac{\xi}{\Delta}\right]_0^{\hbar\omega_D} = -\Delta^2 N(E_F)\operatorname{arsinh}\frac{\hbar\omega_D}{\Delta} \quad (12.83)$$

Inserting therein the expression (12.65) for the gap parameter Δ, we obtain for the potential energy

$$E_{Pot} = -\frac{\Delta^2}{g}V < 0 \quad (12.84)$$

Thus, the transition from the normal conducting to the superconducting state potential energy is released.

12.3.4 Energy Balance:

Adding the kinetic and the potential energy contributions (12.81) and (12.84) of the condensation energy we get

$$E_s - E_n = V N(E_F)(\hbar\omega_D)^2\left\{1-\sqrt{1+\left(\frac{\Delta}{\hbar\omega_D}\right)^2}\right\} \quad (12.85)$$

Thus, indeed, the condensation energy (12.85) turns out to be negative. In case of a weak coupling $gN(E_F) \ll 1$ we have $\Delta \ll \hbar\omega_D$ according to (12.67). This allows to approximate (12.85) via

$$E_s - E_n = -VN(E_F)(\hbar\omega_D)^2 \cdot \frac{1}{2}\left(\frac{\Delta}{\hbar\omega_D}\right)^2 = -\frac{1}{2}VN(E_F)\Delta^2 < 0 \quad (12.86)$$

Here $VN(E_F)\Delta/2$ represents the number of Cooper pairs at the Fermi edge and Δ stands for the energy gain per Cooper pair. Thus, in conclusion, we managed to calculate within the realm of the BCS theory the condensation energy.

12.3.5 Critical Magnetic Field:

Equating the phenomenological expression (12.69) of the condensation energy with the microscopic one (12.86), we obtain for the critical magnetic field:

$$H_c = \sqrt{\frac{N(E_F)\,\Delta^2}{\mu_0}} \qquad (12.87)$$

Note that the density of states at the Fermi edge $N(E_F)$ is experimentally accessible by measuring the temperature dependence of the electronic heat capacity above the critical magnetic field, i.e. for the normal conducting state. According to the Sommerfeld theory for electrons, see e.g. the solid-state physics book by Ashcroft and Mermin, one has

$$C = \frac{\pi^2}{3} k_B^2 T N(E_F) \qquad (12.88)$$

Thus $N(E_F)$ directly follows from measuring $(C/T)/T$. In addition, measuring the critical magnetic field H_c at zero temperature then allows to determine the gap parameter Δ from (12.87). Finally, combining (12.67) and (12.87), we can read off the isotope effect

$$H_c(0) \sim \Delta(0) \sim \hbar\omega_D \sim \frac{1}{\sqrt{M}} \qquad (12.89)$$