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Advanced Condensed Matter Theory

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This script is still in development.

Abstract

Strong correlations are important for the understanding of many phenomena in modern condensed matter physics. Examples are high temperature superconductivity (Nobel prize 1987 http://www.nobel.se/physics/laureates/1987/index.html), the fractional quantum Hall effect (Nobel prize 1998 http://www.nobel.se/physics/laureates/1998/index.html) or quite recently topological phase transitions in two dimensions (Nobel prize 2016 http://www.nobel.se/physics/laureates/2015/index.html). The theory for strong correlations needs new concepts and methods to describe such phenomena and to solve the corresponding models. The aim of this course is to provide these methods, to introduce the models, and to help understanding the phenomena in strongly correlated systems. Not the only one but the most important model to describe strongly correlated Fermions is the Hubbard model. In the modern theory of strong correlations it plays the same role as the Ising model in statistical physics: It serves as a standard model to describe and understand most of the phenomena in strongly correlated systems. The Hubbard model was initially introduced to describe the physical behaviour of transition metals, to understand magnetic phenomena in itinerant electron systems (ferromagnetism, anti-ferromagnetism, ferrimagnetism), to describe the Mott transition, and to describe π-electron systems in quantum chemistry. In one space dimension it describes a Luttinger liquid. Although the model has a very simple structure, the behaviour depends strongly on the parameters, the interaction strength, the density, and the underlying lattice. In this course we try to give an overview over the physics of strongly correlated electrons and the Hubbard model.

The students are expected to know quantum mechanics and statistical physics. Some knowledge in condensed matter physics is helpful as well.

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I am grateful to Johannes Hölck. He carefully read the manuscript, found lots of errors, and had several ideas for improvements.

About this text

The manuscript is available as pdf. Links for citations are coloured in dark red, links within the text in dark blue, links to external material in dark green.

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1 Interacting Fermions and Bosons

1.1 The Hubbard model

As mentioned in the abstract, the Hubbard model serves as a standard model for strongly correlated electrons. The Hamiltonian of the Hubbard model is given by

$$H = H_{\text{kin}} + H_{\text{WW}} = \sum_{x,y,\sigma} t_{x,y} c^\dagger_{x,\sigma} c_{y,\sigma} + U \sum_x c^\dagger_{x\uparrow} c^\dagger_{x\downarrow} c_{x\downarrow} c_{x\uparrow} \tag{1.1}$$

The model describes electrons in a tight binding approximation on a lattice. x, y denote the lattice sites. $\sigma \in \{\uparrow, \downarrow\}$ denotes the spin of the electron. $c^\dagger_{x\sigma}$ is a creation operator for an electron with spin σ on lattice site x, $c_{x\sigma}$ is the corresponding annihilation operator. The first part of the Hamiltonian describes the hopping of electrons on the lattice, t_{xy} is the hopping amplitude. The second part describes the interaction between the electrons. Usually we assume the interaction to be repulsive, i.e. $U > 0$.

The model was proposed independently by J. Hubbard [25] for the description of transition metals, by J. Kanamori [28] for the description of itinerant ferromagnetism, and by M.C. Gutzwiller [19] for the description of the metal-insulator transition. In Quantum Chemistry, the model is popular as well, and was introduced ten years earlier [58, **?**, 60]. Under the name Pariser-Parr-Pople model it has been used to describe extended π-electron systems. Recently, it has been used to describe high temperature superconductors.

Today, the bosonic Hubbard model is of some interest as well. Its Hamiltonian is

$$H = H_{\text{kin}} + H_{\text{WW}} = \sum_{x,y} t_{x,y} c^\dagger_x c_y + \frac{U}{2} \sum_x n_x (n_x - 1) \tag{1.2}$$

where now $c^\dagger_x$, c_x are creation and annihilation operators for bosons.

For students who are not familiar with the notation used in (1.1,1.2), we introduce creation and annihilation operators in the next section. Students who are familiar with this notation may skip that and may continue reading from section 1.3.

1.2 Quantum Systems with many Particles

In reality, almost any system contains many particles interacting with each other. A single particle can be described by a wave function, which is an element of the single particle Hilbert space. The Hilbert space of two or more distinguishable particles is a product of the Hilbert spaces for single particles. For identical particles, the situation is different. Here, the type of the particles is essential, they may be either fermions or bosons. The multi particle wave function for bosons has to be symmetric, for fermions it has to be anti-symmetric against permutations of particles. The goal of the subsequent sections is to obtain a compact notation for such multi particle states using creation or annihilation operators for particles. We introduce them first separately for bosons and fermions.

Many of the concepts in this chapter may be found in standard text books like [56].

1.2.1 Creation and Annihilation Operators for Fermions

Let $\{\phi_i(\vec{r}, \sigma)\}$ be an orthonormal basis of single particle states. We denote the coordinate and the spin by $q = (\vec{r}, \sigma)$. In the case of fermions, a basis of N-particle states can be build out of Slater determinants of the

single particle states:

$$|i_1,i_2,...,i_N\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{i_1}(q_1) & \phi_{i_1}(q_2) & ... & \phi_{i_1}(q_N) \\ \phi_{i_2}(q_1) & \phi_{i_2}(q_2) & ... & \phi_{i_2}(q_N) \\ \vdots & \vdots & & \vdots \\ \phi_{i_N}(q_1) & \phi_{i_N}(q_2) & ... & \phi_{i_N}(q_N) \end{vmatrix} \tag{1.3}$$

This state can be written in the form

$$|i_1,i_2,...,i_N\rangle = \frac{1}{\sqrt{N!}} \sum_{P\in S_N} (-1)^P \prod_{j=1}^{N} \phi_{i_j}(q_{P(j)}) \tag{1.4}$$

Because of the construction as a determinant, the state is anti-symmetric if one permutes a pair of indices, as it should be for fermions.

$$|i_1,...,i_\alpha,...,i_\beta,...,i_N\rangle = -|i_1,...,i_\beta,...,i_\alpha,...,i_N\rangle \tag{1.5}$$

Normalisation:

$$\langle i_1,i_2,...,i_N|i_1,i_2,...,i_N\rangle = 1 \tag{1.6}$$

Orthogonality

$$\langle j_1,j_2,...,j_N|i_1,i_2,...,i_M\rangle = \begin{cases} \sum_P (-1)^P \prod_k \delta_{j_k,i_{P(k)}} & \text{if} N = M \\ 0 & \text{if} N \neq M. \end{cases} \tag{1.7}$$

We now define the creation operator of a particle in the state i by

$$c_i^\dagger |i_1,i_2,...,i_N\rangle = |i,i_1,i_2,...,i_N\rangle \tag{1.8}$$

$c_i^\dagger$ maps states with N onto states with $N+1$ particles. The right-hand side may vanish, this happens if and only if one of the indices $i_k = i$. One has

$$\begin{aligned} c_i^\dagger c_j^\dagger |i_1,i_2,...,i_N\rangle &= |i,j,i_1,i_2,...,i_N\rangle \\ &= -|j,i,i_1,i_2,...,i_N\rangle \\ &= -c_j^\dagger c_i^\dagger |i_1,i_2,...,i_N\rangle \end{aligned} \tag{1.9}$$

This holds for all states, so we have

$$c_i^\dagger c_j^\dagger = -c_j^\dagger c_i^\dagger \tag{1.10}$$

Therefore we have $c_i^\dagger c_i^\dagger = 0$. Furthermore one may write

$$|i_1,i_2,...,i_N\rangle = c_{i_1}^\dagger c_{i_2}^\dagger ... c_{i_N}^\dagger |\text{vak.}\rangle \tag{1.11}$$

For each operator $c_i^\dagger$ we introduce the hermitian conjugate operator c_i:

$$\begin{aligned} &\langle j_1,...,j_M|c_i|i_1,...,i_N\rangle = \langle i_1,...,i_N|c_i^\dagger|j_1,...,j_M\rangle^* \\ &= \langle i_1,...,i_N|i,j_1,...,j_M\rangle^* \\ &= \begin{cases} \delta_{i_1,i}\delta_{i_2,j_1}... - \delta_{i_1,j_1}\delta_{i_2,i} \pm ... \text{ alltogether } N! \text{ permutations}, & \text{if } N = M+1 \\ 0 & \text{if } N \neq M+1. \end{cases} \\ &= \delta_{i_1,i}\langle i_2,...,i_N|j_1,...,j_M\rangle^* - \delta_{i_2,i}\langle i_1,i_3,...,i_N|j_1,...,j_M\rangle^* + ... (N \text{terms}). \end{aligned} \tag{1.12}$$

and therefore

$$c_i|i_1,...,i_N\rangle = \delta_{i_1,i}|i_2,...,i_N\rangle - \delta_{i_2,i}|i_1,i_3,...,i_N\rangle + ... (N \text{terms}). \tag{1.13}$$

and

$$c_i|\text{vak.}\rangle = 0 \tag{1.14}$$

The commutation relations for the creation operators $c_i^\dagger$ can be carried over onto the annihilation operators c_i:

$$c_i c_j = -c_j c_i \tag{1.15}$$

We now introduce the anti-commutator $[A,B]_+ = AB + BA$ for arbitrary operators A and B. Then we may write

$$[c_i^\dagger, c_j^\dagger]_+ = 0, \quad [c_i, c_j]_+ = 0 \tag{1.16}$$

Because of

$$c_i^\dagger c_j |i_1,...,i_N\rangle = \delta_{i_1,j}|i,i_2,...,i_N\rangle - \delta_{i_2,j}|i,i_1,i_3,...,i_N\rangle + ... \tag{1.17}$$

$$c_j c_i^\dagger |i_1,...,i_N\rangle = \delta_{i,j}|i_1,...,i_N\rangle - \delta_{i_1,j}|i,i_2,...,i_N\rangle + \delta_{i_2,j}|i,i_1,i_3,...,i_N\rangle + ... \tag{1.18}$$

we obtain

$$(c_j c_i^\dagger + c_i^\dagger c_j)|i_1,...,i_N\rangle = \delta_{i,j}|i_1,...,i_N\rangle \tag{1.19}$$

and since this holds for any state, we have

$$[c_i^\dagger, c_j]_+ = \delta_{i,j} \tag{1.20}$$

1.2.2 Creation and Annihilation Operators for Bosons

Bosonic wave functions are symmetric. Therefore we could make the ansatz, in analogy to the fermions

$$|i_1,i_2,...,i_N\rangle = \frac{1}{\sqrt{N!}} \sum_P \prod_j \phi_{i_j}(q_{P(j)}) \tag{1.21}$$

But this state is not normalised. Since these wave functions are symmetric against permutations of two indices, they do not vanish if two indices are identical. Let n_i be the number of particles in the state i. Then we have

$$\langle i_1,i_2,...,i_N|i_1,i_2,...,i_N\rangle = \prod_{i\in\{i_1,...,i_N\}} n_i! \tag{1.22}$$

Therefore, the correct normalisation is

$$|i_1,i_2,...,i_N\rangle = \frac{1}{\sqrt{N!\prod_{i\in\{i_1,...,i_N\}} n_i!}} \sum_P \prod_j \phi_{i_j}(q_{P(j)}) \tag{1.23}$$

and therefore

$$\langle j_1,j_2,...,j_N|i_1,i_2,...,i_M\rangle = \begin{cases} \frac{1}{\prod_{i\in\{i_1,...,i_M\}} n_i!} \sum_P \prod_k \delta_{j_k,i_{P(k)}} & \text{if } N=M \\ 0 & \text{if } N\neq M. \end{cases} \tag{1.24}$$

For bosons, the creation operators can be defined as

$$c_i^\dagger |i_1,i_2,...,i_N\rangle = \sqrt{n_i+1}|i,i_1,i_2,...,i_N\rangle \tag{1.25}$$

Here, n_i is the number of particles in the single particle state i contained in $|i_1,i_2,...,i_N\rangle$. This is in complete analogy to the operators one introduces in the typical text-book treatment of the harmonic oscillator.

The hermitian conjugate operators to $c_i^\dagger$ are c_i and we obtain:

$$\begin{aligned} &\langle j_1,...,j_M|c_i|i_1,...,i_N\rangle = \langle i_1,...,i_N|c_i^\dagger|j_1,...,j_M\rangle^* \\ &= \sqrt{n_i+1}\langle i_1,...,i_N|i,j_1,...,j_M\rangle^* \\ &= \frac{\sqrt{n_i+1}}{\prod_{i'\in\{i_1,...,i_N\}} n_{i'}!} \begin{cases} \delta_{i_1,i}\delta_{i_2,j_1}... + \delta_{i_1,j_1}\delta_{i_2,i} + ... \text{ alltogether } N! \text{ permutations}, & \text{if } N=M+1 \\ 0 & \text{if } N\neq M+1. \end{cases} \\ &= \frac{1}{\sqrt{n_i+1}} (\delta_{i_1,i}\langle i_2,...,i_N|j_1,...,j_M\rangle^* + \delta_{i_2,i}\langle i_1,i_3,...,i_N|j_1,...,j_M\rangle^* + ...) \ (N\text{terms}). \end{aligned} \tag{1.26}$$

Here again n_i is the number of particles in the single particle state i contained in $|j_1,...,j_M\rangle$. This means

$$c_i|i_1,...,i_N\rangle = \frac{1}{\sqrt{n_i}}\left(\delta_{i_1,i}|i_2,...,i_N\rangle + \delta_{i_2,i}|i_1,i_3,...,i_N\rangle + ...\right) \ (N\text{terms}) \tag{1.27}$$

where now n_i is the number of particles in the single particle state i contained in $|i_1,...,i_N\rangle$ (one particle more than in $|j_1,...,j_M\rangle$). In complete analogy to the fermionic case treated before, we obtain

$$[c_i^\dagger, c_j^\dagger]_- = 0 \tag{1.28}$$

$$[c_i, c_j]_- = 0 \tag{1.29}$$

$$[c_i, c_j^\dagger]_- = \delta_{i,j} \tag{1.30}$$

where now $[.,.]_-$ is the usual commutator. The creation operators can be used to form the multi particle states:

$$|i_1,i_2,...,i_N\rangle = \frac{1}{\sqrt{\prod_{i\in\{i_1,...,i_N\}} n_i!}} c_{i_1}^\dagger c_{i_2}^\dagger ... c_{i_N}^\dagger |\text{vak.}\rangle \tag{1.31}$$

Summary: Creation and Annihilation Operators

We introduce the variable ζ, which is -1 for fermions, $+1$ for bosons. With the help of this variable, we may write the formula for both types of particles in the compact form

$$|i_1,i_2,...,i_N\rangle = \frac{1}{\sqrt{N!\prod_{i\in\{i_1,...,i_N\}} n_i!}} \sum_P \zeta^P \prod_j \phi_{i_j}(q_{P(j)}) \tag{1.32}$$

$$\langle j_1,j_2,...,j_N|i_1,i_2,...,i_M\rangle = \begin{cases} \frac{1}{\prod_{i\in\{i_1,...,i_M\}} n_i!} \sum_P \zeta^P \prod_k \delta_{j_k,i_{P(k)}} & \text{if } N=M \\ 0 & \text{if } N\neq M. \end{cases} \tag{1.33}$$

$$c_i^\dagger|i_1,i_2,...,i_N\rangle = \sqrt{n_i+1}|i,i_1,i_2,...,i_N\rangle \tag{1.34}$$

$$c_i|i_1,...,i_N\rangle = \frac{1}{\sqrt{n_i}}\left(\delta_{i_1,i}|i_2,...,i_N\rangle + \zeta\,\delta_{i_2,i}|i_1,i_3,...,i_N\rangle + ...\right) \ (N\text{terms}) \tag{1.35}$$

$$[c_i^\dagger, c_j^\dagger]_{-\zeta} = 0 \tag{1.36}$$

$$[c_i, c_j]_{-\zeta} = 0 \tag{1.37}$$

$$[c_i, c_j^\dagger]_{-\zeta} = \delta_{i,j} \tag{1.38}$$

$$|i_1,i_2,...,i_N\rangle = \frac{1}{\sqrt{\prod_{i\in\{i_1,...,i_N\}} n_i!}} c_{i_1}^\dagger c_{i_2}^\dagger ... c_{i_N}^\dagger |\text{vak.}\rangle \tag{1.39}$$

1.2.3 Single particle operators

Let us now discuss the operator

$$\hat{N} = \sum_{i=1}^{N} c_i^\dagger c_i \tag{1.40}$$

One has

$$c_i^\dagger c_i |i_1, ..., i_N\rangle = (\delta_{i_1,i} + \delta_{i_2,i} + ... + \delta_{i_N,i})|i_1, ..., i_N\rangle \tag{1.41}$$

and therefore

$$\hat{N}|i_1, ..., i_N\rangle = N|i_1, ..., i_N\rangle \tag{1.42}$$

$\hat{N}$ is the particle number operator. It is a single particle operator, since it may operate on single particle states. Any single particle operator T (for instance the kinetic energy or a potential) operates on the single particle basis. One has

$$T|i_1\rangle = \sum_{i=1}^{N} t_{i,i_1}|i\rangle \tag{1.43}$$

We consider first operators which are diagonal in the chosen basis

$$T|i\rangle = t_i|i\rangle \tag{1.44}$$

For N-particle states we have similarly

$$T|i_1, ..., i_N\rangle = \sum_j t_{i_j}|i_1, ..., i_N\rangle \tag{1.45}$$

The operator acts on each particle independently. We now want to show that T can be written as

$$T = \sum_i t_i c_i^\dagger c_i \tag{1.46}$$

With this form of T we calculate

$$T|i_1, i_2, ..., i_N\rangle = T\frac{1}{\sqrt{n_{i_1}+1}}c_{i_1}^\dagger|i_2, ..., i_N\rangle = \frac{1}{\sqrt{n_{i_1}+1}}[T, c_{i_1}^\dagger]|i_2, ..., i_N\rangle + \frac{1}{\sqrt{n_{i_1}+1}}c_{i_1}^\dagger T|i_2, ..., i_N\rangle \tag{1.47}$$

and further on

$$[T, c_{i_1}^\dagger] = \sum_i t_i[c_i^\dagger c_i, c_{i_1}^\dagger] = t_{i_1}c_{i_1}^\dagger \tag{1.48}$$

$$\begin{aligned} T|i_1, i_2, ..., i_N\rangle &= t_{i_1}|i_1, i_2, ..., i_N\rangle + c_{i_1}^\dagger T|i_2, ..., i_N\rangle \\ &= \sum_j t_{i_j}|i_1, ..., i_N\rangle \end{aligned} \tag{1.49}$$

which shows that the representation (1.46) of T is correct.

We will deal with single particle operators which are non diagonal. Since any hermitian operator can be diagonalised with the help of a unitary transformation, we have to know how a unitary transformation acts on the creation and annihilation operators. Let us introduce a new basis $|\alpha\rangle = \sum_i u_{\alpha i}|i\rangle$ where $U = (u_{\alpha i})$ with $u_{\alpha i} = \langle i|\alpha\rangle$ is a unitary matrix. Let $c_\alpha^\dagger$ be the new creation operators. We have

$$\begin{aligned} c_\alpha^\dagger|\text{vak.}\rangle &= |\alpha\rangle \\ &= \sum_i u_{\alpha i}|i\rangle \\ &= \sum_i u_{\alpha i}c_i^\dagger|\text{vak.}\rangle \\ &= \sum_i \langle\alpha|i\rangle^* c_i^\dagger|\text{vak.}\rangle \end{aligned} \tag{1.50}$$

and therefore we let

$$c_\alpha^\dagger = \sum_i \langle i|\alpha\rangle\, c_i^\dagger \tag{1.51}$$

$$c_i^\dagger = \sum_i \langle \alpha|i\rangle\, c_\alpha^\dagger \tag{1.52}$$

$$c_\alpha = \sum_i \langle \alpha|i\rangle\, c_i \tag{1.53}$$

$$c_i = \sum_i \langle i|\alpha\rangle\, c_\alpha \tag{1.54}$$

Then we have

$$\begin{aligned} T &= \sum_i t_i c_i^\dagger c_i \\ &= \sum_{i,\alpha,\beta} t_i \langle \alpha|i\rangle \langle i|\beta\rangle\, c_\alpha^\dagger c_\beta \\ &= \sum_{\alpha,\beta} t_{\alpha,\beta} c_\alpha^\dagger c_\beta \end{aligned} \tag{1.55}$$

This is the general form of a single particle operator.

Examples:

- Potential: $V(\vec{r})$

$$t_{i,j} = \int d^3r\, \phi_i^*(\vec{r}) V(\vec{r}) \phi_j(\vec{r}) \tag{1.56}$$

- Kinetic energy:

$$t_{i,j} = \int d^3r \phi_i^*(\vec{r}) \left(-\frac{\hbar^2}{2m}\right) \phi_j(\vec{r}) \tag{1.57}$$

  In the orthonormal basis $\phi_{\vec{k},\sigma} = \frac{1}{\sqrt{V}} \exp(i\vec{k}\cdot\vec{r})\chi_\sigma$ one obtains

$$T = \sum_{\vec{k},\sigma} \frac{\hbar^2\vec{k}^2}{2m} c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma} \tag{1.58}$$

1.2.4 Interactions

The aim of this course is to treat interacting systems. Almost any interaction is an interaction between two particles. Such interactions can be described as two particle operators. Generically, we cannot expect that interactions are diagonal in the multi particle states constructed out of a given single particle basis. But, for simplicity, we will start with this case. Let V be the operator of the interactions, then, in this basis, we have

$$V|i,j\rangle = V_{ij}|i,j\rangle. \tag{1.59}$$

$|i,j\rangle$ is a two particle state. For matrix elements of states with N particles, we obtain

$$\begin{aligned} \langle j_1 \dots j_N|V|i_1 \dots i_N\rangle &= \sum_P \zeta^P \frac{1}{2} \sum_{k\neq k'} \langle j_{P_k}, j_{P_{k'}}|V|i_k, i_{k'}\rangle \prod_{l\neq k,k'} \langle j_{P_l}|i_l\rangle \\ &= \left(\frac{1}{2}\sum_{k\neq k'} V_{i_k,i_{k'}}\right) \langle j_1 \dots j_N|i_1 \dots i_N\rangle \end{aligned} \tag{1.60}$$

Here $\frac{1}{2}\sum_{k\neq k'}$ is the sum over all pairs of particles in the states $|i_1 \dots i_N\rangle$. For $i \neq i'$, the number of pairs of particles in the states i and i' is $n_i n_{i'}$. For $i = i'$, it is $n_i(n_i - 1)$. The number of pairs therefore is

$$\begin{aligned} n_i n_j - \delta_{i,j} n_i &= c_i^\dagger c_i c_j^\dagger c_j - \delta_{i,j} c_i^\dagger c_i \\ &= \zeta c_i^\dagger c_j^\dagger c_i c_j \\ &= c_i^\dagger c_j^\dagger c_j c_i \end{aligned} \tag{1.61}$$

Therefore we have

$$V = \frac{1}{2}\sum_{i,j} V_{i,j} c_i^\dagger c_j^\dagger c_j c_i = \frac{1}{2}\sum_{i,j} \langle i,j|V|i,j\rangle c_i^\dagger c_j^\dagger c_j c_i \tag{1.62}$$

Transforming this into a general basis, we obtain

$$V = \frac{1}{2}\sum_{i,j,k,l} \langle i,j|V|k,l\rangle c_i^\dagger c_j^\dagger c_l c_k \tag{1.63}$$

This is the general form of any two particle operator. Each two particle interaction can be written in that form.

The representation of any operator, e.g. the Hamiltonian of a given model, with the help of creation and annihilation operators is thus a simple short form of writing down the matrix elements of that operator in a multi particle basis that has been constructed from a single particle basis by either forming completely anti-symmetric states, Slater determinants, in the case of fermions or completely symmetric states in the case of bosons. The advantage of this representation is the simple algebraic relation ship between the creation and annihilation operators in the form of commutation relations (bosons) or anti-commutation relations (fermions). Many calculations are much easier in this representation.

1.3 Coherent States

Creation and annihilation operators map states of one Hilbert space onto states of another Hilbert space. A state with N particles is mapped to a state with $N \pm 1$ particles. Successive application of creation and annihilation operators yields states out of Hilbert spaces with an arbitrary number of particles. The direct sum of all Hilbert spaces with N particles, $N = 0, \dots, \infty$ is called Fock space. The entire Fock space can be spanned by applying creation operators onto the vacuum. In many cases it is useful to work in the Fock space instead of a Hilbert space with a fixed number of particles. This is esp. the case, if the number of particles is not a good quantum number, as e.g. in the case of phonons, or if one treats a problem in a grand canonical ensemble.

Up to now we used the N-particle states built out of single particle states as a basis of the Fock space. There is another, actually over-complete set of states which proved to be useful, coherent states. These are eigenstates of the annihilation operators.

First of all, it is easy to see that a creation operator cannot have an eigenstate. Suppose that such an eigenstate exists. It would be a sum of states of a different number of particles. Within this sum, there would be necessarily a state with the lowest number of particles. The creation operator acting on this state would increase the lowest number of particles by one. Therefore this sum of states cannot be an eigenstate.

A corresponding argument does not exist for the annihilation operator, since in the Fock space, there is no state with a maximal number of particles. Suppose that we have got an eigenstate of the annihilation operator, i.e.

$$c_i|\phi\rangle = \phi_i|\phi\rangle. \tag{1.64}$$

For bosons, annihilation operators commute. Therefore their eigenvalues are usual complex numbers. We shall see later that for fermions, this is not the case.

1.3.1 Coherent States for Bosons

A state with n_i bosons in the single particle states $|i\rangle$, $i = 1,\ldots,N$ can be written in the form

$$|n_1,n_2,\ldots,n_N\rangle = \prod_{i=1}^{N}\left(\frac{1}{\sqrt{n_i!}}(c_i^\dagger)^{n_i}\right)|\text{vak.}\rangle \tag{1.65}$$

One has

$$c_i|n_1,n_2,\ldots,n_N\rangle = \sqrt{n_i}|n_1,n_2,\ldots,n_i-1,\ldots,n_N\rangle \tag{1.66}$$

For the coherent state $|\phi\rangle$, we make the ansatz

$$|\phi\rangle = \sum_{n_1,n_2,\ldots,n_N}\phi_{n_1,n_2,\ldots,n_N}|n_1,n_2,\ldots,n_N\rangle \tag{1.67}$$

The condition $c_i|\phi\rangle = \phi_i|\phi\rangle$ yields

$$\phi_i\phi_{n_1,\ldots,n_i,\ldots,n_N} = \sqrt{n_i+1}\,\phi_{n_1,\ldots,n_i+1,\ldots,n_N} \tag{1.68}$$

and therefore

$$\phi_{n_1,n_2,\ldots,n_N} = \prod_{i=1}^{N}\frac{\phi_i^{n_i}}{\sqrt{n_i!}} \tag{1.69}$$

Finally we obtain

$$\begin{aligned}|\phi\rangle &= \sum_{n_1,n_2,\ldots,n_N}\prod_{i=1}^{N}\left(\frac{\phi_i^{n_i}}{n_i!}(c_i^\dagger)^{n_i}\right)|\text{vak.}\rangle \\ &= \exp(\sum_{i=1}^{N}\phi_i c_i^\dagger)|\text{vak.}\rangle\end{aligned} \tag{1.70}$$

A creation operator acting on this state yields

$$\begin{aligned}c_i^\dagger|\phi\rangle &= c_i^\dagger\exp(\sum_i\phi_i c_i^\dagger)|\text{vak.}\rangle \\ &= \frac{\partial}{\partial\phi_i}|\phi\rangle\end{aligned} \tag{1.71}$$

Now we calculate the scalar product of two coherent states:

$$\begin{aligned}\langle\psi|\phi\rangle &= \sum_{n_1,\ldots,n_N}\sum_{m_1\ldots m_N}\prod_i\left(\frac{\psi_i^{*m_i}\phi_i^{n_i}}{\sqrt{m_i!n_i!}}\right)\langle m_1,\ldots,m_N|n_1,\ldots,n_N\rangle \\ &= \sum_{n_1,\ldots,n_N}\prod_i\left(\frac{\psi_i^{*n_i}\phi_i^{n_i}}{n_i!}\right) \\ &= \exp(\sum_i\psi_i^*\phi_i)\end{aligned} \tag{1.72}$$

One can show that coherent states are overcomplete. This property is very important. We now show that

$$\int D[\phi]\exp(-\sum_i\phi_i^*\phi_i)|\phi\rangle\langle\phi| = 1 \tag{1.73}$$

where we use the notation

$$D[\phi] = \prod_i\frac{d(\Re\phi_i)d(\Im\phi_i)}{\pi} \tag{1.74}$$

To show this, we calculate the commutator

$$[c_i, |\phi\rangle\langle\phi|] = (\phi_i - \frac{\partial}{\partial \phi_i^*})|\phi\rangle\langle\phi| \tag{1.75}$$

One obtains

$$[c_i, \int D[\phi] \exp(-\sum_i \phi_i^* \phi_i)|\phi\rangle\langle\phi|] = \int D[\phi] \exp(-\sum_i \phi_i^* \phi_i)(\phi_i - \frac{\partial}{\partial \phi_i^*})|\phi\rangle\langle\phi| \tag{1.76}$$

Partiell integration of the second term on the right hand side shows, that the commutator vanishes. Therefore, the operator $\int D[\phi] \exp(-\sum_i \phi_i^* \phi_i)|\phi\rangle\langle\phi|$ commutes with all annihilation operators c_i. Therefore, it must be a number. To calculate that number, we take it's expectation value in the vacuum. We obtain

$$\int D[\phi] \exp(-\sum_i \phi_i^* \phi_i)\langle \text{vac.}|\phi\rangle\langle\phi|\text{vac.}\rangle = \int D[\phi] \exp(-\sum_i \phi_i^* \phi_i) = 1 \tag{1.77}$$

This shows the completeness.

A trace of an arbitrary operator A can be expressed as

$$\text{Tr}A = \int D[\phi] \exp(-\sum_i \phi_i^* \phi_i)\langle\phi|A|\phi\rangle \tag{1.78}$$

Similarly, we can expand an arbitrary state $|f\rangle$ in terms of coherent states

$$|f\rangle = \int D[\phi] \exp(-\sum_i \phi_i^* \phi_i)\langle\phi|f\rangle|\phi\rangle \tag{1.79}$$

The expression

$$f(\phi^*) := \langle\phi|f\rangle \tag{1.80}$$

is the representation of $|f\rangle$ in terms of coherent states, like $f(x) = \langle x|f\rangle$ is called coordinate representation of $|f\rangle$. In this representation, the annihilation operator is simply the derivative

$$\langle\phi|c_i|f\rangle = \langle f|c_i^\dagger|\phi\rangle^* = \left(\frac{\partial}{\partial \phi_i}\langle f|\phi\rangle\right)^* = \frac{\partial f(\phi^*)}{\partial \phi_i^*} \tag{1.81}$$

and the creation operator is the multiplication operator

$$\langle\phi|c_i^\dagger|f\rangle = \langle f|c_i|\phi\rangle^* = (\phi_i\langle f|\phi\rangle)^* = \phi_i^* f(\phi^*) \tag{1.82}$$

so that we write

$$c_i = \frac{\partial}{\partial \phi_i^*}, \quad c_i^\dagger = \phi_i^* \tag{1.83}$$

This representation fulfils the usual commutation relations. As a consequence, the Hamiltonian, which is usually expressed by creation and annihilation operators in some form $H(\{c_i^\dagger, c_i\})$ can be written as $H(\{\phi_i^*, \frac{\partial}{\partial \phi_i^*}\})$ in the coherent state representation and the eigenvalue equation is

$$H(\{\phi_i^*, \frac{\partial}{\partial \phi_i^*}\})f(\phi^*) = Ef(\phi^*) \tag{1.84}$$

Matrix elements of an operator $A(\{c_i^\dagger, c_i\})$ are

$$\langle\phi|A(\{c_i^\dagger, c_i\})|\psi\rangle = A(\{\phi_i^*, \psi_i\}) \exp(\sum_i \phi_i^* \psi_i) \tag{1.85}$$

where one has to take into account that all creation operators must be placed left of all annihilation operators (normal ordering).

The expectation value of the number operator $n_i = c_i^\dagger c_i$ is therefore $\phi_i^* \phi_i$ and the expectation value of the number of particles is $\bar{N} = \sum_i \phi_i^* \phi_i$. Furthermore

$$\frac{\langle\phi|(\hat{N} - \bar{N})^2|\phi\rangle}{\langle\phi|\phi\rangle} = \sum_i \phi_i^* \phi_i = \bar{N} \tag{1.86}$$

so that the relative deviation of the particle number from it's expectation value is $\propto \bar{N}^{-1/2}$.

1.3.2 Grassmann Algebra

We saw that coherent states for bosons may be useful. In the following we will often make use of coherent states. The goal of the present section is to introduce coherent states for fermions. To do this we need to deal with objects which anti-commute. Such objects are called Grassmann variables. One can define usual operations for them, they form a so called Grassmann algebra. The goal of this subsection is to introduce the main ideas behind this concept. An excellent introduction (in German) on Grassmann variables is the script by Franz Wegner [76].

A Grassman algebra is built up from a set of generating elements $\{\xi_i, i = 1,\ldots,N\}$. It contains all polynomials of these generating elements with complex coefficients. The fundamental rule is

$$\xi_i\xi_j + \xi_j\xi_i = 0 \tag{1.87}$$

and therefore

$$\xi_i^2 = 0 \tag{1.88}$$

In the following, we use an enlarged Grassmann algebra, that is formed by the generators $\{\xi_i, \xi_i^*, i = 1,\ldots,N\}$. The symbolic operation * obeys the following rules

$$(\xi_i)^* = \xi_i^* \tag{1.89}$$

$$(\xi_i^*)^* = \xi_i \tag{1.90}$$

$$(\xi_i\xi_j)^* = \xi_j^*\xi_i^* \tag{1.91}$$

We now consider functions of the variables ξ_i and ξ_i^*. These are polynomials of ξ_i and ξ_i^*, where in each monom, a factor ξ_i occurs only once, since its square vanishes. Known functions are defined by their Taylor expansion, which terminates automatically. E.g. one has $\exp(\xi_i) = 1 + \xi_i$.

Having defined functions, the next point is to define derivatives. One has

$$\frac{\partial}{\partial\xi_i}\xi_i = 1 \tag{1.92}$$

For a product of variables, one has first to interchange the variables so that the variable and the derivative are close to each other. For example, one has

$$\frac{\partial}{\partial\xi_i}\xi_j^*\xi_k\xi_l\xi_i = \frac{\partial}{\partial\xi_i}(-\xi_i\xi_j^*\xi_k\xi_l) = -\xi_j^*\xi_k\xi_l \tag{1.93}$$

The derivative of an expression with respect to a variable vanishes, if the expression does not contain the variable. Similarly, all other known rules like the product rule hold, except for additional signs which occur due to the exchanging of variables. Like variables, derivatives anti-commute:

$$\frac{\partial}{\partial\xi_i}\frac{\partial}{\partial\xi_j} = -\frac{\partial}{\partial\xi_j}\frac{\partial}{\partial\xi_i} \tag{1.94}$$

Next we define integrals. Clearly, there is no integral which is analogue to the usual Riemann integral for real numbers. The idea is to define the integral as a linear mapping of functions to real numbers, which behaves similar to integrals of usual integrable functions which vanish at infinity. Furthermore we need that the integral of a total differential vanishes. There are various possibilities to define the integral, a typical convention is

$$\int d\xi\, 1 = 0 \tag{1.95}$$

$$\int d\xi\, \xi = 1 \tag{1.96}$$

The same must be true for the ξ_i^*. But one has to pay attention concerning anti-commutation and signs. For instance, we have for

$$f(\xi_1,\xi_2) = a_0 + a_1\xi_1 + a_2\xi_2 + a_{12}\xi_1\xi_2 \tag{1.97}$$

$$\int d\xi_2 f(\xi_1,\xi_2) = a_2 - a_{12}\xi_1 \tag{1.98}$$

and

$$\int d\xi_1 d\xi_2 f(\xi_1,\xi_2) = -a_{12} \tag{1.99}$$

but

$$\int d\xi_2 d\xi_1 f(\xi_1,\xi_2) = a_{12} \tag{1.100}$$

The expressions $d\xi_i$ anti-commute like the variables ξ_i itself. With these definitions, arbitrary integrals can be calculated, for instance one obtains

$$\int d\xi^* d\xi \exp(-\xi^*\xi) = \int d\xi^* d\xi (1-\xi^*\xi) = 1 \tag{1.101}$$

We now define a scalar product for functions of Grassmann variables. Let f and g be functions of $\xi_1,\ldots,\xi_N$, then we define

$$\langle f|g\rangle = \int D[\xi] \exp(-\sum_i \xi_i^*\xi_i) f^*(\xi_1,\ldots,\xi_N) g(\xi_1^*,\ldots,\xi_N^*) \tag{1.102}$$

where

$$D[\xi] = \prod_i (d\xi_i^* d\xi_i) \tag{1.103}$$

Using Grassmann variables we can now construct coherent states for fermions.

1.3.3 Coherent states for fermions

First, we need a convention about the behaviour of a product of Grassmann variables and creation and annihilation operators for fermions. It is natural to choose

$$[c_i,\xi_j]_+ = [c_i^\dagger,\xi_j]_+ = [c_i,\xi_j^*]_+ = [c_i^\dagger,\xi_j^*]_+ = 0 \tag{1.104}$$

for all i,j. As an ansatz for the coherent state we take

$$|\xi\rangle = \exp(-\sum_i \xi_i c_i^\dagger)|\text{vak.}\rangle = \prod_i (1-\xi_i c_i^\dagger)|\text{vak.}\rangle \tag{1.105}$$

The second expression can be obtained from the first by taking into account that all the expressions $\xi_i c_i^\dagger$ commute with each other so that the exponential of the sum is a product of exponentials. Furthermore each annihilation operator c_j commutes with $\xi_i c_i^\dagger$ if $i \neq j$. For $i = j$ we have

$$c_i \xi_i c_i^\dagger = -\xi_i c_i c_i^\dagger = -\xi_i (1 - c_i^\dagger c_i) \tag{1.106}$$

This now yields

$$c_i|\xi\rangle = \xi_i|\xi\rangle \tag{1.107}$$

which is indeed the defining property for coherent states.

Let us now calculate, how a creation operator acts on a coherent state.

$$\begin{aligned} c_i^\dagger|\xi\rangle &= c_i^\dagger(1-\xi_i c_i^\dagger)\prod_{j\neq i}(1-\xi_j c_j^\dagger)|\text{vak.}\rangle \\ &= c_i^\dagger\prod_{j\neq i}(1-\xi_j c_j^\dagger)|\text{vak.}\rangle \\ &= -\frac{\partial}{\partial\xi_i}(1-\xi_i c_i^\dagger)\prod_{j\neq i}(1-\xi_j c_j^\dagger)|\text{vak.}\rangle \\ &= -\frac{\partial}{\partial\xi_i}|\xi\rangle \end{aligned} \tag{1.108}$$

For the scalar product of two coherent states we obtain

$$\langle\xi|\chi\rangle = \langle\text{vak.}|\prod_i(1-c_i\xi_i^*)(1-\chi_i c_i^\dagger)|\text{vak.}\rangle = \prod_i(1+\xi_i^*\chi_i) = \exp(\sum_i \xi_i^*\chi_i) \tag{1.109}$$

Next we want to show the completeness relation

$$\int D[\xi]\exp(-\sum_i \xi_i^*\xi_i)|\xi\rangle\langle\xi| = 1 \tag{1.110}$$

To do this, we define

$$E = \int D[\xi]\exp(-\sum_i \xi_i^*\xi_i)|\xi\rangle\langle\xi| \tag{1.111}$$

and show that

$$\langle i_1,\ldots,i_n|E|j_1,\ldots,j_m\rangle = \langle i_1,\ldots,i_n|j_1,\ldots,j_m\rangle \tag{1.112}$$

holds. First, one obtains

$$\langle i_1,\ldots,i_n|\xi\rangle = \langle\text{vak.}|c_{i_n}\ldots c_{i_1}|\xi\rangle = \xi_{i_n}\ldots\xi_{i_1} \tag{1.113}$$

and therefore

$$\langle i_1,\ldots,i_n|E|j_1,\ldots,j_m\rangle = \int D[\xi]\prod_i(1-\xi_i^*\xi_i)\xi_{i_n}\ldots\xi_{i_1}\xi_{j_1}^*\ldots\xi_{j_m}^* \tag{1.114}$$

Furthermore, we have

$$\int d\xi_i^* d\xi_i(1-\xi_i^*\xi_i)\xi_i\xi_i^* = 1 \tag{1.115}$$

$$\int d\xi_i^* d\xi_i(1-\xi_i^*\xi_i)\xi_i = 0 \tag{1.116}$$

$$\int d\xi_i^* d\xi_i(1-\xi_i^*\xi_i)\xi_i^* = 0 \tag{1.117}$$

$$\int d\xi_i^* d\xi_i(1-\xi_i^*\xi_i) = 1 \tag{1.118}$$

This first of all means that one gets a non-vanishing contribution only if $n=m$ and $\{i_1,\ldots,i_n\}=\{j_1,\ldots,j_m\}$. If this condition is fulfilled, the only thing that remains is to permute the ξ_{i_k} so that they occur in the same order as the $\xi_{j_k}^*$. The result is simply the sign, one gets, if one calculates the scalar product in (1.112). This shows the completeness relation. Using it, we directly obtain

$$\text{Tr}A = \int D[\xi]\exp(-\sum_i \xi_i^*\xi_i)\langle-\xi|A|\xi\rangle \tag{1.119}$$

where the additional minus sign in $\langle-\xi|$ occurs because we have to exchange $|\xi\rangle$ with $\langle\xi|$, so that each Grassmann variable gets an additional minus sign. Due to the completeness relation one has also

$$|f\rangle = \int D[\xi]\exp(-\sum_i \xi_i^*\xi_i)\langle-\xi|f\rangle|\xi\rangle \tag{1.120}$$

and we can define the expression

$$f(\xi^*) := \langle -\xi | f \rangle \tag{1.121}$$

like in the bosonic case as the coherent representation of a state $|f\rangle$. One obtains directly

$$\begin{aligned} \langle -\xi | c_i | f \rangle &= (\langle f | c_i^\dagger | -\xi \rangle)^* \\ &= \frac{\partial}{\partial \xi_i^*} \langle f | -\xi \rangle^* \\ &= \frac{\partial}{\partial \xi_i^*} f(\xi^*) \end{aligned} \tag{1.122}$$

and similarly

$$\langle -\xi | c_i^\dagger | f \rangle = -\xi_i^* f(\xi^*) \tag{1.123}$$

The creation operators $c_i^\dagger$ and the annihilation operators c_i for fermions in the coherent representation are therefore simply $-\xi_i^*$ and $\frac{\partial}{\partial \xi_i^*}$. The anticommuation relations are clearly fulfilled. Like in the bosonic case, we obtain for a normal ordered (creation operators left of all annihilation operators) operator $A(\{c_i^\dagger, c_i\})$

$$\langle \xi | A(\{c_i^\dagger, c_i\}) | \chi \rangle = A(\{\xi_i^*, \chi_i\}) \langle \xi | \chi \rangle \tag{1.124}$$

An important point is that these are not real numbers. For instance, the expectation value of the number operator is $\sum_i \xi_i^* \xi_i$ and this is not a real number. In contrast to the bosonic case, fermionic coherent states are not elements of the usual Fock space. Nevertheless they are useful.

Summary: Coherent States

Let $|\phi\rangle$ be a coherent state for bosons or fermions. Like above, we introduce $\zeta = 1$ for bosons and $\zeta = -1$ for fermions. Then we have

$$c_i |\phi\rangle = \phi_i |\phi\rangle. \tag{1.125}$$

$$c_i^\dagger |\phi\rangle = \zeta \frac{\partial}{\partial \phi_i} |\phi\rangle \tag{1.126}$$

$$\langle \psi | \phi \rangle = \exp(\sum_i \psi_i^* \phi_i) \tag{1.127}$$

$$\int D[\phi] \exp(-\sum_i \phi_i^* \phi_i) |\phi\rangle\langle\phi| = 1 \tag{1.128}$$

$$\mathrm{Tr} A = \int D[\phi] \exp(-\sum_i \phi_i^* \phi_i) \langle \zeta\phi | A | \phi \rangle \tag{1.129}$$

$$|f\rangle = \int D[\phi] \exp(-\sum_i \phi_i^* \phi_i) \langle \zeta\phi | f \rangle |\phi\rangle \tag{1.130}$$

$$f(\phi^*) := \langle \zeta\phi | f \rangle \tag{1.131}$$

$$c_i = \frac{\partial}{\partial \phi_i^*}, \quad c_i^\dagger = \zeta \phi_i^* \tag{1.132}$$

$$\langle \phi | A(\{c_i^\dagger, c_i\}) | \psi \rangle = A(\{\phi_i^*, \psi_i\}) \exp(\sum_i \phi_i^* \psi_i) \tag{1.133}$$

The last expression is true for normal ordered operators only.

1.4 Gaussian Integrals

In the following we will often need to compute Gaussian integrals for complex variables or for Grassmann variables. For complex variables, one has

$$\int D[\phi]\exp(-\sum_{i,j}\phi_i^* h_{ij}\phi_j+\sum_i z_i^*\phi_i+\sum_i z_i\phi_i^*)=[\det H]^{-1}\exp(\sum_{i,j}z_i^*(H^{-1})_{ij}z_j) \tag{1.134}$$

where $H=(h_{ij})$ is a matrix with a positive hermitian part. For Grassmann variables we have similarly

$$\int D[\xi]\exp(-\sum_{i,j}\xi_i^* h_{ij}\xi_j+\sum_i \chi_i^*\xi_i+\sum_i \chi_i\xi_i^*)=[\det H]\exp(\sum_{i,j}\chi_i^*(H^{-1})_{ij}\chi_j) \tag{1.135}$$

Let us derive these two relations.

First for complex variables: If H has a positive hermitian part, the inverse H^{-1} is defined. Completing the square as usual, we can introduce a new integration variable $\psi_i=\phi_i-\sum_j(H^{-1})_{ij}z_j$. The left hand side of (1.134) becomes

$$\int D[\psi]\exp(-\sum_{i,j}\psi_i^* h_{ij}\psi_j+\sum_{i,j}z_i^*(H^{-1})_{ij}z_j) \tag{1.136}$$

Next we diagonalise H using a unitary transformation. Let U be this unitary transformation. The we introduce $\varphi_i=\sum_j(U^{-1})_{ij}\psi_j$. We obtain

$$\sum_{i,j}\psi_i^* h_{ij}\psi_j=\sum_i h_i\varphi_i^*\varphi_i \tag{1.137}$$

where h_i are the eigenvalues of H. Furthermore, we have

$$\int\frac{d\Re\phi_i d\Im\phi_i}{\pi}\exp(-h_i\phi_i^*\phi_i)=\frac{1}{h_i} \tag{1.138}$$

which finally yields the desired result.

For Grassmann variables, one can do the same. The problem is, that up to now we have not introduced substitutions of variables in integrals. Let us therefore treat a general integral

$$\int D[\xi]f(\xi_1\dots\xi_N,\xi_1^*\dots\xi_N^*) \tag{1.139}$$

and let us introduce a transformation of the form $\xi_i=\sum_j u_{ij}\eta_j$, $\xi_i^*=\sum_j u_{ij}^*\eta_j^*$. The only non-vanishing contribution in the integral over ξ comes from the term in f which contains each variable exactly once as a factor. Let us denote this last term $f_0\prod_i\xi_i\xi_i^*$. Then, f_0 is the integral. Let us now calculate

$$\int D[\eta]f(\xi_1(\eta)...\xi_N(\eta),\xi_1^*(\eta^*)\dots\xi_N(\eta^*))=f_0\int D[\eta]\prod_i(\sum_j u_{ij}\eta_j\sum_k u_{ik}^*\eta_k^*) \tag{1.140}$$

The polynomial expansion of the right hand side can be calculated. This yields

$$f_0\int D[\eta]\sum_{P,P'}\prod_i u_{iP_i}\eta_{P_i}u_{iP_i'}^*\eta_{P_i'}^* \tag{1.141}$$

where the sum runs over all permutations. Now we can calculate the integral. We obtain

$$f_0\sum_P(-1)^P\prod_i u_{iP_i}\sum_{P'}(-1)^{P'}\prod_i u_{iP_i'}^*=f_0\det U\det U^\dagger=f_0 \tag{1.142}$$

This means that substitutions in integrals over Grassmann variables can be done as usual. For the Gaussian integral, one obtains in the end

$$\int d\eta_i^* d\eta_i\exp(-h_i\eta_i^*\eta_i)=h_i \tag{1.143}$$

This finally yields (1.135).

1.5 Functional-Integral Representaion

In the following we want to deal with a system of interacting particles. We consider first systems where the particle number is a good quantum number. Let us assume that we have a usual two-particle interaction. Then, the Hamiltonian is of the form

$$\hat{H} = \sum_i \varepsilon_i c_i^\dagger c_i + \sum_{i,j,k,l} V_{i,j,k,l} c_i^\dagger c_j^\dagger c_l c_k \tag{1.144}$$

The single particle contribution contains typically the kinetic energy and some single particle potential. We assume, that this contribution can be diagonalised, and we chose the basis for the representation of the Hamiltonian such that it is diagonal. Furthermore, we assume that we have a finite system where the single particle energies ε_i are discrete. Eventually, we may take the thermodynamic limit in the end.

Having such a system, one typically wants to calculate expectation values of some operators $A = A(\{c_i^\dagger, c_i\})$. At finite temperatures, they are

$$\langle A(\{c_i^\dagger, c_i\})\rangle = Z^{-1}\mathrm{Tr}[A(\{c_i^\dagger, c_i\})\exp(-\beta(\hat{H}-\mu\hat{N}))] \tag{1.145}$$

where $\beta = 1/T$ is the inverse temperature, μ is the chemical potential and

$$Z = \mathrm{Tr}\exp(-\beta(\hat{H}-\mu\hat{N})) \tag{1.146}$$

is the grand canonical partition function of the system. The traces are calculated over the entire Fock space. We shall calculate the traces using coherent states. We calculate first the partition function, which yields directly some of the important thermodynamical quantities. We have

$$Z = \int D[\phi]\exp(-\sum_i \phi_i^*\phi_i)\langle\zeta\phi|\exp(-\beta(\hat{H}-\mu\hat{N}))|\phi\rangle \tag{1.147}$$

The first problem now is that $\hat{H}$ and $\hat{N}$ are normal ordered, but $\exp(-\beta(\hat{H}-\mu\hat{N}))$ is not. For small values of ε we have

$$\exp(-\varepsilon(\hat{H}-\mu\hat{N})) =: \exp(-\varepsilon(\hat{H}-\mu\hat{N})) : +O(\varepsilon^2) \tag{1.148}$$

where : . : means that the expression is normal ordered. To see this, simply expand the exponential on both sides. Next we write

$$\exp(-\beta(\hat{H}-\mu\hat{N})) = \left[\exp(-\frac{\beta}{M}(\hat{H}-\mu\hat{N}))\right]^M \tag{1.149}$$

We will choose M sufficiently large so that β/M is small. Then, the term in the parentheses on right hand side is normal ordered up to a small error. We now obtain

$$Z = \int D[\phi]\exp(-\sum_i \phi_i^*\phi_i)\langle\zeta\phi|\exp(-\frac{\beta}{M}(\hat{H}-\mu\hat{N}))\ldots\exp(-\frac{\beta}{M}(\hat{H}-\mu\hat{N}))|\phi\rangle \tag{1.150}$$

where the expectation value contains M factors. Between each pair of factors we put a 1 which we write as

$$\int D[\phi]\exp(-\sum_i \phi_i^*\phi_i)|\phi\rangle\langle\phi| = 1 \tag{1.151}$$

Doing this, we have to change our notation a little bit. Since there are M factors,we need M coherent states. The states are denoted by $|\phi_k\rangle$, $k = 1,\ldots,M$. The variables $|\phi_k\rangle$ depends on are denoted by $\phi_{i,k}$. The first index denotes the single particle states, the second the coherent states. $D[\phi]$ is now the integral over all variables $\phi_{i,k}$ and $\phi_{i,k}^*$. Furthermore, I introduce $\phi_0 = \zeta\phi_M$. Then we obtain

$$Z = \int D[\phi]\exp(-\sum_{i,k}\phi_{i,k}^*\phi_{i,k})\prod_{k=1}^M\langle\phi_k|\exp(-\frac{\beta}{M}(\hat{H}-\mu\hat{N}))|\phi_{k-1}\rangle \tag{1.152}$$

Up to an error of the order $O(M^{-2})$ we can use the formula (1.133). This yields

$$Z = \lim_{M\to\infty} Z_M = \lim_{M\to\infty} \int D[\phi] \exp(-S_M[\phi]) \tag{1.153}$$

$$S_M[\phi] = \varepsilon \sum_{k=1}^{M} \left[\sum_i \phi_{i,k}^* \left(\frac{\phi_{i,k} - \phi_{i,k-1}}{\varepsilon} - \mu \phi_{i,k-1} \right) + H(\{\phi_{i,k}^*, \phi_{i,k-1}\}) \right] \tag{1.154}$$

where $\varepsilon = \beta/M$. Typically one introduces in the limit $M \to \infty$ the function $\phi_i(\tau)$, where $\phi_{i,k} = \phi_i(\varepsilon k)$. Then we may write

$$\frac{\phi_{i,k} - \phi_{i,k-1}}{\varepsilon} = \frac{\phi_i(\varepsilon k) - \phi_i(\varepsilon k - \varepsilon)}{\varepsilon} \to \frac{\partial \phi_i(\tau - 0^+)}{\partial \tau} \tag{1.155}$$

$$\varepsilon \sum_{k=1}^{M} \to \int_0^\beta d\tau \tag{1.156}$$

and

$$S[\phi] = \int_0^\beta d\tau \left(\sum_i \phi_i^*(\tau) (\frac{\partial}{\partial \tau} - \mu) \phi_i(\tau - 0^+) + H(\{\phi_i^*(\tau), \phi_i(\tau - 0^+)\}) \right) \tag{1.157}$$

$$Z = \int_{\phi_i(\beta) = \zeta \phi_i(0)} D[\phi] \exp(-S[\phi]) \tag{1.158}$$

These expressions are called functional integrals. We obtained a functional integral representation of the original model Hamiltonian. Often, it is easy to perform calculations using these expressions. But one should always keep in mind that (1.158), (1.157) are meant as limits of the expressions (1.153), (1.154).

The problem is now to solve these integrals. We will do it first for the non-interacting system.

1.6 The non-interacting system

In a system without interaction one has

$$\hat{H} = \sum_i \varepsilon_i c_i^\dagger c_i \tag{1.159}$$

Therefore

$$S_M[\phi] = \varepsilon \sum_{k=1}^{M} \sum_i \phi_{i,k}^* \left(\frac{\phi_{i,k} - \phi_{i,k-1}}{\varepsilon} + (\varepsilon_i - \mu) \phi_{i,k-1} \right) \tag{1.160}$$

and the integral in (1.153) is a Gaussian integral. We obtain

$$\begin{aligned} Z &= \lim_{M\to\infty} \int D[\phi] \exp\left(-\varepsilon \sum_{k=1}^{M} \sum_i \phi_{i,k}^* \left(\frac{\phi_{i,k} - \phi_{i,k-1}}{\varepsilon} + (\varepsilon_i - \mu) \phi_{i,k-1} \right) \right) \\ &= \lim_{M\to\infty} \prod_i \int D[\phi_i] \exp\left(-\varepsilon \sum_{k=1}^{M} \phi_{i,k}^* \left(\frac{\phi_{i,k} - \phi_{i,k-1}}{\varepsilon} + (\varepsilon_i - \mu) \phi_{i,k-1} \right) \right) \\ &= \lim_{M\to\infty} \prod_i [\det S^{(i)}]^{-\zeta} \end{aligned} \tag{1.161}$$

where $S^{(i)}$ is the $M \times M$-matrix

$$S^{(i)} = \begin{pmatrix} 1 & 0 & & \cdots & 0 & -\zeta a \\ -a & 1 & 0 & & & 0 \\ 0 & -a & 1 & \ddots & & \vdots \\ & 0 & -a & \ddots & 0 & \\ \vdots & & 0 & \ddots & 1 & 0 \\ 0 & & & \cdots & -a & 1 \end{pmatrix} \tag{1.162}$$

with

$$a = 1 - \frac{\beta}{M}(\varepsilon_i - \mu) \tag{1.163}$$

The entry $-\zeta a$ in the upper right corner stems from the condition $\phi_{i,0} = \zeta \phi_{i,M}$. We expand the determinant and perform the limit $M \to \infty$. This yields

$$\begin{aligned} \lim_{M\to\infty} \det S^{(i)} &= \lim_{M\to\infty} [1 + (-1)^M \zeta (-a)^M] \\ &= \lim_{M\to\infty} \left[1 - \zeta \left(1 - \frac{\beta(\varepsilon_i - \mu)}{M} \right)^M \right] \\ &= 1 - \zeta \exp(-\beta(\varepsilon_i - \mu)) \end{aligned} \tag{1.164}$$

The partition function therefore is

$$Z = \prod_i [1 - \zeta \exp(-\beta(\varepsilon_i - \mu))]^{-\zeta} \tag{1.165}$$

This is the well known result for free fermions or bosons. We obtain the corresponding expressions for the occupation numbers as

$$\langle c_i^\dagger c_i \rangle = n_i = -\frac{1}{\beta} \frac{\partial \ln Z}{\partial \varepsilon_i} = \frac{1}{\exp(\beta(\varepsilon_i - \mu)) - \zeta} \tag{1.166}$$

and any further well known results for the free system can be obtained as well (see e.g. L.D. Landau, E.M. Lifschitz, Theoretical Physics, Volume V, Statistical Physics, Chapter V).

For later purposes it is interesting to take a closer look on the last result. We obtain the identity

$$\langle c_i^\dagger c_i \rangle = -\frac{1}{\beta} \frac{\partial \ln Z}{\partial \varepsilon_i} \tag{1.167}$$

by taking a derivative of the partition function $\mathrm{Tr} \exp(-\beta(\hat{H} - \mu \hat{N}))$, expressed by creation and annihilation operators. The derivative can as well be written as calculated from

$$Z = \lim_{M\to\infty} \int D[\phi] \exp\left(-\varepsilon \sum_{k=1}^{M} \sum_i \phi_{i,k}^* \left(\frac{\phi_{i,k} - \phi_{i,k-1}}{\varepsilon} + (\varepsilon_i - \mu)\phi_{i,k-1} \right) \right) \tag{1.168}$$

This yields

$$\frac{\partial Z}{\partial \varepsilon_i} = \lim_{M\to\infty} \int D[\phi] \left[-\varepsilon \sum_{k=1}^{M} \phi_{i,k}^* \phi_{i,k-1} \right] \exp\left(-\varepsilon \sum_{k=1}^{M} \sum_i \phi_{i,k}^* \left(\frac{\phi_{i,k} - \phi_{i,k-1}}{\varepsilon} + (\varepsilon_i - \mu)\phi_{i,k-1} \right) \right) \tag{1.169}$$

$$-\frac{1}{\beta} \frac{\partial \ln Z}{\partial \varepsilon_i} = \frac{1}{\beta} \int_0^\beta d\tau \langle \phi_i^*(\tau) \phi_i(\tau - 0^+) \rangle \tag{1.170}$$

Here, -0^+ in the argument of ϕ denotes that the argument of ϕ has to be infinitesimally smaller than that of ϕ^*. This will be important later. We shall see that the expectation value $\langle \phi_i^*(\tau) \phi_i(\tau') \rangle$ has a discontinuity at $\tau = \tau'$.

There is another important point to mention here: The expectation value of the particle number for fermions in a coherent state is $\phi_i^* \phi_i$, which is no real number. Nevertheless, we can calculate it using the above expression and coherent states.

Later, we need expectation values of the form

$$\langle \phi_i^*(\tau) \phi_j(\tau') \rangle \tag{1.171}$$

and other expressions containing several fields as well. To calculate such an expression, we define a generating function for them:

$$Z_M(J^*, J) = \int D[\phi] \exp\left(-\varepsilon \sum_{k=1}^{M} \sum_i \phi_{i,k}^* \left(\frac{\phi_{i,k} - \phi_{i,k-1}}{\varepsilon} + (\varepsilon_i - \mu)\phi_{i,k-1} \right) + \sum_{k=1}^{M} \sum_i (J_{i,k}^* \phi_{i,k} + J_{i,k} \phi_{i,k}^*) \right) \tag{1.172}$$

Using the generating function one gets

$$\langle \phi^*_{i,k}\phi_{j,l}\rangle = \frac{1}{Z_M}\frac{\partial^2 Z_M(J^*,J)}{\partial J^*_{j,l}\partial J_{i,k}}\bigg|_{J=J^*=0} \tag{1.173}$$

and in the limit $M\to\infty$

$$\langle \phi^*_i(\tau)\phi_j(\tau')\rangle = \frac{1}{Z}\frac{\delta^2 Z(J^*,J)}{\delta J^*_j(\tau')\delta J_i(\tau)}\bigg|_{J=J^*=0} = \frac{\delta^2 \ln Z(J^*,J)}{\delta J^*_j(\tau')\delta J_i(\tau)}\bigg|_{J=J^*=0} \tag{1.174}$$

$$Z(J^*,J) = \lim_{M\to\infty} Z_M(J^*,J) \tag{1.175}$$

It is clear that the generating function can as well be used if one wants to calculate expectation values of expressions containing more than two fields.

For the free system, it is not difficult to calculate $Z_M(J^*,J)$. It is a simple Gaussian integral. First of all we have for the free system

$$Z(J^*,J) = \prod_i Z^{(i)}(J^*_i,J_i) \tag{1.176}$$

where

$$Z^{(i)}(J^*_i,J_i) = \lim_{M\to\infty}\int D[\phi]\exp\left(-\varepsilon\sum_{k=1}^{M}\phi^*_{i,k}\left(\frac{\phi_{i,k}-\phi_{i,k-1}}{\varepsilon}+(\varepsilon_i-\mu)\phi_{i,k-1}\right)+\sum_{k=1}^{M}(J^*_{i,k}\phi_{i,k}+J_{i,k}\phi^*_{i,k})\right) \tag{1.177}$$

This integral is of the form

$$\int D[\phi]\exp\left(-\sum_{k,l=1}^{M}\phi^*_{i,k}S^{(i)}_{k,l}\phi_{i,l}+\sum_{k=1}^{M}(J^*_{i,k}\phi_{i,k}+J_{i,k}\phi^*_{i,k})\right) \tag{1.178}$$

and yields

$$[\det S^{(i)}]^{-\zeta}\exp(\sum_{k,l=1}^{M}J^*_{i,k}(S^{(i)-1})_{k,l}J_{i,l}) \tag{1.179}$$

Therefore we obtain

$$Z_M(J^*,J) = Z_M\prod_i\exp(\sum_{k,l=1}^{M}J^*_{i,k}(S^{(i)-1})_{k,l}J_{i,l}) \tag{1.180}$$

and furthermore

$$\begin{aligned}\langle \phi^*_{i,k}\phi_{j,l}\rangle &= \frac{1}{Z_M}\frac{\partial^2 Z_M(J^*,J)}{\partial J^*_{j,l}\partial J_{i,k}}\bigg|_{J=J^*=0}\\ &= \delta_{i,j}(S^{(i)-1})_{l,k}\end{aligned} \tag{1.181}$$

The inverse is

$$S^{(i)-1} = \frac{1}{1-\zeta a^M}\begin{pmatrix} 1 & \zeta a^{M-1} & \zeta a^{M-2} & \cdots & & \zeta a\\ a & 1 & \zeta a^{M-1} & & & \zeta a^2\\ a^2 & a & 1 & & & \zeta a^3\\ \vdots & a^2 & a & & & \vdots\\ & \vdots & a^2 & \ddots & & \\ a^{M-3} & & \vdots & \ddots & & \zeta a^{M-2}\\ a^{M-2} & a^{M-3} & & & 1 & \zeta a^{M-1}\\ a^{M-1} & a^{M-2} & a^{M-3} & \cdots & a & 1\end{pmatrix} \tag{1.182}$$

where $a = 1 - \frac{\beta}{M}(\varepsilon_i - \mu)$. Therefore we obtain

$$\langle \phi^*_{i,k} \phi_{j,l} \rangle = \delta_{i,j} \frac{a^{l-k}}{1 - \zeta a^M} \tag{1.183}$$

for $l \geq k$ and

$$\langle \phi^*_{i,k} \phi_{j,l} \rangle = \delta_{i,j} \frac{a^{M+l-k}}{1 - \zeta a^M} \tag{1.184}$$

for $l < k$. Let $l = \tau M/\beta$, $k = \tau' M/\beta$ and use as before that in the limit $M \to \infty$ $(1 - x/M)^M \to \exp(-x)$. The we obtain in that limit

$$\langle \phi^*_i(\tau) \phi_j(\tau') \rangle = \delta_{i,j} \exp(-(\varepsilon_i - \mu)(\tau - \tau'))(\theta(\tau' - \tau) + \zeta n_i) \tag{1.185}$$

The above expression

$$n_i = \frac{1}{\beta} \int_0^\beta d\tau \langle \phi^*_i(\tau) \phi_i(\tau - 0^+) \rangle \tag{1.186}$$

can be calculated as before. The expression

$$g_i(\tau - \tau') = \exp(-(\varepsilon_i - \mu)(\tau - \tau'))(\theta(\tau' - \tau) + \zeta n_i) \tag{1.187}$$

is called the single particle propagator.

Expectation values with more than two fields can be calculated similarly. We need such expressions below. An expression of the form

$$\langle \phi^*_{i_1}(\tau_1) \phi^*_{i_2}(\tau_2) \dots \phi^*_{i_n}(\tau_n) \phi_{j_n}(\tau'_n) \phi_{j_{n-1}}(\tau'_{n-1}) \dots \phi_{j_1}(\tau'_1) \rangle \tag{1.188}$$

can be calculated using the derivative

$$\left. \frac{\delta^{2n} \ln Z(J^*, J)}{\delta J^*_{i_1}(\tau_1) \dots \delta J^*_{i_n}(\tau_n) \delta J_{j_n}(\tau'_n) \dots \delta J_{j_1}(\tau'_1)} \right|_{J = J^* = 0} \tag{1.189}$$

As before, the calculation is done for finite M and at the end we perform the limit $M \to \infty$. Taking first the derivatives with respect to all $J_{j,l}(\tau')$, we get for each derivative a factor $\sum_k J^*_{j,k} (S^{(j)-1})_{k,l}$. The derivatives with respect to $J^*_{i,k}$ act on these factors, since all other contributions vanish at the end when we let $J = J^* = 0$. This means that in all these expression we may connect always a variable $J_{j,l}$ with a variable $J^*_{i,k}$ and replace them by a contribution $\delta_{i,j}(S^{(i)-1})_{k,l}$. This holds as well for the variables $\phi^*_{i,k}$ and $\phi_{j,l}$. Therefore, we obtain

$$\begin{aligned} &\langle \phi^*_{i_1}(\tau_1) \phi^*_{i_2}(\tau_2) \dots \phi^*_{i_n}(\tau_n) \phi_{j_n}(\tau'_n) \phi_{j_{n-1}}(\tau'_{n-1}) \dots \phi_{j_1}(\tau'_1) \rangle \\ &\qquad = \sum_P \zeta^P \prod_k \langle \phi^*_{i_k}(\tau_k) \phi_{j_{P(k)}}(\tau'_{P(k)}) \rangle \end{aligned} \tag{1.190}$$

This result is often called Wick's Theorem. In the present calculation, it is a direct consequence of the fact that $Z(J^*, J)$ is a Gaussian integral.

1.7 Perturbation Theory

The results for the non-interacting system can be used to obtain structured perturbative expressions for the interacting system. We first discuss the perturbation expansion for the partition function. Perturbative expressions

for correlation functions can be obtained in a similar way. The partition function of the interacting system can be written as

$$\begin{aligned} Z &= \lim_{M\to\infty} \int D[\phi] \exp\left(-\varepsilon \sum_{k=1}^{M} \phi_{i,k}^* \left(\frac{\phi_{i,k} - \phi_{i,k-1}}{\varepsilon} + (\varepsilon_i - \mu)\phi_{i,k-1} \right) - \varepsilon \sum_{k=1}^{M} V(\{\phi_{i,k}^*, \phi_{i,k-1}\}) \right) \\ &= \lim_{M\to\infty} Z_{0,M} \left\langle \exp\left(-\varepsilon \sum_{k=1}^{M} V(\{\phi_{i,k}^*, \phi_{i,k-1}\}) \right) \right\rangle_{0,M} \\ &= Z_0 \left\langle \exp\left(-\int_0^\beta d\tau V(\{\phi_i^*(\tau), \phi_i(\tau - 0^+)\}) \right) \right\rangle_0 \end{aligned} \tag{1.191}$$

where the index 0 at Z_0 and $\langle . \rangle_0$ denotes the non-interacting system. $V(\{\phi_i^*(\tau), \phi_i(\tau - 0^+)\})$ is a general interaction. A meaningful physical ansatz for the interaction is the Coulomb interaction or similar two-particle interactions. The exponential function in the last term can be written as a series; this yields the perturbation expansion:

$$\begin{aligned} \left\langle \exp\left(-\int_0^\beta d\tau V(\{\phi_i^*(\tau), \phi_i(\tau - 0^+)\}) \right) \right\rangle_0 &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n \\ &\left\langle V(\{\phi_i^*(\tau_1), \phi_i(\tau_1 - 0^+)\}) \ldots V(\{\phi_i^*(\tau_n), \phi_i(\tau_n - 0^+)\}) \right\rangle_0 \end{aligned} \tag{1.192}$$

For a concrete form of the interaction the right hand side becomes a sum of expectation values for products of variables, which can be calculated using Wick's Theorem.

In principle, the perturbation expansion can be calculated for any many-body interaction. In the following, we restrict ourselves to two-particle interactions, which have the general form

$$V(\{\phi_i^*(\tau), \phi_i(\tau - 0^+)\}) = \frac{1}{2} \sum_{i,j,k,l} V_{i,j,k,l} \phi_i^*(\tau) \phi_j^*(\tau) \phi_l(\tau - 0^+) \phi_k(\tau - 0^+) \tag{1.193}$$

I assume that $V_{i,j,k,l}$ is either symmetric (for bosons) or antisymmetric (for fermions) in the first two and in the last two indices. The n-th term in the expansion is then of the form

$$\begin{aligned} \frac{(-1)^n}{2^n n!} \sum_{i_1 j_1 k_1 l_1} \cdots \sum_{i_n j_n k_n l_n} \prod_m V_{i_m j_m k_m l_m} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n \left\langle \phi_{i_1}^*(\tau_1) \phi_{j_1}^*(\tau_1 - 0^+) \phi_{l_1}(\tau_1) \phi_{k_1}(\tau_1 - 0^+) \ldots \right. \\ \left. \phi_{i_n}^*(\tau_n) \phi_{j_n}^*(\tau_n) \phi_{l_n}(\tau_n - 0^+) \phi_{k_n}(\tau_n - 0^+) \right\rangle \end{aligned} \tag{1.194}$$

The expectation value can be written as a sum of products of the form $\langle \phi^* \phi \rangle$. Exactly one ϕ^* and one ϕ belong to a pair. The expectation value of the pair is called a contraction. The sum runs over all possible combinations of contractions. Each contraction $\langle \phi_i^*(\tau) \phi_j(\tau') \rangle$ yields a factor $\delta_{i,j} g_i(\tau - \tau')$. The total sum can be represented in a graphical form. This representation goes back to Feynman, the diagrams are called Feynman diagrams. There are various ways to introduce Feynman diagrams. We choose one to show the main principles, for others we refer to the text books.

A matrix element $V_{i,j,k,l}$ is represented as a point with four lines, two incoming and two outgoing lines. Each line gets an index i, j, k, or l. The lines belonging to i and j belong to creation operators, these are the outgoing lines. The incoming lines have indices k or l, they belong to annihilation operators. A term of n-th order contains n such points. The lines of these points are now connected in such a way, that each outgoing line meets an incoming line. Each point gets an index τ. Each line now corresponds to a factor $\langle \phi_i^*(\tau) \phi_i(\tau') \rangle = g_i(\tau - \tau')$, where τ and τ' belong to the indices of the two points connected by that line. The line has one index i, the original two indices of the incoming and outgoing lines are identical due to the factor δ_{ij} in the expectation value above. Now, an important point is that different combinations of contractions can belong to the same diagram. These combinations of contractions differ only in the order of the indices τ at the vertices. But, in the above expression, we perform the integral over all τ. Therefore all the combinations of

contractions belonging to the same diagram yield the same contribution. The number of different combinations is called the symmetry factor of the diagram. The rules for the diagrams and their contributions to the sum are thus:

1. Draw all diagrams with m points and lines between them so that each line is oriented from one point to another. A point can be connected with itself. At each point, we must have two incoming and two outgoing lines. Two diagrams are different if they cannot be obtained from each other by permuting the points. Mathematically, these diagrams are directed graphs.

2. Calculate the symmetry factor S of the diagram. To do that, each point gets an index τ. S is the number of permutations of the indices which map the diagram to itself.

3. Each line gets an index i. For each line write down a factor $g_i(\tau - \tau')$, where τ is the index of the end point of the line and τ' is the index of the starting point.

4. For each point write done a factor $V_{i,j,k,l}$ where i and j are the indices of the outgoing and k and l are the indices of the incoming lines.

5. Sum over all indices of all lines and integrate over all indices τ of the vertices from 0 to β.

6. Multiply the result with a factor.
$$\frac{(-1)^m \zeta^{n_L}}{2^{n_e} S} \tag{1.195}$$
Here, S is the symmetry factor. n_e is the number of equivalent lines. Two lines are equivalent, if they have the same starting point and the same end point. n_L is the number of loops in the diagram.

7. Adding up all these contributions yields the m-th order of Z/Z_0.

It is instructive to calculate several examples using these rules. Doing that, one notices that many calculations are easier if one calculates $\ln(Z/Z_0)$. The perturbation series for this expression contains only connected diagrams. This fact is often called *Linked Cluster Theorem.* There are several possibilities to prove it. The direct proof is to show that exp(sum of all connected diagrams) yields the sum of all diagrams, thus Z/Z_0.

1.8 Frequency and momentum representation

In most cases it is possible to calculate the above at least partially in frequency and momentum space. If the system is translationally invariant, the single particle Hamiltonian is diagonal in momentum space and the eigenfunctions are plane waves $V^{-1/2}\exp(ikx)$. Here V is the volume of the system. For simplicity we will use periodic boundary conditions. The single particle energies are denoted as ε_k. In a system where the single particle Hamiltonian contains only the kinetic energy, one has $\varepsilon_k = k^2/(2m)$. In a solid, we can start with a lattice model, in that case ε_k is given by the dispersion relation of the lattice.

For the interaction, one has due to momentum conservation

$$V_{k_1 k_2 k_3 k_4} \propto V^{-1} \delta_{k_1+k_2, k_3+k_4} \tag{1.196}$$

The functions ϕ and ϕ^* are either periodic (bosons) or anti-periodic (fermions) functions of τ. Therefore we may write

$$g_k(\tau - \tau') = \frac{1}{\beta} \sum_{\omega_n} \exp(-i\omega_n(\tau - \tau'))\tilde{g}_k(\omega_n) \tag{1.197}$$

where

$$\begin{aligned} \tilde{g}_k(\omega_n) &= \int_0^\beta d\tau \exp((i\omega_n - (\varepsilon_k - \mu))\tau)[\theta(\tau)(1+\zeta n_k) + \zeta\theta(-\tau) n_k] \\ &= \frac{1}{(\varepsilon_k - \mu) - i\omega_n} \end{aligned} \tag{1.198}$$

For bosons one has $\omega_n = \frac{2\pi n}{\beta}$, for fermions $\omega_n = \frac{(2n+1)\pi}{\beta}$. They obey $\exp(i\beta\omega_n) = \zeta$. Due to the (anti-) periodicity, each vertex contains a factor $\delta_{\omega_{n_1}+\omega_{n_2},\omega_{n_3}+\omega_{n_4}}$, where ω_{n_1} and ω_{n_2} belong to the two ϕ^* and ω_{n_3} and ω_{n_4} belong to the two ϕ. The rules above may now be rewritten. One obtains:

1. as above.
2. as above.
3. To each line associate an index k. Momentum conservation at each vertex restricts the possible values. In a diagram with m vertices, we can choose $m+1$ values k for the lines independently, the others are fixed due to momentum conservation. To each line we associate a frequency. Here as well, in diagrams with m vertices we may choose $m+1$ values for ω, the rest is fixed due to the factors $\delta_{\omega_{n_1}+\omega_{n_2},\omega_{n_3}+\omega_{n_4}}$ for each vertex. Each line yields a factor $\tilde{g}_k(\omega_n)$. For lines which connect one vertex with itself, we need an additional factor $\exp(i\omega_n\eta)$. At the end, we take the limit $\eta \to 0^+$.
4. For each vertex, we add a factor $V_{k_1k_2k_3k_4}$. Since momentum conservation has already been taken into account, the factor $\delta_{k_1+k_2,k_3+k_4}$ can be dropped.
5. Take the sum over all k (or $V(2\pi)^{-d}\int d^dk$) and the sum over all ω_n.
6. Multiply the result with an additional factor β^{-m}, where m is the number of vertices.

Since each vertex contains a factor $1/V$ and each sum over k yields a factor V, the final result contains a factor V^{n_c}, where n_c the number of connected components of the diagram. Due to the Linked Cluster Theorem, $\ln(Z/Z_0)$ is the sum of all connected diagrams and therefore $\propto V$. It is an extensive quantity as it should be since the logarithm of the grand canonical partition function is up to a factor $-1/\beta$ the grand canonical potential.

1.9 Calculating Greens Functions

Greens functions can be calculated using a generating function. This is similar to the non-interacting system. The generating function can be defined in a similar way. It is

$$\begin{aligned} G(J^*,J) &= \frac{1}{Z}\int D[\phi]\exp\left(-\int_0^\beta d\tau\left[\sum_i \phi_i^*(\tau)(\frac{\partial}{\partial\tau}-\mu)\phi_i(\tau-0^+)+H(\{\phi_i^*(\tau),\phi_i(\tau-0^+)\})\right]\right) \\ &\quad\times\exp\left(-\int_0^\beta d\tau\sum_i[J_i^*(\tau)\phi_i(\tau-0^+)+\phi_i^*(\tau)J_i(\tau-0^+)]\right) \\ &= \left\langle\exp\left(-\int_0^\beta d\tau\sum_i[J_i^*(\tau)\phi_i(\tau-0^+)+\phi_i^*(\tau)J_i(\tau-0^+)]\right)\right\rangle \end{aligned} \tag{1.199}$$

Here $\langle A\rangle$ is the expectation value of A in the interacting system. The Greens functions are derivatives of $G(J^*,J)$. The calculation can be done again using perturbation theory.

Single particle propagators

Let us now calculate expressions like

$$\langle\phi_i^*(\tau)\phi_j(\tau')\rangle \tag{1.200}$$

The corresponding perturbational series contains diagrams with two outer lines, one incoming and one outgoing corresponding to the two $\phi^{(*)}$ in the propagator. Since this expression contains a division by Z, only connected diagrams occur. The rules are similar to the ones above:

1. Draw all different connected diagrams with 2 outer lines and m vertices. One outer line corresponds to ϕ^*, it ends at a vertex. The other one corresponds to ϕ and starts at a vertex. Two diagrams are different if they cannot be mapped onto each other by a permutation of inner lines and vertices. For each diagram we do the following calculations:
2. Each vertex gets an inner index τ_k. Each line gets an index l. For each inner line we write a factor $g_l(\tau_k - \tau_k')$, if it runs from τ_k to τ_k'. The incoming line yields a factor $g_i(\tau - \tau_k)$, the outgoing line yields a factor $g_j(\tau_k - \tau')$, where τ_k is the corresponding inner vertex. For $m = 0$ one has only a factor $g_j(\tau - \tau')$.
3. For each vertex write down a factor $V_{l_1 l_2 l_3 l_4}$ where l_1 and l_2 are indices of the outgoing, l_3 and l_4 are indices of the incoming lines.
4. Now take the sum over all l, the integral over all τ_i.
5. Multiply the result with a factor $(-1)^m \zeta^{n_L}$ where n_L is the number of loops.

Since the outer lines are fixed, there is no symmetry factor S.

Generating function for connected Greens functions

Next, one may want to calculate higher order Greens functions like

$$\langle \phi_{i_1}^*(\tau_1)\phi_{i_2}^*(\tau_2)\phi_{j_2}(\tau_2')\phi_{j_1}(\tau_1')\rangle \tag{1.201}$$

In 0-th order Wick's Theorem yields

$$\begin{aligned}\langle \phi_{i_1}^*(\tau_1)\phi_{i_2}^*(\tau_2)\phi_{j_2}(\tau_2')\phi_{j_1}(\tau_1')\rangle_0 &= \langle \phi_{i_1}^*(\tau_1)\phi_{j_1}(\tau_1')\rangle_0 \langle \phi_{i_2}^*(\tau_2)\phi_{j_2}(\tau_2')\rangle_0 \\ &- \langle \phi_{i_1}^*(\tau_1)\phi_{j_2}(\tau_2')\rangle_0 \langle \phi_{i_2}^*(\tau_2)\phi_{j_1}(\tau_1')\rangle_0 \end{aligned} \tag{1.202}$$

The perturbative expansion contains contributions where the interaction occurs only in one of the factors $\langle \phi^*\phi\rangle$. Clearly, there are also terms where the interaction is between two factors. This can easily be seen if one draws the corresponding diagrams. One finally obtains

$$\begin{aligned}\langle \phi_{i_1}^*(\tau_1)\phi_{i_2}^*(\tau_2)\phi_{j_2}(\tau_2')\phi_{j_1}(\tau_1')\rangle &= \langle \phi_{i_1}^*(\tau_1)\phi_{j_1}(\tau_1')\rangle \langle \phi_{i_2}^*(\tau_2)\phi_{j_2}(\tau_2')\rangle \\ &- \langle \phi_{i_1}^*(\tau_1)\phi_{j_2}(\tau_2')\rangle \langle \phi_{i_2}^*(\tau_2)\phi_{j_1}(\tau_1')\rangle \\ &+ \langle \phi_{i_1}^*(\tau_1)\phi_{i_2}^*(\tau_2)\phi_{j_2}(\tau_2')\phi_{j_1}(\tau_1')\rangle_c \end{aligned} \tag{1.203}$$

Here, the contribution $\langle \phi_{i_1}^*(\tau_1)\phi_{i_2}^*(\tau_2)\phi_{j_2}(\tau_2')\phi_{j_1}(\tau_1')\rangle_c$ is the sum of all connected diagrams. The other contributions have already been calculated.

Similarly, all higher Greens functions with more than 4 fields can be decomposed into a connected part and unconnected parts that are in turn composed of lower ordered connected diagrams. It is therefore suitable to calculate a generating function for the connected parts only. Similarly to the series for $\ln(Z/Z_0)$ which contains only connected diagrams, we can show that

$$W(J^*, J) = \ln G(J^*, J) \tag{1.204}$$

contains only connected diagrams. An easy way (but not rigorous) to show that is the replica trick. Here, one first looks at the diagrams contributing to $G(J^*,J)^n$ for natural numbers n. To do that, one introduces n copies ϕ_α and ϕ_α^* of the original fields ϕ and ϕ^*. A connected component contains only fields with the same index α since there is no interaction of fields with different indices α. Therefore, each diagram contains simply a factor n^{n_C}, where n_c is the number of connected components of that diagram. Let us now perform the continuation to real n and calculate

$$W(J^*, J) = \lim_{n\to 0} \frac{\partial}{\partial n} G(J^*, J)^n \tag{1.205}$$

Because of the limit $n \to 0$ all contributions vanish where the power of n is larger than 1. Therefore $W(J^*,J)$ contains only diagrams with $n_C = 1$, i.e. only connected diagrams.

Effective potential, effective action...

There are several generating functions similar to $W(J^*,J)$ which contain essentially the same information and are better for one or another reason. I will only mention two of them, the construction of others is similar.

In $W(J^*,J)$ the arguments J^* and J play the role of sources. They can be compared to the role of the magnetic field as an external source in the case of a spin system. The free energy depends on the external source. It is defined as

$$F(h) = -\frac{1}{\beta}\mathrm{Tr}\exp(-\beta H(\{S_i\}) - h\cdot\sum_i S_i) \tag{1.206}$$

The magnetisation is given by

$$M = -\frac{\partial F(h)}{\partial h} \tag{1.207}$$

In statistical physics, one often uses instead of $F(h)$ the Legendre transform

$$G(M) = \inf_h(F(h) + Mh) \tag{1.208}$$

Often, one calculates G from $M(h)$ by inversion $h(M)$ and $G(M) = F(h(M)) + Mh(M)$. From $G(M)$ one gets $F(h)$ back by a similar Legendre transform from M to h. Both contain the same information. The advantage of $G(M)$ compared to $F(h)$ is the better analytical behaviour. In the case of a ferromagnetic phase transition for instance, $M(h)$ jumps as a function of h at $h = 0$. $F(h)$ has no first derivative at $h = 0$. In contrast, $G(M)$ is a smooth function of M, for the ferromagnet it is simply a double well potential.

Similarly, we can calculate the Legendre transform of $W(J^*,J)$. For finite values of J, J^* the expectation values

$$\varphi_j(\tau) = \langle\phi_j(\tau)\rangle_{J,J^*}, \quad \varphi_j^*(\tau) = \langle\phi_j^*(\tau)\rangle_{J,J^*} \tag{1.209}$$

are finite. The Legendre transform is

$$\Gamma(\varphi^*,\varphi) = -W(J^*,J) - \sum_j \int d\tau[\varphi_j^*(\tau)J_j(\tau) + J_j^*(\tau)\varphi_j(\tau)] \tag{1.210}$$

where on the right hand side J and J^* are functions of φ and φ^*. This quantity is often called the effective potential.

A second function, which is useful as well, is the effective action. It is defined as

$$G_{\mathrm{eff}}(\psi^*,\psi) = \ln\left\langle \exp(-\int d\tau V[\phi^*(\tau) + \psi^*(\tau), \phi(\tau - 0^+) + \psi(\tau - 0^+)])\right\rangle_0 \tag{1.211}$$

It plays an important role in renormalisation theory of interacting Fermi systems.

2 Fermi Liquids

The theory of Fermi liquids goes back to Landau. This theory was developed without any connection to the field theoretic methods. Instead, it uses the concept of quasi particles. This concept has been proven to be useful in many different areas of many-particle physics.

In this chapter we first introduce the concept of Fermi liquid theory and derive several physical properties of Fermi liquids. Then we use the methods from the last chapter to show, how Fermi liquid theory can be derived from a microscopic model. Furthermore, we shall see, which instabilities may lead to a breakdown of the Fermi liquid.

The book of Pines and Nozières [59] is an excellent introduction to the theory of Fermi liquids.

2.1 Quasi Particles

Starting point is a gas of non-interacting spin-$\frac{1}{2}$ fermions with N particles in the volume V. The kinetic energy of a particle is $\frac{\vec{k}^2}{2m}$. Due to Pauli's principle, there are only two fermions in a single particle state described by a wave vector $\vec{k}$. The states are filled starting from $\vec{k}=0$. The system is isotropic, the states are filled if $|\vec{k}|<k_F$. Here, k_F is the Fermi wave vector, given implicitly by

$$N=\sum_{|\vec{k}|<k_F} 2 \tag{2.1}$$

The total energy is

$$E=\sum_{\vec{k},\sigma}\frac{\vec{k}^2}{2m}n(\vec{k},\sigma) \tag{2.2}$$

where

$$n(\vec{k},\sigma)=\theta(k_F-|\vec{k}|) \tag{2.3}$$

Let us now assume that we perturb the system a little bit. If the perturbation is small, it leads to a small variation of the occupation numbers $\delta n(\vec{k})$ and therefore to a small change in energy

$$\delta E=\sum_{\vec{k},\sigma}\frac{\vec{k}^2}{2m}\delta n(\vec{k},\sigma) \tag{2.4}$$

If $|\vec{k}|$ is far from k_F, the cost in energy is large. Therefore we may assume that $\delta n(\vec{k})$ is small or vanishes for $|\vec{k}|$ far away from k_F.

Now the interaction is turned on. A Fermi liquid is a Fermi system in which the low lying excitations are similar and evolve from the low lying excitations of the free system adiabatically if the interaction is turned on adiabatically. It may happen, that this concept even fails for arbitrarily small interactions. This happens for instance, if the interaction is attractive, in which case the system becomes superconducting and the ground state is a BCS-state or something similar. Although Fermi liquid theory leads to some stability criteria, it is not possible to derive such an instability from the theory itself. This can be done only via a microscopic derivation of the theory. In the following we assume, that such an instability does not occur.

Typical excitations in a non-interacting Fermi system are particle-, hole-, or particle-hole excitations. Following the general idea of a Fermi liquid, we assume that in the interacting system, the elementary excitations can be described as in the non-interacting case. They can be described by changes $\delta n(\vec{k},\sigma)$ of the occupation numbers. This leads to the concept of quasi particles. It is clear that the interaction yields an interaction

between the quasi particles as well and that therefore these quasi particles have a finite life time. We assume that close to the Fermi surface the life time is long enough so that the concept of the quasi particle is applicable.

Following this reasoning, originally Landau's, we therefore make the ansatz

$$\delta E = \sum_{\vec{k},\sigma} \varepsilon^0_{\vec{k}} \delta n(\vec{k},\sigma) + \frac{1}{2V} \sum_{\vec{k},\vec{k}',\sigma,\sigma'} f(\vec{k},\sigma,\vec{k}',\sigma') \delta n(\vec{k},\sigma) \delta n(\vec{k}',\sigma') + \mathcal{O}((\delta n)^3) \tag{2.5}$$

for a small change in energy. The higher order terms will be neglected in the following. We assume that there is no external magnetic field so that the energies $\varepsilon^0_{\vec{k}}$ do not depend on the spin. The interaction shall be symmetric with respect to spin, so that it depends only on $\sigma \cdot \sigma'$. Let us now consider elementary excitations which do not depend on σ. The energy of an elementary excitation is

$$\varepsilon(\vec{k}) = \frac{\delta E}{\delta n(\vec{k})} = \varepsilon^0_{\vec{k}} + \frac{1}{V} \sum_{\vec{k}',\sigma'} f(\vec{k},\sigma,\vec{k}',\sigma') \delta n(\vec{k}'). \tag{2.6}$$

$\sum_{\sigma'} f(\vec{k},\sigma,\vec{k}',\sigma')$ does not depend on σ. Since the quasiparticles evolve adiabatically from the original particles, the quasiparticle energy has a step for $|\vec{k}| = k_F$. For finite temperatures one has

$$n(\vec{k}) = \frac{1}{\exp(\beta(\varepsilon(\vec{k}) - \mu)) + 1} \tag{2.7}$$

This equation is a self consistency equation for $n(\vec{k})$, since $\varepsilon(\vec{k})$ depends on $n(\vec{k})$.

Since the interaction depends on $\sigma \cdot \sigma'$ it can be written as

$$f(\vec{k},\sigma,\vec{k}',\sigma') = f(\vec{k},\vec{k}') + 4\sigma\sigma'\phi(\vec{k},\vec{k}') \tag{2.8}$$

or

$$f(\vec{k},\sigma,\vec{k}',\sigma') = f_o(\vec{k},\vec{k}') + \delta_{\sigma,\sigma'} f_e(\vec{k},\vec{k}') \tag{2.9}$$

where

$$f_o = f - \phi \tag{2.10}$$

$$f_e = 2\phi \tag{2.11}$$

We use the standard notation where the general interaction coefficient, the spin-symmetric part and further below also the projection of both to the Fermi surface are denoted by f. They can be discriminated by the different arguments. σ and σ' assume the values $\pm\frac{1}{2}$. In most cases it is sufficient to know the interaction for values $\vec{k}$ and $\vec{k}'$ close to the Fermi surface. In the isotropic case, we may assume that the interaction depends only on the angle θ between $\vec{k}$ and $\vec{k}'$. Then we have

$$\begin{aligned} f(\vec{k},\sigma,\vec{k}',\sigma')\Big|_{|\vec{k}|=|\vec{k}'|=k_F} &= f(\theta,\sigma,\sigma') \\ &= f(\theta) + 4\sigma\sigma'\phi(\theta) \\ &= \sum_{L=0}^{\infty} (f_L + 4\sigma\sigma'\phi_L) P_L(\cos\theta) \end{aligned} \tag{2.12}$$

The orthogonality of the Legendre polynomials

$$\frac{2L+1}{2} \int_{-1}^{1} P_L(\cos\theta) P_{L'}(\cos\theta) d(\cos\theta) = \delta_{L,L'} \tag{2.13}$$

yields

$$\left\{ \begin{array}{c} f_L \\ \phi_L \end{array} \right\} = \frac{2L+1}{4\pi} \int d\Omega P_L(\cos\theta) \left\{ \begin{array}{c} f(\vec{k},\vec{k}') \\ \phi(\vec{k},\vec{k}') \end{array} \right\} \Bigg|_{|\vec{k}|=|\vec{k}'|=k_F} \tag{2.14}$$

In many cases it is sufficient to know the coefficients f_L and ϕ_L for small values of L. It is then possible to reduce the theory to a theory with very few parameters. In contrast, in metals, one has a lattice and isotropy breaks down. In that case one needs to know $f(\vec{k},\vec{k}')$ and $\phi(\vec{k},\vec{k}')$ on the Fermi surface. The theory then becomes more complicated.

2.2 Equilibrium Properties of the normal Fermi Liquid

A fundamental parameter of the theory is the effective mass, defined as usual

$$\frac{k_F}{m^*} \equiv \left|\nabla_{\vec{k}} \varepsilon^0_{\vec{k}}\right|_{|\vec{k}|=k_F} = v_F \tag{2.15}$$

Close to the Fermi surface we have

$$\varepsilon^0_k = \mu + (k - k_F)\frac{k_F}{m^*} \tag{2.16}$$

Experimentally the effective mass can be obtained through the specific heat.

Specific heat

Starting from

$$c_V = \frac{1}{V}\left.\frac{\partial E}{\partial T}\right|_V \tag{2.17}$$

we obtain for a small change in temperature

$$\begin{aligned} c_V &= \frac{1}{V}\sum_{\vec{k},\sigma} \frac{\delta E}{\delta n(\vec{k},\sigma)} \frac{\delta n(\vec{k},\sigma)}{\delta T} \\ &= \frac{1}{V}\sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} \frac{\delta n(\vec{k},\sigma)}{\delta T} \\ &= \frac{1}{V}\sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} \frac{\partial n(\vec{k},\sigma)}{\partial \varepsilon_{\vec{k}}} \left(-\frac{\varepsilon_{\vec{k}} - \mu}{T} + \frac{\partial(\varepsilon_{\vec{k}} - \mu)}{\partial T}\right) \end{aligned} \tag{2.18}$$

The term $\sum_{\vec{k}'} f(\vec{k},\vec{k}')\delta n(\vec{k})$ in $\varepsilon_{\vec{k}}$ is $O(T^2)$ and can be neglected. Therefore we may set $\varepsilon_{\vec{k}} = \varepsilon^0_{\vec{k}}$. As for the non-interacting Fermi system we obtain

$$c_V = \frac{1}{3} m^* k_F k_B^2 T \tag{2.19}$$

Typically m^* is larger than m. For liquid ^{3}He at normal pressure one has $m^* = 3m$. But there are as well so called heavy fermion systems, materials like $CeCu_2Si_2$, UPt_3, $CeAl_3$, where m^*/m is of the order 10^2 to 10^3.

Effective mass and interaction

The fact that the effective mass is not equal to m occurs due to the interaction. m^* must therefore depend on the interaction. There are various ways to derive this relationship. We shall use Galilean invariance. To do that, consider a system that moves with a small velocity $\delta\vec{v} = \delta\vec{k}/m$. The energy of the entire system of N_e particles due to this motion is $\delta E = (N_e m)(\delta\vec{v})^2/2$. This energy can be calculated as well using

$$\delta E = \sum_{\vec{k},\sigma} \varepsilon^0_{\vec{k}} \delta n(\vec{k},\sigma) + \frac{1}{2V}\sum_{\vec{k},\vec{k}',\sigma,\sigma'} f(\vec{k},\sigma,\vec{k}',\sigma')\delta n(\vec{k},\sigma)\delta n(\vec{k}',\sigma') \tag{2.20}$$

where $\delta n(\vec{k},\sigma) = n(\vec{k}+\delta\vec{k},\sigma) - n(\vec{k},\sigma)$. The first term yields

$$\begin{aligned} \sum_{\vec{k},\sigma} \varepsilon^0_{\vec{k}} \delta n(\vec{k},\sigma) &= \sum_{\vec{k},\sigma} \varepsilon^0_{\vec{k}} [n(\vec{k}+\delta\vec{k},\sigma) - n(\vec{k},\sigma)] \\ &= \sum_{\vec{k},\sigma} (\varepsilon^0_{\vec{k}-\delta\vec{k}} - \varepsilon^0_{\vec{k}}) n(\vec{k},\sigma) \\ &= \frac{\delta\vec{k}^2}{2m^*} \sum_{\vec{k},\sigma} n(\vec{k},\sigma) \\ &= N_e \frac{\delta k^2}{2m^*} \end{aligned} \tag{2.21}$$

and the second

$$\begin{aligned}
&\frac{1}{2V}\sum_{\vec{k},\vec{k}',\sigma,\sigma'} f(\vec{k},\sigma,\vec{k}',\sigma')\delta n(\vec{k},\sigma)\delta n(\vec{k}',\sigma') \\
&= \frac{1}{2V}\sum_{\vec{k},\vec{k}',\sigma,\sigma'} f(\vec{k},\sigma,\vec{k}',\sigma')[n(\vec{k}+\delta\vec{k},\sigma)-n(\vec{k},\sigma)][n(\vec{k}'+\delta\vec{k},\sigma')-n(\vec{k}',\sigma)] \\
&= \frac{1}{2V}\sum_{\vec{k},\vec{k}',\sigma,\sigma'} f(\vec{k},\sigma,\vec{k}',\sigma')(\delta\vec{k}\cdot\hat{k})(\delta\vec{k}\cdot\hat{k}')\delta(k-k_F)\delta(k'-k_F) \\
&= \frac{V}{2(2\pi)^6}4\int k^2 dk\, d\Omega \int k'^2 dk'\, d\Omega' f(\vec{k},\sigma,\vec{k}',\sigma')(\delta\vec{k}\cdot\hat{k})(\delta\vec{k}\cdot\hat{k}')\delta(k-k_F)\delta(k'-k_F) \\
&= \frac{V\delta k^2}{8\pi^4}k_F^4\int_{-1}^{1} d(\cos\theta)\int_{-1}^{1} d(\cos\theta') f(\theta-\theta')\cos\theta\cos\theta' \\
&= \frac{Vk_F^4}{8\pi^4}\delta k^2\frac{4}{9}f_1
\end{aligned} \tag{2.22}$$

Using the particle density $\rho = (2\pi)^{-3}\sum_\sigma \int d^3k\,\theta(k_F-k) = k_F^3/(3\pi^2)$, we obtain

$$\frac{k_F}{3\pi^2}N_e\frac{\delta k^2}{2}f_1 \tag{2.23}$$

Both expression must lead to the same δE so that

$$\frac{1}{m} = \frac{1}{m^*} + \frac{k_F}{3\pi^2}f_1 \tag{2.24}$$

Often one uses the notation

$$F_L = \rho_F f_L \tag{2.25}$$

$$Z_L = \rho_F \phi_L \tag{2.26}$$

where ρ_F is the density of states at the Fermi level. Using

$$\begin{aligned}
\rho_F &= \frac{1}{V}\sum_{\vec{k},\sigma}\delta(\varepsilon_{\vec{k}}^0-\mu) \\
&= \frac{2}{(2\pi)^3}4\pi\int k^2 dk\,\delta(\varepsilon_{\vec{k}}^0-\mu) \\
&= \frac{m^*k_F}{\pi^2}
\end{aligned} \tag{2.27}$$

we obtain

$$\frac{m^*}{m} = 1+\frac{F_1}{3} \tag{2.28}$$

Compressibility

Compressibility describes the change in pressure if the volume is changed. For a fixed particle number, we have

$$\frac{1}{\chi} = -V\frac{\partial P}{\partial V} = \rho\frac{\partial P}{\partial \rho} \tag{2.29}$$

Compressibility and sound velocity are related through

$$c^2 = \frac{1}{m\rho\chi} \tag{2.30}$$

It is natural to assume that the compressibility depends only on the isotropic average of $f(\vec{k}\sigma,\vec{k}'\sigma')$, i.e.on F_0.

Since the free energy is an extensive quantity, we may write

$$F(T,V,N) = Vf(T,\rho) \tag{2.31}$$

and therefore

$$P = -\frac{\partial F}{\partial V} = -f + \rho\frac{\partial f}{\partial \rho} \tag{2.32}$$

$$\frac{1}{\chi} = \rho^2\frac{\partial^2}{\partial\rho^2}f(T,\rho) \tag{2.33}$$

From

$$\mu = \frac{\partial F}{\partial N} = \frac{\partial f(T,\rho)}{\partial\rho} \tag{2.34}$$

we obtain

$$\frac{1}{\chi} = \rho^2\frac{\partial\mu}{\partial\rho} \tag{2.35}$$

The right hand side can be calculated using

$$\varepsilon(\vec{k}) = \frac{\delta E}{\delta n(\vec{k})} = \varepsilon^0_{\vec{k}} + \frac{1}{V}\sum_{\vec{k}',\sigma'} f(\vec{k},\sigma,\vec{k}',\sigma')\delta n(\vec{k}') \tag{2.36}$$

for values $k = k_F$, since $\mu = \varepsilon(k_F)$. For the compressibility, isotropic values of $\delta n(\vec{k}) = \delta n(k)$ are sufficient.

$$\frac{\partial\mu}{\partial\rho} = \frac{\partial\varepsilon^0_{k_F}}{\partial k_F}\frac{\partial k_F}{\partial\rho} + \sum_{\sigma'}\int\frac{d^3k'}{(2\pi)^3}f(k_F,\vec{k}')\frac{\partial n(k')}{\partial k_F}\frac{\partial k_F}{\partial\rho} \tag{2.37}$$

Using $\rho = k_F^3/(3\pi^2)$ and $\rho\frac{\partial k_F}{\partial\rho} = \frac{k_F}{3}$, furthermore $\frac{\partial\varepsilon^0_{k_F}}{\partial k_F} = \frac{k_F}{m^*}$, $\frac{\partial n(k')}{\partial k_F} = \delta(k'-k_F)$ we obtain

$$\rho\frac{\partial\mu}{\partial\rho} = \frac{k_F^2}{3m^*} + \frac{k_F^2}{(2\pi)^3}\frac{k_F}{3}\sum_{\sigma'}\int d\Omega\, f(\theta,\sigma\sigma') = \frac{k_F^2}{3m^*}(1+F_0) \tag{2.38}$$

and finally

$$\frac{1}{\chi} = \frac{\rho k_F^2}{3m^*}(1+F_0) = \frac{\rho k_F^2}{m}\frac{1+F_0}{3+F_1} \tag{2.39}$$

This shows that χ depends on F_0 as expected and through the effective mass as well on F_1. The compressibility becomes infinite for $F_0 = -1$, the entire system becomes unstable. Therefore we need $F_0 > -1$. This is a special case for the stability criterion $F_L > -(2L+1)$, $Z_L > -(2L+1)$, which can be shown by other means.

Magnetic Susceptibility

Up to now we discussed only spin-independent perturbations. They are connected to the parameters F_L. Now, we discuss spin-dependent perturbations. The most simple case is that of a small magnetic field δH, which yields a small magnetisation δM. The magnetic susceptibility is given by $\chi_M = \frac{\partial M}{\partial H}$. The magnetisation is given by

$$\delta M = \rho(+\frac{1}{2}) - \rho(-\frac{1}{2}) = 2\sum_\sigma \sigma\rho(\sigma) \tag{2.40}$$

We calculate the magnetic susceptibility using the fact that the chemical potential does not depend on the spin σ. Nevertheless, we introduce $\mu(\sigma)$ to be the chemical potential for fermions with spin σ, then we have

$$\mu(\sigma) = \mu_0 - \sigma\delta H + 2\sum_{\sigma'}\frac{\partial\mu(\sigma)}{\partial\rho(\sigma')}\sigma'\delta M \tag{2.41}$$

where the second term is the energy shift due to the external magnetic field and the third term is the energy shift coming from the induced magnetic field. Because of $\mu(\frac{1}{2}) = \mu(-\frac{1}{2})$

$$\delta H = 4 \sum_{\sigma,\sigma'} \frac{\partial \mu}{\partial \rho(\sigma')} \sigma\sigma' \delta M \tag{2.42}$$

$$\frac{1}{\chi_M} = 4 \sum_{\sigma,\sigma'} \frac{\partial \mu}{\partial \rho(\sigma')} \sigma\sigma' \tag{2.43}$$

The calculation is similar to what we did above. We start with

$$\varepsilon(\vec{k},\sigma) = \varepsilon^0_{\vec{k},\sigma} - \sigma\delta h + \frac{1}{V} \sum_{\vec{k}',\sigma'} f(\vec{k},\sigma,\vec{k}',\sigma') \delta n(\vec{k}',\sigma') \tag{2.44}$$

For $k = k_F$, the left hand side must be μ. Therefore

$$\begin{aligned} \frac{\partial \mu}{\partial \rho(\sigma')} &= \frac{\partial k_F}{\partial \rho(\sigma')} \left[\frac{\partial \varepsilon^0_{k\sigma}}{\partial k_F} \delta_{\sigma,\sigma'} + \int \frac{d^3k'}{(2\pi)^3} f(k_F,\sigma,\vec{k}',\sigma') \frac{\partial n(\vec{k}',\sigma')}{\partial k_F} \right] \\ &= \frac{2\pi^2}{k_F^2} \left[\frac{k_F}{m^*} \delta_{\sigma,\sigma'} + \frac{k_F}{2m^*} (F_0 + 4\sigma\sigma' Z_0) \right] \end{aligned} \tag{2.45}$$

$$\frac{1}{\chi_M} = \frac{4\pi^2}{k_F m^*} + \frac{4\pi^2}{k_F m^*} Z_0 \tag{2.46}$$

$$\chi_M = \frac{k_F m^*}{4\pi^2 (1 + Z_0)} \tag{2.47}$$

Again we obtain a stability criterion, namely $Z_0 > -1$. For liquid ^{3}He typical values for Z_0 are between -0.67 for normal pressure and -0.76 at 27 atm. The system is close to a ferromagnetic instability.

Stability

We mentioned already that $F_L, Z_L > -2L - 1$ must hold for the Fermi liquid to be stable. Let us now show that. The Fermi liquid is stable if $E - \mu N$ assumes a minimum. We therefore calculate

$$\delta(E - \mu N) = \sum_{\vec{k},\sigma} (\varepsilon^0_{\vec{k}} - \mu) \delta n(\vec{k},\sigma) + \frac{1}{2V} \sum_{\vec{k},\sigma,\vec{k}',\sigma'} f(\vec{k},\sigma,\vec{k}',\sigma') \delta n(\vec{k},\sigma) \delta n(\vec{k}',\sigma') \tag{2.48}$$

for general $\delta n(\vec{k},\sigma)$. We assume isotropy and low temperatures. Only fluctuations close to the Fermi surface occur. They are of the form

$$\delta n(\vec{k},\sigma) = \delta(k_F - k) \delta k_F(\theta,\sigma) - \frac{1}{2} \frac{\partial \delta(k_F - k)}{\partial k} \delta k_F(\theta,\sigma)^2 \tag{2.49}$$

For first order of $\delta(E - \mu N)$ in $\delta k_F(\theta,\sigma)$ vanishes. The second order contribution is

$$\begin{aligned} \delta(E - \mu N) &= \frac{V}{8} \rho_F v_F^2 \left[\sum_\sigma \int d\cos\theta \, \delta k_F(\theta,\sigma)^2 \right. \\ &\left. + \frac{1}{2} \sum_{\sigma,\sigma'} \int d\cos\theta \int d\cos\theta' (f(\theta - \theta') + 4\sigma\sigma'\phi(\theta - \theta')) \delta k_F(\theta,\sigma) \delta k_F(\theta',\sigma') \right] \end{aligned} \tag{2.50}$$

Expanding

$$\delta k_F(\theta,\sigma) = \sum_L \delta k_L(\sigma) P_L(\cos\theta) \tag{2.51}$$

we obtain

$$\begin{aligned}\delta(E-\mu N) &= \frac{V}{8}\rho_F v_F^2 \sum_L \Big[[\delta k_L(+\frac{1}{2}) + \delta k_L(-\frac{1}{2})]^2 (1+\frac{F_L}{2L+1}) \\ &\quad + [\delta k_L(+\frac{1}{2}) - \delta k_L(-\frac{1}{2})]^2 (1+\frac{Z_L}{2L+1}) \Big] \end{aligned} \tag{2.52}$$

For a minimum, the right hand side must be positive definite, therefore we obtain $F_L, Z_L > -2L-1$.

2.3 Microscopic Derivation

Standard perturbation theory

Let us consider a typical, generic model of interacting fermions.

$$H = \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma} + \frac{1}{2} \sum_{k_1 \ldots \vec{k}_4, \sigma_1 \ldots \sigma_4} V_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4} c^\dagger_{\vec{k}_1\sigma_1} c^\dagger_{\vec{k}_2,\sigma_2} c_{\vec{k}_4,\sigma_4} c_{\vec{k}_3,\sigma_3} \tag{2.53}$$

Perturbation theory to second order yields

$$\begin{aligned} E &= \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} n(\vec{k},\sigma) + \frac{1}{2} \sum_{\vec{k}_1\sigma_1,\vec{k}_2\sigma_2} V_{\vec{k}_1,\vec{k}_2,\vec{k}_1,\vec{k}_2} n(\vec{k}_1,\sigma_1) n(\vec{k}_2,\sigma_2) \\ &\quad + \frac{1}{4} \sum_{k_1 \ldots \vec{k}_4, \sigma_1 \ldots \sigma_4} \delta_{\vec{k}_1+\vec{k}_2,\vec{k}_3+\vec{k}_4} \frac{|V_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4}|^2}{\frac{1}{2m}(k_1^2+k_2^2-k_3^2-k_4^2)} n(\vec{k}_1,\sigma_1) n(\vec{k}_2,\sigma_2)(1-n(\vec{k}_3,\sigma_3))(1-n(\vec{k}_4,\sigma_4)) \\ &\quad + O(V^3) \end{aligned} \tag{2.54}$$

For small variations of $n(\vec{k},\sigma)$ we identify

$$\begin{aligned} \varepsilon^0_{\vec{k},\sigma} &= \varepsilon_{\vec{k}} + \sum_{\vec{k}_1,\sigma_1} V_{\vec{k},\vec{k}_1,\vec{k},\vec{k}_1} n(\vec{k}_1,\sigma_1) \\ &\quad + \frac{1}{2} \sum_{k_1 \ldots \vec{k}_3, \sigma_1 \ldots \sigma_3} \delta_{\vec{k}+\vec{k}_1,\vec{k}_2+\vec{k}_3} \frac{|V_{\vec{k},\vec{k}_1,\vec{k}_2,\vec{k}_3}|^2}{\frac{1}{2m}(k^2+k_1^2-k_2^2-k_3^2)} n(\vec{k}_1,\sigma_1)(1-n(\vec{k}_2,\sigma_2))(1-n(\vec{k}_3,\sigma_3)) \\ &\quad - \frac{1}{2} \sum_{k_1 \ldots \vec{k}_3, \sigma_1 \ldots \sigma_3} \delta_{\vec{k}_1+\vec{k}_2,\vec{k}+\vec{k}_3} \frac{|V_{\vec{k}_1,\vec{k}_2,\vec{k},\vec{k}_3}|^2}{\frac{1}{2m}(k_1^2+k_2^2-k^2-k_3^2)} n(\vec{k}_1,\sigma_1) n(\vec{k}_2,\sigma_2)(1-n(\vec{k}_3,\sigma_3)) \\ &\quad + O(V^3) \end{aligned} \tag{2.55}$$

$$\begin{aligned} \frac{1}{V} f(\vec{k}_1,\sigma_1,\vec{k}_2,\sigma_2) &= V_{\vec{k}_1,\vec{k}_2,\vec{k}_1,\vec{k}_2} \\ &\quad + \frac{1}{2} \sum_{\vec{k}_3,\sigma_3,\vec{k}_4,\sigma_4} \delta_{\vec{k}_1+\vec{k}_2,\vec{k}_3+\vec{k}_4} \frac{|V_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4}|^2}{\frac{1}{2m}(k_1^2+k_2^2-k_3^2-k_4^2)} (1-n(\vec{k}_3,\sigma_3))(1-n(\vec{k}_4,\sigma_4)) \\ &\quad + \frac{1}{2} \sum_{\vec{k}_3,\sigma_3,\vec{k}_4,\sigma_4} \delta_{\vec{k}_1+\vec{k}_2,\vec{k}_3+\vec{k}_4} \frac{|V_{\vec{k}_3,\vec{k}_4,\vec{k}_1,\vec{k}_2}|^2}{\frac{1}{2m}(k_1^2+k_2^2-k_3^2-k_4^2)} n(\vec{k}_3,\sigma_3) n(\vec{k}_4,\sigma_4) \\ &\quad - \sum_{\vec{k}_3,\sigma_3,\vec{k}_4,\sigma_4} \delta_{\vec{k}_1+\vec{k}_3,\vec{k}_2+\vec{k}_4} \frac{|V_{\vec{k}_1,\vec{k}_3,\vec{k}_2,\vec{k}_4}|^2}{\frac{1}{2m}(k_1^2+k_3^2-k_2^2-k_4^2)} n(\vec{k}_3,\sigma_3)(1-n(\vec{k}_4,\sigma_4)) \\ &\quad + O(V^3) \end{aligned} \tag{2.56}$$

In principle, such a calculation can be done. But one has to deal with all the typical problems of standard perturbation theory, esp. small denominators. Furthermore, one has to sum up many terms. Typically, one takes the thermodynamic limit and thereby replaces the sums of $\vec{k}$ by integrals. One then derives integral equations and solves them. A natural way to do such a calculation is to use the formalism of chapter 1. We will not go through all the details but only sketch the main lines of what has to be done.

Self energy

In analogy to the non-interacting propagator in the translationally invariant system we let

$$\left\langle \phi^*_{\vec{k},\sigma}(\tau)\phi_{\vec{k},\sigma}(\tau')\right\rangle = \frac{1}{\beta}\sum_{\omega_n}\exp(-i\omega_n(\tau-\tau'))G_{\vec{k},\sigma}(\omega_n). \tag{2.57}$$

For $G_{\vec{k},\sigma}(\omega_n)$ we may use a perturbative expansion. $G_{\vec{k},\sigma}(\omega_n)$ is the sum of all closed diagrams with two external lines. This sum can be simplified by introducing $\Sigma(k,\vec{i\omega}_n)$ via

$$G_{\vec{k},\sigma}(\omega_n) = \frac{1}{\varepsilon_{\vec{k}} - \mu - i\omega_n + \Sigma(\vec{k},i\omega_n)}. \tag{2.58}$$

$\Sigma(\vec{k},i\omega_n)$ is called self energy. Expanding this expression for $G_{\vec{k},\sigma}(\omega_n)$ yields

$$G_{\vec{k},\sigma}(\omega_n) = \sum_{r=0}^{\infty}(-1)^r \tilde{g}_{\vec{k}}(\omega_n)\left[\Sigma(\vec{k},i\omega_n)\tilde{g}_{\vec{k}}(\omega_n)\right]^r \tag{2.59}$$

This shows immediately that $\Sigma(\vec{k},i\omega_n)$ can be expressed diagrammatically as the sum of all amputated single-particle-irreducible (or 2-connected) diagrams with two external lines. Amputated here means that the factor $\tilde{g}_{\vec{k}}(\omega_n)$ for the external lines is dropped. Single-particle-irreducible (or 2-connected) means that the diagram remains connected if we cut an arbitrary line.

If we know the single particle propagator or equivalently the self energy, we are able to calculate the single particle energies. To do that, we use a continuation of the single particle propagator onto the complex plane and introduce real frequencies ω in both quantities:

$$G^{R/A}_{\vec{k},\sigma}(\omega) = \pm\frac{1}{\varepsilon_{\vec{k}} - \mu - \omega + \Sigma(\vec{k},\omega) \mp i\eta} \tag{2.60}$$

To do that, one typically writes

$$G_{\vec{k},\sigma} = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{\rho(\vec{k},\omega')}{\omega' - i\omega_n} \tag{2.61}$$

and replaces $i\omega_n$ by ω. This continuation is not unique. Since $\exp(i\omega_n\beta) = \zeta$, we may multiply G with a factor $\zeta\exp(i\omega_n\beta)$, without changing anything. This multiplies $G^{R/A}$ with a factor $\zeta\exp(\omega\beta)$. But $G^{R/A}$ are the retarded and advanced Green's functions. The asymptotic behaviour for large ω is well known, it should be $\propto |\omega|^{-1}$. This additional condition makes the continuation to the complex plain unique.

The singularities of $G^{R/A}$ yield the single particle energies.

$$\omega = \varepsilon_{\vec{k}} + \Sigma(\vec{k},\omega) \tag{2.62}$$

Therefore

$$\frac{d\omega}{dk} = \frac{k}{m} + \frac{\partial\Sigma}{\partial k} + \frac{\partial\Sigma}{\partial\omega}\frac{d\omega}{dk} \tag{2.63}$$

Since $\frac{d\omega}{dk} = \frac{k}{m^*}$ one obtains for the effective mass

$$m^* = m\left(1 + \frac{m}{k}\frac{\partial\Sigma}{\partial k}\right)^{-1}\left(1 - \frac{\partial\Sigma}{\partial\omega}\right) \tag{2.64}$$

which has to be calculated for $k = k_F$.

Therefore we must calculate Σ. Starting point is the representation of Σ as a sum of all amputated 2-connected diagrams with two external lines. First order yields

$$\Sigma_1'(\vec{k}) = \frac{1}{\beta V} \sum_{\vec{k}_1 \omega_{n_1}} V_{\vec{k},\vec{k}_1,\vec{k},\vec{k}_1} \tilde{g}_{\vec{k}_1}(\omega_{n_1}) = \sum_{\vec{k}_1} V_{\vec{k},\vec{k}_1,\vec{k},\vec{k}_1} n_{\vec{k}_1} \tag{2.65}$$

This contribution does not depend on ω_n. It yields only a shift of the energy scale and therefore a shift of the chemical potential. $n_{\vec{k}_1} = n(\vec{k}_1) = \theta(\varepsilon_F - \varepsilon_{\vec{k}_1})$ are here the occupation numbers and $\varepsilon_{\vec{k}_1}$ are the original single particle energies of the non-interacting system. With these assumptions, we obtain first order perturbation theory. This result can be improved if we use

$$\Sigma_1(\vec{k}) = \frac{1}{\beta V} \sum_{\vec{k}_1 \omega_{n_1}} V_{\vec{k},\vec{k}_1,\vec{k},\vec{k}_1} G_{\vec{k}_1}(\omega_{n_1}) = \sum_{\vec{k}_1} V_{\vec{k},\vec{k}_1,\vec{k},\vec{k}_1} n_{\vec{k}_1} \tag{2.66}$$

instead of Σ_1'. The difference is that now the occupation number $n_{\vec{k}_1}$ is determined self-consistently. This quantity then represents the Hartree-Fock approximation.

In second order, we obtain

$$\begin{aligned} \Sigma_2'(\vec{k},\omega_n) &= \frac{1}{\beta^2 V^2} \sum_{\vec{k}_1,\omega_{n_1},\vec{k}_2,\omega_{n_2}} V_{\vec{k},\vec{k}_1,\vec{k},\vec{k}_1} V_{\vec{k}_1,\vec{k}_2,\vec{k}_1,\vec{k}_2} \tilde{g}_{\vec{k}_2}(\omega_{n_2}) \tilde{g}^2_{\vec{k}_1}(\omega_{n_1}) \\ &+ \frac{1}{\beta^2 V^2} \sum_{\vec{k}_1,\omega_{n_1},\vec{k}_2,\omega_{n_2}} V_{\vec{k},\vec{k}_1+\vec{k}_2-\vec{k},\vec{k}_1,\vec{k}_2} V_{\vec{k}_1,\vec{k}_2,\vec{k},\vec{k}_1+\vec{k}_2-\vec{k}} \tilde{g}_{\vec{k}_1}(\omega_{n_1}) \tilde{g}_{\vec{k}_2}(\omega_{n_2}) \\ &\quad \tilde{g}_{\vec{k}_1+\vec{k}_2-\vec{k}}(\omega_{n_1}+\omega_{n_2}-\omega_n) \end{aligned} \tag{2.67}$$

The first term again does not depend on ω_n, but the second does.

Instead of the propagators of the non-interacting system we may introduce here the propagators of the interacting system and calculate Σ_2 instead.

Quasi particle energies

Now, we try to solve the equation $\omega = \varepsilon_{\vec{k}} + \Sigma(\vec{k},\omega)$, which yields the singularities of the Green's function. In first order we get a single solution which corresponds to the solution of the non-interacting system. In second order, $\Sigma_2(\vec{k},\omega)$ has singularities. The consequence of these singularities can be understood in an artificial model, where $\Sigma_2(\vec{k},\omega)$ has only two singularities:

$$\Sigma_2(\omega) = \frac{A_1}{\omega - \varepsilon_1} + \frac{A_2}{\omega - \varepsilon_2} \tag{2.68}$$

The Green's function now has the structure

$$\begin{aligned} G_2(\omega) &= \frac{1}{\omega - \varepsilon_0 - \Sigma_2(\omega)} \\ &= \frac{(\omega-\varepsilon_1)(\omega-\varepsilon_2)}{(\omega-\varepsilon_0)(\omega-\varepsilon_1)(\omega-\varepsilon_2) - A_1(\omega-\varepsilon_2) - A_2(\omega-\varepsilon_1)} \end{aligned}$$

For small A_1, A_2, which means weak interaction, we get three singularities close to ε_0, ε_1, and ε_2. The sum of the residua is 1, the residuum of the singularity close to ε_0 is almost 1, the two others are small. In leading order we obtain for the residua

$$1 - \sum_{i=1}^{2} \frac{A_i}{(\varepsilon_0 - \varepsilon_i)^2} \tag{2.69}$$

$$\frac{A_i}{(\varepsilon_0-\varepsilon_i)^2}, \quad i=1,2 \tag{2.70}$$

For the general system, something similar happens. The Greens function has singularities close to the original single particle energies $\varepsilon_{\vec{k}}$ with reduced residua. The singularity close to $\varepsilon_{\vec{k}}$ is the energy of the quasi particle in the Fermi liquid theory.

Interaction of quasi particles

The interaction between the quasi particles is a two-particle property of the system and cannot be calculated from the single particle Greens functions. We therefore need the two-particle Greens functions

$$\left\langle \phi^*_{\vec{k}_1\sigma_1}(\tau_1)\phi^*_{\vec{k}_2\sigma_2}(\tau_2)\phi_{\vec{k}_3\sigma_3}(\tau_3)\phi_{\vec{k}_4\sigma_4}(\tau_4)\right\rangle \tag{2.71}$$

They can be written as

$$\begin{aligned}\left\langle \phi^*_{\vec{k}_1\sigma_1}(\tau_1)\phi^*_{\vec{k}_2\sigma_2}(\tau_2)\phi_{\vec{k}_3\sigma_3}(\tau_3)\phi_{\vec{k}_4\sigma_4}(\tau_4)\right\rangle &= \left\langle \phi^*_{\vec{k}_1\sigma_1}(\tau_1)\phi_{\vec{k}_4\sigma_4}(\tau_4)\right\rangle\left\langle \phi^*_{\vec{k}_2\sigma_2}(\tau_2)\phi_{\vec{k}_3\sigma_3}(\tau_3)\right\rangle \\ &- \left\langle \phi^*_{\vec{k}_1\sigma_1}(\tau_1)\phi_{\vec{k}_3\sigma_3}(\tau_3)\right\rangle\left\langle \phi^*_{\vec{k}_2\sigma_2}(\tau_2)\phi_{\vec{k}_4\sigma_4}(\tau_4)\right\rangle \\ &+ \left\langle \phi^*_{\vec{k}_1\sigma_1}(\tau_1)\phi^*_{\vec{k}_2\sigma_2}(\tau_2)\phi_{\vec{k}_3\sigma_3}(\tau_3)\phi_{\vec{k}_4\sigma_4}(\tau_4)\right\rangle_c\end{aligned} \tag{2.72}$$

where the last contribution is the connected part. The first two terms contain non-interacting quasi particles. The third term yields the effective interaction. It can be written as

$$\begin{aligned}\left\langle \phi^*_{\vec{k}_1\sigma_1}(\tau_1)\phi^*_{\vec{k}_2\sigma_2}(\tau_2)\phi_{\vec{k}_3\sigma_3}(\tau_3)\phi_{\vec{k}_4\sigma_4}(\tau_4)\right\rangle_c &= \sum_{\sigma_1'\sigma_2'\sigma_3'\sigma_4'}\sum_{\vec{k}_1'\vec{k}_2'\vec{k}_3'\vec{k}_4'}\int d\tau_1'\int d\tau_2'\int d\tau_3'\int d\tau_4'\left\langle \phi^*_{\vec{k}_1\sigma_1}(\tau_1)\phi_{\vec{k}_1'\sigma_1'}(\tau_1')\right\rangle \\ &\left\langle \phi^*_{\vec{k}_2\sigma_2}(\tau_2)\phi_{\vec{k}_2'\sigma_2'}(\tau_2')\right\rangle\left\langle \phi^*_{\vec{k}_3'\sigma_3'}(\tau_3)\phi_{\vec{k}_3\sigma_3}(\tau_3')\right\rangle\left\langle \phi^*_{\vec{k}_4'\sigma_4'}(\tau_4)\phi_{\vec{k}_4\sigma_4}(\tau_4')\right\rangle \\ &\Gamma^{(2)}_{\vec{k}_1'\sigma_1',\vec{k}_2'\sigma_2',\vec{k}_3'\sigma_3',\vec{k}_4'\sigma_4'}(\tau_1',\tau_2',\tau_3',\tau_4')\end{aligned} \tag{2.73}$$

$\Gamma^{(2)}$ is now the interaction of the quasi particles. In a perturbative expansion, $\Gamma^{(2)}$ is in first order the bare interaction. In general, $\Gamma^{(2)}$ is the sum of all amputated, single-particle irreducible diagrams with four external lines. In this sense it is similar to the self energy.

The above expression is general. If the system is translationally invariant, there are only contributions with $\vec{k}_i'=\vec{k}_i$, $\sigma_i'=\sigma_i$. Furthermore, we introduce ω_n. The integrals can now be calculated, but one still has to sum over ω_{n_i}. Since energy is conserved, the sums are trivial and one finally obtains

$$\Gamma^{(2)}_{\vec{k}_1\sigma_1,\vec{k}_2\sigma_2,\vec{k}_3\sigma_3,\vec{k}_4\sigma_4}(\omega_{n_1},\omega_{n_2},\omega_{n_3},\omega_{n_4}) = \delta_{K_1+K_2,K_3+K_4}\Gamma_{\sigma_1\sigma_2\sigma_3\sigma_4}(K_1,K_2;K_1-K_3) \tag{2.74}$$

which is also the definition of Γ. Furthermore, $K_i=(\omega_{n_i},\vec{k}_i)$. K_1-K_3 is the momentum transfer due to the interaction. Like the self energy, Γ does not depend on the frequencies ω_n in first order, but only in higher orders. This dependency can be interpreted as a retardation of the interaction.

The spin dependency can be simplified, if one takes into account the $SU(2)$ spin symmetry. Γ can be written as

$$\begin{aligned}\Gamma_{\sigma_1\sigma_2\sigma_3\sigma_4}(K_1,K_2;K) &= \frac{1}{2}(\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}-\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3})\Gamma_s(K_1,K_2;K) \\ &+ \frac{1}{2}(\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}+\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3})\Gamma_t(K_1,K_2;K)\end{aligned} \tag{2.75}$$

where Γ_s is the singlet part and Γ_t is the triplet part of Γ.

In Fermi liquid theory, one considers only effective interactions which depend on the small changes $\delta n(\vec{k},\sigma)$. This means that momentum transfer vanishes. For the quasi particle interaction it is therefore sufficient to consider the contributions where $K=(\omega_n,\vec{k})$ vanishes. Furthermore, we consider the limit of small temperature, which means that it is sufficient to consider the limit $\omega_n \to 0$. And finally we only need Γ where $\vec{k}_i$ are close to the Fermi surface, i.e. $k_i \approx k_F$. In this limit, Γ yields the effective interaction of Fermi liquid theory.

Let us take a look at the perturbation expansion of Γ. First order is the original interaction. For a momentum transfer $= 0$, it yields the first order of the quasi particle interaction as obtained before using ordinary perturbation theory. Similarly, the second order contribution is the same. One can improve this, if one replaces the propagators in the perturbative series by propagators of the interacting system. Γ is then the sum over all two-particle irreducible diagrams. One obtains an integral equation for Γ, which has to be solved. But the problem remains: perturbative expansions contain divergences and expansions do not converge.

3 Renormalisation

3.1 Main idea

We saw that perturbation theory leads to several divergences. A tool to deal with such divergences is renormalisation. Renormalisation is not a specific method but merely a collection of several, but similar methods, either analytic or numeric. Important is to understand the main idea. We treat as an example an interacting, translationally invariant Fermi system.

$$Z = \int D[\phi] \exp\left(S[\phi^*, \phi]\right) \tag{3.1}$$

$$S[\phi^*, \phi] = \sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu)\phi_K^* \phi_K - V[\phi^*, \phi] \tag{3.2}$$

where $K = (\omega_n, \vec{k}, \sigma)$ is a multi index, which contains the wave vector, the frequencies ω_n, and the spin. The interaction is a generic interaction. In the first chapter of this course we saw that the connected propagators can be calculated using the generating function

$$W[J^*, J] = \ln \left\langle \exp(-V[\phi^*, \phi] + \sum_K (J_K^* \phi_K + \phi_K^* J_K)) \right\rangle_0 \tag{3.3}$$

simply by taking derivatives with respect to J_K and J_K^*. We use the notation

$$\langle A[\phi^*, \phi] \rangle_0 = \frac{\int D[\phi] A[\phi^*, \phi] \exp(\sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu)\phi_K^* \phi_K)}{\int D[\phi] \exp(\sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu)\phi_K^* \phi_K)} \tag{3.4}$$

for expectation values of the non-interacting system. The single particle propagator of the non-interacting system is

$$C(K) = \frac{1}{i\omega_n - \varepsilon_{\vec{k}} + \mu} \tag{3.5}$$

and has a divergence at $\omega_n = 0$ and $\varepsilon_{\vec{k}} = \mu$, i.e. for the case which is the interesting divergence for Fermi liquid theory. We expect that this divergence remains, probably shifted and with a reduced residuum, and yields the quasi particle of Fermi liquid theory.

The main idea of renormalisation is simple. We introduce a cut-off Λ and perform all integrals in the expression for W over fields ϕ_K and ϕ_K^* for which $|i\omega_n - \varepsilon_{\vec{k}} + \mu| > \Lambda$. The remaining integrals can again be written as

$$W[J^*, J] = \ln \left\langle \exp(-V_\Lambda[\phi^*, \phi, J^*, J] + \sum_{K: |i\omega_n - \varepsilon_{\vec{k}} + \mu| < \Lambda} (J_K^* \phi_K + \phi_K^* J_K)) \right\rangle_{\Lambda, 0} \tag{3.6}$$

The non-interacting part now depends on Λ since the integration over some of the fields introduce new quadratic contributions. Since the original system is translational invariant, the new quadratic contributions are translational invariant and therefore diagonal. Therefore, the average depends on Λ. The new interaction $V_\Lambda[\phi^*, \phi, J^*, J]$ depends as well explicitly on Λ and on the fields J_K and J_K^* with $|i\omega_n - \varepsilon_{\vec{k}} + \mu| > \Lambda$. In the new integral, divergences are shifted, since the single particle energies $\varepsilon_{\vec{k}}$ and eventually μ as well are shifted. Since we are interested in propagators near the Fermi surface, the fields J_K and J_K^* in $V_\Lambda[\phi^*, \phi, J^*, J]$ are uninteresting. We will never calculate derivatives with respect to these fields. Therefore we may set them to 0 explicitly.

In a next step, we introduce a new cut-off Λ_1 and perform the integral over all fields ϕ_K and ϕ_K^* for which $|i\omega_n - \varepsilon_{\vec{k}} + \mu| > \Lambda_1$. This yields again a new V_{Λ_1} and shifted single particle energies. We iterate this procedure and finally obtain an effective theory which depends only on fields with small values of $|i\omega_n - \varepsilon_{\vec{k}} + \mu|$. This is now the effective theory we are looking for. A priori it is not clear that the procedure converges. For special cases and for not too large interaction, one can eventually prove convergence.

Let us mention that there are various technically different variants of the procedure described above. Instead of a discrete series of steps one can vary the cut-off continuously. Instead of a hard cut-off as described above, one can introduce a soft cut-off (these notions will be explained later). Instead of W one can use a different generating function.

3.2 Effective action

For Fermi systems it is often easier not to use W but

$$G_{\text{eff}}[\psi^*, \psi] = \ln \langle \exp(-V[\phi^* + \psi^*, \phi + \psi]) \rangle_0 \tag{3.7}$$

We mentioned that quantity already in the first chapter. We now discuss it in more detail. First of all, we have

$$\begin{aligned}
Z_0 \langle \exp(-V[\phi^* + \psi^*, \phi + \psi]) \rangle_0 &= \int D[\phi] \exp(\sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu)\phi_K^* \phi_K - V[\phi^* + \psi^*, \phi + \psi]) \\
&= \int D[\phi] \exp(\sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu)(\phi_K^* - \psi_K^*)(\phi_K - \psi_K) - V[\phi^*, \phi]) \\
&= \exp(\sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu)\psi_K^* \psi_K) \\
&\quad \times \int D[\phi] \exp(\sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu)\phi_K^* \phi_K - V[\phi^*, \phi] \\
&\qquad - \sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu)(\phi_K^* \psi_K + \psi_K^* \phi_K)) \\
&= Z_0 \exp(\sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu)\psi_K^* \psi_K + W[C(K)^{-1}\psi_K^*, C(K)^{-1}\psi_K])
\end{aligned} \tag{3.8}$$

and therefore

$$G_{\text{eff}}[\psi^*, \psi] = \sum_K \psi_K^* C(K)^{-1} \psi_K + W[C(K)^{-1}\psi_K^*, C(K)^{-1}\psi_K] \tag{3.9}$$

Since W is the generating function for connected propagators, one can show that G_{eff} is the generating function for connected, amputated propagators. Due to the factors $C(K)^{-1}$ in the argument of W one multiplies the final result with a factor $C(K)^{-1} = (i\omega_n - \varepsilon_{\vec{k}} + \mu)$ for each derivative one takes, so that the factors $C(K)$ for the external lines are cancelled.

G_{eff} is called effective action.

3.3 Renormalisation group equations for G_{eff}

In this subsection we derive the renormalisation group equation for the effective action. In contrast to the above description for W we will use a continuous renormalisation.

Let us introduce the modified propagator

$$C^{\Lambda}(K) = \frac{\Theta_{\Lambda}(K)}{i\omega_n - (\varepsilon_{\vec{k}} - \mu)} \tag{3.10}$$

Here $\Theta_{\Lambda}(K)$ is a cut-off function. The most simple case would be a hard cut-off, e.g.

$$\Theta_{\Lambda}(K) = \theta(|\varepsilon_{\vec{k}} - \mu - i\omega_n| - \Lambda) \tag{3.11}$$

For analytical calculations a cut-off function which is differentiable might be more suitable. Then we have a weak cut-off. For $|\varepsilon_{\vec{k}} - \mu - i\omega_n| \gg \Lambda$ one has $\Theta_\Lambda(K) = 1$ and $C^\Lambda(K) = C(K)$. For $|\varepsilon_{\vec{k}} - \mu - i\omega_n| \ll \Lambda$ one has $\Theta_\Lambda(K) = 0$ and therefore $C^\Lambda(K) = 0$. I define

$$G^\Lambda_{\text{eff}}[\psi^*, \psi] = \ln \frac{\int D[\phi] \exp(\sum_K \phi^*_K (C^\Lambda(K))^{-1} \phi_K - V[\phi^* + \psi^*, \phi + \psi])}{\int D[\phi] \exp(\sum_K \phi^*_K (C^\Lambda(K))^{-1} \phi_K)} \tag{3.12}$$

For values of K with $\Theta_\Lambda(K) = 0$ only $\phi_K = 0$ contributes. G^Λ_{eff} is then given by $-V$. For values of K with $\Theta_\Lambda(K) = 1$, G^Λ_{eff} is given by G_{eff}. G^Λ_{eff} interpolates between $-V$ and G_{eff}. The goal is to derive a differential equation for G^Λ_{eff} which has the initial condition $-V$ and can be solved. We start with

$$F[\psi^*, \psi] = F\left[\frac{\partial}{\partial \eta}, \frac{\partial}{\partial \eta^*}\right] \exp(\sum_K (\eta^*_K \psi_K + \eta_K \psi^*_K))\Big|_{\eta = \eta^* = 0} \tag{3.13}$$

$$\int D[\phi] \exp(\sum_K \phi^*_K (C^\Lambda(K))^{-1} \phi_K + \sum_K (\eta^*_K \phi_K + \eta_K \phi^*_K)) = \exp(\sum_K \eta^*_K C^\Lambda(K) \eta_K) \int D[\phi] \exp(\sum_K \phi^*_K (C^\Lambda(K))^{-1} \phi_K) \tag{3.14}$$

The second equation can be written as

$$\begin{aligned} \left\langle \exp(\sum_K (\eta^*_K \phi_K + \eta_K \phi^*_K)) \right\rangle_{\Lambda,0} &= \frac{\int D[\phi] \exp(\sum_K \phi^*_K (C^\Lambda(K))^{-1} \phi_K + \sum_K (\eta^*_K \phi_K + \eta_K \phi^*_K))}{\int D[\phi] \exp(\sum_K \phi^*_K (C^\Lambda(K))^{-1} \phi_K)} \\ &= \exp(\sum_K \eta^*_K C^\Lambda(K) \eta_K) \end{aligned} \tag{3.15}$$

This yields

$$\begin{aligned} \exp(G^\Lambda_{\text{eff}}[\psi^*, \psi]) &= \langle \exp(-V[\phi^* + \psi^*, \phi + \psi]) \rangle_{\Lambda,0} \\ &= \exp\left(-V\left[\frac{\partial}{\partial \eta}, \frac{\partial}{\partial \eta^*}\right]\right) \left\langle \exp(\sum_K (\eta^*_K (\phi_K + \psi_K) + \eta_K (\phi^*_K + \psi^*_K))) \right\rangle \Big|_{\eta = \eta^* = 0} \\ &= \exp\left(-V\left[\frac{\partial}{\partial \eta}, \frac{\partial}{\partial \eta^*}\right]\right) \exp(\sum_K \eta^*_K C^\Lambda(K) \eta_K + \sum_K (\eta^*_K \psi_K + \eta_K \psi^*_K)) \Big|_{\eta = \eta^* = 0} \\ &= \exp\left(-V\left[\frac{\partial}{\partial \eta}, \frac{\partial}{\partial \eta^*}\right]\right) \exp\left(\sum_K \frac{\partial}{\partial \psi_K} C^\Lambda(K) \frac{\partial}{\partial \psi^*_K}\right) \exp(\sum_K (\eta^*_K \psi_K + \eta_K \psi^*_K)) \Big|_{\eta = \eta^* = 0} \\ &= \exp\left(\sum_K \frac{\partial}{\partial \psi_K} C^\Lambda(K) \frac{\partial}{\partial \psi^*_K}\right) \exp\left(-V\left[\frac{\partial}{\partial \eta}, \frac{\partial}{\partial \eta^*}\right]\right) \exp(\sum_K (\eta^*_K \psi_K + \eta_K \psi^*_K)) \Big|_{\eta = \eta^* = 0} \\ &= \exp\left(\sum_K \frac{\partial}{\partial \psi_K} C^\Lambda(K) \frac{\partial}{\partial \psi^*_K}\right) \exp\left(-V\left[\psi^*_K, \psi_K\right]\right) \end{aligned} \tag{3.16}$$

and

$$\frac{\partial}{\partial \Lambda} \exp(G^\Lambda_{\text{eff}}[\psi^*, \psi]) = \sum_K \frac{\partial}{\partial \psi_K} \frac{\partial C^\Lambda(K)}{\partial \Lambda} \frac{\partial}{\partial \psi^*_K} \exp(G^\Lambda_{\text{eff}}[\psi^*, \psi])$$

finally

$$\begin{aligned} \frac{\partial}{\partial \Lambda} G^\Lambda_{\text{eff}}[\psi^*, \psi] &= \sum_K \frac{\partial}{\partial \psi_K} \frac{\partial C^\Lambda(K)}{\partial \Lambda} \frac{\partial}{\partial \psi^*_K} G^\Lambda_{\text{eff}}[\psi^*, \psi] \\ &\quad + \sum_K \frac{\partial G^\Lambda_{\text{eff}}[\psi^*, \psi]}{\partial \psi_K} \frac{\partial C^\Lambda(K)}{\partial \Lambda} \frac{\partial G^\Lambda_{\text{eff}}[\psi^*, \psi]}{\partial \psi^*_K} \end{aligned} \tag{3.17}$$

This is the differential equation for G^{Λ}_{eff} we were looking for. It is an exact renormalisation group equation. It is clear, that this equation cannot be solved in general. Often, a perturbative expansion is used to solve the equation.

For a further treatment of this equation, one can expand G^{Λ}_{eff} in monomials of factors ψ_K and ψ^*_K and derive differential equations for the expansion coefficients. In the present case it is easier to use an expansion of the form

$$\begin{aligned} G^{\Lambda}_{\text{eff}}[\psi^*,\psi] &= \sum_{m=0}^{\infty} \frac{1}{(m!)^2} \sum_{K_1,\ldots,K_m} \sum_{K'_1,\ldots,K'_m} G^{\Lambda}_m(K'_1,\ldots,K'_m;K_1,\ldots,K_m) \\ &\quad \exp\left(-\sum_K \frac{\partial}{\partial\psi_K} D^{\Lambda}(K) \frac{\partial}{\partial\psi^*_K}\right) \prod_{j=1}^{m} \psi^*_{K_j}\psi_{K_j} \end{aligned} \tag{3.18}$$

where

$$D^{\Lambda}(K) = C(K) - C^{\Lambda}(K) = \frac{1-\Theta_{\Lambda}(K)}{i\omega_n - \varepsilon_{\vec{k}} + \mu} \tag{3.19}$$

The derivative of G^{Λ}_{eff} with respect to Λ yields two contributions, one due to the derivative of the coefficient and one due to the derivative of $D^{\Lambda}(K)$. Since

$$\frac{\partial D^{\Lambda}(K)}{\partial\Lambda} = -\frac{\partial C^{\Lambda}(K)}{\partial\Lambda} \tag{3.20}$$

the second term yields a contribution which has the form of the first term in the renormalisation group equation for G^{Λ}_{eff}. This term does not contribute to the derivative of the coefficient. Only the second term yields a contribution to the differential equations of the coefficients.

It is possible to write down the equations in a graphical form. This form is especially useful for perturbative expansions. Only single-particle irreducible diagrams occur.

We now want to derive the equations to lowest order in a perturbation expansion. The lowest order which yields a contribution to the derivative of G^{Λ}_m is $O(V^2)$. We start with a two-particle interaction, therefore all coefficients G^{Λ}_m with $m > 2$ vanish initially. These coefficients are at least of order $O(V^m)$ with $m > 2$. In $O(V^2)$ it is sufficient to take into account only the coefficients G^{Λ}_2. We obtain

$$\begin{aligned} \frac{\partial}{\partial\Lambda} G^{\Lambda}_2(K'_1,K'_2;K_1,K_2) &= -\sum_{K,K'} \frac{\partial(D^{\Lambda}(K)D^{\Lambda}(K'))}{\partial\Lambda} \Big[\frac{1}{2} G^{\Lambda}_2(K'_1,K'_2;K,K') G^{\Lambda}_2(K,K';K_1,K_2) \\ &\quad - G^{\Lambda}_2(K'_1,K;K_1,K') G^{\Lambda}_2(K',K'_2;K,K_2) \\ &\quad + G^{\Lambda}_2(K'_2,K;K_1,K') G^{\Lambda}_2(K',K'_1;K,K_2)\Big] \end{aligned} \tag{3.21}$$

Since $G^{\Lambda}_2 = -\frac{1}{\beta V}\Gamma^{(2)}$ this can be directly written as an equation for $\Gamma^{(2)}$:

$$\begin{aligned} \frac{\partial}{\partial\Lambda} \Gamma^{(2)}(K'_1,K'_2;K_1,K_2) &= \frac{1}{\beta V} \sum_{K,K'} \frac{\partial(D^{\Lambda}(K)D^{\Lambda}(K'))}{\partial\Lambda} \Big[\frac{1}{2} \Gamma^{(2)}(K'_1,K'_2;K,K') \Gamma^{(2)}(K,K';K_1,K_2) \\ &\quad - \Gamma^{(2)}(K'_1,K;K_1,K') \Gamma^{(2)}(K',K'_2;K,K_2) \\ &\quad + \Gamma^{(2)}(K'_2,K;K_1,K') \Gamma^{(2)}(K',K'_1;K,K_2)\Big] \end{aligned} \tag{3.22}$$

Further simplifications occur if translational invariance and spin symmetry are taken into account. We introduced already the quantities

$$\Gamma^{(2)}_{\vec{k}_1\sigma_1,\vec{k}_2\sigma_2,\vec{k}_3\sigma_3,\vec{k}_4\sigma_4}(\omega_{n_1},\omega_{n_2},\omega_{n_3},\omega_{n_4}) = \delta_{K_1+K_2,K_3+K_4} \Gamma_{\sigma_1\sigma_2\sigma_3\sigma_4}(K_1,K_2;K_1-K_3) \tag{3.23}$$

$$\begin{aligned}\Gamma_{\sigma_1\sigma_2\sigma_3\sigma_4}(K_1,K_2;K) &= \frac{1}{2}(\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}-\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3})\Gamma_s(K_1,K_2;K)\\ &+ \frac{1}{2}(\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}+\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3})\Gamma_t(K_1,K_2;K)\end{aligned} \tag{3.24}$$

where now K contains only $\vec{k}$ and ω_n. The equations for Γ_s and Γ_t are

$$\frac{\partial}{\partial\Lambda}\Gamma_\alpha(K_1,K_2;K)=\sum_{r=1}^{3}\sum_{\alpha',\alpha''=s,t}C^r_{\alpha,\alpha',\alpha''}\beta^r_{\alpha',\alpha''}(K_1,K_2;K) \tag{3.25}$$

$$\beta^1_{\alpha',\alpha''}(K_1,K_2;K)=\frac{1}{2\beta V}\sum_{K'}\frac{\partial(D^\Lambda(K_1-K')D^\Lambda(K_2+K'))}{\partial\Lambda}\Gamma_{\alpha'}(K_1,K_2;K')\Gamma_{\alpha''}(K_1-K',K_2+K';K-K') \tag{3.26}$$

$$\beta^2_{\alpha',\alpha''}(K_1,K_2;K)=-\frac{1}{\beta V}\sum_{K'}\frac{\partial(D^\Lambda(K')D^\Lambda(K'+K))}{\partial\Lambda}\Gamma_{\alpha'}(K_1,K';K)\Gamma_{\alpha''}(K'+K,K_2;K) \tag{3.27}$$

$$\begin{aligned}\beta^3_{\alpha',\alpha''}(K_1,K_2;K)=\frac{1}{\beta V}\sum_{K'}\frac{\partial(D^\Lambda(K')D^\Lambda(K_2-K_1+K'+K))}{\partial\Lambda}&\Gamma_{\alpha'}(K_2,K';K_2+K-K_1)\\ &\times\Gamma_{\alpha''}(K_2-K_1+K+K',K_1;K_2+K-K_1)\end{aligned} \tag{3.28}$$

$$C^1_{sss}=C^1_{ttt}=1,\quad C^1_{\alpha,\alpha',\alpha''}=0 \text{ otherwise} \tag{3.29}$$

$$C^2_{sss}=-C^3_{sss}=-\frac{1}{4},\quad C^2_{s\alpha\alpha'}=-C^3_{s\alpha\alpha'}=\frac{3}{4} \text{ otherwise} \tag{3.30}$$

$$C^2_{ttt}=C^3_{ttt}=\frac{5}{4},\quad C^2_{t\alpha\alpha'}=C^3_{t\alpha\alpha'}=\frac{1}{4} \text{ otherwise} \tag{3.31}$$

In general it is not possible to solve these equations analytically. Furthermore, it is not at all clear that the results do not diverge. It is well known that for sufficiently low temperatures, a divergence occurs which leads to a superconducting instability. The Fermi liquid becomes a super-conductor. This effect is called Kohn-Luttinger effect. It was found by Kohn and Luttinger [31] in a second order perturbative calculation in 1965 and can be treated in a mathematically rigorous way (see a series of work by Knörrer, Trubowitz, Feldman, Sinclair, Salmhofer [9, 62, 10, 63, 11, 12], for a mathematical and comprehensive introduction I refer to the book by Salmhofer [64]). But one can show as well that for weak interaction and not too low temperatures the renormalisation group equations yield a finite solution: the Fermi liquid.

3.4 The Hubbard model I, Renormalization

The Hubbard model is a lattice model for electrons with a short range interaction. The Hamiltonian is

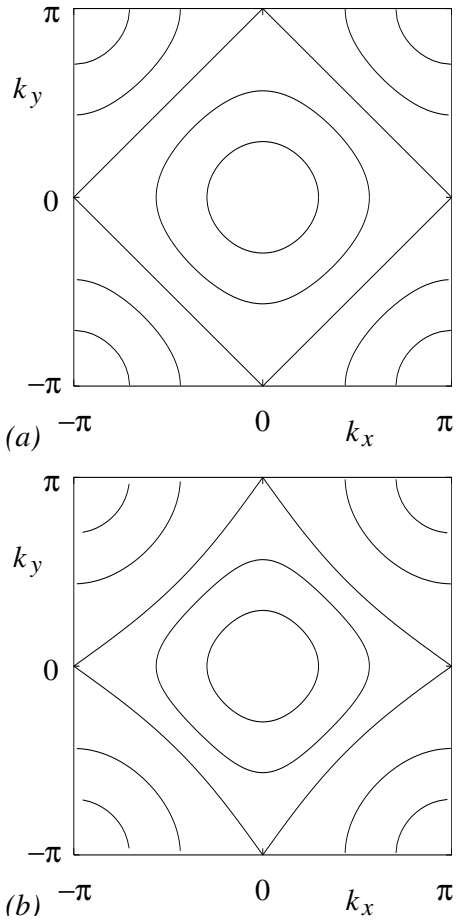
$$H=\sum_{x,y,\sigma}t_{x,y}c^\dagger_{x,\sigma}c_{y,\sigma}+U\sum_x n_{x,\uparrow}n_{x,\downarrow} \tag{3.32}$$

For a translationally invariant lattice with a single energy band we can transform to momentum space and obtain

$$H=\sum_{\vec{k},\sigma}\varepsilon_{\vec{k}}c^\dagger_{\vec{k},\sigma}c_{\vec{k},\sigma}+\frac{U}{N_s}\sum_{\vec{k},\vec{k}',\vec{q}}c^\dagger_{\vec{k},\uparrow}c^\dagger_{\vec{k}',\downarrow}c_{\vec{k}'-\vec{q},\downarrow}c_{\vec{k}+\vec{q},\uparrow} \tag{3.33}$$

where N_s is the number of lattice sites. We discuss general results for this model later. In this subsection we show results of a renormalisation group calculation for the Hubbard model in two dimensions. The results we show have been taken out of the work by Halboth and Metzner [20, 21]. Similar results have been obtained

Figure 3.1: Lines of constant energy $\varepsilon_{\vec{k}}$ in the Brillouin zone for $t' = 0$ (a) and $t' = -0.16$ (b).



by Wegner and coworkers using continuous unitary transformations [18, 22]. Until today, many further results, not only on the square lattice have been obtained, see e.g. the review [45].

Starting point is the Hubbard model on a quadratic lattice with

$$\varepsilon_{\vec{k}} = -2t(\cos k_x + \cos k_y) - 4t'(\cos k_x \cos k_y) \tag{3.34}$$

Here $-t$ is the nearest neighbour hopping, i.e. the value of $t_{x,y}$ for neighboured lattice sites x and y. $-t'$ is the matrix element for next nearest neighbours. For all other distances one has $t_{x,y} = 0$. The $\varepsilon_{\vec{k}}$ can be drawn as lines with constant energy in the (k_x, k_y)-plane, see figure 3.1.

The interaction is

$$V[\phi^*, \phi] = \frac{U}{N_s} \sum_{K,K',Q} \phi^*_{K,\uparrow} \phi^*_{K',\downarrow} \phi_{K'-Q,\downarrow} \phi_{K+Q,\uparrow} \tag{3.35}$$

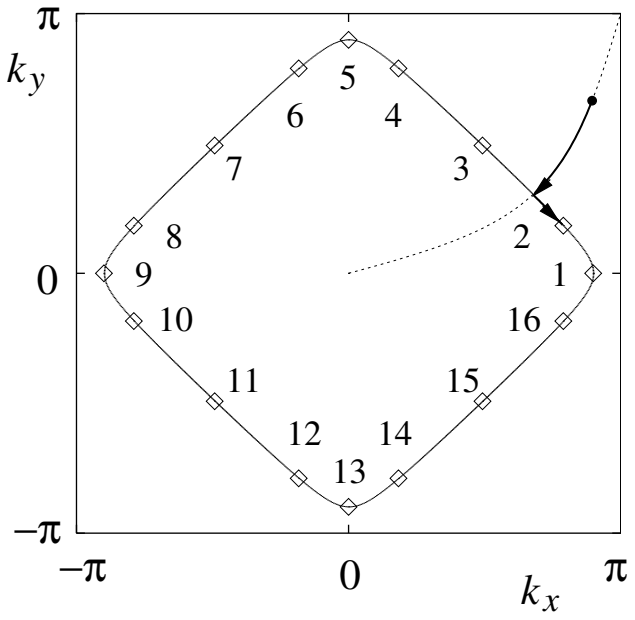
Initially, the matrix elements do not depend on K, K', and Q. In the following, the idea is to derive renormalisation group equations and to solve them numerically. This is done in momentum space. We need several assumptions and approximations. Details are discussed in the course and in the original work by Halboth and Metzner [21, 20].

1. First we need a discretisation in $\vec{k}$-space. If we choose a discretisation with N points in $\vec{k}$-space, we obtain equations for $O(N^3)$ couplings. N must therefore not be too large, a typical value is $N = 16$.

2. We neglect the dependence of Γ on ω_n.

3. Since N is small and since we need precise results close to the Fermi surface, we choose the points in k-space for the discretisation on the Fermi surface. During the calculation, we need values of Γ with

Figure 3.2: The discretisation on the Fermi surface. The numbers are used later as indices.



indices not on the Fermi surface. Therefore we need a projection method which maps these values to values on the Fermi surface. For large Λ this is exact since Γ is constant anyway. For small Λ we have only values of Γ with indices close to the Fermi surface and this approximation should be good as well.

4. Close to the edges of the Fermi surface there should be more points of our discretisation.

The approximation due to the discretisation is

$$\Gamma^{\Lambda}_{\alpha}(\vec{k}_1,\vec{k}_2;\vec{k}'_1,\vec{k}'_2) \approx \Gamma^{\Lambda}_{\alpha}(\vec{k}_{F1},\vec{k}_{F2};\vec{k}'_{F1},\vec{k}_{F1}+\vec{k}_{F2}-\vec{k}'_{F1}) \tag{3.36}$$

Instead of $\vec{k}_F$ we use the angle which fixes the direction of $\vec{k}_F$. One obtains

$$\Gamma^{\Lambda}_{\alpha}(\vec{k}_{F1},\vec{k}_{F2};\vec{k}'_{F1},\vec{k}_{F1}+\vec{k}_{F2}-\vec{k}'_{F1}) = \Gamma^{\Lambda}_{\alpha}(\phi_1,\phi_2;\phi'_1) \tag{3.37}$$

The discretisation that has been used is shown in figure 3.2.

Numerically one calculates the effective interaction and with the help of it several susceptibilities to obtain physically meaningful results. If one of the susceptibilities diverges, this is a sign for an instability of the Fermi liquid. The susceptibility directly yields the type of instability. The following susceptibilities are taken into account:

1. commensurate anti-ferromagnetic spin susceptibility $\chi_S(\pi,\pi)$,
2. incommensurate anti-ferromagnetic spin susceptibilities $\chi_S(\vec{q})$ with $\vec{q}=(\pi-\delta,\pi)$ or $\vec{q}=(1-\delta)(\pi,\pi)$. Here $\delta = 1-N_e/N_s$ is the doping, the distance from a half filled band.
3. commensurate charge susceptibility$\chi_C(\pi,\pi)$,
4. Various singlet pair susceptibilities for s wave pairing (form factor $d(\vec{k})=1$), modified s-wave pairing ($d(\vec{k})=(\cos k_x+\cos k_y)/\sqrt{2}$), d-wave pairing $d_{x^2-y^2}$ (form factor $d(\vec{k})=(\cos k_x-\cos k_y)/\sqrt{2}$) and d_{xy} ($d(\vec{k})=\sin k_x \sin k_y$).

The results we show have been calculated for $U=t$. The susceptibilities are divided by their values for $U=0$ All results are for densities close to half filling and for small values of t'. In the next chapter we shall see that the

Figure 3.3: Flow of the singlet functions Γ_s^Λ for different values of $\vec{k}$. The values are the discretisation points in figure 3.2. Only the most important couplings are shown. The figure below shows the susceptibilities. Calculations are done for $t' = 0$ and $\mu = -0.005$, which corresponds to a density slightly below half filling. The system shows an anti-ferromagnetic instability.

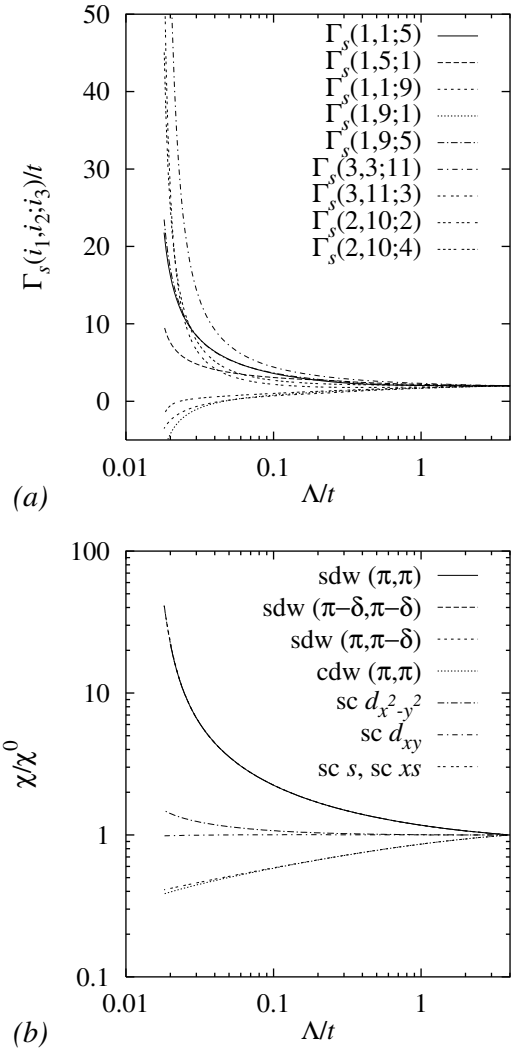
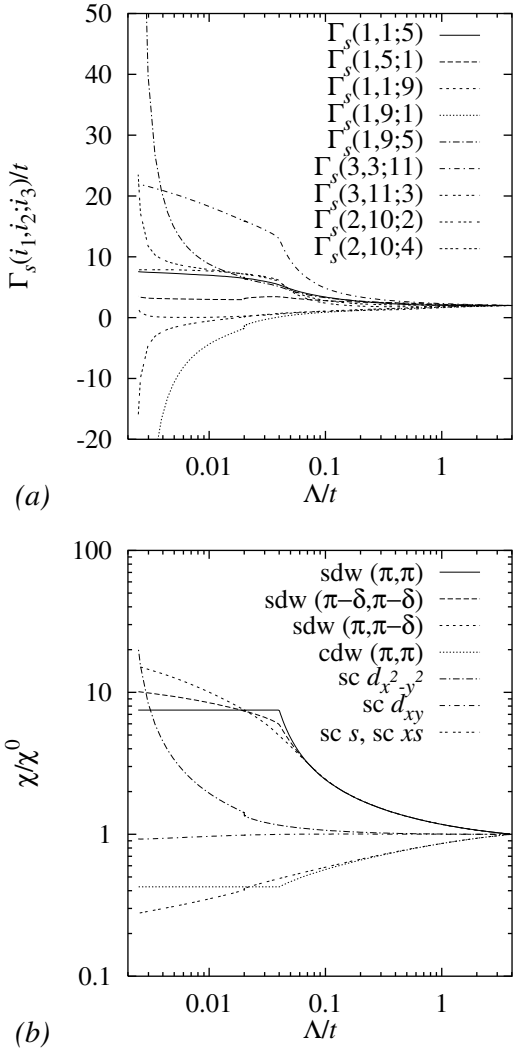


Figure 3.4: Parameters as in 3.3, but $\mu = -0.02$.



Hubbard at half filling is an anti-ferromagnet. The anti-ferromagnetic state should be stable close to half filling. This is shown by the results in figure 3.3. But for lower densities, the anti-ferromagnet becomes unstable. Due to the Kohn-Luttinger instability the system may become super-conducting. This is indeed the case, see figure 3.4. On can see that the spin susceptibilities first grow but then remain constant for smaller values of Λ. Instead, the susceptibility for d-wave super-conductivity dominates. If one performs similar calculation for various parameter sets, one obtains a phase diagram shown in figure 3.5. Figure 3.6 finally shows the critical Λ_c, where the divergence occurs.

It is possible to perform similar calculations for small $t' \neq 0$ as well. Results are similar, the area where the system is anti-ferromagnetic is smaller.

A first impression one gets from these results is that the Hubbard model is never a Fermi liquid. It is either a anti-ferromagnet or a super-conductor. The reason is that the results shown here hold only for low temperatures. For higher temperatures the super-conductor becomes unstable. Only at half filling one may expect that the anti-ferromagnet remains stable for somewhat higher temperatures.

On the other hand it should be made clear that all the calculations presented here have a systematic problem. The renormalisation group equations have been calculated up to second order. This is justified if the interaction is small. But here, we obtain a divergence. Close to the divergence, the interaction is no longer small.

This problem occurs in almost all approaches to the Hubbard model. Often it is not clear whether an approx-

Figure 3.5: Phase diagram for the Hubbard model with small interaction U and close to half filling, $t' = 0$, as obtained from the numerical renormalization group calculations.

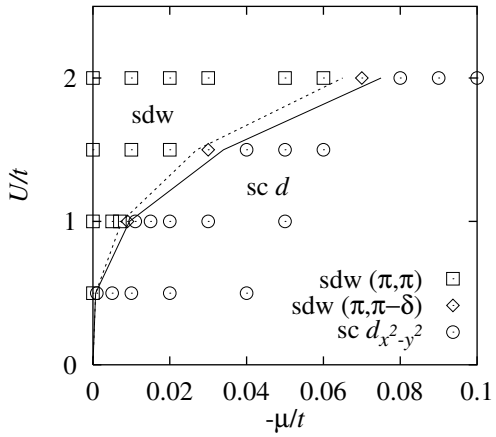
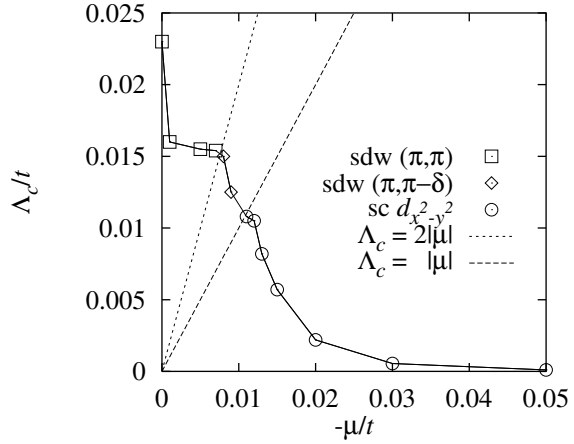


Figure 3.6: The critical Λ_c, where the divergence occurs.



imation is valid or not. A complete picture can only be obtained if several independent approaches are used and if they yield consistent results. Furthermore, exact results are important land marks.

4 The Hubbard model

This chapter is taken from [53]. The emphasis lies on rigorous results for the Hubbard model.

The Hamiltonian of the Hubbard model is given by

$$H = H_{\text{kin}} + H_{\text{int}} = \sum_{x,y\in V,\sigma} t_{xy} c^\dagger_{x,\sigma} c_{y,\sigma} + \sum_x U_x c^\dagger_{x\uparrow} c^\dagger_{x\downarrow} c_{x\downarrow} c_{x\uparrow} \tag{4.1}$$

The model was proposed independently by J. Hubbard [25] for the description of transition metals, by J. Kanamori [28] for the description of itinerant ferromagnetism, and by M.C. Gutzwiller [19] for the description of the metal-insulator transition. In Chemistry, the model is popular as well, and was introduced ten years earlier [58, 60]. Under the name Pariser-Parr-Pople model it has been used to describe extended π-electron systems.

Typically, one assumes that the vertex set V forms a translationally invariant lattice and that U_x is independent of x, *i.e.* $U_x = U$. But more general settings are possible. Especially in the quantum chemical context, V is just a general graph, t_{xy} and U_x depend on the lattice sites.

On a regular lattice, one often assumes nearest neighbour hopping, *i.e.* $t_{xy} = t$ for nearest neighboured sites, $|x-y| = 1$, $t_{xy} = 0$ otherwise. Sometimes, a next nearest neighbour hopping $t_{xy} = t'$ for $|x-y| = 2$ is introduced. In Sect. 3.4 we saw that such a next nearest neighbour hopping may change the physical behaviour of the system drastically.

For small U and in two or more dimensions, one expects that the Hubbard model describes a Fermi liquid. Typically, one is interested in the case where the model describes strongly interacting electrons, *i.e.* correlated electrons. In that situations, the interaction U is as large as or larger than typical values of t_{xy}.

For a general overview on the Hubbard model and on correlated Fermions in general I refer to the book of Fulde [15]. An overview on rigorous results for the Hubbard model can be found in the article of Lieb [40], an overview on ferromagnetism in the Hubbard model in [72].

4.1 Symmetries of the Hubbard model

The Hubbard model has several symmetries:

Gauge symmetry:

$$c^\dagger_{x\sigma} \to \exp(i\alpha) c^\dagger_{x\sigma}, \quad c_{x\sigma} \to \exp(-i\alpha) c_{x\sigma} \tag{4.2}$$

The Hamiltonian remains invariant if this transformation is applied. As a consequence, the particle number $N_e = \sum_{x\sigma} c^\dagger_{x\sigma} c_{x\sigma}$ is conserved. This is a generic property of almost all models in condensed matter theory which describe fermions.

Spin symmetry: With the help of the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4.3}$$

we define local

$$S_{\alpha,x} = \frac{1}{2} \sum_{\sigma,\sigma'} c^\dagger_{x\sigma} (\sigma_\alpha)_{\sigma,\sigma'} c_{x\sigma'}, \quad \alpha = x,y,z, \quad \mathbf{S}_x = (S_{x,x}, S_{y,x}, S_{z,x}) \tag{4.4}$$

and global spin operators.

$$S_\alpha = \sum_x S_{\alpha,x}, \quad \mathbf{S} = (S_x, S_y, S_z) \tag{4.5}$$

Often one uses

$$S_\pm = S_x \pm i S_y, \quad S_+ = \frac{1}{2}\sum_{\vec{n}} c^\dagger_{x\uparrow} c_{x\downarrow}, \quad S_- = S_+^\dagger \tag{4.6}$$

These operators form an $SU(2)$ algebra. The Hamiltonian commutes with these operators, it has a $SU(2)$ -symmetry. We have

$$[S_x, S_y] = i S_z \tag{4.7}$$

H, $\mathbf{S}^2$ and S_z can be diagnosed simultaneously. We denote the eigenvalues of $\mathbf{S}^2$ as $S(S+1)$, where S is the spin of the eigenstate. $S \propto N_e$, *i.e.* an extensive value for S means that the state is ferro- or ferri-magnetic.

Particle-hole transformations: Using the transformation

$$c^\dagger_{x\sigma} \to c_{x\sigma}, \quad c_{x\sigma} \to c^\dagger_{x\sigma} \tag{4.8}$$

the Hamiltonian becomes

$$\begin{aligned} H \to H' &= \sum_{x,y,\sigma} t_{xy} c_{x\sigma} c^\dagger_{y\sigma} + U \sum_x c_{x\uparrow} c_{x\downarrow} c^\dagger_{x\downarrow} c^\dagger_{x\uparrow} \\ &= -\sum_{x,y,\sigma} t_{xy} c^\dagger_{y\sigma} c_{x\sigma} + U \sum_x (1 - c^\dagger_{x\uparrow} c_{x\uparrow})(1 - c^\dagger_{x\downarrow} c_{x\downarrow}) \\ &= -\sum_{x,y,\sigma} t_{xy} c^\dagger_{x\sigma} c_{y\sigma} + U \sum_x c^\dagger_{x\uparrow} c^\dagger_{x\downarrow} c_{x\downarrow} c_{x\uparrow} + U(|V| - N_e) \end{aligned} \tag{4.9}$$

$|V|$ is the number of vertices.

Thus, the particle hole transformation is not a symmetry, but it can be used to obtain eigenstates from other eigenstates.

For a bipartite lattice, *i.e.* a lattice, which decays into two sub-lattices A and B so that $t_{xy} = 0$ if both x and y belong to the same sub-lattice, it is possible to introduce the following transformation:

$$c^\dagger_{x\sigma} \to c^\dagger_{x\sigma} \text{ if } x \in A, \quad c^\dagger_{x\sigma} \to -c^\dagger_{x\sigma} \text{ if } x \in B \tag{4.10}$$

This transformation changes the sign of the kinetic energy. Applying this transformation together with the particle-hole transformation at half filling (*i.e.* $N_e = |V|$) maps the Hamiltonian onto itself. Thus, we have another symmetry for this class of lattices, a particle-hole symmetry.

The transformation (4.10) alone is of some importance since it can be used to change the sign of the hopping matrix elements. Typically, it is assumed that $t_{xy} < 0$ is the natural choice of the sign, at least for nearest neighbours. For bipartite lattices the sign can be changed. In general, the assumption $t_{xy} < 0$, although popular, has no compelling reason. [37]

On bipartite lattices at half filling, one can use the particle-hole symmetry to obtain a second $SU(2)$ symmetry. The generators are

$$\hat{S}_z = \frac{1}{2}(N_e - |V|), \quad \hat{S}_+ = \sum_{x\in A} c^\dagger_{x\uparrow} c^\dagger_{x\downarrow} - \sum_{x\in B} c^\dagger_{x\uparrow} c^\dagger_{x\downarrow}, \quad \hat{S}_- = \hat{S}_+^\dagger \tag{4.11}$$

These generators can be obtained from the original $SU(2)$ generators by performing a particle-hole transformation together with a transformation of type (4.10) for spin down only. The model has thus a $SU(2) \times SU(2) = SO(4)$ symmetry at half fillings. In discussions concerning high temperature superconductivity, even an approximate $SO(5)$-symmetry has been proposed.

The additional symmetry of the Hubbard model on a bipartite lattice at half filling ($N_e = |V|$) is essential for several of the rigorous results which are valid in this case. The two most important is Lieb's theorem [36], see Sect. 4.2.1, and the uniform density theorem, Sect. 4.2.5.

Lattice symmetries: On translationally invariant lattices, the model has the symmetries of the lattice.

The one-dimensional case: The one dimensional Hubbard model has an infinite set of invariants. A special form of the Bethe ansatz yields exact eigenstates of the Hamiltonian. This was first shown by E. Lieb and F. Wu [39]. The ground state is part of that Bethe ansatz eigenstates. Not all the eigenstates of the one-dimensional Hubbard model are Bethe ansatz states. But it was shown by Essler, Korepin, and Schoutens [8], that for even $|V|$, where the lattice is bipartite, all other eigenstates can be obtained by applying the operators $S_\pm$, $\hat{S}_\pm$ to the Bethe ansatz states.

For an exactly solvable model one should expect an infinite set of invariants. A first attempt to find those is a paper by Heilmann and Lieb [23]. Later Shastry [65], Olmedilla and Wadati [57], and Grosse [17] presented a large set of such invariants.

The one-dimensional Hubbard model has been investigated by many people, the literature is vast, and a complete overview would be a course in its own. I will not discuss the one-dimensional Hubbard model in this course.

4.2 Some rigorous results

Most of the rigorous results on the Hubbard model concern the magnetic behaviour in the ground state, *i.e.* at $T = 0$. I discuss the most important rigorous result in the following subsections.

For each of the theorems mentioned below I try to explain the main idea of the proof. For the mathematical details I refer to the original papers.

4.2.1 Lieb's Theorem

In 1989, E. Lieb [36] proved an important theorem and an even more important corollary on the Hubbard model. The theorem is about the attractive Hubbard model. It holds for arbitrary hoppings t_{xy}, with the only assumption that the graph of the hopping matrix is connected. The interaction U_x may depend on x.

Theorem (Lieb 1989) Let H be the Hamiltonian in (4.1) with real t_{xy}, the graph of $T = (t_{xy})$ should be connected, and negative $U_x < 0$. Let the particle number N_e be even. Then, the ground state is unique and has a total spin $S = 0$.

For the proof, I refer to the original paper by Lieb. He uses a technique called spin reflection positivity. For some details see the remarks below.

On a bipartite lattice, using a particle-hole transformation for spin-down only, together with a transformation (4.10), the kinetic energy remains the same but the signs of U_x are switched. In that way, one can obtain a result for the repulsive Hubbard model. Since S_z with the above transformation transforms to $\hat{S}_z$, one obtains a result for $\hat{S}_z = 0$, *i.e.* $N_e = |V|$, *i.e.* half filling. Therefore, the following corollary holds

Corollary Let H be the Hamiltonian in (4.1) with real t_{xy}, the graph of t_{xy} should be connected and bipartite, and positive $U_x = U > 0$. Let the particle number $N_e = |V|$. Then, the ground state is unique in the subspace $S_z = 0$. The total spin is $S = \frac{1}{2}||A| - |B||$.

The last statement $S = \frac{1}{2}||A| - |B||$ does not follow directly from the theorem because the theorem makes no statement about $\hat{S}$. It can be understood in two ways.

The first is to look at weak interactions. For a bipartite lattice, the spectrum of $T = (t_{xy})_{xy \in V}$ is symmetric with respect to 0. For any eigenvalue ε there exists an eigenvalue $-\varepsilon$. Half filling now means that for arbitrary weak interaction all single particle eigenstates with energies $\varepsilon < 0$ are completely filled with two electrons and that the eigenstates with $\varepsilon = 0$ are filled with one electron. For the latter, Hund's rule [50] applies which means that all electrons have the same spin. The degeneracy of the eigenvalue 0 is $||A| - |B||$, therefore we obtain the a total spin $S = \frac{1}{2}||A| - |B||$.

The second idea is to look at strong interactions and to use a unitary transformation $\exp(R)$ to transform the Hamiltonian to a form where the number of doubly occupied sites is conserved. The ansatz is

$$R = \sum_{x,y,\sigma} s_{x,y,\sigma} c^\dagger_{x,\sigma} c_{y,\sigma} \tag{4.12}$$

We assume that U is large and expand $\exp(R) H \exp(-R)$ to obtain

$$H \to H_{\text{int}} + H_{\text{kin}} + [R, H_{\text{int}}] + [R, H_{\text{kin}}] + \frac{1}{2}[R,[R,H_{\text{int}}]] + \cdots \tag{4.13}$$

The kinetic energy H_{kin} can be written as

$$H_{\text{kin}} = H_{\text{kin},0} + H_{\text{kin},1} \tag{4.14}$$

$H_{\text{kin},0}$ does not change the number of doubly occupied sites, $H_{\text{kin},1}$ changes it by ± 1. We have

$$H_{\text{kin},1} = \sum_{x,y,\sigma} t_{xy} (n_{x,-\sigma} - n_{y,-\sigma})^2 c^\dagger_{x,\sigma} c_{y,\sigma} \tag{4.15}$$

We choose R so that

$$H_{\text{kin},1} + [R, H_{\text{int}}] = 0 \tag{4.16}$$

This yields

$$H \to H_{\text{eff}} = H_{\text{int}} + H_{\text{kin},0} - \frac{1}{2}[R,[R,H_{\text{int}}]] + \cdots \tag{4.17}$$

We have

$$[R, H_{\text{int}}] = -U \sum_{x,y,\sigma} r_{x,y,\sigma} (n_{x,-\sigma} - n_{\vec{n}y,-\sigma}) c^\dagger_{x,\sigma} c_{y,\sigma} \tag{4.18}$$

and therefore

$$r_{x,y,\sigma} = \frac{t_{xy}}{U} (n_{x,-\sigma} - n_{y,-\sigma}) \tag{4.19}$$

Let P_0 be the projector onto states for which each site is occupied by one electron, which is the ground state at half filling and U arbitrarily large. If we restrict the Hilbert space to these states, we get

$$\begin{aligned}
H_{\text{eff}} &= P_0 R H R P_0 \\
&= U P_0 R^2 P_0 \\
&= U P_0 \sum_{x,y,\sigma} \frac{t_{xy}}{U} (n_{x,-\sigma} - n_{y,-\sigma}) c^\dagger_{x,\sigma} c_{y,\sigma} \sum_{x',y',\sigma'} \frac{t_{x',y'}}{U} (n_{x',-\sigma'} - n_{y',-\sigma'}) c^\dagger_{x,\sigma'} c_{y',\sigma'} P_0 \\
&= -\frac{1}{U} P_0 \sum_{x,y,\sigma,\sigma'} t^2_{xy} c^\dagger_{x,\sigma} c_{y,\sigma} c^\dagger_{y,\sigma'} c_{x,\sigma'} P_0 \\
&= \frac{1}{U} P_0 \sum_{x,y,\sigma,\sigma'} t^2_{xy} c^\dagger_{x,\sigma} c_{y,\sigma'} c^\dagger_{y,\sigma'} c_{x,\sigma} P_0 - \frac{1}{U} \sum_{\vec{n},\vec{n}'} t^2_{xy} \\
&= \sum_{x,y} \frac{2t^2_{xy}}{U} \mathbf{S}_x \cdot \mathbf{S}_y P_0 \\
&\quad + \frac{1}{U} P_0 \sum_{x,y,\sigma,\sigma'} t^2_{xy} c^\dagger_{x,\sigma} c_{x,\sigma} c^\dagger_{y,\sigma'} c_{y,\sigma'} P_0 - \frac{1}{U} \sum_{x,y} t^2_{xy} \\
&= \sum_{x,y} \frac{2t^2_{xy}}{U} \mathbf{S}_x \cdot \mathbf{S}_y P_0
\end{aligned} \tag{4.20}$$

This transformation is of importance in its own. It shows that the Hubbard model at half filling and for large U can be mapped to the anti-ferromagnetic Heisenberg model. For the corollary above it has the consequence

that the total spin of the Hubbard model at half filling and for large U is the same as for the Heisenberg model, therefore $S = \frac{1}{2}||A| - |B||$.

Since the ground state is unique for all U, it is sufficient to know the total spin S for small or large U, due to the uniqueness it cannot change.

Lieb's theorem suggests anti-ferromagnetism or ferrimagnetism (depending on whether the two sub-lattices A and B have the same size or not) for the Hubbard model at half filling. But, whereas for the anti-ferromagnetic Heisenberg model long-range order was proven in two dimensions in the ground state and in three dimensions for sufficiently low temperatures, there is no proof for long-range order for the Hubbard model up to now. The methods to prove long-range order for the Heisenberg model cannot be applied to the Hubbard model. The simple reason is that the Hubbard model is richer much more complicated and allows for a much larger number of phenomena. Nevertheless, many results including the renormalisation results (see Sect. 3.4) indicate the existence of long range order for large U.

Lieb's proof uses the fact that for an even number of fermions, there is always a ground state with $S_z = 0$ due to the $SU(2)$ spin symmetry. This means that the ground state can be written in the form $\psi = \sum_{\alpha,\beta} W_{\alpha\beta} \psi_{\alpha,\uparrow} \psi_{\beta,\downarrow}$ where $\psi_{\alpha,\sigma}$ form a orthonormal basis of multi-particle states with $N_e/2$ particles with spin σ. Since t_{xy} and U_x are real, one can assume that the matrix W is self adjoined. The expectation value of the Hamiltonian in the state ψ can be written as a quadratic form $E(W)$ in W and it can be shown that for non-positive interactions $E(W) \geq E(|W|)$. $|W|$ is the positive semi-definite matrix satisfying $W^2 = |W|^2$. It is then easy to see that the ground state corresponding to $|W|$ has $S = 0$. The uniqueness is shown by assuming that a second ground state with some W exists. Then, $R = |W| - W$ is a ground state as well. Some lengthy but easy to understand argument which uses the fact that the graph of T is connected then shows that $W = \pm|W|$ and therefore that the ground state is unique. Compared to many other proofs, Lieb's proof is very elegant and compact, only somewhat more than one page in a letter. I recommend to read it to everybody.

4.2.2 The Mermin-Wagner Theorem

The term Mermin-Wagner Theorem is usually used for a huge class of theorems which state that for lattice models in one or two space dimensions with a continuous symmetry, like an $SU(2)$ symmetry, there is no long range order at finite temperature. Originally, Mermin and Wagner [44] showed in 1966 that in the one- or two-dimensional Heisenberg model there is no long-range order, neither anti-ferromagnetic nor ferromagnetic. This result was extended to the Hubbard model by Walker and Ruijgrok 1968 [75] and by Ghosh 1971 [16]. Further, Hohenberg [24] showed 1967 that there cannot be superconductivity or long range crystalline order in one or two dimensions. The proof for the Hubbard model was considerably simplified and somewhat extended by Koma and Tasaki [32].

The original proof by Mermin and Wagner

Mermin and Wagner consider the Heisenberg model

$$H = -\sum_{x,y \in V} J_{xy} \vec{S}_x \cdot \vec{S}_y - h \sum_{x \in V} S_{x,z} s_x \tag{4.21}$$

with a magnetic field h in z-direction. For the ferromagnetic case they choose $s_x = 1$ for all $x \in V$, for anti-ferromagnetism they choose $s_x = \pm 1$ for the two sublattices of the anti-ferromagnet. The interaction has to be of finite range. We write $s_x = \exp(-i\vec{K} \cdot \vec{r}_x)$. For the ferromagnetic case, $\vec{K} = 0$.

For a two-dimensional lattice with lattice sites V they show that

$$|s_z| < \frac{\text{const.}}{T^{1/2}} \frac{1}{|\ln |h||^{1/2}} \tag{4.22}$$

and in one dimension

$$|s_z| < \frac{\text{const.}}{T^{2/3}} |h|^{2/3} \tag{4.23}$$

where $s_z = S_z/|V|$ is the z component of the total spin per lattice site.

To show these result, they make use of the Bogoliubov inequality.

$$\frac{1}{2}\langle [A,A^\dagger]_+\rangle\langle [[C,H],C^\dagger\rangle \geq k_B T|\langle [C,A]\rangle|^2 \tag{4.24}$$

Here, $\langle X\rangle$is the usual expectation value at finite temperature, i.e.

$$\langle X\rangle = \frac{1}{Z}\mathrm{Tr}X\exp(-\beta H) \tag{4.25}$$

where $\beta = 1/k_B T$ is the inverse temperature and $Z = \mathrm{Tr}\exp(-\beta H)$ is the partition function. The Bogoliubov inequality holds for any operators for which the expectation values are defined.

To prove the Bogoliubov inequality, we first introduce

$$(A,B) = \sum_{i,j}{}' \langle i|A|j\rangle^* \langle i|B|j\rangle \frac{w_i - w_j}{E_i - E_j} \tag{4.26}$$

Here, i denote the eigenstates of H, E_i are the eigenvalues, and $w_i = Z^{-1}\exp(-\beta E_i)$. The sum excludes pairs of states with the same energy. First, note that

$$0 < \frac{w_i - w_j}{E_i - E_j} < \frac{1}{2}\beta(w_i + w_j) \tag{4.27}$$

and therefore

$$(A,A) \leq \frac{1}{2}\beta\langle [A,A^\dagger]_+\rangle \tag{4.28}$$

Further, (A,B) satisfies all the properties of an inner product and therefore fulfils Schwartz inequality

$$(A,A)(B,B) \geq |(A,B)|^2 \tag{4.29}$$

The Bogoliubov inequality now follows if one chooses $B = [C^\dagger, H]$.

Let us now apply the Bogoliubov inequality to prove the Mermin-Wagner theorem. We assume translational invariance and introduce the Fourier transformed quantities

$$\vec{S}(\vec{k}) = \sum_{x\in V}\exp(-i\vec{k}\cdot\vec{r}_x)\vec{S}_x \tag{4.30}$$

$$J(\vec{k}) = \sum_{x\in V}\exp(-i\vec{k}\cdot(\vec{r}_x - \vec{r}_0)J_{0x} \tag{4.31}$$

for some arbitrary lattice site 0. $\vec{r}_x$ is the vector pointing to the lattice site x. The back transformation is

$$\vec{S}_x = \frac{1}{|V|}\sum_{\vec{k}}\exp(i\vec{k}\cdot\vec{r}_x)\vec{S}(\vec{k}) \tag{4.32}$$

$$J_{xy} = \frac{1}{|V|}\sum_{\vec{k}}\exp(i\vec{k}\cdot(\vec{r}_x - \vec{r}_y))J(\vec{k}) \tag{4.33}$$

where the sums are taken over the first Brillouin zone.

We now use Bogoliubov's inequality with $C = S_+(\vec{k})$ and $A = S_-(-\vec{k}-\vec{K})$. We obtain

$$\begin{aligned}\frac{1}{2}\langle [S_x(\vec{k}+\vec{K}), S_-(-\vec{k}-\vec{K})]_+\rangle \quad &\geq \quad |V|^2 k_B T s_z \left\{ \frac{1}{|V|}\sum_{\vec{k}'}[J(\vec{k}) - J(\vec{k}'-\vec{k})]\right. \\ &\times \quad \left.\langle S_z(-\vec{k}')S_z(\vec{k}') + \frac{1}{4}[S_+(\vec{k}'), S_-(-\vec{k}')]_+\rangle + \frac{|V|}{2}hs_z\right\}^{-1}\end{aligned} \tag{4.34}$$

The term in the curly bracket can be estimated by

$$\begin{aligned}\frac{1}{|V|}|\sum_x J_x(1-\exp(i\vec{k}\cdot\vec{r}_x)\sum_{\vec{k}'}\exp(-i\vec{k}'\cdot\vec{r}_x)\langle S_z(-\vec{k}')S_z(\vec{k})+\frac{1}{4}[S_+(\vec{k}'),S_-(-\vec{k}')]+\frac{|V|}{2}hs_z \\ <|V|\sum_x|J_x|(1-\cos(\vec{k}\cdot\vec{r}_x))S(S+1)+\frac{|V|}{2}hs_z \\ <\frac{1}{2}|V|[\sum_x \vec{r}_x{}^2|J_x|k^2S(S+1)+hs_z] \end{aligned} \tag{4.35}$$

Replacing the curly bracket by this upper bound and summing over $\vec{k}$ one obtains

$$S(S+1)>2k_BTs_z^2\frac{1}{|V|}\sum_{\vec{k}}[S(S+1)\sum_{x\in V}\vec{r}_x{}^2|J_x|k^2+hs_z] \tag{4.36}$$

Taking the thermodynamic limit, we replace the sum by an integral over a sphere that is entirely contained in the first Brillouin zone. The we obtain in two dimensions

$$s_z^2<\frac{\text{const.}}{k_BT}\frac{\omega}{\ln(1+\omega/|hs_z|}) \tag{4.37}$$

and in one dimension

$$s_z^3<\text{const.}\left(\frac{(|\mathrm{h}|\omega)^{1/2}}{2\mathrm{k_B}\mathrm{T}\tan^{-1}(\omega/|\mathrm{hs_z}|)^{-1/2}}\right) \tag{4.38}$$

which, for small $|h|$ yield (4.22) and (4.23).

Generalisations

Already Mermin and Wagner noted that their proof can be extended to show the absence of long-range crystalline order in one or two dimensions. Walker and Ruijgrok 1968 [75] and Ghosh 1971 [16] extended the result to Hubbard type models, i.e. electrons moving on a lattice with a short-ranged (screened) Coulomb interaction. Further, Hohenberg [24] showed 1967 that there cannot be superconductivity or long range crystalline order in one or two dimensions.

The Theorem was extended to yield limits for the correlation functions. The result by Mermin and Wagner only show that there is no long-range order. More interesting is to understand how the correlation functions decay. The most general result is by Koma and Tasaki. Their proof uses a different method to proof the bounds, which was first used by McBryan and Spencer [43].

Theorem (Koma, Tasaki 1992) For a Hubbard model in one and two dimensions with finite range hopping (*i.e.* $t_{xy}=0$ if the distance $|x-y|$ lies above some finite value) in the thermodynamic limit, the following bounds hold for the correlation functions

$$|\langle c_{x\uparrow}^\dagger c_{x\downarrow}^\dagger c_{y\downarrow}c_{y\uparrow}\rangle|\le\begin{cases}|x-y|^{-\alpha f(\beta)} & \text{for } d=2\\ \exp(-\gamma f(\beta)|x-y|) & \text{for } d=1\end{cases} \tag{4.39}$$

$$|\langle \mathbf{S}_x\cdot\mathbf{S}_y\rangle|\le\begin{cases}|x-y|^{-\alpha f(\beta)} & \text{for } d=2\\ \exp(-\gamma f(\beta)|x-y|) & \text{for } d=1\end{cases} \tag{4.40}$$

for some $\alpha>0$, $\gamma>0$, $f(\beta)>0$ where $\langle.\rangle$ denotes the expectation value at inverse temperature β and $f(\beta)$ is a decreasing function of β which behaves like $f(\beta)\approx 1/\beta$ for $\beta\gg\beta_0$ and $f(\beta)\approx(2/\beta_0)|\ln(\beta)|$ for $\beta\ll\beta_0$. β_0 is some constant.

This result rules out long-range spin-order or superconductivity at finite temperatures in one or two dimensions. The power laws for $d=2$ are certainly not optimal for high temperatures, where one expects an exponential decay of correlation functions. But they are sufficient to exclude long-range order.

Having a power law decay at low temperatures in two dimensions and an exponential decay at large temperatures means that there must be a transition between the two. This transition is called Kosterlitz-Thouless transition [43]. It may occur in two dimensions.

The interesting point of the proof of Koma and Tasaki is that it only needs a $U(1)$ symmetry. Thus, any lattice model with a $U(1)$ symmetry in one or two dimensions cannot have superconducting or magnetic long-range order at finite temperature in one or two dimensions.

The term Mermin-Wagner Theorem is usually used for a huge class of theorems which state that for lattice models in one or two space dimensions with a continuous symmetry, like an $SU(2)$ symmetry, there is no long range order at finite temperature. Originally, Mermin and Wagner [44] showed in 1966 that in the one- or two-dimensional Heisenberg model there is no long-range order, neither anti-ferromagnetic nor ferromagnetic. This result was extended to the Hubbard model by Walker and Ruijgrok 1968 [75] and by Ghosh 1971 [16]. Further, Hohenberg [24] showed 1967 that there cannot be superconductivity or long range crystalline order in one or two dimensions. The proof for the Hubbard model was considerably simplified and somewhat extended by Koma and Tasaki [32].

Theorem (Koma, Tasaki 1992) For a Hubbard model in one and two dimensions with finite range hopping (*i.e.* $t_{xy} = 0$ if the distance $|x-y|$ lies above some finite value) in the thermodynamic limit, the following bounds hold for the correlation functions

$$|\langle c^\dagger_{x\uparrow} c^\dagger_{x\downarrow} c_{y\downarrow} c_{y\uparrow}\rangle| \leq \begin{cases} |x-y|^{-\alpha f(\beta)} & \text{for } d=2 \\ \exp(-\gamma f(\beta)|x-y|) & \text{for } d=1 \end{cases} \tag{4.41}$$

$$|\langle \mathbf{S}_x \cdot \mathbf{S}_y\rangle| \leq \begin{cases} |x-y|^{-\alpha f(\beta)} & \text{for } d=2 \\ \exp(-\gamma f(\beta)|x-y|) & \text{for } d=1 \end{cases} \tag{4.42}$$

for some $\alpha > 0$, $\gamma > 0$, $f(\beta) > 0$ where $\langle . \rangle$ denotes the expectation value at inverse temperature β and $f(\beta)$ is a decreasing function of β which behaves like $f(\beta) \approx 1/\beta$ for $\beta \gg \beta_0$ and $f(\beta) \approx (2/\beta_0)|\ln(\beta)|$ for $\beta \ll \beta_0$. β_0 is some constant.

This result rules out long-range spin-order or superconductivity at finite temperatures in one or two dimensions. The power laws for $d = 2$ are certainly not optimal for high temperatures, where one expects an exponential decay of correlation functions. But they are sufficient to exclude long-range order. This means that a Kosterlitz-Thouless transition may occur. [43].

The interesting point of the proof is that it only needs a $U(1)$ symmetry. Thus, any lattice model with a $U(1)$ symmetry in one or two dimensions cannot have superconducting or magnetic long-range order at finite temperature in one or two dimensions.

The older proof of Ghosh [16] uses the $SU(2)$ spin symmetry and the Bogoliubov inequality and is easy to understand.

The result by Koma and Tasaki is more general, their proof uses a method developed by McBryan and Spencer [43] for classical spin systems and its extension to quantum spin systems by Ito [26]. The proof uses the fact that for an arbitrary observable A one has $\mathrm{Tr}(A\exp(-\beta H)) = \mathrm{Tr}(G(\theta)AG(\theta)^{-1}\exp(-\beta G(\theta)HG(\theta)^{-1}))$. $G(\theta)$ is a local transformation. The right hand side can be bounded using some standard inequalities, namely the Schwartz inequality stating that for hermitian matrices O and P one has $\mathrm{Tr}(\mathrm{OP}) \leq (\mathrm{Tr}(O^*O)\mathrm{Tr}(P^*P))^{1/2}$, and the Golden-Symanzik-Thompson inequality $\mathrm{Tr}\exp(O+P) \leq \mathrm{Tr}(\exp(O)\exp(P))$. Suitable choices for A and $G(\theta)$ then yield the bounds.

In one dimension, with nearest neighbour hopping only, and for finite U_x, the Lieb-Mattis theorem [38] says that the minimal energy in the subspace with fixed spin S is strictly lower than the minimal energy in the subspace with $S+1$. This clearly rules out ferromagnetism in one dimension in the ground state.

4.2.3 Nagaoka's Theorem

The so called Nagaoka Theorem was actually first proven by Thouless [73] 1965 for some special bipartite lattices. The proof of Nagaoka [55], only one year later, is more general and applies to non-bipartite lattices as

well. Therefore, the result is called Nagaoka theorem today. The most general proof is due to Tasaki [68]. It states the following:

Theorem (Tasaki 1989) The Hubbard model (4.1) with non-negative t_{xy}, $N_e = |V| - 1$, and a hard-core repulsion $U_x = \infty$ for all $x \in V$ has a ground state with a total spin $S = \frac{1}{2}N_e$. The ground state is unique except for the usual $(2S+1)$-fold spin degeneracy provided a certain connectivity condition for t_{xy} holds.

This theorem is remarkable, because it states that there is a unique ferromagnetic ground state in the vicinity of half filling, where an anti-ferromagnetic spin order is assumed to be present.

The proof of the theorem uses the Schwarz inequality to show that a ferromagnetic ground state exists. To show the uniqueness, it uses the Perron-Frobenius theorem, which states that for a matrix with only non-negative entries and for which the graph is connected (the matrix is irreducible), the eigenstate with the largest eigenvalue is unique and has non-negative entries. The theorem can be applied here by finding a suitable basis for the multi-particle Hilbert space of the Hubbard model. The connectivity condition in the theorem ensures that the graph of the Hamiltonian in that basis obeys the irreducibility needed in the Perron-Frobenius theorem. Essentially it states that by the hopping of particles, arbitrary permutations of the particles can be realised. This holds for almost any lattice except the one-dimensional chain.

The Nagaoka theorem made people believe that for many lattices, *e.g.* as well for hyper-cubic lattices, a large region in the parameter space (U large and a density close to but not at half filling) exists where the Hubbard model has ferromagnetic ground states. But any attempt to prove that failed so far. Instead, many variational calculations by various groups mainly in the early 90s showed that the Nagaoka state is not very stable. Changing the conditions a bit, either putting more than one hole in the system or lowering U causes the Nagaoka state to become unstable against single spin flips, *i.e.* $E(S = N_e/2 - 1) < E(S = N_e/2)$ (for details see *e.g.* [66]). Exact diagonalisations of small systems yield the same result. On the other hand, for some special non-bipartite lattices, these calculations indicate that the Nagaoka state may be more stable and that a larger region in the parameter space exists where the ground state is ferromagnetic.

4.2.4 Flat-band systems

A first example of a lattice having a flat band is a bipartite lattice with $|A| = n|B|$. A simple example which Lieb [36] used as an illustration for his theorem is the quadratic lattice with additional lattice sites on each edge. If there is only nearest neighbour hopping, the original lattice sites of the quadratic lattice form one of the sub-lattices, say B and the new lattice sites form the second sub-lattice A. There are twice as many lattice sites on A than on B. Each elementary cell contains one lattice site from B and two from A, in total three. We have thus a three band model. Since the lattice is bipartite, the single particle spectrum is symmetric with respect to 0. There is one energy band in the centre which is completely flat. The flat band causes the extensive magnetisation $S = \frac{1}{2}||A| - |B|| = \frac{1}{2}|B|$, as we pointed out already in Sect. 4.2.1. Since this magnetisation is related to the existence of two sub-lattices, the system is ferrimagnetic.

Two years after Lieb first examples of lattices with a flat band at the bottom of the spectrum were published [47, 46, 48, 69, 54]. One class of such lattices are line graphs, the other are decorated lattices. Since the construction of a line graph is elementary and since we need it later, we give a more detailed description here.

Let $G = (V, E)$ be a graph with a vertex set V and an edge set E. Any lattice can be regarded as a graph. The lattice sites are the vertices and there are edges between two vertices if there is a non-vanishing hopping matrix element connecting the two. If we allow only for nearest neighbour hopping, the hopping matrix is (up to a factor t) the adjacency matrix $A(G) = (a_{xy})_{xy \in V}$ of the graph. $a_{xy} = 1$ if $\{x, y\} = e \in E$ is an edge of the graph, 0 otherwise.

The line graph $L(G)$ of a graph G is constructed as follows: The vertex set $V(L(G))$ of the line graph is the edge set $E(G)$ of the original graph and two vertices of the line graph are connected, if the corresponding edges in G have a vertex in common.

Figure (4.1) shows an illustration of the construction of a line graph. Let G be a part of the hexagonal lattice, as shown in black. Now we put a new vertex in the middle of each edge and connect two new vertices if the edges of the original hexagonal lattice have a vertex in common. This procedure yields a new lattice build of

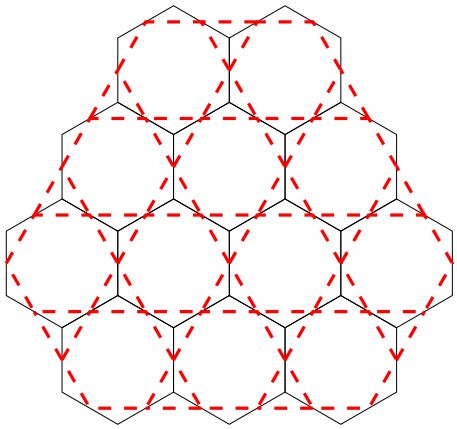


Figure 4.1: The kagomé lattice (red, dashed) as the line graph of the hexagonal lattice (black).

hexagons surrounded by triangles, shown in red. The new lattice constructed that way is the line graph of the hexagonal lattice, it is called kagomé lattice. You may take any lattice or even any graph G and construct the line graph in that way.

Let us now investigate the spectral properties of the adjacency matrix $A(L(G))$ of a line graph. To do this, we first introduce a new matrix $B(G) = (b_{xe})_{x\in V, e\in E}$, the so called edge vertex incidence matrix. The matrix elements $b_{xe} = 1$ if the edge e connects to the vertex x, $b_{xe} = 0$ otherwise. Note that B has $|V|$ columns and $|E|$ rows. Except for a graph without loops or with only one loop, $|E| > |V|$ and the kernel of B has a dimension $\geq |E| - |V|$. The adjacency matrix of the line graph and the incidence matrix of the original graph are related via $A(L(G)) = B(G)^t B(G) - 2$. As a consequence, -2 is a lower bound of the spectrum of $A(L(G))$ and becomes the lowest eigenvalue with degeneracy at least $|E| - |V|$ if $|E| > |V|$. In fact, one can show that the degeneracy is $N_d = |E| - |V| + 1$ if G is bipartite and connected, $N_d = |E| - |V|$ if G is not bipartite and connected.

This fact can now be applied to a lattice. If G is a translationally invariant lattice with one or more energy bands, $L(G)$ is a lattice as well and the lowest energy band lies at energy $-2t$ and is completely flat. A lattice which is a line graph, *e.g.* the kagomé lattice, has a lowest flat band. This makes it easy to construct ground states of the Hubbard model, at least for $N_e \leq N_d$. In that case any state with all electrons having the same spin is a ground state, since this state minimises both the kinetic energy and the interaction. This construction is indeed trivial. The interesting question is whether or not there are other ground states and whether or not they can be characterised completely. This is indeed possible for $N_e = N_d$ as the following theorem shows [46, 47]:

Theorem (Mielke 1991) Let H be the Hubbard model on a line graph $L(G)$ of a two-connected bipartite graph G or a three-connected graph G and let $N_e = N_d$, $U_x > 0$ for all x. Then the ground state has a spin $S = \frac{N_d}{2}$ and is unique up to the $(2S+1)$ -fold degeneracy due to the $SU(2)$ spin symmetry.

The kagomé lattice is obviously an example for this theorem.

The original proof of the theorem uses some graph theoretical notions. We will not present it here since later a more general and simpler result has been shown which does not use the notion of a line graph.

On the other hand, let us discuss the single particle ground states with energy $-2t$ a bit further since they serve for many easy illustrations we may need later. Let p be a self-avoiding closed path $(x_1, x_2, \ldots x_n)$ of even length n on G. It obviously translates to an even path on $L(G)$. Let us now construct the single particle state $\psi_p(e)$ as follows. $\psi_p(e) = 0$ if e lies not on p. On p, $\psi_p(e) = \pm 1$ with alternating sign for subsequent edges of G. It is easy to see that $B\psi_p = 0$. ψ_p is therefore a ground state of $A(L(G))$ with eigenvalue -2. It can be shown that these states form an over-complete basis of the eigenspace of the eigenvalue -2.

If G is a bipartite plane graph, like the hexagonal lattice, each face f is surrounded by a self-avoiding path, let us call it f as well. Let F be the set of faces. Due to Euler's theorem, $|F| = |E| - |V| + 2$. One of the faces is the outer face of the graph, there are exactly $|E| - |V| + 1$ inner faces. It is easy to see that the states ψ_f corresponding to the inner faces f are linearly independent. They thus form a basis (not orthonormal) of the

eigenspace of the ground state energy. Using this construction, it is possible to construct all ground states for $N_e \leq N_d$.

One year later, 1992, Tasaki [69] published a class of decorated lattices with lowest flat bands, for which he proved a similar result. In 1993 [54], we investigated these lattices further and showed how one can construct all ground states with $N_e \leq N_d$ for these decorated lattices. We further showed that for these lattices the characterisation of the ground states can be mapped to a percolation problem. This allows to show that the system remains ferromagnetic with an extensive but not saturated total spin S up to some critical density on that below that density the system is paramagnetic.

This construction is most easily understood for line graphs of planar bipartite graphs, see the kagomé lattice in Fig. 4.1 as an example. For these graphs, the faces yield the single particle ground state. The inner faces form a basis (not orthogonal). Neighboured faces of G have an edge in common. Therefore, putting electrons with different spin on neighboured faces may produce a double occupancy on that edge. This yields to a higher energy. To obtain a ground state, electrons on neighboured faces should have the same spin. But if $N_e < N_d$ not all faces are occupied and one may form non-touching clusters with total spins pointing in different directions. Constructing non-touching clusters of faces is a percolation problem on the dual graph of G. This percolation problem has a percolation threshold, above which one large extended cluster is formed. This cluster has an extensive spin, whereas all other finite clusters have a finite spin. Therefore, above the percolation threshold the system is ferromagnetic. The percolation problem is not the classical percolation problem since each cluster with a spin S has a $2S+1$ fold degeneracy.

After 1993, more classes of lattices with flat bands have been found and investigated. A general result, which covers all these cases, is available as well. It needs a condition on the projector $\rho = (\rho_{xy})_{x,y\in V}$ onto the space of single particle ground states [50, 49, 51].

Theorem (Mielke 1993, 1999) The Hubbard model with an N_d fold degenerate single particle ground state, $U_x > 0$, and $N_e \leq N_d$ electrons has a unique $(2S+1)$-fold degenerate ferromagnetic ground state with $S = N_d/2$ if and only if $N_e = N_d$ and ρ_{xy} is irreducible.

The original proof of this theorem was complicated and used a special construction for a non-orthonormal basis of single particle ground states. The later proof is simpler. First, the following result is shown:

Theorem (Mielke 1999) The Hubbard model with a N_d fold degenerate single particle ground state, $U_x > 0$, and $N_e \leq N_d$ electrons has a multi-particle ground state with $S < N_e/2 - 1$ if it has a single spin flip ground state with $S = N_e/2 - 1$.

In other words: To prove stability of ferromagnetism it is sufficient to show that there is no single spin flip ground state. This is indeed easy if $N_e = N_d$ and ρ_{xy} is irreducible. Therefore, the first theorem is a consequence of the second. Note that the second theorem is not trivial at all. For other lattices, you may easily construct cases where a ferromagnetic state is stable with respect to single spin flips but where it it nevertheless not the ground state of the system.

The last two results are very general, they hold for arbitrary lattices and arbitrary, even complex, hopping matrix elements t_{xy}. This is important because the flat band physics started to attract much attention in the past few years for mainly two reasons. First, using optical lattices it is now possible to investigate these systems experimentally. For instance the kagomé lattice was build using that technique by Jo *et al.* in 2012 [27]. Second, people became interested recently in so called topological flat bands. Here, the flat (often quasi flat) band arises from special choices for the phases of complex t_{xy}.

In 2003, Tanaka and Ueda [67] showed that for the special case of the kagomé lattice, the ferromagnetic ground states remains stable if one introduces a special perturbation that yields a small dispersion to the lowest flat band, provided U is not too small. Similarly, Tasaki [71] showed in 1996, that for some decorated lattices the ferromagnetic ground state remains stable. These results are important because they indicate that flat band ferromagnetism is not something exotic like the Nagaoka ferromagnet.

Another interesting question arises what happens if ρ_{xy} is not irreducible. Batista and Shastry [6] were the first to investigate an example for such a lattice, today many examples are known. One can show the following general results [52]:

Let ρ have the following properties:

1. ρ is reducible. It can be decomposed into N_r irreducible blocks ρ_k, $k = 1,\ldots,N_r$. N_r should be an extensive quantity, *i.e.* $N_r \propto N_d \propto |V|$, so that in the thermodynamic limit the density of degenerate single-particle ground states and the density of irreducible blocks are both finite.
2. Let V_k be the support of ρ_k, *i.e.* the set of vertices for which at least one element of ρ_k does not vanish. $\rho_{k,xy} = 0$ if $x \notin V_k$ or $y \notin V_k$. One has $V_k \cap V_{k'} = \emptyset$ if $k \neq k'$ because of the fact that ρ_k are irreducible blocks of the reducible matrix ρ and $\bigcup_k V_k \subseteq V$.
3. We choose the basis B such that the support of each basis states $\psi_i(x) \in B$ is a subset of exactly one V_k. We denote the number of states belonging to the cluster V_k as ν_k. One has $\sum_k \nu_k = N_d$.
4. $\nu_{\max} = \max_k\{\nu_k\}$ is $O(1)$, *i.e.* not an extensive quantity.

With these properties one can show

Theorem (Mielke 2012) For Hubbard models with a lowest single-particle eigenenergy 0 which is N_d-fold degenerate and for which the projector onto the eigenspace of 0 fulfils the properties on the previous slide, the following results hold for $N_e \leq N_d$:

1. The ground state energy is 0.
2. Let A_x be an arbitrary local operator, *i.e.* an arbitrary combination of the four creation and annihilation operators $c^\dagger_{x\sigma}$ and $c_{x\sigma}$. The correlation function $\rho_{A,xy} = \langle A_x A_y\rangle - \langle A_x\rangle\langle A_y\rangle$ has a finite support for any fixed x and vanishes if x and y are out of different clusters V_k. The system has no long-range order.
3. The system is paramagnetic.
4. The entropy at zero temperature $S(c)$ is an extensive quantity, $S(c) = O(N_e)$. It increases as a function of $c = N_e/N_d$ from 0 for $c = 0$ to some maximal value $S_{\max} \geq \sum_k[(\nu_k - 1)\ln 2 + \ln(\nu_k + 2)]$ and then decays to $S(1) = \sum_k \ln(\nu_k + 1)$.

These models have therefore no long range order. The most interesting aspect is the finite entropy at zero temperature.

4.2.5 Uniform density theorem

The uniform density theorem [41, 42, **?**] is valid on a bipartite lattice and at half filling. The proof makes use of the particle-hole symmetry which is valid in that case. It states

Theorem (MacLachlan 1959, 1961; Lieb, Loss, McCann 1993) For the Hubbard model on a bipartite lattice and at half filling, either in a canonical ensemble with $N_e = |V|$ at $T > 0$ or in the ground state at $T = 0$ or in a grand canonical ensemble with $\mu = 0$, the density matrix $\rho_{\sigma,xy} = \langle c^\dagger_{x\sigma} c_{y\sigma}\rangle$ has the property

$$\rho_{\sigma,xy} = \frac{1}{2}\delta_{xy} \text{ if } x,y \in A \text{ or } x,y \in B \tag{4.43}$$

The theorem may appear to be trivial if one has a translationally invariant lattice in mind. The point is, it holds for arbitrary t_{xy} and arbitrary U_x on an arbitrary bipartite graph, translational invariance is not used and not necessary. The theorem is therefore of large importance in quantum chemistry, *i.e.* for the Pariser-Parr-Pople variant of the Hubbard model.

4.2.6 Further rigorous results

There are further rigorous results on the Hubbard model. Many of them deal with the absence of ferromagnetism or at least with the absence of a fully polarised ground state under certain conditions. For details I refer to [37, 70, 72].

5 High-Temperature Superconductivity: Doped Mott-Insulators

5.1 Preliminary Remarks

High-temperature superconductors were first discovered by J.G. Bednorz and K.A. Müller from the IBM research center in Rüschlikon, Switzerland in 1986. 1987 the received the Nobel prize http://www.nobel.se/physics/laureates/1987/. After the discovery of these materials the interest in correlated electron systems has grown a lot. The Hubbard model, sometimes with some further interactions included, was first used to describe the behaviour of this systems in the normal, non-superconducting state. Quite early, people assumed that the pairing mechanism in high-temperature superconductors is not caused by phonons but by electronic excitations, e.g. spin waves. If this was true, a purely electronic model should be able to explain high-temperature superconductivity.

The goal of this chapter is to introduce some of the basic ideas and concepts used to explain high-temperature superconductivity. We restrict ourselves to the discussion of purely electronic models, i.e. the Hubbard model and its variants. Other aspects of the theory of high-temperature superconductivity will not be discussed.

An overview on the theory of high-temperature superconductivity can be found in the review article by P.A. Lee, N. Nagosa und X.-G. Wen [34]. A large part of the material presented here is taken from that article.

Materials which show high-temperature superconductivity have a rich phase diagram. Besides the superconducting phase, many other phases have been found depending on doping and temperature. Most of the aspects are not yet fully understood. The common aspects of this class of materials are:

1. A common structure element, planes of CuO_2.
2. Undoped materials are insulators.
3. In the undoped case, the conduction band is half filled. Thus, the materials are Mott insulators.
4. In the undoped case, the materials show long-range anti-ferromagnteic order, which vanishes under doping.

5.2 Models of High-Temperature Superconductors

As already mentioned, on common structure element are the CuO_2-planes. Depending on the material, further oxygen atoms are present, so that e.g. octahedra are formed with Cu in the center. These octahedra are distorted (Jahn-Teller effect). The distance between Cu and O in the planes is typically smaller. The planes form a three dimensional structure with other atoms sitting between the planes. One expects that most of the physics of high-temperature superconductors can be understood by looking at a model for electrons moving in the planes. It is clearly possible to add further terms to such a model to make it more realistic.

5.2.1 Single-particle Hamiltonian

The most simple single-particle Hamiltonian one can look at is

$$H_0 = \varepsilon_A \sum_{x\in A} n_x + \varepsilon_B \sum_{y\in B} n_y + t \sum_{<x\in A, y\in B>,\sigma} (c^\dagger_{x\sigma} c_{y\sigma} + c^\dagger_{y\sigma} c_{x\sigma}) \tag{5.1}$$

Here, A and B are the two sub-lattices of the CuO_2–plane (A for Cu, B for O), $\varepsilon_{A,B}$ are the different single particle energies on the two sub-lattices and t is the hopping matrix element. The notation $< .,. >$ menas, that the two lattice sites should be neighboured. Only nearest neighbour hopping is taken into account. Each elementary cell contains three atoms, the single particle Hamiltonian (5.1) has therefore three energy bands. The elementary cells form a square lattice.

Due to the structure of the 3d-orbitals of Cu one often chooses a different sign for the hopping in different directions. But a gauge transformation can be applied so that all hoppings have the same sign. We therefore choose t to be the same in both directions.

After a Fourier transformation one obtains

$$H_0 = \sum_k \sum_{a,b=1}^{3} h_{ab}(k) c^\dagger_{k,a,\sigma} c_{k,b,\sigma} \tag{5.2}$$

The indices a,b are the band indices of the three band. The matrix $H(k) = (h_{ab}(k))_{a,b=1,2,3}$ has the structure

$$H(k) = \begin{pmatrix} \varepsilon_A & 2t\cos(k_x/2) & 2t\cos(k_y/2) \\ 2t\cos(k_x/2) & \varepsilon_B & 0 \\ 2t\cos(k_y/2) & 0 & \varepsilon_B \end{pmatrix}$$

and can be easily diagonalised. The eigenvalues are

$$\varepsilon_{1,2}(k) = \frac{\varepsilon_A+\varepsilon_B}{2} \pm \sqrt{\left(\frac{\varepsilon_A-\varepsilon_B}{2}\right)^2 + 4t^2(\cos^2(k_x/2)+\cos^2(k_y/2))} \tag{5.3}$$

$$\varepsilon_3(k) = \varepsilon_B \tag{5.4}$$

Notice that for the special cases $\varepsilon_A = \varepsilon_B = 0$, the lattice is bipartite. It is just the Lieb lattice with a flat band in the middle of the spectrum and two bands symmetrically above and below. The introduction of the on-site energies shifts the bands and deforms the two non-flat bands.

In the case of high-temperature superconductors, the two lower bands are completely filled and the upper band is half filled in the undoped case, since the two p-orbitals in O are filled with two electrons each and the d-orbitals in Cu are filled with one electron each. The model has five electrons per elementary cell or equivalently one hole. Looking only at the single-particle model, the undoped system should be a metal. Since it is a anti-ferromagnetic insulator, the interaction is essential, the systems are therefore correlated systems.

The simple single-particle model can be extended by introducing a further hopping matrix element t_{BB} between next-nearest neighboured B–lattice sites.As a consequence, the flat band gets a dispersion and the two other bands are modified a bit. But, since the essential physics happens in the conduction band, the generic properties should not change.

5.2.2 Interactions

As already mentioned, simply to explain the undoped ground state of the materials, we need an interaction. The most important interactions are on-site interactions. Taking these into account, one gets a Hubbard model. It should be sufficient to explain the ati-ferromagnetic insulating ground state. Often, interactions for electrons on neighboured sites are introduced as well. The full model to describe these systems is therefore given by the interactions

$$H_{\mathrm{WW}} = U_A \sum_{x\in A} n_{x\uparrow} n_{x\downarrow} + U_B \sum_{y\in B} n_{y\uparrow} n_{y\downarrow} + U_{AB} \sum_{<x\in A, y\in B>} n_x n_y \tag{5.5}$$

and the kinetic energy

$$\begin{aligned} H_{\mathrm{kin}} &= \varepsilon_A \sum_{x\in A} n_x + \varepsilon_B \sum_{y\in B} n_y + t \sum_{<x\in A, y\in B>,\sigma} (c^\dagger_{x\sigma} c_{y\sigma} + c^\dagger_{y\sigma} c_{x\sigma}) \\ &\quad + t' \sum_{<y\in B, y'\in B>,\sigma} c^\dagger_{y\sigma} c_{y'\sigma} \end{aligned} \tag{5.6}$$

so that the full Hamiltonian reads

$$H = H_{\rm kin} + H_{\rm WW} \tag{5.7}$$

This model contains six independent energy parameters: The three interactions U_A, U_B, and U_{AB}, and the three parameters of the kinetic term $\Delta = \varepsilon_A - \varepsilon_B$, t and t'. Since the A-lattice sites represent the Cu atoms and since the $3d$–orbitals of ionised Cu re relatively small, a double occupation of the A-lattice sites costs a lot of energy and we expect the parameter U_A to be the largest.

With this idea in mind we could first take the limit of very large U_A. In the limit $U_A \to \infty$ we have one hole per elementary cell. The lB-lattice sites are occupied by two electrons, the A-lattice sites by one and hopping is strongly suppressed since it would create a double occupancy on an A-lattice site. If U_A is large but finite, virtual processes are possible, where two electrons on neighboured A-lattice sites are exchanged. This requires four hoppings and the intermediate states have energy differences $U_A - U_B + \Delta$, $U_B - \Delta$ and $\Delta - U_B$. In complete analogy to the Hubbard model at large U we can transform the present model to an antiferromagnetic Heisenberg model with an exchange interaction $J = -\frac{4t^4}{(U_A - U_B + \Delta)(U_B - \Delta)^2}$. Hopping t' and interactions U_{AB} play only a role at higher orders and are expected to be smaller than the other energies. Therefore, to leading order, we obtain a Heisenberg model which describes the anti-ferromagnetic ordering of the high-temperature superconductors in the undoped regime.

5.2.3 An effective single-band model

Since the essential physics takes place in the conduction and, one should be able to derive an effective single-band model. This is indeed the case. Starting point is the above Hamiltonian, which we now write as

$$H = H_0 + H_+ + H_- \tag{5.8}$$

H_+ transfers one electron from B to A, $H_- = H_+^\dagger$ transfers one electron from A to B. H_0 contains all the terms which let the number of electrons on the two sublattices constant.

We now introduce flow equations to transform that Hamiltonian. Let

$$\eta = H_- - H_+ \tag{5.9}$$

$$\frac{dH}{d\ell} = [\eta, H] = [H_-, H_0] - [H_+, H_0] - 2[H_+, H_-] \tag{5.10}$$

$$\frac{dH_0}{d\ell} = -2[H_+, H_-] \tag{5.11}$$

$$\frac{dH_+}{d\ell} = -[H_+, H_0] \tag{5.12}$$

$$\frac{dH_-}{d\ell} = [H_-, H_0] \tag{5.13}$$

η is an anti-hermitian operator, the differential equation therefore describes a continuous unitary transformation. For details on flow equations and continuous unitary transformations, I refer to the book by S. Kehrein [29]. (5.8) is the starting point of this continuous unitary transformation. During the transformation, further terms are generated in the Hamiltonian. In the end, for large ℓ, H_+ vanishes and we obtain an effective Hamiltonian which contains no terms that change the number of electrons on the two sublattices. We approximate the Hamiltonian as follows: H_+ should contain all possible matrix elements which transfer one electron from a lattice site A to a neighboured lattice site B.

$$H_+ = \sum_{<x\in A, y\in B>,\sigma} (t + t_{2A} n_{x-\sigma} + t_{2B} n_{y-\sigma} + t_{2AB} n_{x-\sigma} n_{y-\sigma}) c^\dagger_{x\sigma} c_{y\sigma} \tag{5.14}$$

Restricting H_+ to these terms, H_0 contains only terms with three nearest neighboured sites. I use the notation $< x \in A, y \in B, x' \in A >$ etc. One obtains

$$\begin{aligned}
H_0 &= \varepsilon_A \sum_{x\in A} n_x + \varepsilon_B \sum_{y\in B} n_y + U_A \sum_x n_{x\uparrow} n_{x\downarrow} + U_B \sum_y n_{y\uparrow} n_{y\downarrow} \\
&+ J_{AB} \sum_{<x\in A, y\in B>} [\frac{1}{2} n_x n_y - 2\vec{S}_x \cdot \vec{S}_y] + K_{AB} \sum_{<x\in A, y\in B>} [n_{x\uparrow} n_{x\downarrow} n_y - n_{y\uparrow} n_{y\downarrow} n_x] \\
&+ t_A \sum_{<x\in A, x'\in A>\sigma} c^\dagger_{x\sigma} c_{x'\sigma} + t_{AA} \sum_{<x\in A, x'\in A>\sigma} (n_{x-\sigma} + n_{x'-\sigma}) c^\dagger_{x\sigma} c_{x'\sigma} \\
&+ t_B \sum_{<y\in B, y'\in B>\sigma} c^\dagger_{y\sigma} c_{y'\sigma} + t_{BB} \sum_{<y\in B, y'\in B>\sigma} (n_{y-\sigma} + n_{y'-\sigma}) c^\dagger_{y\sigma} c_{y'\sigma} \\
&+ \sum_{<x\in A, y\in B, x'\in A>\sigma\tau} \sigma\tau [\tilde{K}_{AB} + \tilde{K}_{2AB}(n_{x-\sigma} + n_{x'-\tau}) + \tilde{K}_{3AB} n_{x-\sigma} n_{x'-\tau}] c^\dagger_{x\sigma} c^\dagger_{y-\sigma} c_{y-\tau} c_{x'\tau} \\
&+ \sum_{<y\in B, x\in A, y'\in B>\sigma\tau} \sigma\tau [\tilde{K}_{BA} + \tilde{K}_{2BA}(n_{y-\sigma} + n_{y'-\tau}) + \tilde{K}_{3BA} n_{y-\sigma} n_{y'-\tau}] c^\dagger_{y\sigma} c^\dagger_{x-\sigma} c_{x-\tau} c_{y'\tau}
\end{aligned}$$

Some of the terms in H_0 vanish at $\ell = 0$, they are not part of the initial model. But they are generated during the transformation.

U_A is the by far largest parameter in the initial model and we expect it to be the largest parameter for large ℓ. Therefore, we expect that the holes (one per elementary cell in the undoped case, less than one in the doped case) sit on the lattice sites A. Further, ε_A is smaller than ε_B and the difference becomes even larger as a funtions of ℓ. Since in the limit $\ell \to \infty$ $H_\pm$ vanish, it is sufficient to look at H_0. Since in H_0 all lattices sites B are doubly occupied and since there is no hopping from A to B, we may drop all the terms in H_0 which contain B-lattice sites. We therefore obtain the effective Hamiltonian

$$H_{\text{eff}} = \varepsilon_A \sum_{x\in A} n_x + U_A \sum_x n_{x\uparrow} n_{x\downarrow} \tag{5.15}$$

$$+ t_A \sum_{<x\in A, x'\in A>\sigma} c^\dagger_{x\sigma} c_{x'\sigma} + t_{AA} \sum_{<x\in A, x'\in A>\sigma} (n_{x-\sigma} + n_{x'-\sigma}) c^\dagger_{x\sigma} c_{x'\sigma} \tag{5.16}$$

The first three terms form a standard Hubbard model on a square lattice, the last term destroys the particle-hole symmetry. This should have been expected since the original Hamiltonian has no particle-hole symmetry.

The parameters in H_{eff} can be calculated using the flow equations. Doing this, one has to take into account that some of the terms we dropped in the calculation couple back to the terms we kept, if one replaces the particle-number operators n_y for $y \in B$ by their expectation values (i.e. by 2). This makes the actual calculation a bit more complicated but it is still feasible.

5.2.4 $t-J$ model

We already saw that the Hubbard model for large U can be mapped to an anti-ferromagnetic Heisenberg model at half filling. The same is true for the Hamiltonian (5.15,5.16). High-temperature superconductors are doped anti-ferromagnets. Doping introduces holes in the anti-ferromagnet, which can hop. To desribe this situation effectively, one often uses the so called $t-J$ model. The Hamiltonian reads

$$H = t \sum_{<x,y>\sigma} (1 - n_{x-\sigma}) c^\dagger_{x\sigma} c_{y\sigma} (1 - n_{y-\sigma}) + J \sum_{<x,y>} S_x S_y \tag{5.17}$$

and can be obtained from the Hamiltonian (5.15,5.16) by a further unitary transformation valid for large U_A similar to the one leading to (4.20). S_x are the local spin operators we introduced before. It is important to note that the Hilbertspace of the model described by (5.17) does not contain doubly occupied sites .

The $t-J$ model can as well be derived from the simple Hubbard model or from (5.15,5.16) or directly from the three-band model. As discussed above, the coupling J is of the order $\frac{4t^4}{(U_A - U_B + \Delta)(U_B - \Delta)^2}$.

5.3 Frustrated spin systems

5.3.1 Some general ideas

At half filling, the ground state of (5.17) is expected to have anti-ferromagnetic long-range order. Small doping can destroy anti-ferromagnetic order. In high-temperature superconductors, only 1% doping is sufficient to destabilise the anti-ferromagnetic order. This implies the following questions:

1. How does the spin-system look like at small doping?
2. How do the holes move in the spin systems?
3. If kind of effective interactions between holes are introduced due to the spin fluctuations?

ad 1.: The basic idea was formulated by Anderson, Baskaran, and Zhou [2, 3, 4, 5]. They propose that the spin system is in a resonating valence bond (RVB) state. There are many authors who followed that idea and there are therefore many different formulations. In the undopted regime, all those states are variational states with an energy only slightly above the ground state energy. In the following subsection we describe a rather general approach. Among them, there are states with and without anti-ferromagnetic long-range order. The states without long-range order show a local ordering, which is not unexpected.

ad 2.: A hole which moves in a local anti-ferromagnetic background destroys this background locally. This may hinder the movement of the hole.

ad 3.: If two holes move together in a correlated fashion. the second hole may heal the locally disturbed anti-ferromagnetic background. Therefore, one may develop the idea that a correlated movement of holes in an anti-ferromagnetic background is energetically favourable compared to an uncorrelated movement. This effect can be described by an effective attractive interaction between holes.

To better understand these ideas, one first has to understand the physics of the ground state of anti-ferromagnetic spin systems in two dimensions.

5.3.2 RVB-states

Let us first discuss the concept of RVB-states, which allows for the description of ordered, locally ordered or disordered spin systems, the *valence bond* (VB) or *resonating valence bond* (RVB) states. There is a couple of lattices for which one can show that the ground state of a Heisenberg model can be described using this concept.

We first introduce a singlet pair of spins

$$|(x,y)\rangle = \frac{1}{\sqrt{2}}(|\uparrow_x\downarrow_y\rangle - |\downarrow_x\uparrow_y\rangle) \tag{5.18}$$

on lattice sites x and y. We now choose a coverage P of pairs which cover the entire lattice (we assume $|\Lambda|$ to be pair) and form the singlet state

$$|P\rangle = \prod_{(x,y)\in P} |(x,y)\rangle \tag{5.19}$$

This state is called a VB-state. One can show that all VB-states form an overcomplete basis of the singlet space. This means that any singlet state can be written as

$$|\Psi\rangle = \sum_P A(P) \prod_{(x,y)\in P} |(x,y)\rangle \tag{5.20}$$

Since the states $|P\rangle$ are overcomplete, the representation of a singlet state in this form is not unique.

The representation (5.20) is useful because it leads to variational ansatzes for the ground state of the system. A popular variational ansatz is

$$|\Psi\rangle = \sum_P \prod_{(x,y)\in P} a(|x-y|)\,|(x,y)\rangle \tag{5.21}$$

i.e.

$$A(P) = \prod_{(x,y)\in P} a(|x-y|) \tag{5.22}$$

Such a state is called an RVB-state.

In concrete calculations we start with a given lattice. In the following we take the square lattice. It is a bipartite lattice. The two sublattices have the same number of lattice sites. We let

$$a(|x-y|) = 0 \tag{5.23}$$

if x and y are on the same sublattice. For bipartite lattices this is a natural ansatz.

Let us now calculate the overlap of two VB states.

$$\langle P' \,|P\rangle \tag{5.24}$$

where both P and P' contain only sinlet pairs on lattice sites which come from the two different sublattices. Let us first consider an easy example:

$$\begin{aligned}
\langle (x_1,y_2)(x_2,y_1)|(x_1,y_1)(x_2,y_2)\rangle &= \frac{1}{4}(\langle\uparrow_{x_1}\downarrow_{y_2}| - \langle\downarrow_{x_1}\uparrow_{y_2}|)(\langle\uparrow_{x_2}\downarrow_{y_1}| - \langle\downarrow_{x_2}\uparrow_{y_1}|)(|\uparrow_{x_1}\downarrow_{y_1}\rangle - |\downarrow_{x_1}\uparrow_{y_1}\rangle)(|\uparrow_{x_2}\downarrow_{y_2}\rangle - |\downarrow_{x_2}\uparrow_{y_2}\rangle) \\
&= \frac{1}{4}(\langle\uparrow_{x_1}\downarrow_{y_2}|\,\langle\uparrow_{x_2}\downarrow_{y_1}|\,|\uparrow_{x_1}\downarrow_{y_1}\rangle\,|\uparrow_{x_2}\downarrow_{y_2}\rangle + \langle\downarrow_{x_1}\uparrow_{y_2}|\,\langle\downarrow_{x_2}\uparrow_{y_1}|\,|\downarrow_{x_1}\uparrow_{y_1}\rangle\,|\downarrow_{x_2}\uparrow_{y_2}\rangle) \\
&= 2\frac{1}{2^2}
\end{aligned} \tag{5.25}$$

$$\begin{aligned}
\langle (x_1,y_1)(x_2,y_2)|(x_1,y_1)(x_2,y_2)\rangle &= \frac{1}{4}(\langle\uparrow_{x_1}\downarrow_{y_1}| - \langle\downarrow_{x_1}\uparrow_{y_1}|)(\langle\uparrow_{x_2}\downarrow_{y_2}| - \langle\downarrow_{x_2}\uparrow_{y_2}|)(|\uparrow_{x_1}\downarrow_{y_1}\rangle - |\downarrow_{x_1}\uparrow_{y_1}\rangle)(|\uparrow_{x_2}\downarrow_{y_2}\rangle - |\downarrow_{x_2}\uparrow_{y_2}\rangle) \\
&= \frac{1}{4}(\langle\uparrow_{x_1}\downarrow_{y_1}| - \langle\downarrow_{x_1}\uparrow_{y_1}|)(|\uparrow_{x_1}\downarrow_{y_1}\rangle - |\downarrow_{x_1}\uparrow_{y_1}\rangle)(\langle\uparrow_{x_2}\downarrow_{y_2}| - \langle\downarrow_{x_2}\uparrow_{y_2}|)(|\uparrow_{x_2}\downarrow_{y_2}\rangle - |\downarrow_{x_2}\uparrow_{y_2}\rangle) \\
&= 2^2\frac{1}{2^2}
\end{aligned} \tag{5.26}$$

Similar calculations can be done for the general case as well. We obtain

$$\langle P' \,|P\rangle = 2^{n_L - N_s/2} \tag{5.27}$$

where n_L is the number of loops one obtains when drawing $\langle P' \,|P\rangle$ on the lattice and N_s is the number of lattice sites. Up to cyclic permutation a loop C is a sequence of lattice sites, $C = (x_1,y_1,x_2,y_2,\ldots,x_n,y_n)$. In our construction, the lattice sites are alternatingly elements of A and B. $\langle P' \,|P\rangle$ contains each lattice site of the lattice exactly once, therefore it forms a covering $\{C_i, i = 1,\ldots,n_L\}$ of the lattice with loops. The norm of the variational state $|\Psi\rangle$ is

$$Z_\Psi = \sum_{\{C_i\}} \prod_i f(C_i) \tag{5.28}$$

where

$$f(C) = 2 \prod_{(x,y)\in C} \frac{a(|x-y|)}{\sqrt{2}} \tag{5.29}$$

The correlation function is

$$\langle P' \big| S_{3,x} S_{3,x'} \,|P\rangle = \frac{1}{4} 2^{n_L - N_s/2} \tag{5.30}$$

where $x \in A$ and $x' \in A$ are on the same loop, otherwise the right hand side is zero, and

$$\langle P' \big| S_{3,x} S_{3,y} \,|P\rangle = -2^{n_L - N_s/2} \tag{5.31}$$

for $x \in A$ and $y \in B$ where again both lattice sites must belong to the same loop. This means that the entire problem can be mapped to a problem of loops on a lattice.For each loop we introduce a probability

$$\rho(C) = Z_\Psi^{-1} f(C) Z_{\Psi \setminus C} \tag{5.32}$$

that the loop C occurs on the lattice. One has

$$\rho(C) = \frac{\partial \ln Z_\Psi}{\partial \ln f(C)} \tag{5.33}$$

The correlation function

$$\rho_{z,z'} = 4 s_{z,z'} \frac{\langle \Psi | S_{3,z} S_{3,z'} | \Psi \rangle}{Z_\Psi} \tag{5.34}$$

is

$$\rho_{z,z'} = \sum_{C::z,z' \in C} \rho(C) \tag{5.35}$$

where $s_{z,z'} = 1$ if both lattice sites are on the same sublattice, $s_{z,z'} = -1$ otherwise, The quantity

$$\ell = \sum_{z'} \rho_{z,z'} = N_s^{-1} \sum_{z,z'} \rho_{z,z'} \tag{5.36}$$

is the average loop length. If this quantity is extensive, i.e. $\ell \propto N_s$, the system has long range order.

5.3.3 The Néel state

To test whether the above concept is useful we want to investigate whether the Néel state can be described within the RVB concept and whether usual spin wave theory works as well. The Néel state is a state with maximal order. We obtain this ate if we let $a(|x-y|) = 1$ for all $x \in A$, $y \in B$.

Let us first calculate Z_Ψ. We have

$$Z_\Psi = \frac{1}{2^{N_s/2}} \sum_{\{C_i\}} 2^{n_L} \tag{5.37}$$

The sum runs over all loop coverages of the lattice. Let n_i be the number of loops of length $2i$, then we have

$$\sum_i n_i = n_L \tag{5.38}$$

$$\sum_i i n_i = N_s/2 \tag{5.39}$$

The number of coverages of the lattice with n_1 loops of length 2, n_2 loops of length 4, etc is

$$\frac{(\frac{N_s}{2})!^2}{\prod_i i^{n_i} n_i!} \tag{5.40}$$

Therefore we have

$$Z_\Psi = \frac{1}{2^{N_s/2}} (\frac{N_s}{2})!^2 \sum_{\{n_i\}:\sum_i i n_i = N_s/2} \prod_i \frac{2^{n_i}}{i^{n_i} n_i!} = \frac{1}{2^{N_s/2}} (\frac{N_s}{2})! (\frac{N_s}{2}+1)! \tag{5.41}$$

The average loop length is

$$\ell = Z_\Psi^{-1} \frac{1}{2^{N_s/2}} (\frac{N_s}{2})!^2 \sum_{\{n_i\}:\sum_i i n_i = N_s/2} (\frac{4}{N_s} \sum_i i^2 n_i) \prod_i \frac{2^{n_i}}{i^{n_i} n_i!} = \frac{2}{3}(N_s/2+2) \tag{5.42}$$

All the sums can be calculated for the formula gin in the chapter on combinatorics in the *Handbook of Mathematical Functions*, by Abramowitz, Stegun [1]. Since all lattice sites are equivalent, we have

$$\rho_{z,z'} = \frac{N_s+1}{3(N_s-1)} \tag{5.43}$$

for $z \neq z'$. Naively, one may have expected that the Néel state has $\rho_{z,z'} = 1$. But since the state must be $SU(2)$-symmetric, we obtain $\rho_{z,z'} = \frac{1}{3}$.

5.3.4 Short-range correlations

Another extreme case are state where $a(|x-y|) = 1$ for neighboured states, $a(|x-y|) = 0$ otherwise. These states are called dimer states. They have no long-range order, the average loop length is not $\propto N_s$. Unfortunately, excat results for these states are not available. One does not know whether these states have an exponential or an algebraic decay. There are good arguments for both.

5.3.5 The two-dimensional Heisenberg model

Liang, Douçot, and Anderson [35] did variational calculations for the Heisenberg model on a square lattice. Their results have been improved by several authors. The variational state wth the lowest energy one knows has an energy per lattice site of $-0.6688J$ and $a(|x-y|) \propto |x-y|^{-4}$. The state has long-range order, $\rho_{z,z'}$ tends to 0.12 for large distances. The authors point outthat there are states with only a slightly higher energy and without long-range order. This is not unexpected since we know that for any finite temperature, the long range order disappears. This is the Mermin-Wagner theorem. Also, introducing frustration will suppress long-range order.

The problem can as well be treated analytically using an argument by Flory from the theory of polymers. The coverage of loops can be interpreted as a set of loops with repulsive interaction. The repulsive interaction within a loop tends to blow up the loop whereas the repulsive interaction between loops tends to compress a loop. Both effects work in different directions. If one assumes that both effects cancel each other, we may neglect the loop interaction entirely. Doing that yields the exact result for the Néel state. There are good reasons to assume that this argument yields qualitatively good results for dimensions $d \geq 3$ and that it becomes exact in the limit $d \to \infty$. In one dimension the argument is definitely wrong. In two dimension, the situation is unclear. Wegner [77] applied it to the two-dimensional Heisenberg model. he obtained for the correlation function $\rho_{z,z'} \to 0.13$, which is very close to the result by Liang, Douçot, and Anderson [35], but the energy per lattice site is $E = -1.0056J$. For the energy, the short range correlations are important and they are certainly no well described by the Flory argument.

5.4 Field theoretic description

5.4.1 Fermions and Schwinger bosons

Spin operators can be expressed using fermionic or bosonic operators. The fermionic representation is clear, we used it before.

$$S_{3,x} = \frac{1}{2}(c^\dagger_{x+}c_+ - c^\dagger_{x-}c_{x-}) \tag{5.44}$$

$$S_{+,x} = c^\dagger_{x+}c_{x-} \tag{5.45}$$

$$S_{-,x} = c^\dagger_{x-}c_{x+} \tag{5.46}$$

$$S_{1,x} = \frac{1}{2}(S_{+,x} + S_{-,x}) \tag{5.47}$$

$$S_{2,x} = \frac{1}{2i}(S_{+x} - S_{-x}) \tag{5.48}$$

The commutation relation for the spin operators are fulfilled if

$$c^\dagger_{x+}c_{x+} + c^\dagger_{x-}c_{x-} = 1 \tag{5.49}$$

The number of particles on a lattice site must be one. (5.49) implies that the interpretation of the usual commutation relations must be restricted on the Hilbert space in which all states fulfil the constraint. Applying a

bare creation or annihilation operator to an element of that Hilbert space creates a state which is no longer an element on that Hilbert space. Thus, all matrix elements of the creation or annihilation operator in the restricted Hilbert space vanish. Let us consider as an example $[c_{x+}, n_x] = c_{x+}$. On the left hand side, in the restricted Hilbert space, $n_x = 1$. But we we set $n_x = 1$ in this equation the left hand side is zero. This is correct, since, as stated above, all matrix elements of the creation or annihilation operator in the restricted Hilbert space vanish. In the restricted Hilbert space only operators occur where in each product the number of creation and annihilation operators is the same. Taking this restriction into account, the usual commutation relations between the creation or annihilation operators are still correct, i.e. $[c_{x\sigma}, c^\dagger_{x'\sigma'}] = \delta_{x,x'}\delta_{\sigma,\sigma'}$. Later, we will use similar constraints with more operators involved, there, the same is true.

Similarly, we can use bosons to represent spin operators. Let $b_{x\sigma}$ and $b^\dagger_{x\sigma}$ be annihilation and creation operators for bosons on the lattice site x. σ takes the values ± 1. We let

$$S_{3,x} = \frac{1}{2}(b^\dagger_{x+}b_{x+} - b^\dagger_{x-}b_{x-}) \tag{5.50}$$

$$S_{+,x} = b^\dagger_{x+}b_{x-} \tag{5.51}$$

$$S_{-,x} = b^\dagger_{x-}b_{x+} \tag{5.52}$$

and let

$$b^\dagger_{x+}b_{x+} + b^\dagger_{x-}b_{x-} = 1 \tag{5.53}$$

One obtains

$$\begin{aligned} S^2_{3,x} + \frac{1}{2}(S_{+,x}S_{-,x} + S_{-,x}S_{+,x}) &= \frac{1}{4}(b^\dagger_{x+}b_{x+} - b^\dagger_{x-}b_{x-})^2 \\ &\quad + \frac{1}{2}(b^\dagger_{x+}b_{x-}b^\dagger_{x-}b_{x+} + b^\dagger_{x-}b_{x+}b^\dagger_{x+}b_{x-}) \\ &= \frac{1}{4}(b^\dagger_{x+}b_{x+} + b^\dagger_{x-}b_{x-})^2 \\ &\quad + \frac{1}{2}(b^\dagger_{x+}b_{x+} + b^\dagger_{x-}b_{x-}) \\ &= \frac{3}{4} \end{aligned} \tag{5.54}$$

$$[S_{3,x}, S_{\pm,x}] = \pm S_{\pm x} \tag{5.55}$$

$$[S_{+,x}, S_{-,x}] = b^\dagger_{x+}b_{x-}b^\dagger_{x-}b_{x+} - b^\dagger_{x-}b_{x+}b^\dagger_{x+}b_{x-} = 2S_{3,x} \tag{5.56}$$

and the Hamiltonian in this representation is

$$\begin{aligned} H &= \frac{1}{2}\sum_{x,y} J_{x,y}\left[\frac{1}{4}(a^\dagger_{x+}a_{x+} - a^\dagger_{x-}a_{x-})(a^\dagger_{y+}a_{y+} - a^\dagger_{y-}a_{y-})\right. \\ &\quad \left. + \frac{1}{2}(a^\dagger_{x+}a_{x-}a^\dagger_{y-}a_{y+} + a^\dagger_{x-}a_{x+}a^\dagger_{y+}a_{y-})\right] \end{aligned} \tag{5.57}$$

where the additional condition $a^\dagger_{x+}a_{x+} + a^\dagger_{x-}a_{x-} = 1$ has to be taken into account. a and $a^\dagger$ are fermionic or bosonic operators. The projection operator commutes with the Hamiltonian. In a more compact form, the Hamiltonian can be written as

$$H = \frac{1}{4}\sum_{x,y,\sigma,\tau} J_{x,y}(\zeta a^\dagger_{x\sigma}a^\dagger_{y\tau}a_{y\sigma}a_{x\tau} - \frac{1}{2}) \tag{5.58}$$

with $\zeta = +1$ for bosons and $\zeta = -1$ for fermions. Up to a constant $-\frac{1}{2}\sum_{x,y} J_{x,y}$ the Hamiltonian is

$$H = \frac{\zeta}{4}\sum_{x,y} J_{x,y} P_{x,y} \tag{5.59}$$

where the operator $P_{x,y}$ exchanges two particles on the two lattice sites x and y. The eigenstates of H are symmetric with respect to permutations of two bosons. For a two-particle state there are two possible cases

1. For bosons: symmetric in lattice and spin space. For fermions: antisymmetric in lattice and spin space.

$$a^\dagger_{x+} a^\dagger_{y+}|0\rangle, \quad \frac{1}{\sqrt{2}}(a^\dagger_{x+} a^\dagger_{y-} + a^\dagger_{x-} a^\dagger_{y+})|0\rangle, \quad a^\dagger_{x-} a^\dagger_{y-}|0\rangle \tag{5.60}$$

   These are triplet states.

2. For bosons: antisymmetric in lattice and spin space. For fermions: symmetric in lattice and spin space.

$$\frac{1}{\sqrt{2}}(a^\dagger_{x+} a^\dagger_{y-} - a^\dagger_{x-} a^\dagger_{y+})|0\rangle \tag{5.61}$$

   This is the singlet state..

An RVB-state can now be written as

$$|\Psi\rangle = \sum_P \prod_{(x,y)\in P} \frac{a(|x-y|)}{\sqrt{2}}(a^\dagger_{x+} a^\dagger_{y-} - a^\dagger_{x-} a^\dagger_{y+})|0\rangle \tag{5.62}$$

5.4.2 Field theoretic formulation

As introduced in the first chapter of this course, a fermionic or bosonic model can be written in a Lagrangian formulation with Grassmann or complex fields. The only difference is that in the present formulation an additional condition has to be taken into account. For the present model, the action can be written as

$$S = \int_0^\beta d\tau L \tag{5.63}$$

$$L = \sum_{x,\sigma} \phi^*_{x,\sigma}(\tau)(\partial_\tau - \mu)\phi_{x,\sigma}(\tau) - i\sum_x \lambda_x(\tau)(\sum_\sigma \phi^*_{x,\sigma}(\tau)\phi_{x,\sigma}(\tau) - 1) + V(\{\phi^*_{x,\sigma}(\tau), \phi_{x,\sigma}(\tau)\}) \tag{5.64}$$

where

$$V(\{\phi^*_{x,\sigma}(\tau), \phi_{x,\sigma}(\tau)\}) = \frac{\zeta}{4}\sum_{x,y,\sigma,\sigma'} J_{x,y}\phi^*_{x,\sigma}(\tau)\phi^*_{y,\sigma'}(\tau)\phi_{y,\sigma}(\tau)\phi_{x,\sigma'}(\tau) \tag{5.65}$$

A constant has been dropped. $\lambda_x(\tau)$ is a real Lagrangian multiplier field. The integration over $\lambda_x(\tau)$ guaranties that the additional condition

$$\sum_\sigma \phi^*_{x\sigma}(\tau)\phi_{x\sigma'}(\tau) = 1 \tag{5.66}$$

is fulfilled. Because of the additional condition, the chemical potential can in principle be dropped. In what follows we take only couplings between neighboured sites into account. The potential is then

$$V(\{\phi^*_{x,\sigma}(\tau), \phi_{x,\sigma}(\tau)\}) = \frac{\zeta J}{4}\sum_{x,i,\sigma,\sigma'} \phi^*_{x,\sigma}(\tau)\phi^*_{x+e_i,\sigma'}(\tau)\phi_{x+e_i,\sigma}(\tau)\phi_{x,\sigma'}(\tau) \tag{5.67}$$

The index i runs over the directions. Using a Hubbard-Stratonovich transformation, the action becomes quadratic in the fields ϕ and ϕ^*. They can be integrated out and we obtain an effective theory which contains the Hubbard-Stratonovich fields and the Lagrange parameter λ_x. This effective action can then be treated in a saddle point or mean field approach. We can as well study fluctuations around the saddle point. An important property of this effective action is that is possesses a local gauge invariance. The reason is simple: There are local conserved quantities, namely the particle numbers. Let us now perform the different steps sketched so far.

Hubbard-Stratonovich transformation. The Hubbard-Stratonovich transformation is nothing but a Gaussian integral. One has

$$\exp(-\frac{J}{2}z^*z) \propto \int d\chi d\chi^* \exp(-\frac{2}{J}\chi^*\chi + \chi^* z + z^*\chi) \tag{5.68}$$

V can be written as

$$\begin{aligned} V(\{\phi^*_{x,\sigma}(\tau),\phi_{x,\sigma}(\tau)\}) &= \frac{\zeta J}{2}\sum_{x,i,\sigma,\sigma'}\phi^*_{x,\sigma}(\tau)\phi^*_{x+e_i,\sigma'}(\tau)\phi_{x+e_i,\sigma}(\tau)\phi_{x,\sigma'}(\tau) \\ &= \frac{J}{2}\sum_{x,i}(\sum_{\sigma}\phi^*_{x,\sigma}(\tau)\phi_{x+e_i,\sigma}(\tau))(\sum_{\sigma}\phi^*_{x+e_i,\sigma}(\tau)\phi_{x,\sigma}(\tau)) \end{aligned} \tag{5.69}$$

and therefore

$$\begin{aligned} \exp(-V(\{\phi^*_{x,\sigma}(\tau),\phi_{x,\sigma}(\tau)\})) \propto \int D[\chi(\tau)]D[\chi^*(\tau)]\exp\Bigg(&-\frac{2}{J}\sum_{x,i}\chi^*_{x,i}(\tau)\chi_{x,i}(\tau) \\ &+\sum_{x,i}(\chi^*_{x,i}(\tau)(\sum_{\sigma}\phi^*_{x+e_i,\sigma}(\tau)\phi_{x,\sigma}(\tau)) + \chi_{x,i}(\tau)(\sum_{\sigma}\phi^*_{x,\sigma}(\tau)\phi_{x+e_i,\sigma}(\tau))\Bigg) \end{aligned} \tag{5.70}$$

This yields the new action

$$\begin{aligned} L' &= \sum_{x,\sigma}\phi^*_{x,\sigma}(\tau)(\partial_\tau-\mu)\phi_{x,\sigma}(\tau) - i\sum_x\lambda_x(\tau)(\sum_{\sigma}\phi^*_{x,\sigma}(\tau)\phi_{x,\sigma}(\tau)-1) \\ &\quad -\frac{2}{J}\sum_{x,i}\chi^*_{x,i}(\tau)\chi_{x,i}(\tau) \\ &\quad +\sum_{x,i}\left(\chi^*_{x,i}(\tau)\sum_{\sigma}\phi^*_{x+e_i,\sigma}(\tau)\phi_{x,\sigma}(\tau) + \chi_{x,i}(\tau)\sum_{\sigma}\phi^*_{x,\sigma}(\tau)\phi_{x+e_i,\sigma}(\tau)\right) \end{aligned} \tag{5.71}$$

The integral over ϕ and ϕ^* is a Gaussian integral and can be calculated. Before doing this, let us look at the symmetries of L'.

Locale gauge symmetry. With

$$\chi_{x,i}(\tau) = \rho_{x,i}(\tau)\exp(iA_{x,i}(\tau)) \tag{5.72}$$

the local gauge transformation is

$$\phi_x(\tau) \to \phi_x(\tau)\exp(i\varphi_x(\tau)) \tag{5.73}$$

$$\lambda_x(\tau) \to \lambda_x(\tau) + \partial_\tau\varphi_x(\tau) \tag{5.74}$$

$$A_{x,i}(\tau) \to A_{x,i}(\tau) - \varphi_{x+e_i}(\tau) + \varphi_x(\tau) \tag{5.75}$$

This transformation yields

$$L' \to L' + i\sum_x\partial_\tau\varphi_x(\tau) \tag{5.76}$$

and

$$S \to S + i\sum_x\int_0^\beta d\tau\partial_\tau\varphi_x(\tau) = S + i\sum_x(\varphi_x(\beta)-\varphi_x(0)) = S$$

since $\varphi_x(\tau)$ is a bosonic field and therefore periodic in τ. We can even generalise the periodic boundary condition for $\varphi_x(\tau)$ by letting

$$\varphi_x(\beta) = \varphi_x(0) + 2\pi m_x$$

The system is even symmetric under a larger group of gauge transformations. As a consequence of the symmetry, we may choose a special gauge. The main point is that the gauge only needs to guaranty that the condition

$$\sum_{\sigma} \phi^*_{x\sigma}(\tau)\phi_{x\sigma'}(\tau) = 1$$

holds for on value of τ. It is then automatically fulfilled for any τ. For example, we may choose

$$\lambda_x(\tau) = \lambda_x \delta(\tau - \tau_0)$$

Saddle point approximation. One can introduce a parameter to the model which has the effect that in a certain limit the saddle point approximation becomes exact. This allows for a systematic expansion around the saddle point. To do this, we look at a model which has an $SU(N)$ symmetry instead of the usual $SU(2)$ symmetry. The Hamiltonian can then be written as

$$H = \frac{1}{N}\sum_{x,y} J_{x,y} \sum_{\alpha,\beta=1}^{N} \hat{S}^{\beta}_{\alpha}(x)\hat{S}^{\alpha}_{\beta}(y) \tag{5.77}$$

where $\hat{S}^{\beta}_{\alpha}(x)$ are the generators of the $SU(N)$ algebra. As a representation we choose

$$\hat{S}^{\beta}_{\alpha}(x) = \sum_{a=1}^{n_c} c^{\dagger}_{\alpha a}(x)c^{\beta a}(x) - \delta^{\beta}_{\alpha}\frac{n_c}{2} \tag{5.78}$$

with the additional conditions

$$\sum_{\alpha=1}^{N} c^{\dagger}_{\alpha a}(x)c^{\alpha b}(x) = \begin{cases} \delta^b_a m & x \in A \\ \delta^b_a (N-m) & x \in B \end{cases} \tag{5.79}$$

We assume a bipartite lattice with the sublattices A and B. For $N = 2$ there is only one value $m = 1$ and we obtain a representation of the $SU(2)$. The spin in the representation is $s = n_c/2$. For $n_c = 1$ we obtain the above representaion. In the following, I restrict the calculation to the case $n_c = 1$, N even and $m = N/2$. Other cases may be iteresting as well. for example the limit $n_c \to \infty$ yields a spin wave approximation. For the Lagrangian density we obtain

$$\begin{aligned} L' &= \sum_{x,\alpha} \phi^*_{x,\alpha}(\tau)(\partial_\tau - \mu)\phi_{x,\alpha}(\tau) - i\sum_x \lambda_x(\tau)(\sum_\alpha \phi^*_{x,\alpha}(\tau)\phi_{x,\alpha}(\tau) - \frac{N}{2}) \\ &\quad -\frac{N}{J}\sum_{x,i}\chi^*_{x,i}(\tau)\chi_{x,i}(\tau) \\ &\quad +\sum_{x,i}\left(\chi^*_{x,i}(\tau)\sum_\alpha \phi^*_{x+e_i,\alpha}(\tau)\phi_{x,\alpha}(\tau) + \chi_{x,i}(\tau)\sum_\alpha \phi^*_{x,\alpha}(\tau)\phi_{x+e_i,\alpha}(\tau)\right) \end{aligned} \tag{5.80}$$

For $N = 2$ this is the above expression. We now integrate the (in this representation fermionic) fields ϕ and ϕ^* and obtain

$$S_{\text{eff}}[\lambda,\chi,\chi^*] = N\bar{S}[\lambda,\chi,\chi^*] \tag{5.81}$$

$$\begin{aligned} \bar{S}[\lambda,\chi,\chi^*] &= \mathrm{Tr}\ln\left((\partial_\tau - \mu - \mathrm{i}\lambda_{\mathrm{x}}(\tau))\delta_{\mathrm{x,y}}\delta_{\tau,\tau'} + (\chi_{\mathrm{x,i}}(\tau)\delta_{\mathrm{y,x+e_i}} + \chi^*_{\mathrm{x-e_i,i}}(\tau)\delta_{\mathrm{y,x-e_i}})\delta_{\tau,\tau'}\right) \\ &\quad -\int d\tau\left(\frac{1}{J}\sum_{x,i}\chi^*_{x,i}(\tau)\chi_{x,i}(\tau) - \frac{i}{2}\sum_x \lambda_x(\tau)\right) \end{aligned} \tag{5.82}$$

The effective action is $\propto N$ and therefore, for large N the saddle point approximation becomes exact and we may even think of a $1/N$ expansion. The saddle point equations are

$$\frac{\delta \bar{S}}{\delta \rho_{x,i}(\tau)} = 0 \tag{5.83}$$

$$\frac{\delta \bar{S}}{\delta A_{x,i}(\tau)} = 0 \tag{5.84}$$

$$\frac{\delta \bar{S}}{\delta \lambda_{x}(\tau)} = 0 \tag{5.85}$$

It is difficult to find an exact solution of these equations. Only solutions for various subspaces are known.

In the following we consider some solutions of the equations on a square lattice. When we introduced the local gauge transformation, we saw that the phase of χ and λ has the interpretation of an electromagnetic potential. The absolute value of χ represents the density. At constant density and for 0 magnetic field, one obtains the solution which was first proposed by Baskaran, Zou and Anderson. The energy is

$$E_{\mathrm{BZA}} = \frac{4NN_s}{J}\bar{\rho}^2 - \frac{16}{\pi^2}NN_s\bar{\rho} \tag{5.86}$$

with the minimum $E = -16NN_sJ/\pi^4 = -0.164NN_sJ$ for $\bar{\rho} = 2J/\pi^2$. At constant density and constant magnetic field $\neq 0$ we obtain so called flux phase states with a lower energy, namely

$$E_{\mathrm{Flussphase}} = \frac{4NN_s}{J}\bar{\rho}^2 - 8NN_s\bar{\rho}\int_{|p_i|\leq\frac{\pi}{2}} \frac{d^2p}{(2\pi)^2}\sqrt{\sin^2 p_1 + \sin^2 p_2} \tag{5.87}$$

The minimum is $E = -0.230NN_sJ$. Further, there are dimer states with an even lower energy

$$E = \frac{4NN_s}{J}\bar{\rho}^2 - NN_s\bar{\rho} \tag{5.88}$$

and a minimum $E = -JNN_s/4$ at $\bar{\rho} = J/4$. But this energy is still higher than the variational energy of the RVB states for $N = 2$ ($E = -0.6688JN_s$). But the $1/N$ corrections are missing here. A problem of all the states is that in all of them the local gauge symmetry is broken. Thus, the status of the theory is still open.

Flux phases. Flux phases are states with $\lambda = 0$ and with a τ independent χ. With these assumptions we obtain the effective Hamiltonian

$$H = -\sum_{x,j,\alpha} \bar{\rho}_{x,j}\left(c^{\dagger}_{x,\alpha}\exp(iA_{x,j})c_{x+e_j,\alpha} + \mathrm{h.c.}\right) + \frac{N}{J}\sum_{x,j}\bar{\rho}^2_{x,j} \tag{5.89}$$

Flux phase states have a fixed $\bar{\rho}_{x,j} = \bar{\rho}$. The flux phase problem can be solved by first finding the minimum of H at fixed $\bar{\rho}$ by varying $A_{x,j}$ and in a second step finding the minimum by varying $\bar{\rho}$. Here we have to take into account that the number of fermions is equal to the number of lattice sites, we are at half filling. In the following we consider again a square lattice. We choose a vector potential $A_{x,j}$ that corresponds to a flux ϕ through each elementary cell of the square lattice. This is the situation of a constant magnetic field. The ground state energy is then

$$E_0 = -\bar{\rho}\,\mathrm{Tr}|\mathrm{T}| + \frac{4\mathrm{NN_s}}{\mathrm{J}}\bar{\rho}^2 \tag{5.90}$$

where $T = (t_{x,y})$ is the matrix

$$t_{x,y} = \exp(iA_{x,j})\delta_{y,x+e_j} \tag{5.91}$$

and the flux phase condition is

$$A_{x,2} + A_{x+e_2,1} - A_{x+e_1,2} - A_{x,1} = \phi \tag{5.92}$$

Let $|T|$ be the positive definite matrix for which $|T|^2 = T^2$. Tr|T| is the sum of the absolute values of the eigenvalues of T. A special solution, for which the flux phase condition is fulfilled, is

$$A_{x,1} = \frac{\phi}{2}, \quad A_{x,2} = (-1)^{x_1}\frac{\phi}{2} \tag{5.93}$$

Using this gauge, we obtain four sublattices. For the eigenfunctions of T, we make the ansatz

$$\psi_x = \exp(ikx)a_i \tag{5.94}$$

for x in the sublattice $i = 1,\ldots,4$. This yields a eigenvalue equation for a_i with a 4×4-matrix. The eigenvalues can be calculated, as well as Tr|T|. The minimum occurs at

$$\phi = \pi \tag{5.95}$$

and for the eigenvalues we obtain

$$\pm 2\sqrt{\sin^2 k_1 + \sin^2 k_2} \tag{5.96}$$

This yields the above formula for the ground state energy. The optimal value $\phi = \pi$ for the flux is more general than what can be seen from this simple calculations. For instances one can show that for this flux we also obtain a minimm of $\det T$. Further, the result can be generalised to planar bipartite graphs. A planar bipartite graph consist of $n$polygons with n edges. The optimal flux through such a polygon is $\pi(n-2)/2$. Further one can construct flux phase states with a density less than 1.

5.5 The doped anti-ferromagnet: The $t-J$ modell

If we dope an anti-ferromagnet, the long range order may be weakened or even eliminated completely. We already saw that a suitable model for a doped anti-ferromagnet is the $t-J$ model

$$H_{t-J} = \sum_{x,y,\sigma} t_{x,y}(1-n_{x,-\sigma})c^\dagger_{x,\sigma}c_{y\sigma}(1-n_{y,-\sigma}) + \sum_{x,y} J_{x,y}\vec{S}_x\cdot\vec{S}_y \tag{5.97}$$

where we now use a fermionic representation of the spins,

$$S_{3,x} = \frac{1}{2}(c^\dagger_{x+}c_+ - c^\dagger_{x-}c_{x-}) \tag{5.98}$$

$$S_{+,x} = c^\dagger_{x+}c_{x-}, \quad S_{-,x} = c^\dagger_{x-}c_{x+} \tag{5.99}$$

$$S_{1,x} = \frac{1}{2}(S_{+,x}+S_{-,x}), \quad S_{2,x} = \frac{1}{2i}(S_{+x}-S_{-x}) \tag{5.100}$$

The spin interaction in the Hamiltonian is the usual Heisenberg interaction. The kinetic part allows for a hopping of a spin from one lattice site to another. The factors $(1-n_{x,-\sigma})(1-n_{y,-\sigma})$ guaranty that there are never two electrons on a lattice site. Above we derived the $t-J$ from a one band or three band Hubbard model using unitary transformations and the limit of strong repulsion. There are other ways to motivate this model. We take it here as a model of its own interest and not as a limiting case of another model.

The main effect we expect in the $t-J$ model is a weakening of the anti-ferromagnetic order and in connection with that a possible attractive effective interaction between the holes.

There are various methods that have been used so far to investigate the $t-J$ model. In one dimesion it is exactly solvable for a special value of t/J. In higher dimensions the motion of a single hole in the spin background was studied quite early. A finite concentration of holes is not yet completely understood. The methods used in this course can be applied if one introduces auxiliary fields like for the Heisenberg model. For a single lattice site the model has three states: $|0\rangle_x$, the empty lattice site, $|+\rangle_x$ and $|-\rangle_x$ with an electron on the

site with a spin $\sigma = \pm$. We represent the spins using fermionic operators $f^\dagger_{x,\sigma}$ and $f_{x,\sigma}$ as before, empty sites using bosons $b^\dagger_x$ and b_x. The creation or annihilation operator for an electron is then represented as

$$c^\dagger_{x,\sigma} = b_x f^\dagger_{x,\sigma}, \quad c_{x,\sigma} = b^\dagger_x f_{x,\sigma} \tag{5.101}$$

We need the additional condition

$$b^\dagger_x b_x + \sum_\sigma f^\dagger_{x,\sigma} f_{x,\sigma} = 1 \tag{5.102}$$

on each lattice site. The kinetic part of the Hamiltonian reads

$$H_t = \sum_{x,y,\sigma} t_{x,y} f^\dagger_{x,\sigma} f_{y,\sigma} b^\dagger_y b_x \tag{5.103}$$

A different possibility is, as mentioned before for the Heisenberg model, to represent the spins by bosonic operators $b^\dagger_{x,\sigma}$ and $b_{x,\sigma}$. The hole operator then has to be represented by fermionic operators $a^\dagger_x$ and a_x. We have

$$c^\dagger_{x,\sigma} = a^\dagger_x b_{x,\sigma}, \quad c_{x,\sigma} = a^\dagger_x b_{x,\sigma} \tag{5.104}$$

$$a^\dagger_x a_x + \sum_\sigma b^\dagger_{x,\sigma} b_{x,\sigma} = 1 \tag{5.105}$$

$$H_t = \sum_{x,y,\sigma} t_{x,y} b^\dagger_{x,\sigma} b_{y,\sigma} a^\dagger_y a_x \tag{5.106}$$

The two approaches are called slave boson or slave fermion approach. The hole excitations are often called holons, the spin excitations spinons. Holes may condensate, which was interpreted as a first hint for a high T_c superconductor. This idea seems to be wrong. The transitions is just an artefact of the representation.

As the Heisenberg model the $t-J$ can be treated using a field-theoretic approach. The only difference is the additional field for the holes. One has here as well a local gauge symmetry, and one has the local conditions which can be taken into account using a Lagrangian multiplier. Using a Hubbard-Stratonovich transformation it is possible to decouple the interaction. The fields corresponding to the operators $f^\dagger_{x,\sigma}$ and $f_{x,\sigma}$ or $b^\dagger_{x,\sigma}$ and $b_{x,\sigma}$ can then be integrated out. One obtains an action that depends on the Hubbard-Stratonovich field and the Lagrangian multiplier. The action has again a local gauge symmetry. Investigating the influence of holes further, it turns out that the flux phase state is stabilised. On the square lattice, the optimal flux per unit cell is πn where n is the electron density.

We choose the ansatz (5.101). The exchange interaction then has the form

$$\vec{S}_x \cdot \vec{S}_y = -\frac{1}{4} \sum_{\sigma,\sigma'} f^\dagger_{x\sigma} f_{y\sigma} f^\dagger_{y\sigma'} f_{x\sigma'} - \frac{1}{4} (f^\dagger_{x+} f^\dagger_{y-} - f^\dagger_{x-} f^\dagger_{y+})(f_{y-x} f_{x+} - f_{y+} f_{x-}) + \frac{1}{4} \sum_\sigma (f^\dagger_{x\sigma} f_{x\sigma} + f^\dagger_{y\sigma} f_{y\sigma})$$

The derivation is easy, one just uses the representation of the spin operators by fermions and the representation (5.101) of the fermionic operators. One then eliminates the bosonic operators $b^{(\dagger)}_x$ using (5.102). In a similar way, the density-density interaction can be written as

$$n_x n_y = (1 - b^\dagger_x b_x)(1 - b^\dagger_y b_y)$$

Often, the term $b^\dagger_x b^\dagger_y b_y b_x$ is neglected because of the low hole concentration. The remaining quartic terms are decoupled using the Hubbard-Stratonovich transformation, as already mentioned. We obtain

$$\begin{aligned} L_1 \quad = \quad & \frac{1}{4} \sum_{xy} J_{xy} (|\chi_{xy}|^2 + |\Delta_{xy}|^2) + \sum_{x\sigma} f^*_{x\sigma} (\partial_\tau - i\lambda_x) f_{x\sigma} \\ & - \frac{1}{4} \left[\sum_{xy\sigma} J_{xy} \chi^*_{xy} f^*_{x\sigma} f_{y\sigma} + \text{c.c.} \right] + \frac{1}{4} \left[\sum_{xy} J_{xy} \Delta_{xy} (f^*_{x+} f^*_{y-} - f^*_{x-} f^*_{y+}) + \text{c.c.} \right] \\ & + \sum_x b^*_x (\partial_\tau - i\lambda_x + \mu) b_x - \sum_{xy\sigma} t_{xy} b_x b^*_y f^*_{x\sigma} f_{y\sigma} \end{aligned}$$

S is invariant under local gauge transformations

$$f_{x\sigma} \to \exp(i\theta_x) f_{x\sigma}, \quad b_x \to \exp(i\theta_x) b_x$$

$$\chi_{xy} \to \exp(-i\theta_x)\chi_{xy}\exp(i\theta_y)$$

$$\Delta_{xy} \to \exp(i\theta_x)\Delta_{xy}\exp(i\theta_y)$$

$$\lambda_x \to \lambda_x + \partial_\tau \theta_x$$

Often one writes L_1 in the form

$$\begin{aligned} L_1 &= \frac{1}{8}\sum_{xy} \mathrm{Tr} J_{xy} U_{xy}^\dagger U_{xy} + \frac{1}{8}\sum_{xy\sigma}(\Phi_{x\sigma}^\dagger U_{xy}\Phi_{y\sigma} + \text{c.c.}) \\ &+ \sum_{x\sigma} f_{x\sigma}^*(\partial_\tau - i\lambda_x) f_{x\sigma} + \sum_x b_x^*(\partial_\tau - i\lambda_x + \mu) b_x - \sum_{xy\sigma} t_{xy} b_x b_y^* f_{x\sigma}^* f_{y\sigma} \end{aligned}$$

where

$$\Phi_{x+} = \begin{pmatrix} f_{x+} \\ f_{x-}^* \end{pmatrix}, \quad \Phi_{x-} = \begin{pmatrix} f_{x-} \\ -f_{x+}^* \end{pmatrix}$$

$$U_{xy} = \begin{pmatrix} -\chi_{xy}^* & \Delta_{xy} \\ \Delta_{xy}^* & \chi_{xy} \end{pmatrix}$$

In this representation, and at half filling ($\mu = 0$, $b = 0$) S is invariant under

$$\Phi_{x\sigma} \to V_x \Phi_{x\sigma}$$

$$U_{xy} \to V_x U_{xy} V_y^\dagger$$

where V_x are local $SU(2)$ matrices. Therefore, besides the local gauge symmetry, the model even has a local $SU(2)$-symmetry.

Various authors proposed different mean field solutions to this model. They correspond to different saddle point approximations. In these saddle point approximations, the following variables play a crucial role

$$\chi_{xy} = \sum_\sigma \langle f_{x\sigma}^* f_{y\sigma} \rangle$$

$$\Delta_{xy} = \langle f_{x+}^* f_{y-}^* - f_{x-}^* f_{y+}^* \rangle$$

The first represents the RVB-state proposed by Baskaran, Zou, and Anderson. The ansatz is $\chi_{xy} = \chi$ real and $\Delta_{xy} = 0$. The spectrum is that of a ferionic model

$$H_{BZA} = -\frac{\chi}{2}\sum_{xy\sigma} J_{xy} f_{x\sigma}^\dagger f_{y\sigma}$$

There are other states with low energies. Among them, there is a super-conducting d-wave state and a flux phase state, both with the same variational energy and the same dispersion relation for low lying excitations. Both are equivalent and can be obtained from each other using the local $SU(2)$-symmetry. Totally, one obtains four different mean fields phase: a Fermi liquid ($\chi \neq 0$, $b \neq 0$), a spin-gap phase ($\chi \neq 0$, $\Delta \neq 0$), d-wave superconductivity ($\chi \neq 0$, $b \neq 0$, $\Delta \neq 0$), a strange metal ($\chi \neq 0$), and at higher temperature the RVB-state. The mean-field theory represents the experimental situation quite well.

Partially, these considerations can be made mathematically precise, see the work by J. Fröhlich and P. Marchetti [14]. But the resulting field theory is difficult and has not yet been fully investigated and understood.

6 The fractional quantum Hall effect

6.1 Introduction

The quantum Hall effect was found 1980 by von Klitzing and published in a paper by von Klitzing, Dorda, and Pepper [30], Klaus von Klitzing received in 1985 the Nobel prize. For a general introduction I refer to [61]. The quantum Hall effect can be observed in two dimensional electron systems in a strong perpendicular magnetic field. Under certain conditions one observes a conductivity tensor of the form

$$\sigma = \begin{pmatrix} 0 & -n\frac{e^2}{h} \\ n\frac{e^2}{h} & 0 \end{pmatrix} \tag{6.1}$$

The Hall conductivity is thus $\sigma_H = n\frac{e^2}{h}$. For the usual quantum Hall effect, n is an integer. The most remarkable point is the experimental precision with which this number can be obtained. The relative precision is $3 \cdot 10^{-7}$ or even better. Therefore, the quantum Hall effect can be used to determine the fine structure constant $\frac{e^2}{\hbar c} \approx \frac{1}{137}$ with a very high precision since c is fixed. In the fractional quantum Hall effect n is a fraction with a typically small odd denominator. The precision is less but still high. The theory has to explain why the effect occurs and why the experimental precision is so high. This is remarkable since the two dimensional electron system is formed at the interface between two semi-conductors, e.g. in a Si-MOSFET or in a GaAs/GaAlAs hetero structure. At the interface between two semi-conductors one has lots of imperfections, disorder, so that such a high precision is really astonishing.

The Hall effect

The most simple theory takes quantum effects only in a semi-classical approximation into account. The theory is based on the assumption that the two dimensional electrons have a mean free path ℓ_0 or equivalently a mean free flight time τ_0. Both are related because the electron move at the Fermi velocity , i.e. $\ell_0 = v_F \tau_0$. In an electric field $\vec{E}$ an electron is accelerated between two collisions. The velocity between two collision increases by $\Delta\vec{v} = -e\vec{E}\tau_0/m$. Adding up the contributions of all electrons, one obtains the current density $\vec{j} = \sigma_0\vec{E}$ where

$$\sigma_0 = \rho e^2 \tau_0 / m \tag{6.2}$$

Quantum effects are included only via an effective mass m and via the mean free flight time τ_0.

If we apply in addition a magnetic field, the Lorentz force acts on the electrons and we obtain

$$\vec{j} = \sigma_0\vec{E} - \frac{\sigma_0}{\rho ec}\vec{j}\times\vec{B} \tag{6.3}$$

In a two dimensional system we therefore obtain

$$\sigma^{-1} = \begin{pmatrix} \sigma_0^{-1} & \frac{B}{\rho ec} \\ -\frac{B}{\rho ec} & \sigma_0^{-1} \end{pmatrix} \tag{6.4}$$

The conductivity is therefore

$$\sigma_{xx} = \frac{\sigma_0}{1+\omega_c^2\tau_0^2}, \quad \sigma_{xy} = \frac{\rho ec}{B} + \frac{\sigma_{xx}}{\omega_c\tau_0} \tag{6.5}$$

where $\omega_c = \frac{eB}{mc}$ is the cyclotron frequency. Note that in the limit $\tau_0 \to \infty$ one obtains the result for free electrons.

Experimental realisation

As already mentioned, the quantum Hall effect is observed at the interface of two semi-conductors, to be precise, at the interface of a semi-conductor (e.g. doped Si, GaAlAs) and an insulator (SiO_2, GaAs). The typical systems are Si-MOSFETs or GaAs-GaAlAs hetero structures. The basic idea is relatively simple: Via a gate one applies an electric field perpendicular to the interface so that electrons move to the interface. Since they cannot enter the insulator, they form a two dimensional electron gas at the interface. At the interface, the energy band is lower than in the bulk so that electrons concentrate at the interface. They form an inversion layer. The electrons are bound in the direction perpendicular to the interface, but they can move rlatively freely parallel to the interface. Due to defects and impurities, esp. in the doped semi-conductor, the mean free path is expected to be short.

Landau levels

We now apply a magnetic field perpendicular to the interface. We first neglect all impurities and interactions, we just look at a free electron in two dimensions with a perpendicular megnetic field. The Hamiltonian is

$$H = \frac{\hbar^2}{2m}\left[\left(\frac{1}{i}\frac{\partial}{\partial x} - \frac{eB}{\hbar c}y\right)^2 - \frac{\partial^2}{\partial y^2}\right] \tag{6.6}$$

where we chose a Landau gauge $A_x = -yB$, $A_y = 0$. Since x does not appear as a variable in the Hamiltonian, we can use the ansatz

$$\psi \propto \exp(ikx)\phi(y) \tag{6.7}$$

for the eigenfunctions. This leads to the eigenvalue equation

$$\frac{\hbar\omega_c}{2}\left(-l_B^2\frac{\partial^2}{\partial y^2} + \left(\frac{y}{l_B} - l_B k\right)^2\right)\phi = E\phi \tag{6.8}$$

where $l_B = (\hbar c/eB)^{1/2}$ is the magnetic length. This is the eigenvalue equation of a shifted harmonic oscillator. The solutions are therefore

$$\phi_{n,k} \propto H_n(y/l_B - l_B k)\exp(-(y - l_B^2 k)/2l_B^2) \tag{6.9}$$

$$E_{nk} = \hbar\omega_c(n + 1/2) \tag{6.10}$$

and the eigenvalues do not depend on k. We therefore obtain a huge degeneracy. The degenerate eigenvalues are called Landau levels. The number of states in a Landau level is $F/2\pi l_B^2$, where F is the area of the system. Boundary effects are neglected here. The density of states is given by

$$n_B = \frac{1}{2\pi l_B^2} = \frac{eB}{hc} \tag{6.11}$$

The single-particle states constructed in that way are localised in y-direction and extended in x-direction. But the high degeneracy allows to take arbitrary linear combinations of states with the same eigenvalue. Therefore, one can as well construct eigenstates that are localised in x-direction and extended in y-direction or that are localised in both directions.

If a Landau level is completely filled, the Fermi energy lies between two Landau levels in a region without states. That means that there is no scattering and no diffusion, i.e. $\tau_0 = \infty$. The filling factor

$$\nu = \frac{\rho}{n_B} \tag{6.12}$$

is an even number and for the conductivity tensor one obtains

$$\sigma^{-1} = \begin{pmatrix} \sigma_0^{-1} & \frac{B}{\rho ec} \\ -\frac{B}{\rho ec} & \sigma_0^{-1} \end{pmatrix} = \begin{pmatrix} 0 & \frac{h}{\nu e^2} \\ -\frac{h}{\nu e^2} & 0 \end{pmatrix} \tag{6.13}$$

A second argument yields the same result. Is uses the Lorentz invariance. A system with a magnetic field $\vec{B}$ and a perpendicular electric field $\vec{E}$ can be transformed to another system with a Lorentz transformation with velocity

$$\vec{v} = c\frac{\vec{E} \times \vec{B}}{B^2} \tag{6.14}$$

which contains no electric field and therefore no macroscopic current. In the original system, the current density is therefore

$$\vec{j} = -\rho e\vec{v} \tag{6.15}$$

which yields the same conductivity tensor. Therefore, without imperfections, defects or impurities one always obtains

$$\sigma_{xx} = 0, \quad \sigma_{xy} = \frac{\rho ec}{B} = \nu\frac{e^2}{h} \tag{6.16}$$

The question now is, what is the influence of disorder.

6.2 The integer quantum Hall effect

In this section we will discuss two different arguments which may explain the plateaus one observes experimentally in the integer quantum Hall effect. The main goal is a qualitative understanding of the effect, not the theoretical details. We are mainly interested in the fractional quantum Hall effect, where interactions play a crucial role.

6.2.1 Disorder

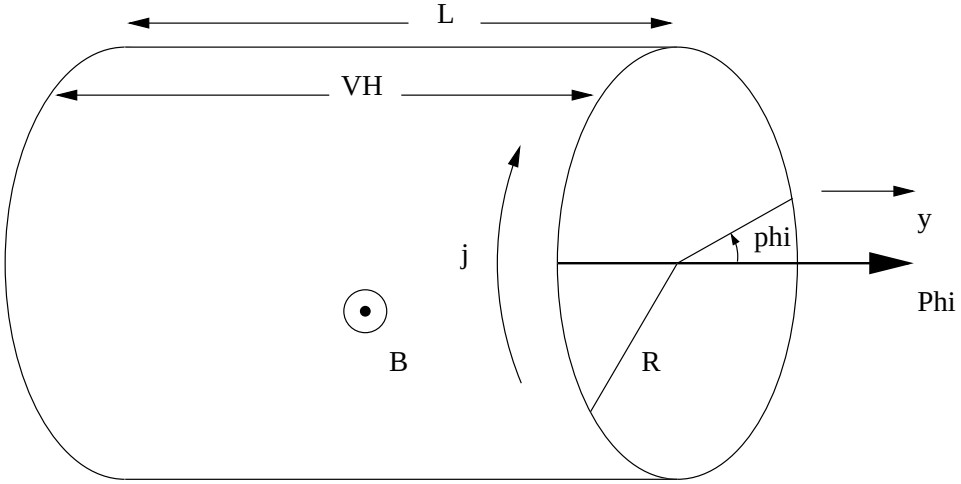
The integer quantum Hall effect can be explained on a very basic level as follows: We saw that a completely filled Landau level yields a contribution of $\frac{e^2}{h}$ to σ_{xy}. The question is now, what happens for a partially filled Landau level. We have many imperfections, defects and impurities, in the system. What is the effect of disorder? Generically, disorder leads to localisation, this is the so called Anderson localisation. P. W. Anderson received the Nobel prize (together with Mott and van Fleck) in 1977 for his contribution to the theory of localisation. Suppose that the disorder is not too large. Typically, one describes a disordered system by a potential $V(x,y)$. Suppose that the typical energy differences of the potential are small compared to $\hbar\omega_c$. Then, in a first order perturbational treatment, one has to diagonalise the Hamiltonian

$$H_0 = P_0 V(x,y) P_0 \tag{6.17}$$

where P_0 is the projector onto a Landau level. We take the Landau level which contains the Fermi energy. A potential $V(x,y)$ that describes disorder is often realised as a random potential. Such a potential lifts the degeneracy of the Landau level and tends to localise the electrons. Electrons close to deep minima or maxima of the potential will be stronger localised and will have an energy far away from the original energy of the Landau level. On the other hand, we know that the complete Landau level must still yield a contribution $\frac{e^2}{h}$ to the Hall conductivity. This contribution cannot com from localised states. It must come from extended states which we expect to find in the middle of the broadened Landau level. If we now change the filling factor, e.g. by changing the magnetic field, the Fermi energy will move through the spectrum. There are regions in the spectrum where all states are localised and do not contribute to the current. In these regions we should observe a zero diagonal conductivity and a Hall conductivity which is an integer multiple $\frac{e^2}{h}$.

It is of course possible to formulate this argument in a mathematically more precise way. A field theoretic formulation can be found in Chapter 5 by A. M. M. Pruisken in [61].

Figure 6.1: The cylinder geometry



6.2.2 Laughlins gauge argument

Let us choose the vector potential to be

$$A_x = -By + \frac{\Phi}{2\pi R}, \quad A_y = 0 \tag{6.18}$$

so that the Hamiltonian reads

$$H = \frac{\hbar^2}{2m}\left[\left(\frac{1}{i}\frac{\partial}{\partial x} - \frac{eB}{\hbar c}y + \frac{e\Phi}{2\pi R\hbar c}\right)^2 - \frac{\partial^2}{\partial y^2}\right] + V(x,y) \tag{6.19}$$

Further, we assume periodic boundary conditions in x-direction, i.e.

$$x = \varphi R \tag{6.20}$$

where $0 < \varphi \leq 2\pi$. This corresponds to a cylinder geometry. The potential $V(x,y)$ contains the Hall voltage V_H applied in y-direction, a boundary potential depending only on y, and the disorder potential coming from the impurities. For $V = 0$ the energy levels are the Landau levels characterised by the Landau index n. Within a Landau level one introduces a second index. The eigenfunctions are

$$\psi_{n,k} \propto \exp(ikx) H_n(y/l_B - l_B(k + \frac{e\Phi}{2\pi R\hbar c})) \exp(-(y - l_B^2(k + \frac{e\Phi}{2\pi R\hbar c})/2l_B^2) \tag{6.21}$$

where $k = l/R$, $l \in Z$ because of the periodic boundary conditions. We can write as well

$$\psi_{n,l} \propto \exp(2\pi i l\varphi) H_n\left(\frac{y}{l_B} - \frac{l_B}{R}(l + \frac{e\Phi}{hc})\right) \exp\left(-\frac{1}{2}\left(\frac{y}{l_B} - \frac{l_B}{R}(l + \frac{e\Phi}{hc})\right)^2\right) \tag{6.22}$$

The eigenvalues do not depend on l or Φ. We now introduce a potential $V_0(y)$ that fixes the boundary. It is still possible to describe the states by the two indices n and l, but now the eigenvalues may depend on l and Φ. The dependency $E_{n,l}(\Phi)$ is not arbitrary. The x-dependency of the wave function is not affected by $V_0(y)$ and the Hamiltonian depends only on $l + \frac{e\Phi}{hc}$, therefore we have $E_{n,l}(\Phi) = E_n(l + e\Phi/hc)$ and

$$E_{n,l}(\Phi + \frac{hc}{e}) = E_{n,l+1}(\Phi) \tag{6.23}$$

$V_0(y)$ is only at the boundary different from 0. The states are therefore still localised in y-direction close to $\frac{l_B^2}{R}(l + \frac{e\Phi}{hc})$ and only those states where the localisation is close to the boundary will be affected by the potential.

Therefoe, only states close to the boundary will have an energy significantly different from $\hbar\omega_c(n+\frac{1}{2})$. The contribution of a state to the current in x-driection is

$$I_{n,l} = -c\frac{dE_{n,l}(\Phi)}{d\Phi} \tag{6.24}$$

Only the states close to the boundary have a significant dependency on Φ. They yield a contribution to the current. The total current is the sum over all contributions $I_{n,l}$ weighted with the occupation number. Averaging over Φ yields

$$\begin{aligned} I &= \frac{e}{h}\int_0^{hc/e} d\Phi \sum_{n,l} n_{n,l} I_{n,l} \\ &= -\frac{e}{h}\sum_{n,l} n_{n,l}(E_{n,l}(hc/e) - E_{n,l}(0)) \\ &= -\frac{e}{h}\sum_{n=0}^{\nu}(E_{n,l_{max}}(0) - E_{n,l_{min}}(0)) \\ &= \frac{e^2}{h}\nu V_H \end{aligned} \tag{6.25}$$

Therefore $\sigma_H = I/V_H$ is an integer multiple of e^2/h. This argument remains correct if one introduces disorder to the system. In that case, the eigenenergies $E_{n,l}(\Phi)$ depend separately on l and Φ and not only on $l + \frac{e\Phi}{hc}$. But the Hamiltonian is still periodic in Φ and therefore we may still apply the above argument. The disorder will localise most of the eigenstates, but some of them must still carry a current. With this argument it becomes clear that in this geometry the current carrying states are those close to the boundary.

Experimental systems always have a boundary, also in x-direction. If one introduces a boundary potential in x-direction as well, the argument cannot be applied directly but one still expects that the current is carried by states which are extended around the boundary. On the other hand, it is as well possible to formulate the theory with periodic boundary conditions in both directions. In that case there are no boundary states but there are still states carrying the current.

6.3 The fractional quantum Hall effect

The fractional quantum Hall effect was found by Tsui, Störmer and Gossard at the end of 1981 and published in 1982 [74]. First theoretical approaches followed immediately, the main theoretical achievement was the work by Laughlins [33] who described the ground state of the interacting many-electron system as a quantum fluid. The Nobel Prize in Physics 1998 was awarded to Robert B. Laughlin, Horst L. Störmer, Daniel C. Tsui for their discovery and theoretical work on the fractional quantum Hall effect.

6.3.1 Wave functions

Lowest Landau level

Models with non-interacting electrons as introduced in the last section cannot explain the fractional quantum Hall effect. For the fractional quantum Hall effect, the interaction between electrons is important. The Hamiltonian is

$$H = \sum_j \left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla_j + \frac{e}{c}\vec{A}_j\right)^2 + V_1(\vec{r}_j)\right] + \frac{1}{2}\sum_{j\neq k} V(|\vec{r}_j - \vec{r}_k|) \tag{6.26}$$

$V_1(\vec{r})$ is a single particle potential. In the simplest way it describes a homogeneous background. In a more complete model in contains the effect of the lattice, of imperfections, of the boundary, etc. The interaction $V(|\vec{r}|)$ is typically isotropic. An ansatz would be the Coulomb interaction

$$V(|\vec{r}|) = \frac{e^2}{|\vec{r}|} \tag{6.27}$$

or a screened interaction, which may be more suitable in the case we have in mind. The electrons move in a strong magnetic field. We assume that the spin of the electrons is polarised and can therefore be ignored. This is a suitable approximation if the filling factor $\nu \leq 1$. For the vector potential we choose a symmetric gauge

$$\vec{A} = \frac{B}{2}(y\vec{e}_x - x\vec{e}_y) \tag{6.28}$$

m is the effective mass, it depends on the material we are looking at. For GaAs hetero structures $m = 0.07m_e$ is a typical value. In the following I take as a first ansatz a constant background potential V_1 which can be put to 0. The single particle Hamiltonian now reads

$$\begin{aligned} H &= \frac{1}{2}\hbar\omega_c \left[\left(-il_B \frac{\partial}{\partial x} - \frac{y}{2l_B} \right)^2 + \left(-il_B \frac{\partial}{\partial y} + \frac{x}{2l_B} \right)^2 \right] \\ &= \frac{1}{2}\hbar\omega_c [z^* z + z^* \partial_{z^*} - z\partial_z - \partial_z \partial_{z^*}] \end{aligned} \tag{6.29}$$

where

$$z = \frac{1}{2l_B}(x - iy), \quad z^* = \frac{1}{2l_B}(x + iy) \tag{6.30}$$

$$\partial_z = l_B \left(\frac{\partial}{\partial_x} + i\frac{\partial}{\partial_y} \right), \quad \partial_{z^*} = l_B \left(\frac{\partial}{\partial_x} - i\frac{\partial}{\partial_y} \right) \tag{6.31}$$

We define

$$a^\dagger = \frac{1}{\sqrt{2}}(z^* - \partial_z) \tag{6.32}$$

$$a = \frac{1}{\sqrt{2}}(z + \partial_{z^*}) \tag{6.33}$$

where $[a, a^\dagger] = 1$, and obtain

$$H = \hbar\omega_c (a^\dagger a + \frac{1}{2}) \tag{6.34}$$

A wave function in the lowest Landau level obeys the condition

$$a\psi = 0 \tag{6.35}$$

$$z\psi + \partial_{z^*}\psi = 0 \tag{6.36}$$

with the general solution

$$\psi = f(z)\exp(-z^* z) \tag{6.37}$$

$f(z)$ is an arbitrary analytic function depending on z. We assume that $\hbar\omega_c$ is the by far largest energy scale and that $\nu < 1$. The Hilbert space can then be restricted to the lowest Landau level. A general multi-particle wave function in the lowest Landau level has the form

$$\Psi = f(z_1, \ldots, z_{N_e})\exp(-\sum_i z_i^* z_i) \tag{6.38}$$

where f is again an analytic function.

Construction of a single particle basis and angular momentum

Before we discuss a variational ansatz for the many particle ground state, let us introduce a suitable single particle basis. The Hamiltonian has a rotational symmetry, it commutes with the angular momentum L_z parallel to the magnetic field. One has

$$\begin{aligned} L_z &= ix\frac{\partial}{\partial y} - iy\frac{\partial}{\partial x} \\ &= z\partial_z - z^*\partial_{z^*} \end{aligned} \tag{6.39}$$

$$L_z f(z)\exp(-z^*z) = zf'(z)\exp(-z^*z) \tag{6.40}$$

The eigenstates of L_z are therefore

$$\psi_m = z^m \exp(-z^*z) \tag{6.41}$$

with the eigenvalue m. The ψ_m for a complete and orthogonal system of states within the lowest Landau level, since they are the eigenfunctions of the operator L_z. Introducing a suitable normalisation the set $\{\psi_m, m = 1,\ldots,\infty\}$ forms an orthonormal basis of the single-particle Hilbert space. $|\psi_m(z,z^*)|^2$ is rotational invariant and has a maximum at $|z|^2 = m$. To deal with a finite system, we restrict the Hilbert space to values $m \leq M$, the filling factor is then $\nu = N_e/M$. This corresponds to a disk geometry with a soft boundary.

A many particle wave function

$$\Psi = f(z_1,\ldots,z_{N_e})\exp(-\sum_i z_i^* z_i) \tag{6.42}$$

is an eigenfunction of L_z, if $f(z_1,\ldots,z_{N_e})$ is a homogeneous polynomial in the variables.

Laughlins ansatz for the ground state

Because of the projection to the lowest Landau level the only important contribution in the Hamiltonian is the interaction. There is no single particle Hamiltonian any more. Laughlins idea is that the electrons should avoid each other as good as possible. We therefore look for an ansatz which is homogeneous and where the electrons have a large distance between each other. An ansatz, which was very successful in the description of liquid He_3 is the Jastrow ansatz. It has the form

$$\prod_{j<k} f(\vec{r}_j - \vec{r}_k) \tag{6.43}$$

In our case this means

$$\Psi = \prod_{j<k} f(z_j - z_k)\exp(-\sum_i z_i^* z_i) \tag{6.44}$$

This wave function must have the following properties

- It should be an eigenfunction ofL_z. Therefore $f(z) \propto z^m$.
- It should be antisymmetric with respect to permutaions of two particles. Therefore, m must be odd.

This means that the Jastrow ansatz yields

$$\Psi = \Psi_m = \prod_{j<k}(z_j - z_k)^m \exp(-\sum_i z_i^* z_i) \tag{6.45}$$

Ψ_m is a wave function with an angular momentum $L_z = mN_e(N_e-1)/2$. The highest power which occurs for a single argument z_j is $M = m(N_e-1)$. As a consequence, the filling factor of the wave function is $\nu = 1/m$. For a fixed density, i.e. a fixed filling factor, the Jastrow ansatz has no free parameter, the wave function is fixed.

The question is whether Ψ_m is a good ansatz for the ground state of the Hamiltonian, and if yes, why. To clarify this we look at two different calculations which have been done quite early after the publication of this ansatz by Laughlin. The first is the diagonalisation of the Hamiltonian for small numbers of particles. An exact

diagonalisation allows to calculate the overlap of the true ground state with Ψ_m. A good overview of such calculations can be found in the book by T. Chakraborty and O. Pietiläinen [7]. It turns out that the overlap is better for short range interactions and that for the bare Coulomb interaction the overlap is about 99% per particle. The calculation have been done with up to 7 electrons for $\nu = 1/3$. The Hilbert space dimension is $\begin{pmatrix} 21 \\ 7 \end{pmatrix}$, the diagonalisations are done using a Lanczos algorithm.

The numerical calculations show that for short range interactions the overlap is even better. Since the electrons in our case have all the same spin, a short range interaction of Hubbard type, which would be $V(r) = V_0\delta(r)$ in the continuum, has no effect. The Pauli principle interdicts two electrons with the same spin at the same place. The shortest possible interaction is therefore

$$V(r) = V_2\nabla^2\delta(r) \tag{6.46}$$

One can show that Ψ_m is the exact ground state for such a short range interaction. We will come back to this point. It supports the view that Ψ_m describes the ground state wave function quite well.

Let us mention that it is possible to formulate a Laughlin type wave function as well for systems with periodic boundary conditions. This is useful because in such a case the gauge argument formulated by Laughlin for the integer quantum Hall effect can be applied. We discuss periodic boundary conditions below.

Properties of Ψ_m

Let us first discuss the case $m = 1$.

$$\Psi_1 = \prod_{j<k}(z_j - z_k)\exp(-\sum_i z_i^* z_i) \tag{6.47}$$

The factor $\prod_{j<k}(z_j - z_k)$ is a so called Vandermonde determinant. One has

$$\prod_{j<k}(z_j - z_k) = (-1)^{N_e(N_e-1)/2}\sum_P (-1)^P \prod_i z^i_{P(i)} \tag{6.48}$$

Up to a normalisation factor, Ψ_1 is the Slater determinant of the N_e single particle basis states ψ_m, $m = 1,\ldots,N_e$. Therefore, Ψ_1 is the exact ground state of the system for filling factor $\nu = 1$.

Let us now discuss general wave functions Ψ_m. One has

$$|\Psi_m|^2 = \exp(-\beta\phi_m(z_1,\ldots,z_{N_e})) \tag{6.49}$$

This is the distribution function of the electrons. It can be interpreted as a classical gas with a free energy $\phi_m(z_1,\ldots,z_{N_e})$. We choose $\beta = 2/m$ and obtain

$$\phi_m(z_1,\ldots,z_{N_e}) = -m^2\sum_{j<k}\ln|z_j - z_k| + m\sum_{l=1}^{N_e}|z_l|^2 \tag{6.50}$$

This is the free energy of a classical two-dimensional one-component plasma with charge m. The general free energy of a classical two-dimensional one-component plasma is

$$\phi_m(z_1,\ldots,z_{N_e}) = -e^2\sum_{j<k}\ln|z_j - z_k| + \frac{\pi}{2}\rho_0 e\sum_{l=1}^{N_e}|z_l|^2 \tag{6.51}$$

Here, the first term represents the two-dimensional Coulomb repulsion of the particles and the second term represents the attractive interaction with a homogeneous background with a charge density ρ_0. In our case we have

$$\rho_0 = \frac{2}{\pi} \tag{6.52}$$

The plasma is neutral, the particle density is

$$\rho = \frac{2}{\pi m} \tag{6.53}$$

Th physical properties of the two-dimensional single-component plasma is well understood. For not too large m it forms an incompressible fluid. It has a homogeneous density. The most important quantity to look at is the pair correlation function

$$g(z_1, z_2) = \frac{N_e(N_e-1)}{\rho^2} \frac{\int d^2z_3 \ldots d^2z_{N_e} |\Psi_m|^2}{\int d^2z_1 \ldots d^2z_{N_e} |\Psi_m|^2} \tag{6.54}$$

g describes the correlation of two particles. For a translational invariant and isotropic system, it depends only on $r = |z_1 - z_2|$. For large r the function tends to 1. For small r it decays like $\propto r^{2m}$. The interaction energy is

$$E_{WW} = \frac{1}{2} \int d^2z g(|z|) V(|z|) \tag{6.55}$$

Taking into account the homogeneous background, the total energy is

$$E = \frac{1}{2} \int d^2z (g(|z|) - 1) V(|z|) \tag{6.56}$$

For a short range interaction $V(z) = V_2 \nabla^2 \delta(z)$ we have $E = E_{WW}$. If $g(r)$ decays faster than r^2 one obtains $E = 0$. Since E is non-negative, Ψ_m is a ground state of the system, as stated above. Further, one can show that Ψ_m is the only ground state for $m = 3$. For $m = 5$ it is not unique but it becomes unique if a second term is introduced to the interaction $V(z) = (V_2 \nabla^2 + V_4 (\nabla^2)^2) \delta(z)$. Similar results can be shown for larger values of m. This explains the above proposition that Ψ_m is the exact ground state of the system for short range interactions.

The function $g(r)$ shows the typical characteristics of an incompressible fluid. It vanishes sufficiently fast at $r = 0$, has a single maximum at some characteristic value of r and tends to 1 without further oscillations for large r. For a crystal $g(r)$ shows oscillations. For $m = 1$ we can calculate $g(r)$ exactly, one obtains

$$g(r) = 1 - \exp(-r^2) \tag{6.57}$$

The wave function Ψ_m therefore describes for not too large m an incompressible quantum fluid. For an incompressible quantum fluid one expects an energy gap between the ground state and the low lying excitations. Let us now look at the low lying excitations.

6.3.2 Elementary excitations

We use the quasi-particle concept to describe the elementary excitations. We constrict quasi-particles and -holes. Let ε_p and ε_h be the energy of a quasi-particle or -hole respectively. Then, $\varepsilon = \varepsilon_p + \varepsilon_h$ is the excitation energy of an uncharged excitation. In Laughlin's original formulation, he created quasi-particles or -holes by changing M instead of N_e. Let us first discuss a quasi-hole. It can be obtained by increasing M.

For a given wave function Ψ, M is determined by the number of zeros the wave function has as a function of a single particle coordinate z_i. Increasing M means increasing the number of zeros. The simplest state is one with an additional zero, i.e. a state with $M+1$ zeros. We let

$$\Psi_m^{(-)} = S_{z_0} \Psi_m \tag{6.58}$$

$$S_{z_0} = \prod_{j=1}^{N_e} (z_j - z_0) \tag{6.59}$$

The wave function $S_{z_0}^m \Psi_m$ corresponds to a wave function with filling factor $1/m$ and $N_e + 1$ electrons, where one electron at z_0 is taken out. $\Psi_m^{(-)}$ ca therefore be interpreted as a hole where a $1/m$ fraction of an electron was removed. The state is a state with a fractional charge. The quasi-hole generated at z_0 via S_{z_0} has the charge e/m. The same holds true for the classical two-dimensional one-component plasma. The multiplication with

S_{z_0} corresponds to adding $-m\sum_j \ln|z_j - z_0|$ to ϕ_m, and therefore to a missing charge of 1, whereas the particles forming the plasma have a charge m.

Because of the translational invariance of the system the energy of the quasi-hole does not depends on z_0. One can determine the energy either by diagonalising small systems numerically like for the ground state or by calculating the expectation value of the Hamiltonian in the state $\Psi_m^{(-)}$, which as well must be done numerically. The typical energy of the quasi-hole is $0.025e^2/l_B$. At typical field strength $B \approx 10-20T$ the excitation energy corresponds to a temperature of $4-8K$. This is in good agreement with the experimental fact that the fractional quantum Hall effect can be observed ate temperature below $1K$.

It is a bit more difficult to construct wave functions for quasi-particles. Laughlins proposal was to use

$$\Psi_m^{(+)} = \exp(-\sum_j |z_j|^2) \prod_{j=1}^{N_e} \frac{\partial}{\partial z_j} \prod_{k<l} (z_k - z_l)^m \tag{6.60}$$

for a quasi-particle at the origin. The numerical calculations show that this is a less good approximation. Nevertheless, the basic physical idea connected to this ansatz is the same as for quasi-holes.

The excitation energies for quasi-particles or quasi-holes are finite, as it should be for an incompressible quantum fluid. Similarly to the integer quantum Hall effect, one may now argue that the quasi-particles or holes in the system behave like usual electrons in the integer quantum hole effect. The only difference is the charge, which is $1/m$ times the original charge. This argument can then be used to explain why there are plateaus in the Hall conductivity at integer multiples of e^2/hm.

6.3.3 Periodic boundary conditions

The ideas presented so far can be formulated in a system with periodic boundary conditions as well. The mathematical formulation is more evolved, because one has to deal with doubly-periodic analytic functions. Such functions do not exists. Instead, one needs quasi-periodic functions, so called θ-functions. The representation uses projective representations of the translation group. Within this representation it can be shown that an additional particle or hole in the system is indeed localised and thereby on can explain the existence of a plateau in the Hall conductivity.

6.4 Universality

In a seminal paper, Fröhlich and Kerler [13] showed that there is a completely different way to explain the integer and fractional quantum Hall effect. In this last section, I briefly sketch their view and I try to connect it to what we learned so far. Starting point is classical electrodynamics.

6.4.1 Classical electrodynamics in quantum Hall systems

In this subsection we look at the classical electrodynamics of a two-dimensional electron gas which has a conductivity tensor of the form

$$\sigma = \begin{pmatrix} 0 & -\sigma_H \\ \sigma_H & 0 \end{pmatrix} = \sigma_H \varepsilon \tag{6.61}$$

where $\varepsilon = (\varepsilon_{\alpha\beta})_{\alpha,\beta=1,2}$ with $\varepsilon_{12} = -\varepsilon_{21} = 1$, $\varepsilon_{11} = \varepsilon_{22} = 0$. We introduce the current density $\vec{j} = (j^1, j^2)$ and the charge density j^0. The electric field is $\vec{E} = (E_1, E_2)$ and we introduce a field-strength tensor F. It is anti-symmetric and has the elements $F_{0\alpha} = E_\alpha$, $F_{12} = -B$. B is the magnetic field perpendicular to the two-dimensional plane the electrons move in. Further, let $x^0 = ct$ and x^1, x^2 be the coordinates, $x = (x^0, x^1, x^2)$, and

$$\partial_\alpha = \frac{\partial}{\partial x^\alpha} \tag{6.62}$$

The current density is given by

$$j^{\alpha}(x) = \sigma_H \varepsilon^{\alpha\beta} E_{\beta}(x) \tag{6.63}$$

The continuity condition is

$$\partial_{\alpha} j^{\alpha} = 0 \tag{6.64}$$

and Faradays law has the form

$$\frac{\partial B}{\partial x^0}(x) + \nabla \times \vec{E}(x) = 0 \tag{6.65}$$

or

$$\varepsilon^{\alpha\beta\gamma} \partial_{\alpha} F_{\beta\gamma}(x) = 0 \tag{6.66}$$

Taking the continuity condition and Faradays law, we obtain

$$\sigma_H \partial_0 B = -\sigma_H \nabla \times \vec{E} = -\nabla \cdot \vec{j} = \partial_0 j^0 \tag{6.67}$$

and therefore

$$j^0(x) = \sigma_H B(x) \tag{6.68}$$

Taking this equation together with the material equations for $\vec{j}$ we may put everything together in the compact form

$$J_{\alpha\beta}(x) = \sigma_H F_{\alpha\beta}(x) \tag{6.69}$$

where

$$J_{\alpha\beta}(x) = \varepsilon_{\alpha\beta\gamma} j^{\gamma}(x) \tag{6.70}$$

$\varepsilon_{\alpha\beta\gamma}$ is the complete anti-symmetric tensor. The continuity equation now takes the form

$$\varepsilon^{\alpha\beta\gamma} \partial_{\alpha} J_{\beta\gamma}(x) = 0 \tag{6.71}$$

As a consequence, σ_H must be locally independent of x! Further, lines where σ_H changes must carry a current. The continuity equation implies that for the current tensor $J_{\alpha\beta}$ and as well for the field-strength tensor $F_{\alpha\beta}$ we can introduce a vector potential

$$F_{\alpha\beta} = \partial_{\alpha} A_{\beta} - \partial_{\beta} A_{\alpha} \tag{6.72}$$

$$J_{\alpha\beta} = \partial_{\alpha} a_{\beta} - \partial_{\beta} a_{\alpha} \tag{6.73}$$

and we obtain

$$\partial_{\alpha}(a_{\beta} - \sigma_H A_{\beta}) - \partial_{\beta}(a_{\alpha} - \sigma_H A_{\alpha}) = 0 \tag{6.74}$$

This relation can be derived from the action

$$S_{CS}(a - \sigma_H A) = \int_{R \times \Omega} d^3x \varepsilon^{\alpha\beta\gamma}(a_{\alpha} - \sigma_H A_{\alpha}) \partial_{\beta}(a_{\gamma} - \sigma_H A_{\gamma}) \tag{6.75}$$

S_{CS} is called Chern-Simons action. This action is independent of the choice of coordinates.

The status of the ideas presented so far is as follows: Whereas the continuity equation and Faradays law hold exactly, the material equation $J = \sigma_H F$ is experimentally varified only on sufficiently large time and length scales. We therefore cannot exclude that in addition to the Chern-Simons action S_{CS} the total action contains a further term S_I which should be symmetric under time reversal and which should conserve parity. The total action will therefore be

$$S(a,A) = S_{CS}(a - \sigma_H A) + S_I(a,A) \tag{6.76}$$

where the behaviour on long time and length scales is determined by S_{CS}.

6.4.2 Quantisation

The current density j is a quantum mechanical operator, to be precise an operator valued distribution, therefore the vector potential a must be an operator as well. The same is true for A, at least in principle. Since we do not want to treat QED, it is in our case sufficient to take A as a classical field. The remaining task is now to quantise the action $S(a,A)$ where A will be treated as an external, classical field. The quantisation can be performed using a path integral. We use Euclidean path integrals and introduce the coordinates

$$a_0 \to -ia_0, \quad A_0 \to -iA_0, \quad \partial_0 \to -i\partial_0, \quad dx^0 \to idx^0 \tag{6.77}$$

Further, we introduce the vector potential A_c for the external constant magnetic field so that the total as vector potential $\tilde{A} = A_c + A$ contains A_c and A, coming from local sources. The Euclidean measure dP_A, which describes the ground state of the system with the action S is then given by

$$dP_A(a) := Z(A_c + A)^{-1} \exp(-\frac{1}{\hbar} S^E(a,A)) D[a] \tag{6.78}$$

where

$$S^E(a,A) = -i\kappa S_{CS}(a - \sigma_H A) + S_I(a,A) \tag{6.79}$$

$$D[a] = \prod_x \prod_{\alpha=0}^{2} da_\alpha(x) \tag{6.80}$$

and $Z(A_c + A)$ is the partition function, chosen such that $\int dP_A(a) = 1$. The action $S^E(a,A)$ should be derived form a microscopic theory, but such a derivation does not yet exist. The field theoretical formulation of the non-interacting electron system presented e.g. in the chapter 5 by Pruisken in [61] for the integer quantum Hall effect is of that form. But using just the structure of the action one can already derive some properties. The Euclidean partition function $Z(A_c + A)$ should be invariant under gauge transformations and the electron wave function must be unique. Both properties can only be fulfilled if σ_H takes values

$$\sigma_H = \pm \frac{1}{2l+1} \frac{e^2}{h} \tag{6.81}$$

This was shown by Fröhlich and Kerler [13]. The authors further show that one may allow for more than one current. Let $J^{(i)}$ be a set of currents, for each the condition

$$J^{(i)} = \sigma_H^{(i)} F \tag{6.82}$$

must hold. This then explains the experimentally observed values of σ_H.

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