Lecture notes
Quantum Theory of Solids

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Foreword to the digitalized lecture notes

Digitialized lecture notes for the course "TFY4210 - Quantum Theory of Many-Particle Systems" held by Prof. Asle Sudbø spring 2020. These notes follow that of the hand written lecture notes, which are based upon the lecture notes for the course "FY8302 - Quantum Theory of Solids", written in 1996 or so.

There may be a few extra comments to the text and / or figures that is based on the lectures themselves.

Course website: https://www.ntnu.edu/studies/courses/TFY4210

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1 Introduction

Many-particle systems are systems where interactions between the particle-constituents of the system are important. When quantum effects are important, we talk about quantum many-body systems. The sort of systems we will consider in this course are made up of aggregate states of various atoms, and may typically be separated, a priori, into interacting states of electrons and ions:

1. Electrons interacting among themselves.
2. Ions interacting among themselves.
3. Interactions between electrons and ions.

What we seek to explain, is what determines the various physical states such a system may take up. Why are some materials metals, insulators, superfluids, superconductors, ferromagnets, antiferromagnets? The plethora of states appears quite bewildering. A major objective of this course is to see how to give a unifying description of all these systems, a "theory of everything" (almost).

In principle, the answer to the above question is obtained by solving the Schrödinger-equation for the many-body quantum-mechanical state $|\psi\rangle$:

$$H|\psi\rangle = i\hbar \frac{\partial |\psi\rangle}{\partial t} \tag{1.1}$$

H: Operator that generates dynamics. Here, H is the Hamiltonian of the system, this H consists of three parts:

1. H_{e-e} : Describes the electrons with interactions among themselves.
2. H_{i-i} : Describes the ions with interactions among themselves.
3. H_{e-i} : Describes the interactions between ions and electrons.

The Hamiltonian we consider will furthermore describe a priori non-relativistic systems, which means we can separate H into kinetic energy, T, and potential energy, V,

$$H = T + V \tag{1.2}$$

$$H_{e-e} = \sum_i \frac{\vec{p_i}^2}{2m} + \sum_{i,j} V_{e-e}^{Coulomb}(\vec{r_i} - \vec{r_j}) \tag{1.3}$$

m : Electron mass
$\vec{p_i}$: Electron momentum
$\vec{r_i}$: Electron coordinate
$V_{e-e}^{Coulomb}(\vec{r}) = \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}$ $-e$: Electron charge (e defined as positive)
ε_0 : Vacuum-permittivity

$$H_{i-i} = \sum_i \frac{\vec{P_i}^2}{2M} + \sum_{i,j} V_{i-i}^{Coulomb}(\vec{R_i} - \vec{R_j}) \tag{1.4}$$

M : Ion mass
$\vec{P_i}$: Ion momentum
$\vec{R_i}$: Ion coordinate
$V_{i-i}^{Coulomb}(\vec{R}) = \frac{Z^2e^2}{4\pi\varepsilon_0}\frac{1}{R}$
Ze : Ionic charge

$$H_{e-i} = \sum_{i,j} V_{e-i}^{Coulomb}(\vec{R_i} - \vec{r_j}) \tag{1.5}$$

$V_{e-i}^{Coulomb}(\vec{R}) = \frac{-Ze^2}{4\pi\varepsilon_0}\frac{1}{R}$

NB! Note that the kinetic energy of the entire system is the sum of kinetic energies of each individual particle. The potential energy of the system is the sum of potential energy of pairs of particles, this later statement is an approximation. In principle, we can include three-, four-, five-, ... body interactions, but these will be ignored to a good approximation. Thus, the total Hamiltonian for a many-body system is a sum of one-particle terms and two-particle terms. This is an enormous simplification. NB!! There exists physical systems in condensed matter physics where this may not be a good approximation.

Observables are represented by operators $\hat{O}$. A measurable quantity is then

$$\left\langle \hat{O} \right\rangle = \langle\psi| \hat{O} |\psi\rangle , \tag{1.6}$$

which is the expectation value of $\hat{O}$ in the many-body quantum state. $|\psi\rangle$ is computed at zero temperature $T = 0$; i.e. $|\psi\rangle$ is a ground state. Often, we would like to compute expectation-values of $\hat{O}$ at $T > 0$. This can be done by introducing a statistical parameter

$$\beta = \frac{1}{k_b T}; \tag{1.7}$$

k_b : Boltzman's constant.

Partition function:

$$\mathcal{Z} = Tr\left(\mathrm{e}^{-\beta H}\right) \tag{1.8}$$

$$\left\langle \hat{O} \right\rangle_T = \frac{1}{Z} Tr\left(\hat{O}\mathrm{e}^{-\beta H}\right) \tag{1.9}$$

Thermal average involves also excited states.

The systems are assumed to be overall charge-neutral. The above Hamiltonian is formulated as a classical Hamiltonian in terms of coordinates and momenta of electrons and ions. We are seeking a quantum formulation of such a system, which means we need to find a useful formalism of operators and states in order to proceed.

For the systems that will be considered in this course, quantum particles come in two varieties:

i) Fermions.

ii) Bosons.

We first proceed by setting up a formulation for fermions (electrons are fermions).

2 Many-particle states, fermions

2.1 N-particle vacuum state

Many-particle states will be built up by constructing a basis using products of single-particle states. Let λ be some set of quantum numbers that uniquely specifies a single-particle quantum state.

Example: λ could be the set of quantum numbers of the hydrogen-atom.
$\lambda = (n, l, m, \sigma)$

n : Main quantum number.
l : Orbital angular momentum quantum number.
m : Quantization of angular momentum along z-axis.
σ : Spin quantum number.

Motion in 3 dimensions $\implies$ 3 quantum numbers : (n, l, m)
Spin: 1 quantum number.

Corresponding state:	$\|n_\lambda\rangle$
Adjoint state:	$\langle n_\lambda \| = (\|n_\lambda\rangle)^\dagger$

Vacuum-state (unoccupied state): $|0_\lambda\rangle$
Introduce creation and annihilation operators.

Creation:	$c_\lambda^\dagger$
Annihilation:	c_λ

$$
\begin{aligned}
|1_\lambda\rangle &= c_\lambda^\dagger \, |0_\lambda\rangle \\
|0_\lambda\rangle &= c_\lambda \, |1_\lambda\rangle \\
0 &= c_\lambda \, |0_\lambda\rangle
\end{aligned}
$$

In general, we will use a set og quantum numbers that are convenient. Exactly what this means in practice will become clear later, when we start looking at specific systems.

Many-body state:

$$|N\rangle = |n_{\lambda_1}, n_{\lambda_2}, n_{\lambda_3}, ..., n_{\lambda_N}\rangle$$

N-particle vacuum-state:

$$
\begin{aligned}
&|0\rangle = |0_{\lambda_1}, 0_{\lambda_2}, ..., 0_{\lambda_N}\rangle \\
&|N\rangle : \text{Fock-basis}
\end{aligned}
\tag{2.1}
$$

We regard fermions as quantized excitations of a matter field, in the same way as we regard photons as quantized excitations of an electromagnetic field.

Field operators for a fermion: $\psi^\dagger(x,t)$: Creates a fermion in some quantum state at point $(\vec{r},s)=x$ at time t.

$$\psi^\dagger(x,t)=\sum_\lambda c_\lambda^\dagger(t)\varphi_\lambda^*(x) \tag{2.2}$$

$\varphi_\lambda(\vec{r},s)$: Wave-function for quantum state with quantum numbers $\underline{\lambda}$.

Quantization:

$$\{\psi^\dagger(x,t),\psi(x,t)\}=\delta(\vec{r}-\vec{r'})\delta(s,s') \tag{2.3}$$

Note that t is the same in $\psi^\dagger$ and ψ!

$$\{A,B\}=AB+BA \tag{2.4}$$

The set of wavefunctions $\varphi_\lambda(\vec{r})$ are assumed to constitute a complete set i.e. any function $f(\vec{r})$ can be expressed in terms of $\{\varphi_\lambda(\vec{r})\}$

$$f(\vec{r},s)=\sum_\lambda a_\lambda\varphi_\lambda(\vec{r},s) \tag{2.5}$$

$\{\varphi_\lambda(\vec{r},s)\}$ is furthermore assumed to be orthonormalized

$$\sum_{\vec{r},s}\varphi_\lambda^*(\vec{r},s)\varphi_{\lambda'}(\vec{r},s)=\delta_{\lambda,\lambda'}, \tag{2.6}$$

where

$$\delta_{\lambda,\lambda'}=\begin{cases}1; & \lambda=\lambda'\\ 0; & \lambda\neq\lambda'\end{cases}$$

$$\begin{aligned}\sum_{\vec{r}}\varphi_{\lambda'}^*(\vec{r},s)f(\vec{r},s)&=\sum_\lambda\sum_{\vec{r}}\varphi_{\lambda'}^*(\vec{r},s)\varphi_\lambda(\vec{r},s)\\&=\sum_\lambda\delta_{\lambda,\lambda'}\\&=\lambda'\end{aligned}$$

$$\begin{aligned}f(\vec{r},s)&=\sum_\lambda\sum_{\vec{r'},s}\varphi_\lambda^*(\vec{r'},s')f(\vec{r},s')\varphi_\lambda(\vec{r},s)\\&=\sum_{\vec{r'},s'}\left[\sum_\lambda\varphi_\lambda^*(\vec{r'},s')\varphi_\lambda(\vec{r},s)\right]f(\vec{r'},s')\\&=\sum_{\vec{r'},s'}\delta(\vec{r}-\vec{r'})\delta_{s,s'}f(\vec{r'},s')\end{aligned}$$

2.2 Completeness relation

$$\sum_{\lambda} \varphi_{\lambda}^{*}(\vec{r}, s)\varphi_{\lambda}(\vec{r}, s) = \delta(\vec{r} - \vec{r'})\delta_{s,s'} \tag{2.7}$$

Futhermore:

$$\begin{aligned} \{\psi^{\dagger}(x', t), \psi(x, t)\} &= \delta_{x',x} \\ &= \sum_{\lambda_1} \sum_{\lambda_2} \{c_{\lambda_1}^{\dagger}, c_{\lambda_2}\}(\vec{r}, s)\varphi_{\lambda_1}^{*}(\vec{r}, s)\varphi_{\lambda_2} \end{aligned} \tag{2.8}$$

If $\{c_{\lambda_1}^{\dagger}, c_{\lambda_2}\} = \delta_{\lambda_1,\lambda_2}$ then equation (2.8) is satisified.

$$\{c_{\lambda_1}^{\dagger}, c_{\lambda_2}\} = \delta_{\lambda_1,\lambda_2} \tag{2.9}$$

In addition:

$$\{\psi^{\dagger}(x', t), \psi^{\dagger}(x, t)\} = 0 \implies \{c_{\lambda'}^{\dagger}, cd_{\lambda}\} = 0 \tag{2.10}$$

$$\{\psi(x', t), \psi(x, t)\} = 0 \implies \{c_{\lambda'}, c_{\lambda}\} = 0 \tag{2.11}$$

$$c_{\lambda}^{\dagger} c_{\lambda}^{\dagger} |0\rangle = 0 \tag{2.12}$$

Cannot create more than one fermion in one single-particle state. (Pauli-principle) $\implies$

$$\begin{aligned} c_{\lambda} c_{\lambda} |n_{\lambda}\rangle &= 0 \\ \{c_{\lambda_1}^{\dagger}, c_{\lambda_2}\} &= \delta_{\lambda_1,\lambda_2} \\ \lambda_1 \neq \lambda &: \\ |n_{\lambda_1} n_{\lambda_2}\rangle &= - |n_{\lambda_2} n_{\lambda_1}\rangle \end{aligned}$$

A fermionic two-particle sstate is antisymmetric under interchange of the constituent single-particle states.

> The next step is now to express operators representing observables in terms of creation and destruction operators. This is called second quantization.

2.3 Operators

Definitions:

1. One-particle operator is an operator representing an observable of the following classical form

$$U = \sum_{i=1}^{N} U_i(\vec{r_i}, \vec{p_i}). \tag{2.13}$$

U_i depends only on the coordinate and momentum of one particle $(\vec{r_i}, \vec{p_i})$.

2. Two-particle operator is an operator representing an observable of the following classical form

$$V = \sum_{i,j} V_{ij}(\vec{r_i}, \vec{p_i}, \vec{r_j}, \vec{p_j}). \tag{2.14}$$

V_{ij} depends on the coordinates and momenta of two particles, $(\vec{r_i}, \vec{p_i})$ and $(\vec{r_j}, \vec{p_j})$. For the situations we will consider V_{ij} will depend only on $\vec{r_i}$ and $\vec{r_j}$, not $\vec{p_i}, \vec{p_j}$.

Matrix elements of single-particle operators.

$$\hat{U} \left|N\right\rangle = \sum_i \hat{U}_i \left|N\right\rangle$$

$\hat{U}_i$ Only works on *one* element in $|N\rangle$:

$$\hat{U}_i = \hat{U}_i \left| n_{\lambda_1}, \cdots, n_{\lambda_i}, \cdots, n_{\lambda_N} \right\rangle$$

Works on this element only

Examples of one-particle operators:

1. Kinetic energy T

$$\hat{T} = \sum_{i=1}^{N} \frac{\hat{p_i}^2}{2m} \left|N\right\rangle, \tag{2.15}$$

spin-independent (does not involve spin-coordinate).

2. Crystal potential that electrons move through in a solid

$$\hat{V} = \sum_i \hat{V}_i \left|N\right\rangle \tag{2.16}$$

$$\hat{V_i} = \sum_j \hat{V}_{ij}(\vec{r_i} - \vec{R_j}), \tag{2.17}$$

spin-independent, (no spin-coordinate).
$\vec{r_i}$: Electron-coordinate
$\vec{R_j}$: Ion-coordinate

The matrix element of a 1-p operator sandwiched between two many-particle states:

$$\begin{aligned}
\langle N'|\,\hat{U}\,|N\rangle &= \sum_i \langle N'|\,\hat{U}_i\,|N\rangle \\
&= \sum_i \Big\langle n'_1,\cdots,\ n'_i\ ,\cdots,n'_N\Big|\ \underbrace{\hat{U}_i}_{\text{i-th element}}\ \Big|n_1,\cdots,\ n_i\ ,\cdots,n_N\Big\rangle \\
&= \sum_i \Big\langle \tilde{N}'\Big|\tilde{N}\Big\rangle\,\langle n'_i|\,U_i\,|n_i\rangle \qquad (2.18)\\
\Big|\tilde{N}\Big\rangle &= \prod_{k\neq i}|n_k\rangle \\
\Big|\tilde{N}'\Big\rangle &= \prod_{k\neq i}|n'_k\rangle
\end{aligned}$$

Normalization:

$$\begin{aligned}
\frac{\langle N'|\,\hat{U}\,|N\rangle}{\langle N'|N\rangle} &= \sum_i \frac{\Big\langle \tilde{N}'\Big|\tilde{N}\Big\rangle}{\Big\langle \tilde{N}'\Big|\tilde{N}\Big\rangle}\cdot\frac{\langle n'_i|\,\hat{U}_i\,|n_i\rangle}{\langle n'_i|n_i\rangle} \\
&= \sum_i \frac{\langle n'_i|\,\hat{U}_i\,|n_i\rangle}{\langle n'_i|n_i\rangle} \qquad (2.19)
\end{aligned}$$

> One-particle operators are defined by matrix-elements in a one-particle Hilbert-space $\{|n_i\rangle\}$, $i=1,\cdots,N$.

Matrix elements of two-particle operators

$$\hat{V}\,|N\rangle = \sum_{i,j}\ \underbrace{\hat{V}_{ij}\ \Big|n_1,\cdots,\ n_i\ ,\cdots,\ n_j\ ,\cdots,n_N\Big\rangle}_{\text{Works only on these two elements}} \qquad (2.20)$$

Example: Coulomb-interactions
Matrix element:

$$\langle N'|\,\hat{V}\,|N\rangle = \sum_{i,j}\big\langle n'_1,\cdots,n'_i,\cdots,n'_j,\cdots,n'_N\big|\,\hat{V}_{ij}\,|n_1,\cdots,n_i,\cdots,n_j,\cdots,n_N\rangle \qquad (2.21)$$

$$= \sum_{i,j}\ \prod_{k\neq(i,k)}\langle n'_k|n_k\rangle\,\big\langle n'_i,n'_j\big|\,\hat{V}_{ij}\,|n_i,n_j\rangle \qquad (2.22)$$

Normalization:

$$\frac{\langle N'|\,\hat{V}\,|N\rangle}{\langle N'|N\rangle} = \sum_{ij} \frac{\langle n_i', n_j'|\,\hat{V}_{ij}\,|n_i, n_j\rangle}{\langle n_i', n_j'|n_i, n_j\rangle} \tag{2.23}$$

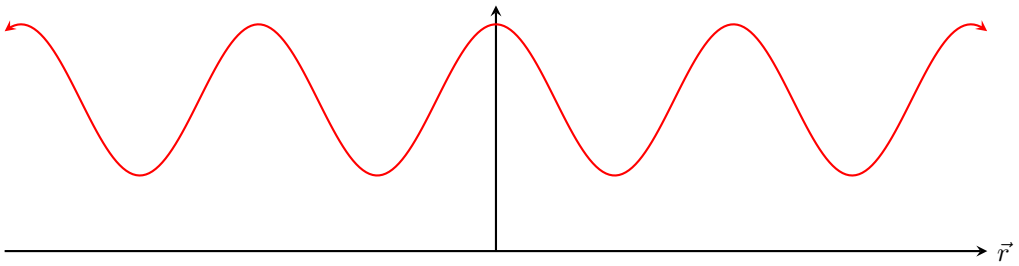
> Matrix elements of two-particle operators are computed in a Hilbert-space of two-particle states.

For the 2-particle operators we consider

$$\hat{V}_{ij} = \hat{V}_{ji}, \qquad i \neq j \tag{2.24}$$
$$\text{If } i = j \implies \hat{V}_{ij} = 0,$$

because otherwise a 2-particle operator would operate on a 1-particle state, which it does not.

Interacting electron gas in a periodic crystal potential $U(\vec{r})$



$$H = \sum_i \left[\frac{\vec{p_i}^{\,2}}{2m} + U(\vec{r_i})\right] + \sum_{ij} V_{e-e}^{C}(\vec{r_i} - \vec{r_j}) \tag{2.25}$$

This is, in general, a very hard problem to solve. In particular, it is the Coulomb-term which makes it really hard.

One-particle term:

$$H_1 = \sum_i H_1(\vec{r_i}, \vec{p_i}) \tag{2.26}$$

$$H_1(\vec{r_i}, \vec{p_i}) = \frac{\vec{p_i}^{\,2}}{2m} + U(\vec{r_i}) \tag{2.27}$$

Two-particle term:

$$H_2 = \sum_{ij} V_{e-e}^{C}(\vec{r_i} - \vec{r_j} \tag{2.28}$$

We will first work out the second-quantized form of the two terms in $H_1(\vec{r_i}, \vec{p_i})$.

We define $\varphi_\lambda(\vec{r}, s)$ as follows: Solutions to the single-particle Schrödinger-equation

$$H_1\varphi_\lambda = \varepsilon_\lambda\varphi_\lambda \tag{2.29}$$

$$H_1 = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\vec{r}); \qquad \vec{\nabla}^2 : \text{Laplace-operator} \tag{2.30}$$

The task is now to find a second-quantized form of H_1 which will yield the same matrix elements as 2.30.

Consider:

$$\langle\lambda_1| H_1 |\lambda_2\rangle ; \qquad \langle\lambda_1|\lambda_2\rangle = \delta_{\lambda_1,\lambda_2} \tag{2.31}$$

Completeness relation:

$\langle\vec{r}, s|\lambda_1\rangle = \varphi_{\lambda_1}$ (some wavefunction)

Normalized states: $\langle\lambda|\lambda\rangle = 1$

$$\sum_\lambda \varphi^*_\lambda(\vec{r}, s)\varphi_\lambda(\vec{r'}, s') = \delta(\vec{r} - \vec{r'})\delta_{s,s'} \tag{2.32}$$

$$\sum_{\vec{r},s} \varphi^*_{\lambda'}(\vec{r}, s)\varphi_\lambda(\vec{r}, s) = \delta_{\lambda,\lambda'} \tag{2.33}$$

$$\langle\lambda|\lambda'\rangle = \delta_{\lambda,\lambda'} \implies \sum_{\vec{r},s} |\vec{r}, s\rangle \langle\vec{r}, s| = 1; \quad \sum_x |x\rangle \langle x| = 1 \tag{2.34}$$

Now we use this version of the completeness relations to evaluate the matrix element $\langle\lambda_1| H_1 |\lambda_2\rangle$

$$\begin{aligned}\langle\lambda_1| H_1 |\lambda_2\rangle &= \sum_{\vec{r},s}\sum_{\vec{r'},s'} \langle\lambda_1|\vec{r}, s\rangle \langle\vec{r}, s| H_1 |\vec{r'}, s'\rangle \langle\vec{r'}|\lambda_2\rangle \\ &= \sum_{\vec{r},s}\sum_{\vec{r'},s'} \varphi^*_{\lambda_1}(\vec{r}, s) \langle\vec{r}, s| H_1 |\vec{r'}, s'\rangle \varphi_{\lambda_2}(\vec{r'}, s')\end{aligned} \tag{2.35}$$

$$H_1 = \frac{\vec{p}^2}{2m} + U(\vec{r}) \qquad \text{Classical} \tag{2.36}$$

$$\vec{p} = \frac{\hbar}{i}\vec{\boldsymbol{\nabla}}; \qquad \vec{\boldsymbol{\nabla}} : \text{Gradient operator} \tag{2.37}$$

$$H_1 = -\frac{\hbar^2\vec{\nabla}^2}{2m} + U(\hat{r}) \qquad \text{Quantum mechanical} \tag{2.38}$$

$$U(\hat{r})|r\rangle = U(\vec{r})|r\rangle \tag{2.39}$$

$\vec{r}$: Position : eigenvalue of the position operator

$$\hat{r}\,|\vec{r},s\rangle = \vec{r}\,|\vec{r},s\rangle \tag{2.40}$$
$$U(\hat{r})\,|\vec{r},s\rangle = U(\vec{r})\,|\vec{r},s\rangle \tag{2.41}$$

$$\langle\vec{r},s|\,H_1\,|\vec{r'},s'\rangle = \left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\vec{r})\right]\delta_{\vec{r},\vec{r'}}\delta_{s,s'} \tag{2.42}$$

$$\begin{aligned}\langle\lambda_1|\,H_1\,|\lambda_2\rangle &= \sum_{\vec{r},s}\varphi^*_{\lambda_1}(\vec{r},s)\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\vec{r})\right]\varphi_{\lambda_2}(\vec{r},s) \\ &\equiv \varepsilon_{\lambda_1,\lambda_2}\end{aligned} \tag{2.43}$$

$\varphi_\lambda(\vec{r},s)$: Some complete set of functions, by assumption.

Let us now give an alternative form of H_1, which will yield the same matrix elements.
Anzats:

$$H_1 = \sum_{\lambda_1,\lambda_2} h_{\lambda_1,\lambda_2} c^\dagger_{\lambda_1} c_{\lambda_2} \tag{2.44}$$

where h_{λ_1,λ_2} is some complex number. Then:

$$\begin{aligned}\langle\lambda_1|\,H_1\,|\lambda_2\rangle &= \langle 0|\,c_{\lambda_1}\left(\sum_{\lambda'_1,\lambda'_2} h_{\lambda'_1,\lambda'_2} c^\dagger_{\lambda'_1} c_{\lambda'_2}\right) c^\dagger_{\lambda_2}\,|0\rangle \\ &= \sum_{\lambda'_1,\lambda'_2} h_{\lambda'_1,\lambda'_2}\,\langle 0|\,c_{\lambda_1} c^\dagger_{\lambda'_1} c_{\lambda'_2} c^\dagger_{\lambda_2}\,|0\rangle \\ &= \sum_{\lambda'_1,\lambda'_2} h_{\lambda'_1,\lambda'_2}\,\langle 0|\,(\delta_{\lambda_1,\lambda'_1} - c^\dagger_{\lambda'_1} c_{\lambda_1})(\delta_{\lambda_2,\lambda'_2} - c^\dagger_{\lambda_2} c_{\lambda'_2})\,|0\rangle \\ &= \sum_{\lambda'_1,\lambda'_2} h_{\lambda'_1,\lambda'_2}\delta_{\lambda_1,\lambda'_1}\delta_{\lambda_2,\lambda'_2}\,\langle 0|0\rangle \qquad (c_\lambda\,|0\rangle = 0) \\ &= h_{\lambda_1,\lambda_2}\end{aligned} \tag{2.45}$$

Choose $h_{\lambda_1,\lambda_2} = \varepsilon_{\lambda_1,\lambda_2} \implies$ Same matrix-elements for

$$H_1 = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\hat{r}) \tag{2.46}$$

and

$$\boxed{H_1 = \sum_{\lambda_1,\lambda_2} \varepsilon_{\lambda_1,\lambda_2} c^\dagger_{\lambda_1} c_{\lambda_2}} \tag{2.47}$$

Thus, 2.47 is a useful 2nd quantized form of H_1.

This expression may be simplified. Consider now a judicial choice of the complete set $\{\varphi_\lambda(x)\}$:
Let φ_λ be defined by

$$\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\vec{r})\right)\varphi_\lambda(x) = \varepsilon_\lambda \varphi_\lambda(x) \tag{2.48}$$

i.e. φ_λ are eigenfunctions of H_1

Then:

$$\begin{aligned}\varepsilon_{\lambda_1,\lambda_2} &= \sum_x \varphi^*_{\lambda_1}(x)\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\vec{r})\right)\varphi_{\lambda_2}(x) \\ &= \sum_x \varphi^*_{\lambda_1}(x)\varepsilon_{\lambda_2}\varphi_{\lambda_2}(x) \\ &= \varepsilon_{\lambda_2}\sum_x \varphi^*_{\lambda_1}(x)\varphi_{\lambda_2}(x) \\ &= \varepsilon_{\lambda_2}\delta_{\lambda_1,\lambda_2}\end{aligned} \tag{2.49}$$

giving that,

$$H_1 = \sum_{\lambda_1} \varepsilon_{\lambda_1} c^\dagger_{\lambda_1} c_{\lambda_1} \tag{2.50}$$

This form of H_1 has an intuitively appealing form: $c^\dagger_{\lambda_1} c_{\lambda_1}$ is a number operator. It counts the number of particles in state $|\lambda_1\rangle$.
ε_λ is the single-particle energy in this state. Thus, H_1 is an operator that counts the energy in the system coming from all the possible states of the system.

General one-particle operators:

$$T(x,\vec{p}) = T(x, \frac{\hbar}{i}\vec{\nabla}) \tag{2.51}$$

Could in principle depend on spin-coordinate s !

$$\langle\lambda_1|\, T\,|\lambda_2\rangle = \sum_x \varphi^*_{\lambda_1}(x) T(x, \frac{\hbar}{i}\vec{\nabla})\varphi_{\lambda_2}(x) \tag{2.52}$$

$$\begin{aligned}T &= \sum_{\lambda_1,\lambda_2} \langle\lambda_1|\, T(x,\vec{p})\,|\lambda_2\rangle\, c^\dagger_{\lambda_1} c_{\lambda_2} \\ &= \sum_{\lambda_1,\lambda_2} t_{\lambda_1,\lambda_2} c^\dagger_{\lambda_1} c_{\lambda_2}\end{aligned} \tag{2.53}$$

This expression for H_1 and T in second quantized form applies for any choice of sets of quantum numbers λ.

We next proceed by setting up a general form of second quantized form of 2-particle operators.

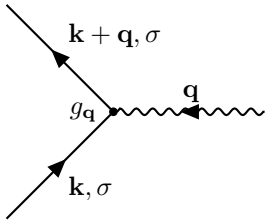


Figure 1: Diagram of electron-phonon vertex

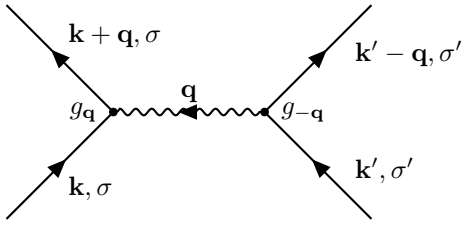


Figure 2: Diagram of the effective electron-phonon interaction

3 Many-particle perturbation theory

TODO: *Start on these notes...*

4 Quasi-particles in interacting electron-systems. Fermi-liquids.

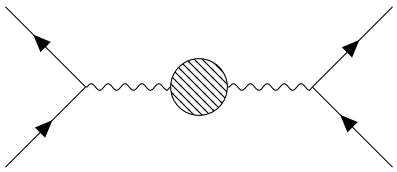
4.1 Fermi-liquids

4.2 Screening of the Coulomb-interaction

4.3 Phonon mediated electron-electron interaction

Due to the electron-phonon coupling depicted in fig. 1, we will get an effective phonon-mediated interaction between electrons, depicted in fig. 2

This is an exchange of a virtual phonon. The above diagram is the effective interaction to second order in g_q if we regard the wavy line ∿∿∿ as a bare phonon Green's function. We could also imagine that we replaced this by



which would include an effective interaction computed correctly up to order $\mathcal{O}(g^4)$. In fact, we might replace $D_0 + D_0\Pi D_0 + \dots$ by D! Thus computing the effective interaction up to infinite order in g. Another, often used approach would be to replace ~~~~ by **TODO:** *SETT INN DIAGRAM*

Here, we have resummed a subset of diagrams to infinite order in g in order to get an effective interaction between electrons. Under the assumption that g is weak, we will keep terms only to $\mathcal{O}(g^2)$.

$$V_{\text{eff}}(q,\omega) = |g_q^2| \frac{2\omega_q}{\omega^2 - \omega_q^2} \tag{4.1}$$

Thus, the interaction part of the Hamiltonian becomes

$$\mathcal{H} = \sum_{\substack{k,k',q \\ \sigma,\sigma'}} V_{\text{tot}}(q,\omega) c^\dagger_{k+q,\sigma} c^\dagger_{k'-q,\sigma'} c_{k',\sigma'} c_{k,\sigma} \tag{4.2}$$

$$V_{\text{tot}}(q,\omega) = \frac{e^2}{4\pi\varepsilon q^2} + V_{\text{eff}}(q,\omega), \tag{4.3}$$

where the first term is the Coulomb-interaction. Furthermore, ω is the energy transfer between scattering electrons when they exchange a phonon

$$\omega = \varepsilon_{k+q} - \varepsilon_k \tag{4.4}$$

TODO: *Sett inn figur*

Note the singularities in V_{tot} when $|\omega| \to \omega_q$. In particular, note the negative singularity when $|\omega| \to \omega_q^-$. This singularity persists when Coulomb-repulsion is included. For most frequencies, the Coulomb-interaction completely dominates. However, in a narrow ω-region close to ω_q, the extremely weak electron-phonon coupling will always beat the Coulomb-interaction! This frequency is slightly smaller than ω_q. For small ω, V_{tot} is repulsive. For large ω, V_{tot} is repulsive. For $|\omega| \lesssim \omega_q$, V_{tot} is attractive.

Let us try to give a physical picture for this: When an electron moves past an ion, they interact. The electron pulls slightly on the heavy, positively charged ion. Electrons are light, and move much faster than the heavy ions. The electron this moves quickly out of the scattering zone, while the ion relaxes slowly back to its equilibrium position. The ion in its out-of-equilibrium position represents excessive positive charge in that position, which can pull another electrn towards it. This is effectively a charge-dipole interaction. If the second electron "waits" a little for the first electron to get away (thus reducing Coulomb-repulsion) but does not wait for too long (such that the ion has relaxed back to its equilibrium position), then the second electron can be attracted the scattering region. Effectively, the second electron is attracted to the scattering region because the first electron was there. This is an effective electron-electron attraction. It only works if the electron waits a little, but not for too long. A minimum time

corresponds to a maximum frequency, while a maximum time corresponds to a minimum frequency. This implies that V_{tot} is attractive if $\omega_{\text{min}} < \omega < \omega_{\text{masx}}$, as depicted in **TODO:** *Sett in figurer og referanse til figuren (s.7)* We may view the effective electron-electron attrraction as a result of an electron locally deforming an elastic medium. Think of a rubber membrane that you put a little metal sphere on. The membrane is stretched, dipping down where you put the first sphere. If you put another little sphere on the membrane, it will fall into the dip, i.e. it will be attracted to the first particle. This is also how gravity works: A mass deforms space-time (an elastic medium) and thus attracts another mass.

Disclaimer: The above two analogs are classical. There will be an important quantum effect coming into play here, which we will come back to. here, it will suffice to not that, classically, one can keep adding particles to the dip, such that all particles will be gathered in the same one, forming a large heavy object. This is not how it works quantum mechanically with fermions. Note also that in V_{tot}, and the two different simplified models for $\bar{V}$, they are only attractive up to a maximum ω, i.e. only after a minimum amount of time. The second particle has to wait a minimum amount of time for the interaction to be attractive. This is called retardation.

> The electrons avoid the Coulomb-interactions by avoiding each other, not in space, but in time.

4.4 Magnon mediated electron-electron interaction

We have seen how a boson (a phonon) with a linear coupling to electrons could give an effective attractive interaction aming electrons. What is we couple the electrons linearly to other bosons? One obvious thing to investigate, is to consider the coupling of electrons to magnons. For simplicity, we consider itinerant electrons coupled to spin-fluctuations in a ferromagnetic insulatior. (FMI) The question is if the spin-fluctuations of the FMI can give rise to an attractive interaction aming electrons. We therefore consider a system of itinerant electrons with Hamiltonian

$$\mathcal{H}_{\text{el}} = \sum_{k,\sigma} (\varepsilon_k - \mu) c^\dagger_{k\sigma} c_{k\sigma}. \tag{4.5}$$

In this system, we envisage a regular lattice of localized spins with ferromagnetic coupling, with Hamiltonian

$$\mathcal{H}_{\text{spin}} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{4.6}$$

The localized spins are denoted by capital letter $\mathbf{S}$. The coupling between the localized spins (FMI) and the itinerant electron spins $\mathbf{s}_i$ (lower case) is given by

$$\mathcal{H}_{\text{el-spin}} = -J_{sd} \sum_i \mathbf{S}_i \cdot \mathbf{s}_i. \tag{4.7}$$

As a minimal model, we have assumed that the electrons are hopping around on the same regular lattice that the localized spins are located. Using the Holstein-Primakoff transformation, ignoring the classical ground-state energy, and expressing operators in momentum space, we have

$$\mathcal{H}_{\text{spin}} = \sum_q \omega_q a_q^\dagger a_q \tag{4.8}$$

$$\omega_q = 2JS(z - \gamma(\mathbf{q}))) \tag{4.9}$$

$$\gamma(\mathbf{q}) = \sum_\delta \mathrm{e}^{i\mathbf{q}\cdot\delta}, \tag{4.10}$$

where δ connects site i to all its nearest neighbors. One important fact ato make note of at once, is that $\omega_q \sim q^2$ for small q. For the phonon-case, with acoustical phonons, $\omega_q \sim q$. Thus ω_q for small q is much smaller for ferromagnetic magnons than acoustical phonons. We will return to this point. Consider next the electron-spin coupling:

$$\mathcal{H}_{\text{el-spin}} = -J_{sd} \sum_i \mathbf{S}_i \cdot \mathbf{s}_i \tag{4.11}$$

$$= -J_{sd} \sum_i (S_{iz}s_{iz} + S_{ix}s_{ix} + S_{iy}s_{iy}) \tag{4.12}$$

$$= -J_{sd} \sum_i \left(S_{iz}s_{iz} + \frac{1}{2}\left(S_{i+}s_{i-} + S_{i-}s_{i+}\right)\right), \tag{4.13}$$

where $S_{i\pm} = S_{ix} \pm iS_{iy}$, $S_{iz} = S - a_i^\dagger a_i$, $S_{i+} = \sqrt{2S}a_i$, $S_{i-} = \sqrt{2S}a_i^\dagger$. $\mathbf{s}_i = \frac{1}{2}c_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{i\beta}$ with implicit summation over repeated indices α, β.

$$\implies s_{iz} = \frac{1}{2}(c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}) = \frac{1}{2}\sum_\sigma \sigma c_{i\sigma}^\dagger c_{i\sigma}$$

$$\sigma^x = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right) \qquad \sigma^y = \left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right) \qquad \sigma^z = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$$

$$\sigma^\pm = \sigma^z \pm i\sigma^y \qquad \sigma^+ = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix} \qquad \sigma^- = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}$$

Thus, we have

$$\begin{aligned} \mathcal{H}_{\text{el-spin}} = &-J_{sd}S \sum i, \sigma\sigma c_{i\sigma}^\dagger c_{i\sigma} + J_{sd} \sum_{i,\sigma} \sigma a_i^\dagger a_i c_{i\sigma}^\dagger c_{i\sigma} \\ &- \frac{J_{sd}\sqrt{2S}}{2} \sum_i \left(a_i c_{i\downarrow}^\dagger c_{i\uparrow} + a_i^\dagger c_{i\uparrow}^\dagger c_{i\downarrow} \right) \end{aligned} \tag{4.14}$$

For the remainder of the calculation, we focus on the linear coupling of magnons to electrons, and ignore the second term. Thus, we focus on el-el interaction mediated by the vertices in fig. 3.

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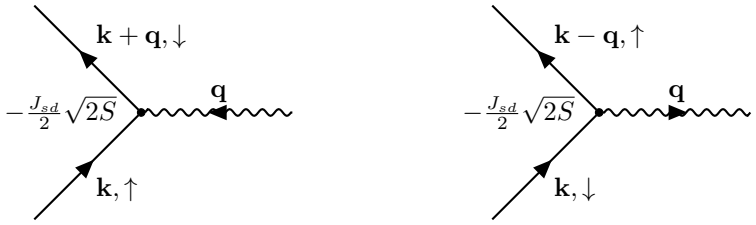


(a) Spin-1 magnon is dumped into electron, flipping $\downarrow\rightarrow\uparrow$

(b) Spin-1 magnon is excited, taking with it a spin-1, flipping $\uparrow\rightarrow\downarrow$

Figure 3: The two interaction vertices of interest

5 The Cooper-problem

6 The Bardeen-Cooper-Scheiffer theory of superconductivity

This is essentially the many-particle version of the Cooper-problem. Superconductivity: **TODO:** *Sett inn figur*

Note that a non analytic function like this usually suggests that there is some phase-transition in the system, so we are essentially looking at a phase transition of the electron gas. T_C : A sharply defined temperature

$$\rho(T) = \begin{cases} 0 & \text{if } T < T_C \\ \text{nonzero} & \text{if } T > T_C \end{cases} \tag{6.1}$$

T_C is denoted the critical temperature. Superconductivity was discovered experimentally in 1911 by Heike Kammerlingh Onnes in Leiden, measuring low-T $\rho(T)$ in ultra pure Mercury (Hg). This was 15 years before the discovery of quantum mechanics. It turns out that the phenomena is purely a quantum effect. So in 1911, there was no hope of giving a correct explanation for what is happening. It took 46 years to figure out what is going on. The most important reasons for this, is that apart from having to invent quantum mechanics first, completely novel and radical ideas had to be formulated in order to solve the problem[1]. Historically, one important clue to figuring out what is happening, was the experimental observations that T_C varied with ion mass. (Isotope substitution on elemental superconductors). This indicated that lattice-vibrations somehow were involved in the early discovered superconductors. (Recall that electron-phonon-coupling $\sim \frac{1}{\sqrt{M}}$). This "isotope-effect" was announced in 1950 on elemental Mercury, and the measured shift in T_C was 0.01K, something that

[1]From in the lecture: illustration of the Meissner effect. The Higgs providing a mass to the em-field in the metal blob drawn is the expectation value of the Cooper pair operator. Superconductivity is that the photon acquires a mass through the Higgs field, which is a cooper pair. Lots of analogs to the standard model.

required very careful and precise measurements. We may guess what will happen with T_C by appealing to what we found in the Cooper-problem, where we surmised a Cooper-pair dissociation temperature $T^* \sim \Delta$ and

$$\Delta = 2\hbar\omega_0 \mathrm{e}^{-\frac{1}{\lambda}} \tag{6.2}$$

ω_0: A typical phonon-frequency, if we assume that the effective attractions originates with e-ph coupling. $\omega_0 \sim \frac{1}{\sqrt{M}} \rightarrow T^* \sim \frac{1}{\sqrt{M}}$. This means that $\sqrt{M}T_C$ =constant! This relation is validated very well in experiments on elemental superconductors such as Hg, Sn, and Tl. Previously, we have derived an effective e-e interaction, including Coulomb-interactions and e-ph–e interactions, $\tilde{V}_{\text{eff}}$.

$$\begin{aligned}\mathcal{H} = &\sum_{k,\sigma} (\varepsilon_k - \mu)\, c^\dagger_{k\sigma} c_{k\sigma} \\ &+ \sum_{\substack{k,k',q \\ \sigma,\sigma'}} \tilde{V}_{\text{eff}} c^\dagger_{k+q,\sigma} c^\dagger_{k'-q,\sigma'} c_{k',\sigma'} c_{k,\sigma}\end{aligned} \tag{6.3}$$

Notice the global U(1)-symmetry of this Hamiltonian. This is on the standard form for a second-quantized electron-gas, now including the (potentially singular) effects of e-ph- coupling

$$\tilde{V}_{\text{eff}} = \frac{2|g_q|^2\omega_q}{\omega^2 - \omega_q^2} + V_{\text{Coulomb}}(q) \tag{6.4}$$

TODO: *Sett inn figure*

ω : Energy-transfer in scattering. $\omega = \varepsilon_{k+q} - \varepsilon_k, \quad \varepsilon_{k'} = \varepsilon_{k'-q} + \omega$. The effect of the repulsive interaction can be calculated pertubatively. In any case, this repulsion is not a singular perturbation. We therefore set it aside for the moment, and consider

$$\tilde{V}_{\text{eff}} = \frac{2|g_q|^2\omega_q}{\omega^2 - \omega_q^2}. \tag{6.5}$$

This interaction as attractive (< 0) if

$$(\varepsilon_{k+q} - \varepsilon_k)^2 < \omega_q^2$$

or

$$(\varepsilon_{k'-q} - \varepsilon_{k'})^2 < \omega_q^2$$

We now focus on those scattering processes that give attraction between electrons. The processes giving repulsion do nothing more than what the Coulomb interaction does. We will include these effects later on. We now simplify this in a series of steps. The scattering caused by the weak e-ph-e coupling can only take place in a thin shell around the Fermi-surface. Thus $\varepsilon_k, \varepsilon_{k'}, \varepsilon_{k+q}, \varepsilon_{k'-q}$ must all lie within a thin shell around the Fermi surface. Let us take a look at the relevant kinematics seen in fig. 4. We see that in general, the state with

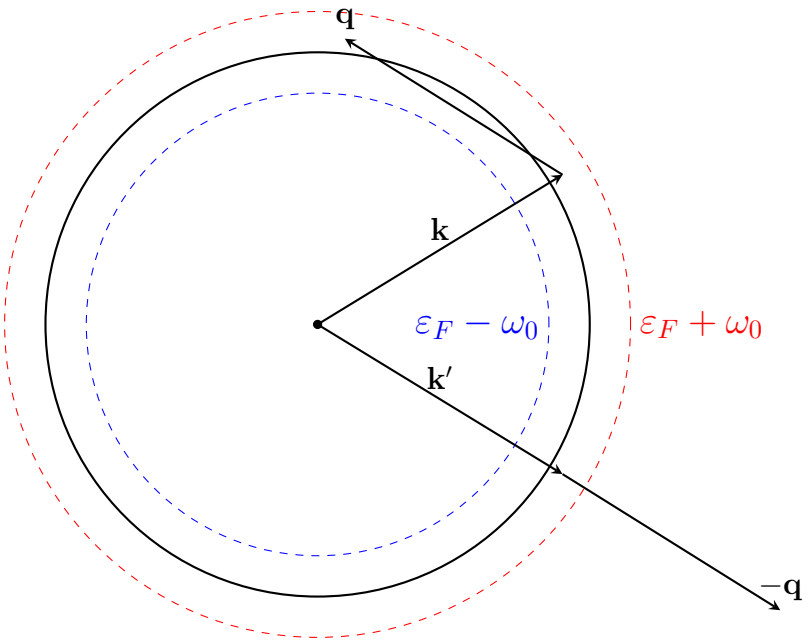


Figure 4: Thin shell around the Fermi surface.

momenta $k' - q$ will lie outside the shell, even if $\varepsilon_k, \varepsilon_{k'}, \varepsilon_{k+q}$ lie within the shell. There is an important special case where $\varepsilon_{k'-q}$ will always lie within shell if $\varepsilon_k, \varepsilon_{k'}, \varepsilon_{k+q}, \varepsilon_{k'-q}$ is within shell, namely the case when $k' = -k$. This choice will this maximize the scattering phase-space for attractive interactions. We will retain only such terms: $k' = -k$.

A second simplification: $\sigma' = -\sigma$. The spatial extent of attractive interaction is small. We may essentially think of it (in real space) as an attractive Hubbard-interaction. Thus, we end up with the following simplified Hamiltonian

$$\mathcal{H} = \sum_{k,\sigma} (\varepsilon_k - \mu) c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k,q,\sigma} \tilde{V}_{\text{eff}} c^\dagger_{k+q,\sigma} c^\dagger_{-(k+q),-\sigma} c_{-k,-\sigma} c_{k\sigma}. \tag{6.6}$$

Now redefine variables $k \to k'$, $\quad k+q \to k$, $\quad \tilde{V}_{\text{eff}} \to V_{k,k'}/2$ (spin independent interaction). Thus we can write eq. (6.6) as

$$\mathcal{H} = \sum_{k,\sigma} (\varepsilon_k - \mu) c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k,k'} V_{k,k'} c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} c_{-k',\downarrow} c_{k,\uparrow}, \tag{6.7}$$

with $V_{k,k'}$ being attractive if k, k' lie in a small vicinity of the Fermi-surface, and zero otherwise. eq. (6.7) is the so called BCS-model of superconductivity. Althought it has been motivated by an attractive e-ph-e interaction, the above model is in fact more general than that, and can be applied to any system

with an effective (somehow) attractive electron-electron interaction. This model in spirit is very much like the model we looked at for the Cooper-problem. The difference is that $V_{k,k'}$ in the BCS-model works between all electrons in a thin shell around the Fermi-surface, while the Cooper-problem only considered interactions between two such electrons. The Hamiltonian can not be treated exactly. Moreover, from the Cooper-problem, there is every reason to believe that in order to get correct eigenvalues, we cannot use perturbations theory. We must therefore treat $\mathcal{H}$ both approximately and non-perturbatively. This is what we will do next. We will transform this many-body problem to a self-consistent one-particle problem. This is done very much like what we do when we perform a mean-field approximation on spin-systems:

$$\begin{aligned} c_{-k\downarrow}c_{k\uparrow} &= \underbrace{\langle c_{-k\downarrow}c_{k\uparrow}\rangle}_{\equiv b_k} + \underbrace{c_{-k\downarrow}c_{k\uparrow} - \langle c_{-k\downarrow}c_{k\uparrow}\rangle}_{\delta b_k} \\ &= b_k + \delta b_k. \end{aligned} \tag{6.8}$$

Here, b_k is a statistical average [2]. Note that giving the b's a finite expectation value breaks the $\{}mathrm{U}(1)$-symmetry of the system. There is no way to gradually break this symmetry, it either happens or not. Note also that these expectations values are not on the usual $\langle c^\dagger c\rangle$-form, and the question now is to answer whether such expectation values can exist or not. Now insert the definitions in eq. (6.8) and the Hermitian conjugate into eq. (6.7) and ignore terms $\mathcal{O}((\delta b)^2)$ Consider the interaction term:

$$\begin{aligned} \sum_{k,k'} V_{k,k'} c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} c_{-k',\downarrow} c_{k,\uparrow} &= \sum_{k,k'} V_{k,k'} \left(b^\dagger_k + \delta b^\dagger_k\right)\left(b_{k'} + \delta b_{k'}\right) \\ &= \sum_{k,k'} V_{k,k'} \left(b^\dagger_k b_{k'} + b^\dagger_k \delta b_{k'} + \delta b^\dagger_k b_{k'}\right) + \mathcal{O}((\delta b)^2) \\ &\simeq \sum_{k,k'} V_{k,k'} \left(b^\dagger_k b_{k'} + b^\dagger_k c_{-k'\downarrow} c_{k'\uparrow} + b_{k'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} - 2 b^\dagger_k b_{k'}\right). \end{aligned}$$

Next, definge

$$\Delta_k \equiv -\sum_{k'} V_{kk'} b_{k'} \tag{6.9a}$$

$$\Delta^\dagger_k \equiv -\sum_{k} V_{kk'} b^\dagger_k. \tag{6.9b}$$

Inserting these in definitions into the Hamiltonian gives

$$\begin{aligned} \mathcal{H} = \sum_{k,\sigma} (\varepsilon_k - \mu) c^\dagger_{k\sigma} c_{k\sigma} - \sum_k \left[\Delta_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + \Delta^\dagger_k c_{-k\downarrow c_{k\uparrow}}\right] \\ + \sum_k \Delta_k b^\dagger_k. \end{aligned} \tag{6.10}$$

[2] with respect to the "correct" Hamiltonian.

This is the mean-field approximation to the BCS-model, where b_k (and hence Δ_k) must be determined self-consistently, by minimizing the free energy of the system. We return to that below, but first we must diagonalize the Hamiltonian in eq. (6.10). Note that we now have terms like $c^\dagger c$, $c^\dagger c^\dagger$, and cc in $\mathcal{H}$, reminiscent of what we had with boson-operators for the case of quantum antiferromagnets. We will now proceed along a similar route, but with the important difference that we are now considering fermions. Introduce new fermion-operators

$$\eta_k = u_k c_{k\uparrow} + v_k c^\dagger_{-k\downarrow} \tag{6.11a}$$

$$\gamma_k = u_k c_{-k\downarrow} - v_k c_{k\uparrow} \tag{6.11b}$$

These operators are fermionic quasi-particles as linear combinations of spin-up and spin-down particles. Thus spin is not a correct quantum number for the new fermions. Note the minus sign in eq. (6.11b). This transformations is required to preserve fermionic commutation relations, for instance

$$\left\{\eta_k, \eta^\dagger_{k'}\right\} = \delta_{kk'}, \tag{6.12}$$

η_k, γ_k anticommute,

$$\left\{\eta_k, \gamma^\dagger_{k'}\right\} = 0$$

.

$$u_k u_{k'} \delta_{kk'} + v_k v_{k'} \delta_{kk'} = \delta_{kk'},$$

with the +-sign originating in anti-commutation relations. Thus $u_k^2 + v_k^2 = 1$. We reach the same conclusion with $\{\gamma_k, \gamma_{k'}\} = \delta_{kk'}$. This relation is the reason for the minus sign in front of v_k in eq. (6.11b)!

$$\begin{pmatrix} \eta_k \\ \gamma_k \end{pmatrix} = \overbrace{\begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix}}^{\equiv M} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} \tag{6.13}$$

With these signs, $\det M = u_k^2 + v_k^2 = 1$

$$M = \begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix} \qquad M^T = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \qquad M^{-1} = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \tag{6.14}$$

Thus, M is a unitary transformation with the constraint $u_k^2 + v_k^2 = 1 \implies |u_k|, |v_k| \leq 1$. This is very different from the "squeezing" transformation we

used in the quantum AFM-case. Going back to eq. (6.11), we have

$$\begin{pmatrix}\eta_k\\ \gamma_k\end{pmatrix} = \begin{pmatrix}u_k & v_k\\ -v_k & u_k\end{pmatrix}\begin{pmatrix}c_{k\uparrow}\\ c^\dagger_{-k\downarrow}\end{pmatrix} \tag{6.15a}$$

$$\begin{pmatrix}\eta^\dagger_k\\ \gamma^\dagger_k\end{pmatrix} = \begin{pmatrix}u_k & v_k\\ -v_k & u_k\end{pmatrix}\begin{pmatrix}c^\dagger_{k\uparrow}\\ c_{-k\downarrow}\end{pmatrix} \tag{6.15b}$$

$$\begin{pmatrix}c_{k\uparrow}\\ c^\dagger_{-k\downarrow}\end{pmatrix} = \begin{pmatrix}u_k & -v_k\\ v_k & u_k\end{pmatrix}\begin{pmatrix}\eta_k\\ \gamma_k\end{pmatrix} \tag{6.15c}$$

$$\begin{pmatrix}c^\dagger_{k\uparrow}\\ c_{-k\downarrow}\end{pmatrix} = \begin{pmatrix}u_k & -v_k\\ v_k & u_k\end{pmatrix}\begin{pmatrix}\eta^\dagger_k\\ \gamma^\dagger_k\end{pmatrix} \tag{6.15d}$$

Insert this into the Hamiltonian eq. (6.10),

$$\begin{aligned}\mathcal{H} = \sum_k \Big\{ &\Big(\varepsilon_k - \mu\Big)\Big(u_k\eta^\dagger_k - v_k\gamma^\dagger_k\Big)\Big(u_k\eta_k - v_k\gamma_k\Big)\\ &+ \Big(\varepsilon_k - \mu\Big)\Big(v_k\eta_k + u_k\gamma_k\Big)\Big(v_k\gamma^\dagger_k + u_k\gamma^\dagger_k\Big)\\ &- \Delta_k\Big(u_k\eta^\dagger_k - v_k\gamma^\dagger_k\Big)\Big(v_k\eta_k + u_k\gamma_k\Big)\\ &- \Delta^\dagger_k\Big(u_k\eta^\dagger_k + u_k\gamma^\dagger_k\Big)\Big(u_k\eta_k - v_k\gamma_k\Big) + \Delta_k b^\dagger_k\Big\}\end{aligned} \tag{6.16}$$

As in the quantum antiferromagnet-case, we now collect terms of different types:

$$\eta^\dagger_k\eta_k : \left(\varepsilon_k - \mu\right)u_k^2 - u_k v_k\left(\Delta_k + \Delta^\dagger_k\right) \tag{6.17a}$$

$$\gamma^\dagger_k\gamma_k : \left(\varepsilon_k - \mu\right)v_k^2 + +u_k v_k\left(\Delta_k + \Delta^\dagger_k\right) \tag{6.17b}$$

$$\eta_k\eta^\dagger_k : \left(\varepsilon_k - \mu\right)v_k^2 \tag{6.17c}$$

$$\gamma_k\gamma^\dagger_k : \left(\varepsilon_k - \mu\right)u_k^2 \tag{6.17d}$$

$$\gamma^\dagger_k\eta_k : -2\left(\varepsilon_k - \mu\right)u_k v_k + \Delta_k v_k^2 - \Delta^\dagger_k u_k^2 \tag{6.17e}$$

$$\eta^\dagger_k\gamma_k : -2\left(\varepsilon_k - \mu\right)u_k v_k - \Delta_k u_k^2 + v_k^2\Delta^\dagger_k \tag{6.17f}$$

Using the anticommutation relations in eq. (6.12), and the corresponding for γ_k, we may express eqs. (6.17a) and (6.17b) as

$$\eta^\dagger_k\eta_k : \left(\varepsilon_k - \mu\right)\left(u_k^2 - v_k^2\right) - u_k v_k\left(\Delta_k + \Delta^\dagger_k\right) \tag{6.18a}$$

$$\gamma^\dagger_k\gamma_k : \left(\varepsilon_k - \mu\right)\left(v_k^2 - u_k^2\right) + u_k v_k\left(\Delta_k + \Delta^\dagger_k\right) \tag{6.18b}$$

These are the same, except opposite sign. Adjust u_k, v_k such that the coefficients in front of eq. (6.17e) and **??** are zero. Fortunately, these two equations are just

complex conjugate of each other, so if one is fulfilled, so is the other. If we set these two to 0, we have

$$-2\left(\varepsilon_k-\mu\right)u_k v_k = u_k^2\Delta_k - v_k^2\Delta_k^\dagger \tag{6.19}$$
$$-2\left(\varepsilon_k-\mu\right)u_k v_k = u_k^2\Delta_k^\dagger - v_k^2\Delta_k^\dagger. \tag{6.20}$$

By adding these two equations, we get

$$-4\underbrace{\left(\varepsilon_k-\mu\right)}_{\equiv\tilde{\varepsilon}_k}u_k v_k = \left(u_k^2-v_k^2\right)\left(\Delta_k+\Delta_k^\dagger\right)$$
$$\Delta_k+\Delta_k^\dagger = 2\,\mathrm{Re}\{\Delta_k\}\equiv 2\tilde{\Delta}_k$$
$$-2\tilde{\varepsilon}_k u_k v_k = \left(u_k^2-v_k^2\right)\tilde{\Delta}_k$$

Since we have $u_k^2+v_k^2=1$, we may write

$$u_k = \cos\theta$$
$$v_k = \sin\theta$$
$$-\tilde{\varepsilon}_k\sin 2\theta = \tilde{\Delta}_k\cos 2\theta$$

$$\tan 2\theta = -\frac{\tilde{\Delta}_k}{\tilde{\varepsilon}_k} \tag{6.21}$$

This is an equation for θ, and thus u_k, v_k, which gives coefficients of $\gamma_k^\dagger\eta_k, \eta_k^\dagger\gamma_k$ equal to zero. Choose $\tilde{\Delta}_k \geq 0$

$$\tan 2\theta < 0; \quad \tilde{\varepsilon} > 0$$
$$\tan 2\theta > 0; \quad \tilde{\varepsilon} < 0$$
$$\frac{\sin^2(2\theta)}{\cos^2(2\theta)} = \left(\frac{\tilde{\Delta}_k}{\tilde{\varepsilon}_k}\right)^2 \equiv b^2$$
$$\cos^2(2\theta) = \frac{1}{1+b^2}$$
$$\cos(2\theta) = \begin{cases} \frac{-1}{\sqrt{1+b^2}}; & \tilde{\varepsilon} > 0 \\ \frac{1}{\sqrt{1+b^2}}; & \tilde{\varepsilon} < 0 \end{cases}$$

Coefficient in front of $\eta_k^\dagger \eta_k$:

$$\begin{aligned}
\tilde{\varepsilon}_k \cos 2\theta - \tilde{\Delta}_k \sin 2\theta &= \cos(2\theta)\left(\tilde{\varepsilon}_k + \left(\frac{\tilde{\Delta}_k}{\tilde{\varepsilon}_k}\right)^2\right) \\
&= -\frac{\operatorname{sign}\tilde{\varepsilon}_k}{\tilde{\varepsilon}_k}\frac{\left(\tilde{\varepsilon}_k^2 + \tilde{\Delta}_k^2\right)}{(1+b^2)^{\frac{1}{2}}} \\
&= -\frac{\operatorname{sign}\tilde{\varepsilon}_k}{\frac{\tilde{\varepsilon}_k}{|\tilde{\varepsilon}_k|}}\left(\tilde{\varepsilon}_k^2 + \tilde{\Delta}_k^2\right)^{\frac{1}{2}} \\
&= -\left(\tilde{\varepsilon}_k^2 + \tilde{\Delta}_k^2\right)^{\frac{1}{2}}
\end{aligned}$$

Coefficient in front of $\gamma_k^\dagger \gamma_k$: $\left(\tilde{\varepsilon}_k^2 + \tilde{\Delta}_k^2\right)^{\frac{1}{2}}$. Thus, we have finally diagonalized the Hamiltonian

$$\mathcal{H} = \sum_k \left[2\left(\varepsilon_k - \mu\right) + \Delta_k b_k^\dagger + E_k\left(\gamma_k^\dagger \gamma_k - \eta_k^\dagger \eta_k\right)\right], \tag{6.22}$$

where the summation over spins has been made, and with

$$E_k \equiv \left(\tilde{\varepsilon}_k^2 + \tilde{\Delta}_k^2\right)^{\frac{1}{2}}. \tag{6.23}$$

b_k and $\tilde{\Delta}_k$ are as yet undetermined. They will have to be determined by minimizing the free energy of this system. The long-lived fermionic excitation are described by $(\eta_k, \eta_k^\dagger)$, $(\gamma_k, \gamma_k^\dagger)$. **TODO:** *Sjekk at fortegnene er riktige på eta/gamma*

$$\mathcal{H} = E_0 + \sum_k E_k\left(\gamma_k^\dagger \gamma_k - \eta_k^\dagger \eta_k\right) \tag{6.24}$$

$$E_0 = \sum_k \left[2\left(\varepsilon_k - \mu\right) + \Delta_k b_k^\dagger\right] \tag{6.25}$$

If we have a fermionic system with a Hamiltonian

$$\mathcal{H} = \sum_k (\varepsilon_k - \mu) c_k^\dagger c_k,$$

the grand canonical partition function is given by

$$\mathcal{Z}_g = \prod_k \left(1 + \mathrm{e}^{-\beta(\varepsilon_k - \mu)}\right). \tag{6.26}$$

Is the present case, this gives

$$\mathcal{Z}_g = \mathrm{e}^{-\beta E_0} \prod_k \left(1 + \mathrm{e}^{\beta E_k}\right)\left(1 + \mathrm{e}^{-\beta E_k}\right). \tag{6.27}$$

In the limit of large number of particles, all ensembles are equivalent. To expedite th computations, we will consider $\mathcal{Z}_g$ ti be equal to $\mathcal{Z} = \mathrm{e}^{-\beta F}$, where F is the Helmholz free energy for a system.

$$F = E_0 - \frac{1}{\beta}\sum_k \left[\ln\left(1+\mathrm{e}^{-\beta E_k}\right) + \ln\left(1+\mathrm{e}^{\beta E_k}\right)\right] \tag{6.28}$$

We now minimize with respect to Δ_k or $b_k^\dagger$ for a particular value of k. It does not matter which one of these we use. We look for

$$\frac{\partial F}{\partial \Delta_k} = 0, \tag{6.29}$$

or

$$b_k^\dagger - \frac{1}{\beta}\left(\frac{1}{1+\mathrm{e}^{-\beta E_k}}(-\beta)\frac{\partial E_k}{\partial \Delta_k}\mathrm{e}^{-\beta E_k} + \frac{1}{1+\mathrm{e}^{\beta E_k}}(\beta)\frac{\partial E_k}{\partial \Delta_k}\mathrm{e}^{\beta E_k}\right) = 0$$

$$\begin{aligned} b_k^\dagger &= \frac{\partial E_k}{\partial \Delta_k}\left(\frac{\mathrm{e}^x}{1+e^x} - \frac{\mathrm{e}^{-x}}{1+e^{-x}}\right) \\ &= \frac{\partial E_k}{\partial \Delta_k}\cdot\tanh\left(\frac{x}{2}\right); \quad x = \beta E_k \\ \frac{\partial E_k}{\partial \Delta_k} &= \frac{\Delta_k}{\sqrt{\tilde{\varepsilon}_k^2 + \Delta_k^2}}, \end{aligned}$$

where we have set Δ_k to be real, such that $\tilde{\Delta}_k = \Delta_k$.

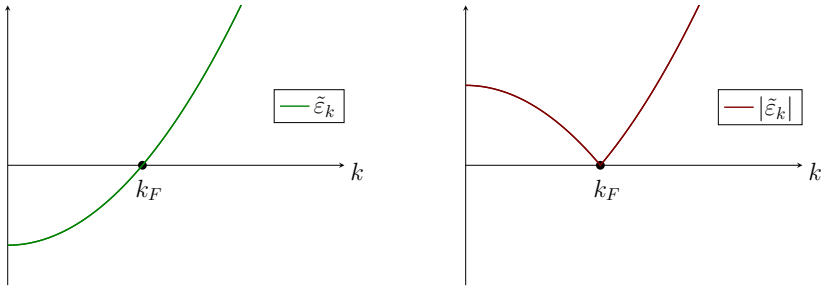
$$b_k^\dagger = \frac{\Delta_k}{\sqrt{\tilde{\varepsilon}_k^2 + \Delta_k^2}}\tanh\left(\frac{\beta E_k}{2}\right) \tag{6.30}$$

We close this to an equation for Δ_k by using the definitions in eq. (6.9) to obtain

$$\Delta_k = -\sum_{k'} V_{kk'}\Delta_{k'}\chi_{k'} \tag{6.31}$$

$$\chi_k = \frac{1}{(\tilde{\varepsilon}_k^2 + \Delta_k^2)^{\frac{1}{2}}}\tanh\left(\frac{\beta E_k}{2}\right) \tag{6.32}$$

This is the so-called BCS gap-equation. The reason for this name that it is an equation for Δ_k, which represents a gap in the excitation-spectrum. To see this, we first consider the excitation spectrum at $\Delta_k = 0$, depicted in fig. 5 Note that on the Fermi-surface ($k = k_F$), there is zero gap in the excitation spectrum $\Delta_k = 0$. From fig. 6, we see that Δ_k represents a gap on the Fermi-surface in the excitation spectrum of the Bogoliubov fermions. We will now solve eq. (6.31) for the same model for $V_{kk'}$ that we used in the Cooper problem, namely a



(a) $\tilde{\varepsilon}_k$ (b) $|\tilde{\varepsilon}_k|$

Figure 5: Typical excitation spectrum at $\Delta_k = 0$.

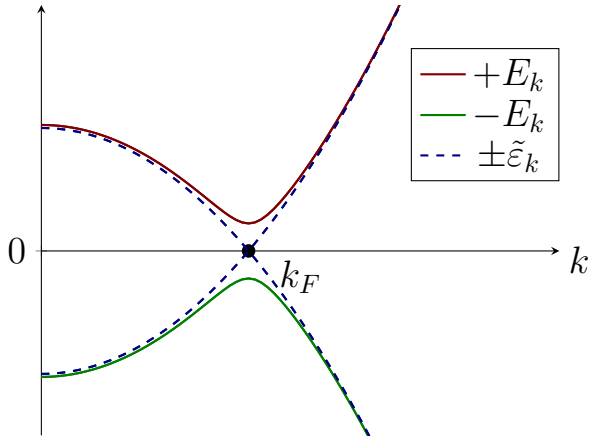


Figure 6: $\Delta_k \neq 0$ represents a gap in the excitation spectrum at the Fermi surface, here greatly exaggerated. The difference in the minimum of $+E_k$ and the maximum of $-E_k$ is $2\Delta_k$. This gap always tracks the Fermi surface.

constant attractive potential in a thin shell around the Fermi-surface. With the understanding that k, k' lie within this thin shell, we have

$$\Delta_k = V \sum_{k'} \Delta_{k'} \chi_{k'} \tag{6.33}$$

This means that Δ_k is independent of k, and we can divide by $\Delta = \Delta_k$ and get

$$1 = V \sum_{k'} \frac{1}{(\tilde{\varepsilon}_{k'}^2 + \Delta^2)^{\frac{1}{2}}} \tanh\left(\frac{\beta E_{k'}}{2}\right). \tag{6.34}$$

Now use

$$\sum_k g(\tilde{\varepsilon}_k) = \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \sum_k \delta(\varepsilon - \tilde{\varepsilon}_k) g(\tilde{\varepsilon}) = \int_{-\infty}^{\infty} \mathrm{d}\varepsilon N(\varepsilon) g(\varepsilon), \tag{6.35}$$

$$1 = V \int_{-\omega_0}^{\omega_0} \mathrm{d}\varepsilon \frac{N(\varepsilon)}{\sqrt{\varepsilon^2 + \Delta^2}} \tanh\left(\frac{\beta\sqrt{\varepsilon^2 + \Delta^2}}{2}\right) \tag{6.36}$$

Note: ε must lie within a thin energy-shell around the Fermi surface! We have denoted the width of this shell $2\omega_0$

$$-\omega_0 < \varepsilon < \omega_0$$

when energies ε are measured relative μ. Consider now $N(\varepsilon)$ a rather slowly varying function of ε in the thin shell around the Fermi-surface, such that $N(\varepsilon) \simeq N(\varepsilon_F) = N(\mu)$. Introduce $\lambda \equiv V N(\varepsilon_F)$, such that

$$1 = \lambda \int_{-\omega_0}^{\omega_0} \mathrm{d}\varepsilon \frac{1}{\sqrt{\varepsilon^2 + \Delta^2}} \tanh\left(\frac{\beta\sqrt{\varepsilon^2 + \Delta^2}}{2}\right). \tag{6.37}$$

eq. (6.37) is difficult to solve, but we will look at two special cases, at $T = 0$ and $T = T_C$.

i) $T = 0$

At $T = 0$, $\tanh\left(\frac{\beta\sqrt{\varepsilon^2+\Delta^2}}{2}\right) = 1$, such that [3]

$$1 = \lambda \int_0^{\omega_0} \frac{\mathrm{d}\varepsilon}{\sqrt{\varepsilon^2 + \Delta^2}} \tag{6.38}$$

$$= \lambda \int_0^{\frac{\omega_0}{\Delta}} \frac{\mathrm{d}x}{\sqrt{x^2 + 1}} \tag{6.39}$$

$$= \lambda \sinh^{-1}\left(\frac{\omega_0}{\Delta}\right) \tag{6.40}$$

$$= \lambda \ln\left(\frac{\omega_0}{\Delta} + \sqrt{\left(\frac{\omega_0}{\Delta}\right) + 1}\right) \tag{6.41}$$

$$\implies \frac{\omega_0}{\Delta} = \sinh\left(\frac{1}{\lambda}\right) = \frac{1}{2}\left(\mathrm{e}^{\frac{1}{\lambda}} - \mathrm{e}^{\frac{-1}{\lambda}}\right) \tag{6.42}$$

[3] The subsequent λ is now redefined by a factor 2, not any more considering per-spin density of states.

Now consider $\lambda \ll 1 \implies \frac{2\omega_0}{\Delta} \simeq \mathrm{e}^{\frac{1}{\lambda}}$. Reinserting $\hbar$ we obtain

$$\Delta = 2\hbar\omega_0 \mathrm{e}^{\frac{-1}{\lambda}}. \tag{6.43}$$

Notice the similar expression in eq. (6.43) **TODO:** *Sett inn utrryk for Δ fra Cooper-problemet.*

ii) The critical temperature

We see from the gap-equation that as T increases, the tanh-factor decreases. Thus, to obtain a solution to the gap-equation requires smaller Δ. As T increases, Δ decreases. Sooner or later, we will reach a temperature whre $\Delta \to 0^+$. This will be the critical temperature, T_C, which is determined by the equation

$$1 = \lambda \int_0^{\omega_0} \mathrm{d}\varepsilon \, \frac{\tanh\left(\frac{\beta\varepsilon}{2}\right)}{\varepsilon}. \tag{6.44}$$

Introducing $x = \frac{\beta\varepsilon}{2}$,

$$\begin{aligned} \frac{1}{\lambda} &= \int_0^{\frac{\beta\omega_0}{2}} \frac{\mathrm{d}x}{x} \tanh(x) \\ &= \ln(x)\tanh(x)\big|_0^{\frac{\beta\omega_0}{2}} - \int_0^{\frac{\beta\omega_0}{2}} \mathrm{d}x \, \frac{\ln(x)}{\cosh^2(x)}. \end{aligned}$$

Again, we consider $\lambda \ll 1 \implies \frac{\beta\omega_0}{2} \gg 1$. In the last term, we may replace the upper limit by ∞.

$$\frac{1}{\lambda} \simeq \ln\left(\frac{\beta\omega_0}{2}\right) - \underbrace{\int_0^{\infty} \mathrm{d}x \, \frac{\ln(x)}{\cosh^2(x)}}_{=\ln\left(\frac{\pi}{4}\mathrm{e}^{-\gamma}\right)\equiv\ln(C)}, \tag{6.45}$$

where $\gamma \simeq 0.5772156649$ is the Euler-Mascheroni constant.

$$\frac{1}{\lambda} = \ln\left(\frac{\beta\omega_0}{2C}\right) \tag{6.46}$$

$$\frac{\beta\omega_0}{2C} = \mathrm{e}^{\frac{1}{\lambda}} \tag{6.47}$$

$$k_B T_C = \frac{2}{\pi}\mathrm{e}^{\gamma}\omega \mathrm{e}^{\frac{-1}{\lambda}} \tag{6.48}$$

Note how extremely sensitive both Δ and $k_B T_C$ is to λ! Note also that the depend on λ in the same way. So if we take their ratios, this dependence cancels, as does the prefactor.

$$\frac{2\Delta(T=0)}{k_B T_C} = \frac{4\omega_0 \mathrm{e}^{\frac{-1}{\lambda}}}{\frac{2}{\pi}\mathrm{e}^{\gamma}\omega_0 \mathrm{e}^{\frac{-1}{\lambda}}} \tag{6.49}$$

$$= 2\pi\mathrm{e}^{-\gamma} \simeq 3.53, \tag{6.50}$$

which is a universal number! This prediction of the theory turned out to be remarkably accurate for real superconductors where $\lambda \ll 1$. Examples are Hg, Al, Sn. For Pb, the ratio is somewhat larger, and this is attributed to the fact that λ is larger than in Hg, Al, Sn. The opening up of a gap on the Fermi-surface means that the electron many-body state is protected from scattering by this gap. As a result, the resistivity of the electron gas drops abruptly to 0 at $T = T_C$.

Superconductivity-onset is thus a phase-transition associated with the opening of a gap Δ_k on the Fermi-surface.

Often, this gap Δ_k is referred to as an order-parameter of the system.
The original Hamiltonian is invariant under the transformation

$$c_{k\sigma} \to \mathrm{e}^{i\theta} c_{k\sigma}, \tag{6.51}$$

where θ is a global phase factor. This is therefore a symmetry of the problem, a global $U(1)$-symmetry as mentioned above. Δ_k is nonzero if and only if b_k is nonzero. The quantity

$$\langle b_k \rangle = \langle c_{-k\downarrow} c_{k\uparrow} \rangle \tag{6.52}$$

is, however, not invariant under this global U(1)-transformation. Thus, in the superconducting state, the U(1)-symmetry of $\mathcal{H}$ is spontaneously broken.

7 The Meissner Effect