Advanced Quantum Theory

Andreas Mielke

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1 Quantum theory of matter

This chapter contains mainly introductory material needed later. Most of the material presented here can be found in standard text books on quantum mechanics or advanced quantum mechanics, e.g. the book by Dick [5].

1.1 Recapitulation: Schrödinger equation, central potentials, angular momentum

The fundamental equation in standard quantum mechanics is the Schrödinger equation

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

with the Hamiltonian H and the time dependent wave function ψ. Formally, ψ is an element of a Hilbert space and H is a hermitian operator acting on that Hilbert space.

One of the first examples one treats in quantum mechanics is the problem of a single particle in a central potential. An example is the simple motion of a single particle, an electron, in a $1/r$ potential, which is typically treated as a simple model for the hydrogen atom and is exactly solvable. In that case, the wave function depends on the three coordinates of the particle, in Cartesian coordinates $\psi = \psi(x_1, x_2, x_3, t)$, and the Hamiltonian is

$$H = \frac{1}{2m}p^2 + V(r) \tag{1.2}$$

where $r^2 = \sum_i x_i^2$ is the distance of the particle from the origin and $p = \frac{1}{i}\nabla$ is the momentum operator. Obviously, the system of a particle in a central potential is rotationally invariant. By Noether's theorem, the angular momentum is a conserved quantity and the operator of the angular momentum $L = (L_1, L_2, L_3)$ with $L_j = \sum_{k,l} \epsilon_{j,k,l} x_k p_l$ commutes with the Hamiltonian, $[H, L] = 0$. The operator L is also the generator of rotations, $\exp(i\theta \cdot L)$ with $\theta = (\theta_1, \theta_2, \theta_3)$ is a rotation around the axis given by the direction of θ with the angle $|\theta|$. The operators L_j obey the commutation relations $[L_j, L_k] = i\sum_l \epsilon_{j,k,l} L_l$. As a consequence, only L^2 and one component of L, e.g. L_3 can be diagonalised simultaneously. For the problem of a single particle in a central potential, the eigenfunctions are the spherical harmonic functions $Y_{l,m}$ with $l \in \mathbb{N}$, $m \in \{-l, \ldots, l\} \subset \mathbb{Z}$.

1.2 The $su(2)$-algebra

The rotation group is actually the group $SO(3)$. It has a matrix representation in the space of real orthogonal 3×3 matrices. The properties of representations of the group can be derived using the commutation relations $[L_j, L_k] = i\sum_l \epsilon_{j,k,l} L_l$. We choose L_3 and L^2 to be diagonal and introduce $L_\pm = L_1 \pm iL_2$. One obtains

$$[L_3, L_\pm] = \pm L_\pm \tag{1.3}$$

$$[L_+, L_-] = 2L_3 \tag{1.4}$$

$$L^2 = \frac{1}{2}(L_+L_- + L_-L_+) + L_3^2 \tag{1.5}$$

Since L_3 is hermitian, it has real eigenvalues m. We denote the corresponding eigenfunctions as $|m\rangle$. The commutation relations imply

$$L_\pm|m\rangle = c_\pm(m)|m \pm 1\rangle \tag{1.6}$$

and

$$c_+(m-1)c_-(m) = 2m + c_-(m+1)c_+(m) \tag{1.7}$$

Further, $L_+^\dagger = L_-$ implies $c_-(m) = c_+(m-1)^*$. Eliminating c_- in the above equation using this relation yields

$$|c_+(m)|^2 = |c_+(m-1)|^2 - 2m \tag{1.8}$$

Since the left hand side is non-negative, there must be a maximal value $m = l$ and $c_+(l) = 0$, $L_+|l\rangle = 0$. As a consequence we have $|c_+(l-1)|^2 = 2l$ and after n iterations

$$|c_+(m-n)|^2 = 2nl - n(n-1) \tag{1.9}$$

Again, since the left hand side is non-negative, there must be a maximal value N for n and $2l = N - 1$, $c_+(l - N) = c_-(-l) = 0$. Therefore we have $N = 2l + 1$ and $-l \le m \le l$. As a consequence of this purely algebraic derivation, $l = \frac{1}{2}(N-1)$ is either integer or half integer. We already know that for the angular momentum operator L only integer values of l are realized, the eigenfunctions are $Y_{l,m}$. The reason is that the algebra allows for

$$\exp(i(\theta + 2\pi\theta/|\theta|) \cdot L) = \pm \exp(i\theta \cdot L) \tag{1.10}$$

whereas for pure rotations only the $+$-sign is realized. The group, which allows the $-$-sign as well is the group $SU(2)$ of unitary 2×2 matrices, the corresponding algebra is called $su(2)$-algebra. For spin $\frac{1}{2}$ a standard representation of the $su(2)$ algebra is given by $\frac{1}{2}\sigma_{x,y,z}$ where $\sigma_{x,y,z}$ are the Pauli matrices, in there standard representation

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_\pm = \sigma_x \pm i\sigma_y \tag{1.11}$$

1.3 Identical particles

When one considers a system of many particles, e.g. balls, in classical mechanics, it is often useful to consider those balls as marked e.g. by a number or colour. Numbering or painting the balls does not change their physical behaviour.

In microscopic systems as they are described by quantum mechanics, this is not possible. Identical particles are strictly indistinguishable. Consider a system with two or more particles. Take any observable A and any state ψ and let P be a permutation operator of the particles. Then the expectation value of the operator should not change, if we permute the particles, i.e.

$$\langle P\psi|A|P\psi\rangle = \langle\psi|A|\psi\rangle \tag{1.12}$$

The left hand side of this equation can be written as $\langle\psi|P^\dagger AP|\psi\rangle$ and since permutation are unitary operators we have $P^\dagger = P^{-1}$. Therefore $\langle\psi|P^{-1}AP|\psi\rangle = \langle\psi|A|\psi\rangle$. Since this must hold for any state ψ, the operator identity $P^{-1}AP = A$ must hold. Multiplying with P from the left, we obtain

$$[P, A] = 0 \tag{1.13}$$

for any observable.

The eigenvalues of P are ± 1. To show that, consider a permutation P of two particles. For this permutation we have $P^2 = 1$. The eigenvalues of this permutation are therefore ± 1. Since any

permutation can be constructed as a product of permutations of two particles, this holds for any permutation. Eigenstates of P are symmetric for the eigenvalue 1 and antisymmetric for eigenvalue -1.

This now means that in quantum mechanics, a many particle state must be either symmetric if one permutes two particles or it must be antisymmetric. Particles with symmetric many particle states are called Bosons, those with antisymmetric states are called Fermions.

1.4 Spin and statistics

Since the angular momentum allows only integer values of the quantum numbers l and m, is was a huge surprise when first Stern and Gerlach found half-integer values. The explanation was provided by Pauli, who proposed an intrinsic angular momentum for the electron, called spin. Later it was shown that all elementary particles have a spin. The spin operators form a $su(2)$-algebra. Further, with the help of relativistic field theory, Fierz, Pauli, and others derived the so called spin-statistics theorem. It states that all particles with a half-integer spin have anti-symmetric wave functions with respect to an exchange of particles, whereas all particles with an integer spin have symmetric wave functions with respect to an exchange of particles. Particles with a half-integer spin are Fermions, those with an integer spin are Bosons.

1.5 Time reversal symmetry

For a good introduction on time reversal symmetry I refer to the second chapter of the book of Haake [11].

In classical physics, time reversal symmetry means that a system is symmetric under the transformation $x \to x$, $t \to -t$, $p \to -p$ and consequently $L \to -L$. In quantum mechanics, if we have a spinless particle and a Hamiltonian of the form

$$H = \frac{p^2}{2m} + V(x) \tag{1.14}$$

the conventional time reversal operation is

$$x \to x, \quad p \to -p, \quad t \to -t, \quad \psi(x,t) \to \psi(x,-t)^* \tag{1.15}$$

This holds in position representation. A general time reversal operator T must be of the form $T = UK$ where K is the operator of complex conjugation and U is a unitary operator. Further, acting with T twice on a wave function should reproduce that wave function, eventually with a phase factor, i.e. $T^2 = u$ with $|u| = 1$. Using the representation $T = UK$ we obtain $u = T^2 = UKUK = UU^*K^2 = UU^*$ and therefore $U = u(U^*)^{-1} = uU^t$. Transposing this equation and inserting U^t on the right hand side yields $U = u^2 U$ and therefore $u^2 = 1$, i.e. $u = \pm 1$. As a consequence, the time reversal operator in quantum mechanics needs to fulfill

$$TxT^{-1} = x \tag{1.16}$$
$$TpT^{-1} = -p \tag{1.17}$$
$$TJT^{-1} = -J \tag{1.18}$$

and

$$\langle \phi | \psi \rangle = \langle T\psi | T\phi \rangle \tag{1.19}$$
$$T^2 = \pm 1 \tag{1.20}$$

Let us now ask how time reversal acts on a spin. For spin $\frac{1}{2}$ we have

$$T\sigma_x T^{-1} = UK\sigma_x KU^\dagger = U\sigma_x U^\dagger = -\sigma_x \tag{1.21}$$

$$T\sigma_y T^{-1} = UK\sigma_y KU^\dagger = -U\sigma_y U^\dagger = -\sigma_y \tag{1.22}$$

$$T\sigma_z T^{-1} = UK\sigma_z KU^\dagger = U\sigma_z U^\dagger = -\sigma_z \tag{1.23}$$

which is solved by $U = i\sigma_y$. Therefore, $T = i\sigma_y K$ and we obtain $T^2 = -1$. This can be generalized to systems with many particles and with arbitrary spin. If the total spin of the system is integer, we have $T^2 = 1$, if it is half integer, we have $T^2 = -1$. For more details on time reversal symmetry, we refer to [11].

1.6 Creation and Annihilation Operators for Fermions

For an excellent introduction of creation and annihilation operator as presented in this chapter I refer to chapter 1 of the book of Negele and Orland [18].

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, for which the states must be antisymmetric if one exchanges two particles, a basis of N-particle states can be build out of Slater determinants of the single particle states:

$$|i_1, i_2, ..., i_N\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{i_1}(q_1) & \phi_{i_1}(q_2) & ... & \phi_{i_1}(q_N) \\ \phi_{i_2}(q_1) & \phi_{i_2}(q_2) & ... & \phi_{i_2}(q_N) \\ \vdots & \vdots & & \vdots \\ \phi_{i_N}(q_1) & \phi_{i_N}(q_2) & ... & \phi_{i_N}(q_N) \end{vmatrix} \tag{1.24}$$

This state can be written in the form

$$|i_1, i_2, ..., i_N\rangle = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \prod_j \phi_{i_j}(q_{P(j)}) \tag{1.25}$$

Because of the construction as a determinant, the state is antisymmetric if one permutes a pair of indices, as it should be for Fermions.

$$|i_1, ..., i_\alpha, ..., i_\beta, ..., i_N\rangle = -|i_1, ..., i_\beta, ..., i_\alpha, ..., i_N\rangle \tag{1.26}$$

Normalization:

$$\langle i_1, i_2, ..., i_N | i_1, i_2, ..., i_N \rangle = 1 \tag{1.27}$$

Orthogonality:

$$\langle j_1, j_2, ..., j_N | i_1, i_2, ..., i_M \rangle = \tag{1.28}$$

$$\begin{cases} \sum_P (-1)^P \prod_k \delta_{j_k, i_{P(k)}} & \text{if } N = M \\ 0 & \text{if } N \neq M. \end{cases} \tag{1.29}$$

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

$$c_i^\dagger |i_1, i_2, ..., i_N\rangle = |i, i_1, i_2, ..., i_N\rangle \tag{1.30}$$

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

$$c_i^\dagger c_j^\dagger |i_1, i_2, ..., i_N\rangle = |i, j, i_1, i_2, ..., i_N\rangle \tag{1.31}$$

$$= -|j, i, i_1, i_2, ..., i_N\rangle \tag{1.32}$$

$$= -c_j^\dagger c_i^\dagger |i_1, i_2, ..., i_N\rangle \tag{1.33}$$

This holds for all states, so we have

$$c_i^\dagger c_j^\dagger = -c_j^\dagger c_i^\dagger \tag{1.34}$$

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

$$|i_1, i_2, ..., i_N\rangle = c_{i_1}^\dagger c_{i_2}^\dagger ... c_{i_N}^\dagger |\text{vac.}\rangle \tag{1.35}$$

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

$$\langle j_1, ..., j_M | c_i | i_1, ..., i_N\rangle = \langle i_1, ..., i_N | c_i^\dagger | j_1, ..., j_M\rangle^* \tag{1.36}$$

$$= \langle i_1, ..., i_N | i, j_1, ..., j_M\rangle^* \tag{1.37}$$

$$= \begin{cases} \delta_{i_1,i}\delta_{i_2,j_1}... - \delta_{i_1,j_1}\delta_{i_2,i} \pm ... \text{ alltogether } N! \text{ permutations,} & \text{if } N = M+1 \\ 0 & \text{if } N \neq M+1. \end{cases} \tag{1.38}$$

$$= \delta_{i_1,i}\langle i_2, ..., i_N | j_1, ..., j_M\rangle^* - \delta_{i_2,i}\langle i_1, i_3, ..., i_N | j_1, ..., j_M\rangle^* + ... (N \text{ terms}). \tag{1.39}$$

and therefore

$$c_i | i_1, ..., i_N\rangle = \delta_{i_1,i}|i_2, ..., i_N\rangle - \delta_{i_2,i}|i_1, i_3, ..., i_N\rangle + ... (N \text{ terms}). \tag{1.40}$$

and

$$c_i |\text{vak.}\rangle = 0 \tag{1.41}$$

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

$$c_i c_j = -c_j c_i \tag{1.42}$$

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

$$[c_i^\dagger, c_j^\dagger]_+ = 0, \quad [c_i, c_j]_+ = 0 \tag{1.43}$$

Because of

$$c_i^\dagger c_j | i_1, ..., i_N\rangle = \delta_{i_1,j}|i, i_2, ..., i_N\rangle - \delta_{i_2,j}|i, i_1, i_3, ..., i_N\rangle + ... \tag{1.44}$$

$$c_j c_i^\dagger | i_1, ..., i_N\rangle = \delta_{i,j}|i_1, ..., i_N\rangle - \delta_{i_1,j}|i, i_2, ..., i_N\rangle + \delta_{i_2,j}|i, i_1, i_3, ..., i_N\rangle + ... \tag{1.45}$$

we obtain

$$(c_j c_i^\dagger + c_i^\dagger c_j)|i_1, ..., i_N\rangle = \delta_{i,j}|i_1, ..., i_N\rangle \tag{1.46}$$

and since this holds for any state, we have

$$[c_i^\dagger, c_j]_+ = \delta_{i,j} \tag{1.47}$$

1.7 Creation and Annihilation Operators for Bosons

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

$$|i_1, i_2, ..., i_N\rangle = \frac{1}{\sqrt{N!}} \sum_P \prod_j \phi_{i_j}(q_{P(j)}) \tag{1.48}$$

But this state is not normalized. 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

$$\langle i_1, i_2, ..., i_N | i_1, i_2, ..., i_N\rangle = \prod_{i \in \{i_1, ..., i_N\}} n_i! \tag{1.49}$$

Therefore, the correct normalization is

$$|i_1, i_2, ..., i_N\rangle = \frac{1}{\sqrt{N! \prod_{i \in \{i_1, ..., i_N\}} n_i!}} \sum_P \prod_j \phi_{i_j}(q_{P(j)}) \tag{1.50}$$

and therefore

$$\langle j_1, j_2, ..., j_N | i_1, i_2, ..., i_M \rangle =$$
$$\begin{cases} \frac{1}{\prod_{i \in \{i_1, ..., i_M\}} n_i!} \sum_P \prod_k \delta_{j_k, i_{P(k)}} & \text{if } N = M \\ 0 \quad \text{if } N \neq M. \end{cases} \tag{1.51}$$

For Bosons, the creation operators can be defined as

$$c_i^\dagger |i_1, i_2, ..., i_N\rangle = \sqrt{n_i + 1} |i, i_1, i_2, ..., i_N\rangle \tag{1.52}$$

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 adjungate operators to $c_i^\dagger$ are c_i and we obtain:

$$\langle j_1, ..., j_M | c_i | i_1, ..., i_N \rangle = \langle i_1, ..., i_N | c_i^\dagger | j_1, ..., j_M \rangle^* \tag{1.53}$$
$$= \sqrt{n_i + 1} \langle i_1, ..., i_N | i, j_1, ..., j_M \rangle^* \tag{1.54}$$
$$= \frac{\sqrt{n_i + 1}}{\prod_{i' \in \{i_1, ..., i_N\}} n_{i'}!} \begin{cases} \delta_{i_1, i} \delta_{i_2, j_1} ... + \delta_{i_1, j_1} \delta_{i_2, i} + ... \text{ alltogether } N! \text{ permutations,} & \text{if } N = M + 1 \\ 0 & \text{if } N \neq M + 1. \end{cases}$$
$$= \frac{1}{\sqrt{n_i + 1}} \left(\delta_{i_1, i} \langle i_2, ..., i_N | j_1, ..., j_M \rangle^* + \delta_{i_2, i} \langle i_1, i_3, ..., i_N | j_1, ..., j_M \rangle^* + ... (N \text{ terms}) \right). \tag{1.55}$$

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

$$c_i |i_1, ..., i_N\rangle = \frac{1}{\sqrt{n_i}} \left(\delta_{i_1, i} |i_2, ..., i_N\rangle + \delta_{i_2, i} |i_1, i_3, ..., i_N\rangle + ... (N \text{ terms}) \right) \tag{1.56}$$

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

$$[c_i^\dagger, c_j^\dagger]_- = 0 \tag{1.57}$$

$$[c_i, c_j]_- = 0 \tag{1.58}$$

$$[c_i, c_j^\dagger]_- = \delta_{i,j} \tag{1.59}$$

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

$$|i_1, i_2, ..., i_N\rangle = \frac{1}{\sqrt{\prod_{i \in \{i_1, ..., i_N\}} n_i!}} c_{i_1}^\dagger c_{i_2}^\dagger ... c_{i_N}^\dagger |\text{vac.}\rangle \tag{1.60}$$

1.8 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

$$|i_1, i_2, ..., i_N\rangle = \frac{1}{\sqrt{N! \prod_{i \in \{i_1,...,i_N\}} n_i!}} \sum \zeta_P^P \prod_j \phi_{i_j}(q_{P(j)}) \tag{1.61}$$

$$\langle j_1, j_2, ..., j_N | i_1, i_2, ..., i_M \rangle =$$
$$\begin{cases} \frac{1}{\prod_{i \in \{i_1,...,i_M\}} n_i!} \sum \zeta_P^P \prod_k \delta_{j_k, i_{P(k)}} & \text{if } N = M \\ 0 \quad \text{if } N \neq M. \end{cases} \tag{1.62}$$

$$c_i^\dagger |i_1, i_2, ..., i_N\rangle = \sqrt{n_i + 1} |i, i_1, i_2, ..., i_N\rangle \tag{1.63}$$

$$c_i |i_1, ..., i_N\rangle = \frac{1}{\sqrt{n_i}} \left(\delta_{i_1, i} |i_2, ..., i_N\rangle + \zeta \delta_{i_2, i} |i_1, i_3, ..., i_N\rangle + ... (N \text{ terms}) \right) \tag{1.64}$$

$$[c_i^\dagger, c_j^\dagger]_{-\zeta} = 0 \tag{1.65}$$

$$[c_i, c_j]_{-\zeta} = 0 \tag{1.66}$$

$$[c_i, c_j^\dagger]_{-\zeta} = \delta_{i,j} \tag{1.67}$$

$$|i_1, i_2, ..., i_N\rangle = \frac{1}{\sqrt{\prod_{i \in \{i_1,...,i_N\}} n_i!}} c_{i_1}^\dagger c_{i_2}^\dagger ... c_{i_N}^\dagger |\text{vac.}\rangle \tag{1.68}$$

1.9 Single particle operators

Let us now discuss the operator

$$\hat{N} = \sum_i c_i^\dagger c_i \tag{1.69}$$

One has

$$c_i^\dagger c_i |i_1, ..., i_N\rangle = (\delta_{i_1, i} + \delta_{i_2, i} + ... + \delta_{i_N, i}) |i_1, ..., i_N\rangle \tag{1.70}$$

and therefore

$$\hat{N} |i_1, ..., i_N\rangle = N |i_1, ..., i_N\rangle \tag{1.71}$$

$\hat{N}$ 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

$$T |i_1\rangle = \sum_i t_{i, i_1} |i\rangle \tag{1.72}$$

We consider first operators which are diagonal in the chosen basis

$$T |i\rangle = t_i |i\rangle \tag{1.73}$$

For N-particle states we have similarly

$$T|i_1,...,i_N\rangle = \sum_j t_{i_j}|i_1,...,i_N\rangle \tag{1.74}$$

The operator acts on each particle independently. We now want to show that

$$T = \sum_i t_i c_i^\dagger c_i \tag{1.75}$$

With this form of T one calculates

$$T|i_1,i_2,...,i_N\rangle = T\frac{1}{\sqrt{n_{i_1}+1}}c_{i_1}^\dagger|i_2,...,i_N\rangle = \frac{1}{\sqrt{n_{i_1}+1}}[T,c_{i_1}^\dagger]|i_2,...,i_N\rangle + \frac{1}{\sqrt{n_{i_1}+1}}c_{i_1}^\dagger T|i_2,...,i_N\rangle \tag{1.76}$$

and further on

$$[T,c_{i_1}^\dagger] = \sum_i t_i[c_i^\dagger c_i, c_{i_1}^\dagger] = t_{i_1}c_{i_1}^\dagger \tag{1.77}$$

$$T|i_1,i_2,...,i_N\rangle = t_{i_1}|i_1,i_2,...,i_N\rangle + c_{i_1}^\dagger T|i_2,...,i_N\rangle \tag{1.78}$$

$$= \sum_j t_{i_j}|i_1,...,i_N\rangle \tag{1.79}$$

which shows that the representation of T is correct.

We will deal with single particle operators which are non diagonal. Since any hermitian operator can be diagonalized 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 $U = (u_{\alpha i})$ is a unitary matrix. Let $c_\alpha^\dagger$ be the new creation operators. We have

$$c_\alpha^\dagger|\text{vac.}\rangle = |\alpha\rangle \tag{1.80}$$

$$= \sum_i u_{\alpha i}|i\rangle \tag{1.81}$$

$$= \sum_i u_{\alpha i}c_i^\dagger|\text{vac.}\rangle \tag{1.82}$$

$$= \sum_i \langle\alpha|i\rangle c_i^\dagger|\text{vac.}\rangle \tag{1.83}$$

and therefore we let

$$c_\alpha^\dagger = \sum_i \langle\alpha|i\rangle c_i^\dagger \tag{1.84}$$

$$c_i^\dagger = \sum_i \langle i|\alpha\rangle c_\alpha^\dagger \tag{1.85}$$

$$c_\alpha = \sum_i \langle i|\alpha\rangle c_i \tag{1.86}$$

$$c_i = \sum_i \langle\alpha|i\rangle c_\alpha \tag{1.87}$$

Then we have

$$
\begin{aligned}
T &= \sum t_i c_i^\dagger c_i & (1.88) \\
&= \sum_{i,\alpha,\beta} t_i \langle \alpha|i \rangle \langle i|\beta \rangle c_\alpha^\dagger c_\beta & (1.89) \\
&= \sum_{\alpha,\beta} t_{\alpha,\beta} c_\alpha^\dagger c_\beta & (1.90)
\end{aligned}
$$

This is the general form of a single particle operator.

Examples:

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

$$
t_{i,j} = \int d^3r \, \phi_i^*(\vec{r}) V(\vec{r}) \phi_j(\vec{r}) \qquad (1.91)
$$

- Kinetic energy:

$$
t_{i,j} = \int d^3r \phi_i^*(\vec{r}) \left(-\frac{\nabla^2}{2m} \right) \phi_j(\vec{r}) \qquad (1.92)
$$

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

$$
T = \sum_{\vec{k},\sigma} \frac{\hbar^2 \vec{k}^2}{2m} c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma} \qquad (1.93)
$$

1.10 Interactions

In this course, we will also 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 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

$$
V|i,j\rangle = V_{ij}|i,j\rangle. \qquad (1.94)
$$

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

$$
\begin{aligned}
\langle j_1 \ldots j_N | V | i_1 \ldots i_N \rangle &= \sum_P \zeta^P \frac{1}{2} \sum_{k \neq k'} \langle j_{P_k}, j_{P_{k'}} | V | i_k, i_{k'} \rangle \prod_{l \neq k,k'} \langle j_{P_l} | i_l \rangle & (1.95) \\
&= \left(\frac{1}{2} \sum_{k \neq k'} V_{i_k, i_{k'}} \right) \langle j_1 \ldots j_N | i_1 \ldots i_N \rangle & (1.96)
\end{aligned}
$$

Here $\frac{1}{2} \sum_{k \neq k'}$ is the sum over all pairs of particles in the states $|i_1 \ldots i_N\rangle$. 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 $\frac{1}{2} n_i (n_i - 1)$. Using

$$
\begin{aligned}
n_i n_j - \delta_{i,j} n_i &= c_i^\dagger c_i c_j^\dagger c_j - \delta_{i,j} c_i^\dagger c_i & (1.97) \\
&= \zeta c_i^\dagger c_j^\dagger c_i c_j & (1.98) \\
&= c_i^\dagger c_j^\dagger c_j c_i & (1.99)
\end{aligned}
$$

we therefore obtain

$$V = \frac{1}{2} \sum_{i,j} V_{i,j} c_i^\dagger c_j^\dagger c_j c_i = \frac{1}{2} \sum_{i,j} \langle i,j|V|i,j \rangle c_i^\dagger c_j^\dagger c_j c_i \tag{1.100}$$

For $i \neq j$ the factor $1/2$ in front takes into account that pairs in the sum are counted twice. For $i = j$, the factor $1/2$ comes from the number of pairs. Transforming this into a general basis, we obtain

$$V = \frac{1}{2} \sum_{i,j,k,l} \langle i,j|V|k,l \rangle c_i^\dagger c_j^\dagger c_l c_k \tag{1.101}$$

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 antisymmetric states, Slater determinants, in the case of Fermions or completely symmetric states in the case of Bosons. The advantage of this representation are the simple algebraic relation ship between the creation and annihilation operators in the form of commutation relations (Bosons) or anti-commutation relation (Fermions). Many calculations are much easier in this representation.

1.11 Quantum states

1.11.1 The density matrix

In quantum mechanics, one typically describes a system using a Hamiltonian, and one tries to calculate or estimate its eigenstates. Let the system be in such an eigenstate, e.g. in the ground state ψ_0. Then one has complete information about the system. One can calculate any expectation value of any observable A simply using $\langle A \rangle = \langle \psi_0|A|\psi_0 \rangle$.

In all more complex realistic cases, one does not have complete knowledge of the system. This is already true in classical mechanics. And there is no way to obtain complete knowledge of a system by doing experiments, simply because of the finite accuracy of any experiment. Therefore, in a realistic description of a system, one cannot have complete knowledge of the system.

How do we introduce such an incomplete knowledge into quantum mechanics? Let us assume that $\{\psi_i, i \geq 0\}$ is a orthonormal basis (ONB) of the Hilbert space of our system, e.g. the ONB formed by the eigenstates of the Hamiltonian. We can describe incomplete knowledge of the system by assigning to each state ψ_i a probability p_i. We will later present some ideas how to estimate these probabilities. In the case of complete knowledge, one of the probabilities is equal to 1, all the others vanish. The expectation value of an observable A would then be

$$\langle A \rangle = \sum_i p_i \langle \psi_i|A|\psi_i \rangle \tag{1.102}$$

We now introduce the operator

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| = \sum_i p_i P_i \tag{1.103}$$

and write the expectation value in the form

$$\langle A \rangle = \mathrm{Tr}\rho A \tag{1.104}$$

The operator ρ is called density matrix. The representation (1.103) is the diagonal representation of it. Since the p_i are probabilities, we have $0 \leq p_i \leq 1$ for all i and $p_i \geq p_i^2$, further $\sum_i p_i = 1$. As a consequence, the density matrix obeys the conditions

$$0 \leq \rho^2 \leq \rho \leq 1 \tag{1.105}$$

$$\mathrm{Tr}\rho = 1 \tag{1.106}$$

1.11.2 Special density matrices

According to Jaynes, the missing information about a state of a system is given by $I = -\sum_i p_i \ln p_i$. If we let $k_B = 1$ it is identical to the entropy. For a quantum system, this can be written as

$$I = -\mathrm{Tr}\rho \ln \rho \tag{1.107}$$

Suppose that we have some additional information about the system, e.g. the expectation value of an operator A. If we want to estimate ρ given this knowledge, we have to maximize I under the condition $\langle A \rangle = \mathrm{Tr}\rho A$. This condition can be taken into account using a Lagrangian multiplier λ. A second condition we always need to take into account is (1.106). We do this using a second Lagrangian multiplier α. Then we get

$$\delta(\mathrm{Tr}\rho \ln \rho + \alpha \mathrm{Tr}\rho + \lambda \mathrm{Tr}\rho \mathrm{A}) = 0 \tag{1.108}$$

which yields

$$\mathrm{Tr}(\ln \rho + 1 + \alpha + \lambda \mathrm{A})\delta\rho = 0 \tag{1.109}$$

Since this must hold for arbitrary variations $\delta\rho$ we obtain

$$\rho = \exp(-1 - \alpha - \lambda A)$$

where α and λ need to be determined using the two conditions.

Let A be the Hamiltonian itself and assume we know its expectation value. Then the density matrix is given by

$$\rho = \frac{1}{Z} \exp(-\beta H) \tag{1.110}$$

where

$$Z = \mathrm{Tr}\exp(-\beta H) \tag{1.111}$$

and β can be identified with the inverse temperature in analogy to classical physics. This is called the canonical ensemble. We can also introduce the grand canonical ensemble, where also the particle number is not known exactly but only its expectation value, or the micro canonical ensemble, where the energy is known precisely.

1.11.3 Time dependent systems

Consider now a time dependent system. Then we would have time dependent states $\psi(t)$ obeying the time dependent Schrödinger equation. Let $P(t) = |\psi(t)\rangle\langle\psi(t)|$ be the projector onto that state. For the projector, we obtain (in the Schrödinger picture)

$$\frac{dP}{dt} = -i[H, P] \tag{1.112}$$

Since the incomplete information one has initially about the system does not change as long as no measurements are done, the probabilities p_i are constant in time and one obtains for the density operator

$$\frac{d\rho}{dt} = -i[H, \rho] \tag{1.113}$$

2 Open quantum systems

The aim of this chapter is to give an overview on open quantum systems. Some details esp. on driven dissipative quantum systems will be treated later. A comprehensive treatment of dissipative quantum systems is given in the book of Weiss [26]. I also refer to the review article by Caldeira and Leggett [3].

2.1 A preliminary study: classical systems

An open system in classical as well as in quantum physics is a system coupled to an environment. Before we enter to quantum systems, let us look at a simple model for a classical open system. The starting point is a Hamilton function of the system coupled to the environment of the form

$$H = H_S + H_B + H_{SB} \tag{2.1}$$

H_S is the Hamiltonian for the system. The environment is a simple heat bath described by H_B and the coupling between the system and the bath is given by H_{SB}. Although the model looks symmetric, it is asymmetric. The heat bath is much larger than the system we are looking at. In most cases we will perform a thermodynamic limit where the heat bath contains infinitely many degrees of freedom whereas the system itself contains typically few degrees of freedom. As a consequence, the heat bath will influence the system but the system will have (almost) no effect on the bath. Further, we will typically have a detailed knowledge about the structure of the system whereas we typically know only very few properties of the bath, like its temperature or some other macroscopic quantities.

What one is typically interested in is the effect of the bath on the dynamics of the system. What we expect is an energy transfer from the system to the bath, in classical mechanics described as friction, and eventually an energy transfer from the bath to the system, which is uncorrelated and causes phenomena like Brownian motion. The aim of this subsection is to derive these phenomena from a model given by (2.1).

In classical physics, in the theory of small vibrations, one expands a system to second order and performs a principal axis transformation. The result is a set of independent harmonic oscillations. With this idea in mind we can describe the bath as a set of independent harmonic oscillators. Let us now as a very simple example consider a classical one-dimensional particle in a potential as our system. Then, the Hamiltonian function is

$$H = \frac{p^2}{2m} + V(q) + \sum_i \left(\frac{p_i^2}{2m_i} + \frac{m_i}{2} \widetilde{\omega}_i^2 q_i^2 \right) + \sum_i \lambda_i (q - q_i)^2 \tag{2.2}$$

The equations of motion are

$$\dot{q} = \frac{\partial H}{\partial p}, \ \dot{p} = -\frac{\partial H}{\partial q}, \ \dot{q}_i = \frac{\partial H}{\partial p_i}, \ \dot{p}_i = -\frac{\partial H}{\partial q_i}. \tag{2.3}$$

and one obtains

$$\dot{q} = \frac{p}{m} \tag{2.4}$$

$$\dot{p} = F(q) - 2 \sum_i \lambda_i(q - q_i) \tag{2.5}$$

$$\dot{q}_i = \frac{p_i}{m_i} \tag{2.6}$$

$$\dot{p}_i = -m_i\tilde{\omega}_i^2 q_i - 2\lambda_i(q_i - q) \tag{2.7}$$

These equations can be investigated further by integrating the equations of motion for the bath variables and inserting the result into the equation of motion for the system. The result is an integro-differential equation for the system which contains the initial conditions of the bath variables as parameters. One then needs to make some assumptions about the statistical properties of these initial conditions. To illustrate the procedure, let us take a simple example, the dissipative harmonic oscillator. The Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{m}{2}\tilde{\omega}^2 q^2 + \sum_i \left(\frac{p_i^2}{2m} + \frac{m}{2}\tilde{\omega}_i{}^2 q_i^2\right) + \sum_i \lambda_i(q - q_i)^2. \tag{2.8}$$

We expand the last term in (2.8) and introduce the quantities $\omega^2 = \tilde{\omega}^2 + \frac{2}{m}\sum_i \lambda_i$, $\omega_i^2 = \tilde{\omega}_i^2 + \frac{2}{m_i}\lambda_i$. ω must be finite, therefore $\sum_i \lambda_i$ must be well defined. Further, similarly to the treatment of the harmonic oscillator in quantum mechanics, it is useful to introduce complex coordinates

$$b = \frac{1}{\sqrt{2}}(\sqrt{m\omega}q + ip/\sqrt{m\omega}) \tag{2.9}$$

$$b_i = \frac{1}{\sqrt{2}}(\sqrt{m_i\omega_i}q_i + ip_i/\sqrt{m_i\omega_i}) \tag{2.10}$$

The transformation back to the original coordinates is

$$q = \frac{1}{\sqrt{2m\omega}}(b + b^*) \tag{2.11}$$

$$p = \frac{1}{i}\sqrt{\frac{m\omega}{2}}(b - b^*) \tag{2.12}$$

and similarly for q_i and p_i. Using these quantities, the Hamiltonian becomes

$$H = \omega b^* b + \sum_i \omega_i b_i^* b_i - \sum_i \frac{\lambda_i}{\sqrt{m\omega m_i \omega_i}}(b + b^*)(b_i + b_i^*) \tag{2.13}$$

We introduce $g_i = \frac{\lambda_i}{\sqrt{m\omega m_i \omega_i}}$ as the new coupling constant in the last term. The Hamiltonian equations of motion are $\dot{b} = -i\frac{\partial H}{\partial b^*}$ and similarly for b_i and their complex conjugates. One obtains

$$\dot{b}_i = -i\omega_i b_i + ig_i(b + b^*) \tag{2.14}$$

$$\dot{b} = -i\omega b + i\sum_i g_i(b_i + b_i^*) \tag{2.15}$$

Integrating the first equation yields

$$b_i = b_{i0}\exp(-i\omega_i t) + ig_i \int_0^t \exp(-i\omega_i(t - t'))(b(t') + b^*(t'))dt' \tag{2.16}$$

We introduce this result into the equation of motion for b and obtain

$$\dot{b} = -i\omega b - 2i\sum_i g_i^2 \int_0^t \sin(\omega_i(t-t'))(b(t')+b^*(t'))dt' + i\sum_i g_i(b_{i0}\exp(-i\omega_i t) + b_{i0}^*\exp(i\omega_i t)) \quad (2.17)$$

The first term is the simple harmonic oscillation of the system. The second term contains a coupling of the system to its previous states. This is a memory effect, the system remembers its past. We will make a plausible assumptions that reduces this memory significantly. It will turn out that this term describes dissipation. The last term depends on the initial conditions of the bath variables, which are typically not known. We will see that it represents a stochastic force.

In a first step we take the thermodynamic limit and we assume that the bath frequencies form a continuous spectrum. As long as the bath is finite, there is no "real" dissipation. We introduce

$$G(\omega') = 2\sum_i g_i^2 \delta(\omega' - \omega_i) \quad (2.18)$$

which is a continuous function. It can be used to rewrite the second term in the equation of motion as

$$\int d\omega' G(\omega') \sin(\omega'(t-t')) = -\frac{d}{dt'}\int d\omega' \frac{G(\omega')}{\omega'}\cos(\omega'(t-t')) = -\frac{d}{dt'}R(t-t') \quad (2.19)$$

The two functions $G(\omega)$ or equivalently $R(t)$ describe the bath and the system-bath-coupling. After a partial integration, the equation of motion can now be written as

$$\dot{b} = -i\omega b + iR(0)(b+b^*) - iR(t)(b(0)+b^*(0)) - i\int_0^t dt' R(t-t')(\dot{b}(t')+\dot{b}^*(t'))$$
$$+ i\sum_i g_i(b_{i0}\exp(-i\omega_i t) + b_{i0}^*\exp(i\omega_i t)) \quad (2.20)$$

The second term yields a shilft of the frequency. The equation is well defined if and only if $2R(0) \leq \omega$. $R(t)$ is a sum of many small oscillating contributions and can therefore be expected to fall of quickly as a function of time. Therefore, the third term only contributes for small t and the fourth term only contributes for $t \approx t'$. Taking the real and the imaginary part of this equation, we obtain the equation for p and q.

$$\dot{q} = \frac{p}{m} \quad (2.21)$$

$$\dot{p} = -m\omega^2 q + 2m\omega R(0)q - 2m\omega R(t)q(0) - \kappa\dot{q} + \sqrt{2m\omega}\sum_i g_i(b_{i0}\exp(-i\omega_i t) + b_{i0}^*\exp(i\omega_i t)) \quad (2.22)$$

which yields

$$m\ddot{q} = -m\omega_{\text{ren}}^2 q - \kappa\dot{q} + F(t) \quad (2.23)$$

with

$$\kappa \approx 2m\omega \int_0^\infty dt R(t) \quad (2.24)$$

$$\omega_{\text{ren}} = \sqrt{\omega^2 - 2\omega R(0)} \quad (2.25)$$

and

$$F(t) = \sqrt{2m\omega}\sum_i g_i(b_{i0}\exp(-i\omega_i t) + b_{i0}^*\exp(i\omega_i t)) \quad (2.26)$$

ω_{ren} should be real, therefore $2R(0) \leq \omega$ must hold as already stated above.

If $R(t)$ falls of quickly, we see that the fourth term in the equation for b directly yields a typical friction. The fifth term contains a time dependent force $F(t)$. It depends on the unknown initial conditions of the bath . We eventually know some statistical properties of the bath. Let us take

$F(t)$ as a stochastic force. If we assume a symmetric distribution of the initial conditions, i.e. the probabilities for e.g. $p_i(0)$ and $-p_i(0)$ are the same, the expectation value of $F(t)$ vanishes. Let us calculate the second moments of $F(t)$.

$$\langle F(t)F(t')\rangle = 2m\omega \sum_{ij} g_i g_j \left\langle (b_{i0}\exp(-i\omega_i t) + b_{i0}^*\exp(i\omega_i t))(b_{j0}\exp(-i\omega_j t') + b_{j0}^*\exp(i\omega_j t'))\right\rangle$$

(2.27)

We can assume that the different bath modes are independent. Then, only the term with $i = j$ contributes to the sum. It contains the expectation values $\langle b_{i0}^* b_{i0}\rangle$ which depend on ω_i. We obtain

$$\langle F(t)F(t')\rangle = 4m\omega \sum_i g_i^2 \langle b_{i0}^* b_{i0}\rangle \cos(\omega_i(t - t'))$$

(2.28)

Because of the equipartition theorem we have

$$\langle b_{i0}^* b_{i0}\rangle = \frac{k_B T}{\omega_i}$$

(2.29)

and we finally obtain

$$\langle F(t)F(t')\rangle = 4m\omega k_B T \sum_i \frac{g_i^2}{\omega_i}\cos(\omega_i(t - t')) = 4m\omega k_B T R(t - t')$$

(2.30)

The second moment of the fluctuating force is therefore directly related to the dissipation. This is the so called fluctuation-dissipation theorem. We already assumed that $R(t)$ falls of quickly as a function of t. We may approximate

$$R(t) \approx \delta(t) \int dt' R(t') = \frac{\kappa}{m\omega}\delta(t)$$

(2.31)

This is clearly in contradiction to the condition $2R(0) \leq \omega$. Indeed $R(t) \propto \delta(t)$ is an assumption which is only valid if we keep ω_{ren} fixed. This is a typical example for renormalization, as it is often used in many different areas of physics. The assumption $R(t) \propto \delta(t)$ is physically reasonable. It simply means that the correlation time τ for $F(t)$, which determines the decay of $R(t)$, is small compared to ω^{-1} or other relevant time scales in the system.

Let us make some final remarks here:

1. The uncorrelated noise with $R(t) \propto \delta(t)$ is called white noise. We obtain white noise if $G(\omega)/\omega$ (or equivalent g_i^2/ω_i) is constant. Since formally $R(0)$ must be finite to have a well defined model, one has to introduce an ultra-violett cutoff ω_c which represents a finite correlation time. In the limit $\omega_c \to \infty$ we obtain white noise. Keeping the theory meaningful in that limit is a typical renormalization problem.

2. The friction constant κ and the second moment of the stochastic force $F(t)$ are parameterized by G and are therefore not independent. The relation ship of the two is a simple version of the fluctuation-dissipation theorem.

3. If the mass of the harmonic oscillator is large, the effect of the fluctuating force becomes small and can be neglected. We then obtain the usual equation of motion with a friction term.

4. It is important to perform the thermodynamic limit. Without it, system plus bath just form a system of coupled oscillators with characteristic eigenmodes.

2.2 Noise in quantum systems

In quantum mechanics, a state is described by a wave function or by a density matrix. If one wants to describe a quantum mechanical system coupled to an environment, a wave function is not suitable. One would need a precise knowledge of the environment, which is not available. Therefore, the description using a density matrix may be better.

If one describes a quantum mechanical system by a density matrix, the equation of motion for the density matrix is

$$\frac{d\rho_S}{dt} = -i[\rho_S, H_S] \tag{2.32}$$

An effective description of a quantum mechanical system coupled to an environment can eventually be obtained by adding further terms to this equation. In analogy to the classical case one has to expect a memory term which contains $\rho(t')$ for times $t' < t$, and a stochastic term. But the situation is not easy since a modified equation of motion for the density matrix has to fulfill certain condition which guaranty that the result is again a density matrix. The necessary conditions for the density matrix are

1. $\rho_S \geq \rho_S^2 \geq 0$.

2. $\text{Tr}\rho_S = 1$.

3. $\langle\phi|\rho_S\phi\rangle \leq 1$ for all ϕ.

These conditions need to be fulfilled for all times and all allowed initial conditions.

Another possibility is to describe the coupled system plus environment by a joined Hamiltonian as in the classical case. Eventually, one can derive either an equation of motion for ρ_S from such a model or at least equations of motion for some observables of interest. As above, a coupled Hamiltonian has the form

$$H = H_S \otimes I_B + I_S \otimes H_B + A_S \otimes A_B \tag{2.33}$$

The indices S denote the system, B the bath (the environment). $I_{S,B}$ are identities on the Hilbert spaces of the system and the bath, resp.. The Hilbert space of the entire system is the direct product of the two Hilbert spaces of system and bath.

The combined density matrix ρ of system and bath obeys the equation

$$\frac{d\rho}{dt} = -i[\rho, H] \tag{2.34}$$

The density matrix of the system can be obtained from ρ by a reduction on the Hilbert space of the system by a partial trace over the states in the Hilbert space of the bath. If we arrive at applying this reduction directly to the equation of the coupled system, we would get an effective equation for ρ_S. The same is true for the equations of motion for observables. The full equation of motion for an observable of the system contains bath operators. If one succeeds to eliminate those, one would have an effective equation of motion for the observable. In this way, we treated the classical dissipative harmonic oscillator. Let us now look at the quantum analogue.

2.2.1 The dissipative harmonic oscillator

With a harmonic approximation for the bath, i.e. using a bath of independent harmonic oscillators and a linear coupling to the system, we have

$$H_S = \frac{p^2}{2m} + \frac{m}{2}\Omega^2 q^2 \tag{2.35}$$

$$H_B = \sum_k \left(\frac{p_k^2}{2m_k} + \frac{m_k}{2} \omega_k^2 q_k^2 \right) \tag{2.36}$$

$$A_S = q \tag{2.37}$$

$$A_B = \sum_k g_k q_k \tag{2.38}$$

as in the classical case. Introducing level operators, or, in the language of the first chapter, bosonic creation and annihilation operators, the Hamiltonian can be written in the form

$$H = \Omega a^\dagger a + \sum_k \omega_k a_k^\dagger a_k + \sum_k \lambda_k (a + a^\dagger)(a_k + a_k^\dagger) \tag{2.39}$$

The equations of motion are

$$\frac{da}{dt} = i\Omega a + i \sum_k \lambda_k (a_k + a_k^\dagger) \tag{2.40}$$

$$\frac{da_k}{dt} = i\omega_k a_k + i\lambda_k (a + a^\dagger) \tag{2.41}$$

As in the classical case we formally integrate the equation for a_k

$$a_k(t) = a_k(0) \exp(i\omega_k t) + i\lambda_k \int_0^t dt' \exp(i\omega_k(t - t'))(a(t') + a^\dagger(t')) \tag{2.42}$$

and obtain

$$\frac{da}{dt} = i\Omega a + i \sum_k \lambda_k (\exp(i\omega_k t) a_k(0) + \exp(-i\omega_k t) a_k^\dagger(0)) \tag{2.43}$$

$$-2i \sum_k \lambda_k^2 \int_0^t dt' \sin(\omega_k(t - t'))(a(t') + a^\dagger(t')) \tag{2.44}$$

Although this equation looks very similar to the corresponding equation in the classical case, the two equation are different. In the quantum case, we have an equation for operators. Fortunately, the operators from a closed algebra, which makes it possible to solve the equation. There are several ways to do that. A direct integration of the equation of motion is possible in principle. It has the disadvantage that it cannot be generalized to more complex quantum systems. Another possibility is to rewrite the system in terms of path integrals [26]. This allows to integrate out the bath variables. A third possibility is to use a Hamiltonian based renormalization approach called flow equations for Hamiltonians [25, 12]. It uses continuous unitary transformations to diagonalize the Hamiltonian. This approach has been applied successfully to a lot of dissipative quantum systems. The exact solution of the dissipative harmonic oscillator using flow equations was first presented in [13]. Using one of these approaches, it is possible to calculate e.g. dynamical correlation functions like $\langle q(t)q(0) \rangle$. One obtains

$$\langle q(t)q(0) + q(0)q(t) \rangle = \frac{1}{8m\Omega} \int d\omega C(\omega)(2n(\omega) + 1)\cos(\omega t) \tag{2.45}$$

with

$$n(\omega) = \frac{1}{\exp(\omega/T) - 1} \tag{2.46}$$

$$C(\omega) = \frac{2J(\omega)(\omega^2 + \Omega^2)}{\left(\Omega^2 - \omega^2 + 4\Omega P \left(\int \frac{d\omega' \, \omega' J(\omega')}{\omega^2 - \omega'^2}\right)\right)^2 + 4\pi^2 \Omega^2 J^2(\omega)} \tag{2.47}$$

$$J(\omega) = \sum_k \lambda_k^2 \delta(\omega - \omega_k) \tag{2.48}$$

$P(.)$ stands for the principal value of the integral. We introduced here the spectral density of the environmental coupling $J(\omega)$. As long as the bath is finite, there is no "real" dissipation. As in classical physics, real dissipation only occurs, if you take the thermodynamic limit. In the thermodynamic limit the spectrum of the bath becomes continuous and $J(\omega)$ becomes a continuous function of ω. Examples will be discussed below in connection with the dissipative two-level system. The formula for $C(\omega)$ shows several things:

1. The first term in the denominator of $C(\omega)$ is a pole term. For vanishing coupling we have $C(\omega) \propto (\delta(\omega - \Omega) + \delta(\omega + \Omega))$. For a finite coupling the maxima are shifted to lower values

$$\Omega_{\text{ren}}^2 = \Omega^2 + 4\Omega P \left(\int \frac{d\omega' \omega' J(\omega')}{\Omega_{\text{ren}}^2 - \omega'^2}\right) \tag{2.49}$$

   As a consequence one needs

$$\Omega^2 + 4\Omega P \left(\int \frac{d\omega' \omega' J(\omega')}{\Omega_{\text{ren}}^2 - \omega'^2}\right) \geq 0 \tag{2.50}$$

   This condition guaranties that the Hamiltonian is bounded from below..

2. The second term yields a damping. As a consequence, there are no poles at $\omega = \pm\Omega_{\text{ren}}$ but maxima.

3. In contrast to the classical case we obtain damping already for $T = 0$. The reason are quantum fluctuations.

4. For finite temperature $C(\omega)(2n(\omega) + 1)$ if proportional to $\frac{T}{\omega}J(\omega)$ for small ω. The case of friction according Stoke's law corresponds to the case $J(\omega) \propto \omega$. Correlation functions fall of exponentially in this case, as in the classical case.

5. For $T = 0$, when only quantum fluctuations are present, we have $n(\omega) = 0$ and therefore $C(\omega) \propto J(\omega)$ for small ω. For $J(\omega) \propto \omega$, we obtain an algebraic decay of the correlation function $\propto t^{-2}$.

6. In quantum mechanics, other baths exist where $J(\omega) \propto \omega^s$ with $s > 1$ or $s < 1$. Phonons in solids have $s = 3$. As a consequence there are quantum baths with a non-exponential damping.

2.2.2 The two-level system

The dissipative two-level system is the paradigm for dissipative quantum systems. In analogy the the harmonic oscillator, the Hamiltonian can be written as

$$\begin{aligned} H &= H_S \otimes I_B + I_S \otimes H_B + A_S \otimes A_B \tag{2.51} \\ &= -\frac{\Delta}{2}\sigma_x + \sum_k \omega_k b_k^\dagger b_k + \frac{1}{2}\sigma_z \sum_k \lambda_k(b_k + b_k^\dagger) \tag{2.52} \end{aligned}$$

The two level system is described by a 2×2-matrix, here σ_x. The coupling to the bath induces transitions between the two states, thereby creating or annihilating a Boson. The bath is again represented by independent Bosons. The model is often called spin-boson model.

In the language of quantum computers, a two level system is a quantum bit. The above model describes a quantum bit coupled to an environment. In quantum computing, the goal is to keep the coupling to the bath as small as possible. But since it can never be reduced to zero, it is important to understand how the quantum bit reacts when coupled to a bath and how different types of baths create a different behaviour.

The spin-boson model has also been used to describe tunneling systems in an environment, for instance impurities in solids or glasses.

The model is for most cases not exactly solvable. An exact solution is known for $J(\omega) = \sum_k \lambda_k^2 \delta(\omega - \omega_k) = \omega$. For other cases, renormalization approaches or field theoretic approaches have been proven useful.

2.2.3 A nucleon in a pion-cloud

Another simple two-level system is given by the Hamiltonian

$$H = \sum_k \omega_k (a_k^\dagger a_k + b_k^\dagger b_k) + g_0 \sum_k (2\omega_k)^{-1/2} [(a_k + b_k^\dagger)\sigma_+ + (a_k^\dagger + b_k)\sigma_-] \tag{2.53}$$

Here, a_k and b_k are bosonic operator represented charged mesons ($\pi^\pm$). They interact with a nucleon, which has two states, a proton or a neutron. By emitting or absorbing a $\pi^\pm$, the nucleon is transferred from a proton to a neutron and back. The transitions are described by the Pauli matrices $\sigma_\pm$. g_0 is a coupling constant and $\omega_k = (k^2 + \mu^2)^{1/2}$, where μ is the meson mass. The model was proposed and investigated first by Ken Wilson in 1965 [27, 28]. It serves as a prototype for a local quantum field theory. The model cannot be treated by perturbation theory because of divergences. Instead, renormalization needs to be used.

2.2.4 Fermionic baths

The cases discussed so far had heat baths formed by Bosons, which is natural if one thinks of vibrations. But in reality there are also fermionic baths. The classical prototype of a model with a fermionic bath is the Kondo model. It describes a magnetic impurity in a Fermi see of band electrons in a solid. The Hamiltonian reads

$$H = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} - 2J \vec{s}(0) \cdot \vec{S} \tag{2.54}$$

where $\vec{S}$ is the spin of the magnetic impurity located at 0 and $\vec{s}(0)$ is the spin of the band electrons at this location,

$$\vec{s}(0) = \frac{1}{2} \sum_{k,k',\sigma,\sigma'} c_{k\sigma}^\dagger (\vec{\sigma})_{\sigma\sigma'} c_{k'\sigma'} \tag{2.55}$$

The Hamiltonian has the same form as a typical system-bath model with a vanishing system part (which may be included if one introduces a local external magnetic field). The system-bath interaction is a usual (typically anti-ferromagnetic, $J < 0$) exchange interaction. Kondo showed that at temperatures below the Kondo temperature

$$T_K = D \exp(\frac{1}{2N(0)J}) \tag{2.56}$$

perturbation theory breaks down. Here, D is the band width and $N(0)$ is the density of states at the Fermi level. The model has been analyzed in detail by Wilson using numerical renormalization. Below the Kondo temperature, the electrons form a singly occupied localized state which forms a singlet with the impurity spin.

A similar model with a fermionic bath is the Anderson impurity model. The Hamiltonian

$$H = \epsilon_d \sum_\sigma c_{d,\sigma}^\dagger c_{d,\sigma} + U c_{d,\uparrow}^\dagger c_{d,\downarrow}^\dagger c_{d,\downarrow} c_{d,\uparrow} + \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum V_k (c_{d,\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{d,\sigma}) \tag{2.57}$$

describes an impurity by the first two terms which is coupled to a band of electrons, the third term, via a hybridization, the fourth term. It can be (approximately) transformed to the Kondo model if the Fermi energy lies somewhere in the band, ϵ_d, the impurity energy, lies well below and $\epsilon_d + U$ lies well above the Fermi energy. Then, the impurity is occupied by a single electron which has spin $\frac{1}{2}$ and is coupled via the hybridization to the band. This produces virtual processes where electrons can move from the impurity to the band an vice versa, which produces an effective exchange interaction between the spin on the impurity and the spins of the band electrons.

2.3 Flow equations for Hamiltonians

A suitable method to treat dissipative quantum systems are continuous unitary transformations, also called flow equations. In this chapter I will first introduce the basic idea. For details I refer to the original papers by Wegner [25] and Glazek and Wilson [8, 9]. For a comparison of the different approaches I refer to an old lecture on the method (in German) [16]. A good introduction can be found in the book by Kehrein [12]. In a second section of this chapter I will present the treatment of the spin-boson model using this method. The method can also be applied to time dependent quantum systems, see the following chapters.

2.3.1 Basic idea

If one wants to diagonalize a matrix numerically one typically applies a sequence of unitary transformations with the goal to reduce or eliminate off-diagonal matrix elements. The basic idea of flow equations is to do that using a continuous unitary transformation. A continuous unitary transformation depends on a parameter ℓ. We denote it as $U(\ell)$ with $U(0) = 1$. The continuous unitary transformation shall be constructed such that $U(\infty)$ diagonalizes the given Hamiltonian or matrix H. This yields a ℓ-dependent matrix

$$H(\ell) = U^\dagger(\ell) H U(\ell). \tag{2.58}$$

If the transformation $U(\ell)$ was known, one could directly calculate $H(\infty)$ and the problem would be solved. This is typically not the case. Therefore we reformulate the unitary transformation as an infinitesimal unitary transformation

$$\frac{dH(\ell)}{d\ell} = [\eta(\ell), H(\ell)]. \tag{2.59}$$

Here η is the generator of the transformation. η is anti-hermitian, $\eta^\dagger = -\eta$. For the matrix elements, one obtains

$$\frac{dh_{k,q}(\ell)}{d\ell} = \sum_p (\eta_{k,p}(\ell) h_{p,q}(\ell) - h_{k,p}(\ell) \eta_{p,q}(\ell)) \tag{2.60}$$

η shall be chosen such that the matrix becomes more and more diagonal with increasing ℓ. A possible condition could be that $\sum_{k \neq q} h_{k,q}^2$ decays monotonically as a function of ℓ. Let $H = H_d + H_r$, $H_d = \text{diag}(H)$.

$$\text{Tr} H_d^2 + \text{Tr} H_r^2 = \text{Tr} H^2 = \text{const.} \tag{2.61}$$

$\sum_{k \neq q} h_{k,q}^2 = \mathrm{Tr} H_r^2$ decays monotonically if $\mathrm{Tr} H_d^2$ increases monotonically.

$$
\begin{aligned}
\frac{d\mathrm{Tr} H_d^2}{d\ell} & = \frac{d}{d\ell} \sum_q h_{q,q}^2 \\
& = 2 \sum_q h_{q,q} \sum_p (\eta_{q,p} h_{p,q} - h_{q,p} \eta_{p,q}) \\
& = 2 \sum_{p,q} \eta_{p,q} h_{p,q} (h_{p,p} - h_{q,q})
\end{aligned}
\tag{2.62}
$$

The right hand side should be non-negative. A possible choice for $\eta_{p,q}$ is $\eta_{p,q} = h_{p,q}(h_{p,p} - h_{q,q})$ or

$$
\eta = [H_d, H_r].
\tag{2.63}
$$

It yields

$$
\frac{dh_{k,q}(\ell)}{d\ell} = \sum_p (h_{k,k}(\ell) + h_{q,q}(\ell) - 2h_{p,p}(\ell)) h_{k,p}(\ell) h_{p,q}(\ell).
\tag{2.64}
$$

$$
\begin{aligned}
\frac{d}{d\ell} \sum_{k \neq q} h_{k,q}^2 & = -\frac{d}{d\ell} \sum_k h_{k,k}^2 \\
& = -2 \sum_{k,q} (h_{k,k} - h_{q,q})^2 h_{k,q}^2 \\
& = -2 \sum_{k,q} \eta_{k,q}^2
\end{aligned}
\tag{2.65}
$$

Since $\sum_{k \neq q} h_{k,q}^2$ decays monotonically but is bounded from below, the derivative must vanish for $\ell \to \infty$ which means

$$
\eta(\ell) = [H_d, H] \to_{\ell \to \infty} 0
\tag{2.66}
$$

This means that with the choice (2.63) we achieved our goal almost. We obtained a matrix that commutes with its diagonal part. That means that for degenerate diagonal matrix elements there may still remain some off-diagonal non-vanishing matrix elements. Let us mention that there are other choices of η which avoid this behaviour, but they are not suitable for the treatment of dissipative quantum systems. It is intuitive to explicitly treat the case of a 2×2-matrix to understand how the method works, we leave this as an exercise.

2.3.2 Flow equations for the spin-boson model

The general Hamiltonian of a system coupled to a bosonic bath can be written as

$$
H = H_S + A \sum_k \lambda_k (b_k + b_k^\dagger) + \sum_k \omega_k : b_k^\dagger b_k : .
\tag{2.67}
$$

where we assume that we take the thermodynamic limit where the function

$$
J(\omega) = \sum_k \lambda_k^2 \delta(\omega - \omega_k)
\tag{2.68}
$$

becomes a continuous function of ω. As long as the bath is finite, there is no "real" dissipation. As in classical physics, see (2.18), real dissipation only occurs, if you take the thermodynamic limit. In the thermodynamic limit the spectrum of the bath becomes continuous. Further, we introduced normal ordering $: b_k^\dagger b_k := b_k^\dagger b_k - n_k$ which is especially important for $T > 0$. Typically,

H_S is a Hamiltonian of a particle in a potential. Let us assume that we have a general coupling $\sum_k W_k(q - q_k)$ with arbitrary functions W_k. For small vibrations, it is sufficient to expand the functions W_k about the minimum. The first non-trivial part is $\sum_k \frac{c_k}{2}(q - q_k)^2$. It yields a term $\propto q^2$ which can be absorbed in H_S and terms $\propto q_k^2$, which are small in the thermodynamic limit since $c_k \propto \lambda_k \propto \frac{1}{\sqrt{N}}$. The mixed term is proportional to qq_k which is exactly the form of the coupling in (2.67). For the spin-boson model we have

$$H_S = -\frac{\Delta}{2}\sigma_x + E_0 \,, \quad A = \frac{1}{2}\sigma_z \tag{2.69}$$

A general choice of η can be

$$\eta = i \sum_k A_k(b_k + b_k^\dagger) + \sum_k B_k(b_k - b_k^\dagger) \tag{2.70}$$

$$
\begin{aligned}
[\eta, H] \;=\; & i \sum_k \omega_k A_k(b_k - b_k^\dagger) + \sum_k \omega_k B_k(b_k + b_k^\dagger) \\
& + i \sum_k [A_k, H_S](b_k + b_k^\dagger) + \sum_k [B_k, H_S](b_k - b_k^\dagger) \\
& + i \sum_{k,q} \lambda_q [A_k, A] : (b_k + b_k^\dagger)(b_q + b_q^\dagger) : + i \sum_k \lambda_k [A_k, A](2n_k + 1) \\
& + \sum_{k,q} \lambda_q [B_k, A] : (b_k - b_k^\dagger)(b_q + b_q^\dagger) : + \sum_k \lambda_k [B_k, A]_+
\end{aligned}
\tag{2.71}
$$

We impose the conditions

$$A_k = -\frac{i}{\omega_k}[B_k, H_S], \tag{2.72}$$

$$\omega_k B_k + i[A_k, H_S] = -\lambda_k A f(\omega_k, \ell). \tag{2.73}$$

For the spin-boson model and for the dissipative harmonic oscillator these equations can be solved explicitely. This allows to prevent the creation of terms in $[\eta, H]$ which contain expressions containing $(b_k - b_k^\dagger)$. The remaining terms are quadratic in the bosonic operators. Since already in the construction of the model such terms have not been included, we neglect these terms in a first step. The flow equations then are

$$\frac{d\lambda_k}{d\ell} = -\lambda_k f(\omega_k, \ell) \tag{2.74}$$

$$\frac{dH_S}{d\ell} = i \sum_k \lambda_k [A_k, A](2n_k + 1) + \sum_k \lambda_k [B_k, A]_+. \tag{2.75}$$

This is still a generic expression. For the spin-boson model we obtain

$$A_k = -\frac{1}{2}\lambda_k f(\omega_k, \ell)\frac{\Delta}{\omega_k^2 - \Delta^2}\sigma_y, \tag{2.76}$$

$$B_k = -\frac{1}{2}\lambda_k f(\omega_k, \ell)\frac{\omega_k}{\omega_k^2 - \Delta^2}\sigma_z. \tag{2.77}$$

$$\frac{\partial J(\omega, \ell)}{\partial \ell} = -2f(\omega, \ell)J(\omega, \ell) \tag{2.78}$$

$$\frac{dH_S}{d\ell} = \frac{1}{2}\int d\omega J(\omega, \ell)f(\omega, \ell)\left(\frac{\Delta}{\omega^2 - \Delta^2}\sigma_x - \frac{\omega}{\omega^2 - \Delta^2}\right). \tag{2.79}$$

The parameters Δ and λ_k are now functions of ℓ. $f(\omega, \ell)$ can still be chosen. To avoid vanishing denominators we choose $f(\omega, \ell) = (\omega - \Delta)^2$. This yields

$$\frac{d\Delta}{d\ell} = -\Delta \int d\omega J(\omega, \ell) \frac{\omega - \Delta}{\omega + \Delta}, \tag{2.80}$$

$$\frac{dE_0}{d\ell} = -\frac{1}{2} \int d\omega \omega J(\omega, \ell) \frac{\omega - \Delta}{\omega + \Delta}. \tag{2.81}$$

The equation for $J(\omega, \ell)$ can be formally integrated

$$J(\omega, \ell) = J(\omega, 0) \exp(-2 \int_0^\ell d\ell'(\omega - \Delta)^2) \tag{2.82}$$

Inserting this in the equation for Δ we obtain

$$\frac{d \ln \Delta}{d\ell} = \frac{1}{2} \int d\omega \frac{\partial J(\omega, \ell)}{\partial \ell} \frac{1}{\omega^2 - \Delta^2} \tag{2.83}$$

For small values of ℓ the integral will be dominated by large values of ω. For large values of ℓ we may assume that Δ approaches its final value $\Delta(\infty)$. This allows us to replace Δ by $\Delta(\infty)$ on the right hand side. This yields

$$\frac{d \ln \Delta}{d\ell} = \frac{1}{2} \frac{d}{d\ell} \int d\omega J(\omega, \ell) \frac{1}{\omega^2 - \Delta^2(\infty)}, \tag{2.84}$$

and finally

$$\ln \frac{\Delta(\infty)}{\Delta} = -\frac{1}{2} \int d\omega \frac{J(\omega, \ell)}{\omega^2 - \Delta^2(\infty)} \tag{2.85}$$

The final form of the Hamiltonian is

$$H(\infty) = -\frac{\Delta(\infty)}{2} \sigma_x + \sum_k \omega_k b_k^\dagger b_k \tag{2.86}$$

Let us discuss some interesting examples:

- The Ohmic bath:
$$J(\omega, 0) = 2\alpha\omega f_c(\omega/\omega_c) \tag{2.87}$$

  with a cutoff function f_c. It corresponds to the case discussed earlier which in the classical example yields a friction proportional to the velocity. We obtain

$$\int d\omega \frac{J(\omega, \ell)}{\omega^2 - \Delta^2(\infty)} \approx 2\alpha \int_0^{\omega_c} d\omega \frac{\omega}{\omega^2 - \Delta^2(\infty)} \approx 2\alpha \ln \frac{\Delta(\infty)}{\omega_c} \tag{2.88}$$

  which yields

$$\frac{\Delta(\infty)}{\Delta(0)} \propto \left(\frac{\Delta(0)}{\omega_c}\right)^{\frac{\alpha}{1-\alpha}} \tag{2.89}$$

  for $\alpha < 1$, $\Delta(\infty) = 0$ for $\alpha > 1$.

- The super-Ohmic bath
$$J(\omega, 0) = K^{1-s}\omega^s f_c(\omega/\omega_c), \quad s > 1 \tag{2.90}$$

$$\int d\omega \frac{J(\omega, \ell)}{\omega^2 - \Delta^2(\infty)} \approx \frac{1}{s-1} \frac{\omega_c^{s-1}}{K^{s-1}} \tag{2.91}$$

$$\Delta(\infty) = \Delta(0) \exp\left(-\frac{1}{2(s-1)} \frac{\omega_c^{s-1}}{K^{s-1}}\right). \tag{2.92}$$

  In this case $\Delta(\infty)$ does not vanish.

For both cases we see strong renormalization effects. These are found in other approaches as well. Due to these effects, a pertubational treatment of the coupling terms is useless. For the Ohmic case, we further see a quantum transition from a state where the system tunnels between the two states with a renormalized tunneling frequency Δ_∞ to a state where the system is localized in one of the two states. This is a Kosterlitz-Thouless transition. These results can as well be obtained by other methods, see e.g. [26], but the current calculation is a lot easier.

2.3.3 Equilibrium correlation functions

An important dynamical quantity for the spin-boson model is the equilibrium correlation function

$$C(t) \stackrel{\text{def}}{=} \frac{1}{2}\langle \sigma_z(t)\sigma_z(0) + \sigma_z(0)\sigma_z(t)\rangle_T \tag{2.93}$$

where $\langle . \rangle_T$ indicates the thermal average at temperature T. Later, we will also discuss the limit $T \to 0$ betrachten. The Hamiltonian has a simple structure in the limit $\ell \to \infty$. Therefore it is useful to calculate $C(t)$ in that limit. This means that we have to apply the continuous unitary transformation to σ_z Let us use the following ansatz for $\sigma_z(\ell)$

$$\sigma_z(\ell) = h(\ell)\sigma_z + \sigma_x \sum_k \chi_k(\ell)(b_k + b_k^\dagger) \ . \tag{2.94}$$

Calculating the commutator $[\eta(\ell), \sigma_z(\ell)]$,we obtain the flow equations

$$\frac{dh}{d\ell} = -\Delta \sum_k \lambda_k \chi_k (2n_k + 1)\frac{\omega_k - \Delta}{\omega_k + \Delta} \tag{2.95}$$

$$\frac{d\chi_k}{d\ell} = \Delta h \lambda_k \frac{\omega_k - \Delta}{\omega_k + \Delta} \tag{2.96}$$

For the correlation function one obtains

$$C(t) = h^2(\infty)\cos(\Delta(\infty)t) + \sum_k \chi_k^2(\infty)(2n_k + 1)\cos(\omega_k t). \tag{2.97}$$

Using the flow equations one can show that

$$\frac{d}{d\ell}(h^2 + \sum_k \chi_k^2) = 0 \tag{2.98}$$

Therefore $h^2 + \sum_k \chi_k^2$ is constant which guaranties $C(0) = 1$. For small $\omega_k \ll \Delta(\infty)$ the coefficients χ_k are propotional to λ_k. The Fourier transform of $C(t)$ is therefore proportional to $J(\omega, 0)$ for small ω which yields the correct long time behaviour.

Analyzing the asymptotic behaviour of the flow equations for $J(\omega, \ell)$ and $\Delta(\ell)$ for large ℓ one can learn a bit more about the correlation function $C(t)$. For $\omega_k = \Delta(\infty)$ the factor $\omega_k - \Delta$ decays $\propto \ell^{-1/2}$ and λ_k decays like $\lambda_k \propto \ell^{-1/4}$. Therefore, h must vanish in the limit $\ell \to \infty$ since otherwise χ_k would diverge which contradicts $h^2 + \sum_k \chi_k^2 = 1$. This yields

$$\sigma_z(\infty) = \sigma_x \sum_k \chi_k(\infty)(b_k + b_k^\dagger) \ . \tag{2.99}$$

$$C(t) = \sum_k \chi_k^2(\infty)(2n_k + 1)\cos(\omega_k t). \tag{2.100}$$

which means that even for $T = 0$ coherence vanishes for long times. (2.99) shows that as a consequence, the observable σ_z decays completely into combinations involving bath operators.

Let us close this section with some remarks:

1. The treatment of the spin boson model is generic and can be applied to many other dissipative quantum systems.

2. The dissipative harmonic oscillator can be solved exactly using flow equations. To do that, the neglected terms quadratic in the bosonic operators must be taken into account.

3. The flow equations for the spin-boson model can be improved by including terms quadratic in the bosonic, this is esp. important for the description of dynamics at $\omega \approx \Delta(\infty)$.

4. The spin-boson model with an Ohmic bath at $\alpha = \frac{1}{2}$ can be solved exactly using flow equations.

3 Time dependent quantum phenomena

If the Hamiltonian of a system is time-dependent, the notion of eigenstates becomes more or less useless. Solutions of the time-dependent Schrödinger equation $\sim \exp(-iEt)$ no longer occur. We need instead a way of solving the time-dependent Schrödinger equation. In this chapter we will first discuss the driven two-level system. Although it is (over-) simplistic, it shows several interesting phenomena. We will then discuss in more detail general periodically driven quantum systems.

Perodically driven systems are already very interesting in classical physics. In most cases where the non-driven system is classically integrable, the driven system is not integrable and may even show chaotic behaviour. For a comprehensive discussion I refer to the book of Haake [11]. See also the review article [10] for many details discussed in this and the subsequent chapter.

Clearly, a driven quantum system cannot be separated from its environment. The discussion of open driven quantum systems is done in the subsequent chapter.

3.1 The driven two-level system

There are several ways to write down a Hamiltonian for a driven two-level system. Here, I will use the representation

$$H(t) = -\frac{\Delta}{2}\sigma_x + h(t)\sigma_z \tag{3.1}$$

You may think of it as an atom with only the two lowest states taken into account coupled to an external field. Another interpretation would be a driven tunneling system, this corresponds to the interpretation often used for the spin-boson model presented in the previous chapter.

Suppose that $h(t)$ is constant in some fixed time intervals, i.e.

$$h(t) = h_n \text{ for } t_n \leq t < t_{n+1}, \quad t_n = n\Delta t \tag{3.2}$$

Let $\psi(t = 0) = \psi_0$ be the initial state, then we obtain

$$\psi(t = t_n) = U_{n-1}U_{n-2}\ldots U_1 U_0 \psi_0 \tag{3.3}$$

where

$$U_n = \exp(-iH(t_n)\Delta t) \tag{3.4}$$

We introduce a time ordering operator T that acts on products of operators and puts them in a time order. For two operators, we have

$$T[A(t)B(t')] = \begin{cases} A(t)B(t') & \text{if } t > t' \\ B(t')A(t) & \text{if } t < t' \end{cases} \tag{3.5}$$

Using the time ordering operator, we can rewrite (3.3) as

$$\psi(t = t_n) = T[\prod_{j=0}^{n-1} U_j]\psi_0 \tag{3.6}$$

The sequence of the U_j's in the product is determined by the time ordering operator. Now notice that

$$U_{j+1}U_j = \exp(-iH(t_{j+1})\Delta t)\exp(-iH(t_j)\Delta t) = \exp(-i(H(t_{j+1}) + H(t_j))\Delta t + O(\Delta t^2)) \quad (3.7)$$

For small (and in the end infinitesimal) Δt we can neglect the quadratic term and therefore write

$$\psi(t = t_n) = T[\exp(-i\Delta t \sum_{j=0}^{n-1} H(t_j))] \quad (3.8)$$

which formally in the limit $\Delta t \to 0$ can be written as

$$\psi(t_n) = U(t_n)\psi_0 \quad (3.9)$$

with

$$U(t) = \lim_{\Delta t \to 0} T[\prod_{j=0}^{n-1} U_j] = T\left[\exp\left(-i\int_0^t dt' H(t')\right)\right] \quad (3.10)$$

The expression (3.10) clearly holds for any time dependent Hamiltonian, not only for the driven two-level system in (3.1). Note that this is only a formal expression which is only defined in the form (3.6) with the limit t $\Delta t \to 0$.

Despite the simplicity of the Hamiltonian (3.1), there is no general solution to the time-dependent Schrödinger equation. An easy case is a constant external field $h(t) = h_0$ for $t < 0$ that is switched of, i.e. $h(t) = 0$ for $t > 0$. Another easy case is that of a kick, i.e. $h(t) = \delta(t)$. We leave those to the exercises.

3.1.1 Periodical driving close to resonance

Let us now discuss the case of periodical driving, i.e. $h(t) = h_0 \cos(\omega t)$. In a first step we expand $\psi(t)$ in the eigenbasis of σ_x

$$\psi(t) = a_1(t)\exp(i\frac{\Delta}{2}t)\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + a_2(t)\exp(-i\frac{\Delta}{2}t)\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (3.11)$$

We have

$$\sigma_x\psi(t) = a_1(t)\exp(i\frac{\Delta}{2}t)\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} - a_2(t)\exp(-i\frac{\Delta}{2}t)\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (3.12)$$

$$\sigma_z\psi(t) = a_1(t)\exp(i\frac{\Delta}{2}t)\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} + a_2(t)\exp(-i\frac{\Delta}{2}t)\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (3.13)$$

which yields the differential equations for the time-dependent coefficients

$$i\frac{da_1}{dt} = a_2 h\exp(-i\Delta t) = \frac{1}{2}h_0 a_2(\exp(i(\omega - \Delta)t) + \exp(-i(\omega + \Delta)t)) \quad (3.14)$$

$$i\frac{da_2}{dt} = a_1 h\exp(i\Delta t) = \frac{1}{2}h_0 a_2(\exp(i(\omega + \Delta)t) + \exp(-i(\omega - \Delta)t)) \quad (3.15)$$

There is no analytical solution to these two equations. To proceed further we assume that $\delta = \omega - \Delta \ll \omega + \Delta$, i.e. we are working in a case close to resonance. In a first step, we assume that $a_{1,2}(t)$ are functions that oscillate slow in time. We can then replace the fast oscillating terms in the two equations by there averages, which vanish. We therefore neglect the fast oscillating terms in the two equations and obtain

$$i\frac{da_1}{dt} = \frac{1}{2}h_0 a_2 \exp(i\delta t) \quad (3.16)$$

$$i\frac{da_2}{dt} = \frac{1}{2}h_0 a_1 \exp(-i\delta t) \tag{3.17}$$

which by eliminating a_2 yields

$$\frac{d^2 a_1}{dt^2} - i\delta \frac{da_1}{dt} + \frac{1}{4}h_0^2 a_1 = 0 \tag{3.18}$$

with the general solution

$$a_1(t) = a_{1+} \exp(i\omega_+ t) + a_{1-} \exp(i\omega_- t) \tag{3.19}$$

where

$$\omega_\pm = \frac{1}{2}\delta \pm \frac{1}{2}\sqrt{\delta^2 + h_0^2} \tag{3.20}$$

For a_2 we obtain

$$a_2(t) = -\frac{2}{h_0}[a_{1+}\omega_+ \exp(-i\omega_- t) + a_{1-}\omega_- \exp(-i\omega_+ t)] \tag{3.21}$$

Suppose, we switch off the external field after a time t_f. The system then is in a mixed state of the two eigenstates of the Hamiltonian with $h = 0$. We now measure the energy. Then, $|a_1(t_f)|^2$ is the probability to find the system in the state with energy $-\frac{1}{2}\Delta$, which is given by

$$|a_1(t_f)|^2 = \frac{h_0^2}{\delta^2 + h_0^2}\sin^2\frac{\sqrt{\delta^2 + h_0^2}}{2}t_f \tag{3.22}$$

The oscillations of this quantity as a function of t_f are called Rabi oscillations, named after the American physicist Isidor Isaac Rabi (Nobel prize 1944). The amplitude of the oscillations id proportional to $(1 + \delta^2/h_0^2)$ which is a typical resonance curve, a so called Lorentzian with a maximum at $\delta = 0$, i.e. $\omega = \Delta$. This resonance is also the basis of NMR (Nobel prize for Bloch and Purcell 1952, Ernst 1991) with its medical application MRT (Nobel prize Lauterbur and Mansfield 2003). There, the two level system is a nuclear spin which is coupled to a time-dependent magnetic field.

3.1.2 Fast driving

For a fast driven system, $\omega \gg \Delta$, we need to modify the ansatz for the wave functions. Since Δ is small, we choose as a basis to expand the states the eigenbasis of σ_z. For $\Delta = 0$ we have

$$\psi(t) = \psi_+(t)\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \psi_-(t)\begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{3.23}$$

with

$$i\frac{d\psi_\pm}{dt} = \pm h(t)\psi_\pm \tag{3.24}$$

The solution is

$$\psi_\pm(t) = \psi_{\pm,0}\exp\left(\mp i\int_0^t dt' h(t')\right) \tag{3.25}$$

$$= \psi_{\pm,0}\exp\left(\mp i\frac{h_0}{\omega}\sin(\omega t)\right) \tag{3.26}$$

Therefore, for small Δ we make the ansatz

$$\psi(t) = c_1(t)\exp\left(-i\frac{h_0}{\omega}\sin(\omega t)\right)\begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_2(t)\exp\left(i\frac{h_0}{\omega}\sin(\omega t)\right)\begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{3.27}$$

and obtain from the Schrödinger equation

$$i\frac{dc_{1,2}}{dt} = -\frac{\Delta}{2}\exp(\pm 2i\frac{h_0}{\omega}\sin(\omega t))c_{2,1} \tag{3.28}$$

As before, for fast oscillations we can replace the time-dependent terms by their time averages. For the exponential functions, the average over one period is

$$\frac{\omega}{2\pi}\int_0^{2\pi/\omega}\exp(2i\frac{h_0}{\omega}\sin(\omega t))dt = J_0(\frac{2h_0}{\omega}) \tag{3.29}$$

where J_0 is the zeroth-order Bessel function. We then obtain

$$i\frac{dc_{1,2}}{dt} = -\frac{\Delta}{2}J_0(\frac{2h_0}{\omega})c_{2,1} \tag{3.30}$$

with the solution

$$c_{1,2}(t) = c_{1,2}^0\exp(\pm i\frac{\Delta}{2}J_0(\frac{2h_0}{\omega})t)$$

This is the behaviour of a usual two-level system with a reduced tunneling frequency $\Delta J_0(2h_0/\omega)$. The fast oscillations slow down the tunneling and can even localize the tunneling particle at values of $2h_0/\omega$ where the Bessel function has zeros. This effect is called coherent destruction of tunneling. See the review article [10] for details. The small oscillations we obtain for $c_{1,2}$ justify a posterio the approximation from (3.28) to (3.30).

3.2 Floquet theory

Let $H(t)$ be a time periodic Hamiltonian, $H(t + \frac{2\pi}{\omega}) = H(t)$. Then, the Floquet theorem states that the time dependent Schrödinger equation

$$i\frac{\partial\psi}{\partial t} = H\psi$$

is solved by

$$\psi_a(t) = u_a(t)\exp(-i\epsilon_a t) \tag{3.31}$$

where $u_a(t) = u_a(t + \frac{2\pi}{\omega})$ is time periodic. The ϵ_a are obtained as eigenvalues of the Floquet operator

$$F = H(t) - i\frac{\partial}{\partial t} \tag{3.32}$$

acting in the Floquet space which is the direct product of the original Hilbert space and the space of time periodic function with period $\frac{2\pi}{\omega}$. Let ϕ_n be an ONB of the original Hilbert space. Let $f_n(t) = \exp(-in\omega t)$ be an ONB in the space of time periodic function with the scalar product

$$\langle f|g\rangle = \frac{\omega}{2\pi}\int_0^{\frac{2\pi}{\omega}}dt f^*(t)g(t) \tag{3.33}$$

Then an ONB in the Floquet space is given by $\psi_{n,m} = \phi_n\exp(-im\omega t)$. The eigenvalue equation for F is

$$Fu_a(t) = [H(t) - i\frac{\partial}{\partial t}]u_a(t) = \epsilon_a u_a \tag{3.34}$$

Note that the state $u_{a,n}(t) = u_a(t)\exp(-in\omega t)$ is an eigenstate of F with eigenvalue $\epsilon_a - n\omega$. But $u_{a,n}(t)$ and $u_{a,0}(t) = u_a(t)$ are physically identical solutions of the Schrödinger equation. Therefore it is sufficient to consider states with

$$-\frac{\omega}{2} \leq \epsilon_a < \frac{\omega}{2} \tag{3.35}$$

3.2.1 The two level system

Let us discuss again the Hamiltonian (3.1). For $\Delta = 0$, (3.34) yields the two uncoupled equations

$$[\pm h(t) - i\frac{d}{dt}]u_\pm = \epsilon_\pm u_\pm \tag{3.36}$$

with the solution

$$u_\pm(t) = \exp(\mp i \int_0^t dt' h(t')) \exp(i\epsilon_\pm t) \tag{3.37}$$

Since due to the Floquet Theorem, $u_\pm(t)$ must be periodic and because of (3.35), $\epsilon_\pm = 0$. The two eigenstates are thus degenerate.

We now consider the case of small Δ. In first order degenerate perturbation theory, we obtain the 2×2-matrix

$$\begin{pmatrix} h_{++} & h_{+-} \\ h_{-+} & h_{--} \end{pmatrix}$$

with

$$h_{s_1 s_2} = -\frac{\Delta}{2}(\sigma_x)_{s_1 s_2} \langle u_{s_1} | u_{s_2} \rangle \tag{3.38}$$

It has the same form as the original tunneling Hamiltonian $-\frac{\Delta}{2}\sigma_x$ but with an effective tunneling matrix element

$$\Delta_{\text{eff}} = \Delta \langle u_- | u_+ \rangle \tag{3.39}$$

For $h(t) = h_0 \cos(\omega t)$ one obtains

$$\Delta_{\text{eff}} = \Delta J_0(\frac{2h_0}{\omega}) \tag{3.40}$$

as in the previous section for fast driving.

There is a second way to interpret the result. The unitary time evolution is in general given by $U(t)$ in (3.10). After n full cycles of driving, we obtain $U(\frac{2\pi}{\omega}n) = T_F^n$ with the so called Floquet map (not to be confused with the Floquet operator in (3.32))

$$T_F = U(\frac{2\pi}{\omega}) \tag{3.41}$$

It is described and used in Detail in [11]. Since T_F is a unitary operator, it can be written as

$$T_F = \exp(-\frac{2\pi}{\omega}iH_{\text{eff}}) \tag{3.42}$$

with a hermitian operator H_{eff}. This defines an effective Hamiltonian H_{eff}. For a given initial state $\psi(t=0)$ we obtain

$$\psi(t = \frac{2\pi}{\omega}n) = T_F^n \psi(0) \tag{3.43}$$

The Floquet map T_F or the effective Hamiltonian thus yields a stroboscopic description of the system. The dynamics given by $U_{\text{eff}}(t) = \exp(-iH_{\text{eff}}t)$ yields an exact description of the dynamics of the system only for those stroboscopic times. The deviation between exact dynamics and effective dynamics is given by

$$U_F(t) = U_{\text{eff}}(t)U^\dagger(t) \tag{3.44}$$

and it is possible to obtain the effective Hamiltonian as

$$H_{\text{eff}} = U_F(t)H(t)U_F^\dagger(t) - iU_F(t)\frac{d}{dt}U_F^\dagger(t) \tag{3.45}$$

We can therefore obtain the effective Hamiltonian by finding a time-dependent unitary transformation $U_F(t)$ such that the resulting Hamiltonian does not depend on time and $U_F(0) = 1$.

For the driven two-level system we make the ansatz

$$U_F(t) = \exp(ia(t)\sigma_z) \tag{3.46}$$

we obtain

$$H_{\text{eff}} = -\frac{\Delta}{2}\cos(2a(t))\sigma_x - \frac{\Delta}{2}\sin(2a(t))\sigma_y + h(t)\sigma_z - \frac{da}{dt}\sigma_z \tag{3.47}$$

We choose $\frac{da}{dt} = h$ and obtain for $h = h_0\cos(\omega t)$

$$H_{\text{eff}} = -\frac{\Delta}{2}\cos(\frac{2h_0}{\omega}\sin(\omega t))\sigma_x - \frac{\Delta}{2}\sin(\frac{2h_0}{\omega}\sin(\omega t))\sigma_y \tag{3.48}$$

We now set

$$\cos(\frac{2h_0}{\omega}\sin(\omega t)) = \sum_k \cos(k\omega t)J_k(\frac{2h_0}{\omega}) \tag{3.49}$$

and neglect the oscillating terms which is a good approximation for large ω as noted before. The second term in the Hamiltonian contains only fast oscillating terms and is therefore neglected entirely. Then we obtain the same effective Hamiltonian with the effective tunneling frequency as before. Let us mention that we get the same result if we use flow equations and assume ω to be large which is obvious since in the case there is no difference to the full unitary transformation (3.46). But flow equations can be used to eliminate the fast oscillating terms to any order and to obtain a more precise expression for the effective Hamiltonian.

3.2.2 Strong correlations in optical lattices

The above treatment of the two level system has a very important application in the current experimental investigation of strongly correlated systems in optical lattices. An optical lattice is a typically two dimensional lattcie formed by the interference of counter-propagating laser beams. This creates a spatially periodic potential in which atoms can be trapped. Cooling them down yields a system similar to a crystal lattice but with the advantage that all parameters can be controlled experimentally. This allows for precise quantum simulations to understand strong correlations in lattices.

The atoms trapped in such a lattice have typically a short range interaction, since they are neutral. This interaction takes place when two atoms sit on the same lattice site and is assumed to be repulsive. Therefore, such a system resembles the Hubbard model, a tight binding model for particles on a lattice with a purely local interaction. The aim of this course is not to study the Hubbard model in detail, for the interested reader I refer to the literature, e.g. [17]. The particles in the lattice form energy bands. The essential parameters are the band width D, the interaction strength U, and the density of particles n. Strong correlations occur when U is larger then D. There are lattices, for instance the kagomé lattice, which have among others a flat band, i.e. $D = 0$. This is a prototype of a strongly correlated system and shows many interesting properties. But unfortunately, the flat band lies at the top of the spectrum. The experimental idea is now to periodically shake the system to eventually obtain effective hopping similar to (3.40). Since the Bessel function changes its sign as a function of the argument, it should be possible to reverse the sign of the hopping and achieve a situation where the flat Band lies at the bottom of the spectrum. This would allow experimental quantum simulations of flat band systems.

To illustrate such a system we consider a one dimensional bosonic Hubbard model

$$H_H = -t\sum_i (b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i) + U\sum_i n_i(n_i - 1) \tag{3.50}$$

The first term is the hopping term. Particles can hop from a site i to its neighboured sites. The second term is the repulsive interaction. Putting more than one particle on a site costs energy U times the number of pairs of particles on that site. To this Hamiltonian we now add a periodic shaking of the form

$$H_S = h \cos(\omega t) \sum_i i n_i \tag{3.51}$$

which corresponds to an oscillating field constant in space. We now proceed as before and try to find an effective Hamiltonian H_{eff}. This can be done using

$$U_F(t) = \exp(i \frac{h}{\omega} \sin(\omega t) \sum_j j n_j) \tag{3.52}$$

which with the same approximation as for the two level system yields (3.50) with an effective hopping

$$t_{\text{eff}} = t J_0(\frac{h}{\omega}) \tag{3.53}$$

This result has been first obtained in [6]. Since in experiments one finds deviations from this result, it may be suitable to obtain higher orders. This can be done using the flow equations from section 2.3. Details may be found in [24].

Applications of optical lattices are e.g. quantum computers and very precise atomic clocks, so called lattice clocks.

3.2.3 The kicked rotator (and Anderson localization)

The kicked rotator is described by the Hamiltonian

$$H(t) = -\frac{1}{2I} \frac{\partial^2}{\partial \theta^2} + \frac{\lambda I}{\tau} V(\theta) \delta(t - n\tau) \tag{3.54}$$

The classical kicked rotator is a prototype for a classically chaotic system. For sufficiently large coupling is shows chaotic behaviour. It is therefore studied as a prototype to investigate the quantum properties of a classically chaotic system. A detailed treatment of the kicked rotator and its relation to Anderson localization (Nobel prize 1977) may be found in Chapter 7 of the book by Haake [11]. In this subsection, I follow mainly the presentation of Haake.

The Hamiltonian (3.54) is periodic in t with period τ. I is the moment of inertia, λ is a dimensionless coupling constant, and $V(\theta)$ is a periodic potential with period 2π. For simplicity we let $I = \tau = 1$. Think of $V(\theta) = \cos(\theta)$.

Instead of a continuous time-periodic function $H(t)$ contains a periodic series of kicks. This makes the dynamics easier to describe. The Floquet map can be written as

$$T_F^+ = \exp(-i\lambda V(\theta)) \exp(\frac{i}{2} \frac{\partial^2}{\partial \theta^2}) \tag{3.55}$$

It describes the stroboscopic time evolution from a state immediately after one kick to a state immediately after the next kick. Similarly, the Floquet map that maps a state immediately before the kick to one immediately before the next kick is

$$T_F^- = \exp(\frac{i}{2} \frac{\partial^2}{\partial \theta^2}) \exp(-i\lambda V(\theta)) \tag{3.56}$$

$$= \exp(i\lambda V(\theta)) T_F^+ \exp(-i\lambda V(\theta)) \tag{3.57}$$

and the two operators are related by a unitary transformation. Thus they have the same eigenvalues. Let

$$T_F^{\pm} u^{\pm} = \exp(-i\phi)u^{\pm} \tag{3.58}$$

be the eigenvalue equation. The eigenstates are related via

$$u^- = \exp(i\lambda V)u^+ \tag{3.59}$$

We now introduce

$$u = \frac{1}{2}(u^+ + u^-) \tag{3.60}$$

and the hermitian operator

$$W = -\tan\frac{\lambda V}{2} \tag{3.61}$$

We have

$$\exp(-i\lambda V) = \frac{1+iW}{1-iW} \tag{3.62}$$

and

$$u = (1+iW)^{-1}u^+ = (1-iW)^{-1}u^- \tag{3.63}$$

which in the end, using the eigenvalue equation, yields

$$(1-iW)u = \exp(i\phi)\exp(\frac{i}{2}\frac{\partial^2}{\partial\theta^2})(1+iW)u \tag{3.64}$$

Writing $u = \sum u_n \exp(-in\theta)$ we obtain

$$u_n - i\sum_r W_{n-r}u_r = \exp(i\phi - \frac{i}{2}n^2)(u_n + i\sum_r W_{n-r}u_r) \tag{3.65}$$

which can be rewritten as

$$\epsilon_n u_n + \sum_{r\neq 0} W_r u_{n+r} = W_0 u_n \tag{3.66}$$

with

$$\epsilon_n = \tan(\frac{\phi}{2} - \frac{n^2}{4}) \tag{3.67}$$

(3.66) looks like a Schrödinger equation of a particle on a one dimensional chain in tight binding representation. $n \in \mathbb{Z}$ represent the lattice sites. u_n is the wave function in position representation. ϵ_n are on-site energies of the particle sitting on the site n. W_r are hopping matrix elements which allow the particle to move from a site n to a site $n+r$. They do not depend on n, the hopping is therefore translational invariant. The interesting point is that the ϵ_n are pseudo random numbers. The quantity $(\phi + \frac{1}{2}n^2)\mathrm{mod}\, 2\pi$ is dense and uniformly distributed in the interval $[0, 2\pi)$. This means that the ϵ_n are distributed according to the density $\rho(\epsilon) = 1/(\pi(1+\epsilon^2))$. If the ϵ_n were true random numbers drawn from that distribution, (3.66) would be the Lloyd model, a special form of the Anderson model with random numbers according to this density. For the Anderson model, the eigenstates are localized. They fall off exponentially as a function of the distance, here n. There is no proof that one obtains localization for the pseudo random numbers, but in all numerical calculations the u_n show the same properties as for usual random numbers. Due to the localization, the diffusive behaviour observed in the classical system is suppressed.

3.3 Adiabatic time dependence and the Berry phase

So far, we often considered fast moving systems. If the system is initially in a given state ψ, the dynamics of the system do not allow the state to adopt to the fast motion. Esp. fast oszillations average out. Such fast motions are called diabatic. Now we will consider slow motions of the Hamiltonian.

Consider a Hamiltonian $H(t)$ that, for a fixed time t can be diagonalized with eigenvalues $\epsilon_n(t)$ and eigenstates $\phi_n(t)$, i.e.

$$H(t)\phi_n(t) = \epsilon_n(t)\phi_n(t) \tag{3.68}$$

The eigenstates form on ONB of the Hilbert space. The motion is called adiabatic if it is slow enough so that it remains in an eigenstate $\phi_n(t)$ if it starts at $\phi_n(t=0)$.

Consider now the following problem: at $t=0$ the system is prepared in the initial state

$$\psi_n(t=0) = \phi_n(t=0) \tag{3.69}$$

With this initial condition, we want to solve the Schrödinger equation

$$i\frac{d\psi_n}{dt} = H(t)\psi_n(t) \tag{3.70}$$

The question is: under which conditions is it possible to directly relate $\psi_n(t)$ to $\phi_n(t)$? If that was possible, and since both are normalized, they can only differ by a phase, we would have

$$\psi_n(t) = \exp(-i\Omega_n(t))\phi_n(t) \tag{3.71}$$

Inserting this ansatz into the Schrödinger equation we obtain

$$\frac{d\Omega_n}{dt}\phi_n + i\frac{d\phi_n}{dt} = \epsilon_n\phi_n \tag{3.72}$$

and therefore

$$\frac{d\Omega_n}{dt} = \epsilon_n - i\langle\phi_n|\frac{d\phi_n}{dt}\rangle \tag{3.73}$$

which can directly be integrated and yields

$$\Omega_n(t) = \int_0^t dt'(\epsilon_n(t') - i\langle\phi_n(t')|\frac{d\phi_n}{dt'}\rangle) \tag{3.74}$$

However, the ansatz (3.71) is generically not a solution of the Schrödinger equation. It is only a solution to the Schrödinger equation if

$$\frac{d\phi_n}{dt} \propto \phi_n \tag{3.75}$$

Otherwise, we would get contributions $\propto \phi_m$, $m \neq n$ in the Schrödinger equation. But if this proportionality holds, we get

$$\frac{1}{i}\frac{d\phi_n}{dt} = (\frac{d\Omega_n}{dt} - \epsilon_n(t))\phi_n \tag{3.76}$$

and therefore

$$\phi_n(t) = \exp(-i\beta_n(t))\phi_n(t=0) \tag{3.77}$$

with

$$\beta_n(t) = i\int_0^t dt'\langle\phi_n(t')|\frac{d\phi_n}{dt'}\rangle \tag{3.78}$$

$\beta_n(t)$ is called the Berry phase [1]. Under which conditions can this approach be applied at least approximately to a given problem? In general, since the ϕ_n form an ONB, we have

$$\frac{d\phi_n}{dt} = \sum_m \langle \phi_m | \frac{d\phi_n}{dt} \rangle \phi_m \tag{3.79}$$

Therefore, the requested proportionality (3.75) holds approximately if

$$|\langle \phi_m | \frac{d\phi_n}{dt} \rangle| \ll |\langle \phi_n | \frac{d\phi_n}{dt} \rangle| \tag{3.80}$$

or in other words, if the initial state $\phi_n(0)$ fulfills

$$H(t')\phi_n(0) \simeq \epsilon_n(t')\phi_n(0) \tag{3.81}$$

for times t' between 0 and t. The latter can be seen by comparing

$$\psi_n(t) = T \exp(-i \int_0^t dt' H(t'))\phi_n(0) \tag{3.82}$$

and the approximation

$$\psi_n(t) = \exp(-i \int_0^t dt' \epsilon_n(t'))\phi_n(0) \tag{3.83}$$

The last statement can be made precise, it is then called adiabatic theorem and states that a physical system remains in its instantaneous eigenstate if the time evolution is slow enough and if there is a gap between the eigenvalue and the rest of the spectrum. To show that, one uses the ONB ϕ_n to expand a solution of the time dependent Schrödinger equation as

$$\psi(t) = \sum_n c_n(t)\phi_n(t) \exp(-i \int_0^t dt' \epsilon_n(t')) \tag{3.84}$$

Substituting this into the Schrödinger equation yields

$$i \sum_n (\dot{c}_n \phi_n + c_n \dot{\phi}_n - i c_n \epsilon_n \phi_n) \exp(-i \int_0^t dt' \epsilon_n(t')) = \sum_n c_n H(t)\phi_n \exp(-i \int_0^t dt' \epsilon_n(t')) \tag{3.85}$$

which simplifies to

$$\sum_n \dot{c}_n \phi_n \exp(-i \int_0^t dt' \epsilon_n(t')) = - \sum_n c_n \dot{\phi}_n \exp(-i \int_0^t dt' \epsilon_n(t')) \tag{3.86}$$

Taking the scalar product with ϕ_m we obtain

$$\dot{c}_m(t) = - \sum_n c_n \langle \phi_m | \dot{\phi}_n \rangle \exp(-i \int_0^t dt' (\epsilon_n(t') - \epsilon_m(t'))) \tag{3.87}$$

On the right hand side, all terms except the one for $n = m$ are oscillatory and cancel out over long time. To make this statement mathematically rigorous is not easy and goes beyond the scope of this lecture.

Trivial examples where the adiabatic theorem holds occur whenever the eigenstate of a system is given by some quantum number that remains constant in time. Take e.g. the harmonic oscillator with a time dependent ω. The eigenstates are described by the quantum number n. If ω changes adiabatically, transitions between states are not induced, the system remains in the eigenstate with the same quantum number and only the energy changes.

In the original work of Berry [1], the case where $H(t)$ depends on t through a set of parameters was discussed and the case, where the system is moved adiabatically on a closed curve in this parameter space. This is the case where $H(t) = H(0)$, and $\phi_n(t)$ is the phase the wave functions picks up when it is moved on a the closed curve. For a more comprehensive review look at [29].

3.3.1 The driven two-level system

Let us take again the driven two-level system with the Hamiltonian now denote as

$$H(t) = \vec{h} \cdot \vec{\sigma} \tag{3.88}$$

with

$$\vec{h} = h(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \tag{3.89}$$

For this Hamiltonian, we obtain

$$\epsilon_\pm(t) = \pm h(t) \tag{3.90}$$

and the eigenvectors are

$$\phi_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ \exp(i\phi)\sin\frac{\theta}{2} \end{pmatrix} \tag{3.91}$$

and the eigenvectors are

$$\phi_- = \begin{pmatrix} \exp(-i\phi)\sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix} \tag{3.92}$$

One obtains

$$\langle\phi_\pm|\frac{d\phi_\pm}{dt}\rangle = \pm i\frac{d\phi}{dt}\sin^2\frac{\theta}{2} \tag{3.93}$$

Consider now a closed curve in the parameter space. Then the Berry phase becomes

$$\beta_\pm = \pm\int_0^t dt' \frac{d\phi}{dt'}\sin^2\frac{\theta}{2} = \pm\int_{\phi(0)}^{\phi(t)} d\phi\sin^2\frac{\theta}{2} \tag{3.94}$$

which for constant θ becomes $\pm 2\pi\sin^2\frac{\theta}{2}$.

The two level system is a caricature of a general system in which, depending on parameters, a degeneracy occurs. The degeneracy for the two level system occurs at $h = 0$. If we have discrete energy states we may reduce the general system to a two level system if the level spacing between the two almost degenerate states is small compared to the distance to the other states. In this sense, the above treatment is generic for a Hamiltonian with a crossing point of two energy levels.

3.3.2 The Aharonov-Bohm effect

Consider two charged particles which move on two different paths from the same starting point to the same end point, e.g. through a double slit. Each of the particles picks up a phase on its path. The difference of the two phases is the phase a particle would pick up if it runs on a closed path consisting of the first and the second reversed. Consider now the case where this closed path encloses a region with a magnetic field. Even if the magnetic field vanishes along the path, the magnetic vector potential will not vanish and influences the particle. This causes a phase the particle pics up, it is given by the charge of the particle and the magnetic flux through the path. This phase is the Berry phase for this setup. Experimentally it has been observed as a shift of the interference pattern of the double slit experiment mentioned above.

To derive this phase, we follow closely the presentation by Berry [1]. He considers a magnetic field consisting of a single flux line of flux Φ. The magnetic field vanishes outside this flux line. The magnetic vector potential does not vanish outside this flux line, because for any curve C around the flux line we have by definition of the flux

$$\int_C d\vec{r} \cdot \vec{A}(\vec{r}) = \Phi \tag{3.95}$$

Consider now a particle in a confining box located at $\vec{R}$. The box shall not contain the flux line. Without a magnetic field the Hamiltonian is

$$H = \frac{1}{2m}\vec{p}^2 + V(\vec{r} - \vec{R}) \tag{3.96}$$

where V is the potential of the confining box. We may assume that V vanishes inside the box and imposes boundary conditions at the boundaries of the box, so that the eigenstates of the particle in the box are standing waves inside the box. We denote the eigenfunctions in position representation by $\psi_n(\vec{r} - \vec{R})$ and the eigenvalues by E_n. If we now turn on the magnetic field with the single flux line, the Hamiltonian becomes

$$H = \frac{1}{2m}(\vec{p} - e\vec{A})^2 + V(\vec{r} - \vec{R}) \tag{3.97}$$

and the eigenfunctions are multiplied by a Dirac phase, i.e. are

$$\psi_{n,\Phi} = \exp(ie \int_{\vec{R}}^{\vec{r}} d\vec{r} \cdot \vec{A})\psi_n(\vec{r} - \vec{R}) \tag{3.98}$$

Let us now assume that we move the box such that $\vec{R}(t)$ moves on a closed circuit C around the flux line such that the box never touches the flux. Then, we obtain

$$\beta = i \int_C d\vec{R} \cdot \langle \psi_{n,\Phi} | \nabla_R \psi_{n,\Phi} \rangle \tag{3.99}$$

The integrand can be calulated as

$$\langle \psi_{n,\Phi} | \nabla_R \psi_{n,\Phi} \rangle = \int d^3r \psi_n^*(\vec{r} - \vec{R}) \left(-ie\vec{A}(\vec{R})\psi_n(\vec{r} - \vec{R}) + \nabla_R \psi_n(\vec{r} - \vec{R}) \right) \tag{3.100}$$

$$= -ie\vec{A}(\vec{R}) \tag{3.101}$$

and therefore

$$\beta = e\Phi \tag{3.102}$$

This result is universal, it only depends on the magnetic flux Φ, not on the special form of C or on any other special setup.

3.3.3 The Landau-Zener-Stückelberg problem

For details of the problem treated in this subsection, see [10], section 3.5, p. 253ff and for applications see [20]. It has also been discussed in the context of the solar neutrino problem [2].

The Landau-Zener-Stückelberg problem deals with the tunneling between two states in a system where two energy levels are approach each other as a function of time. It was proposed in different contexts independently by Landau, Zener, And Stückelberg and is therefore named after these authors.

Since only two states are considered, the problem can again be described by a two-level system. The Hamiltonian is

$$H = -\frac{1}{2}vt\sigma_z - \frac{1}{2}\Delta\sigma_x \tag{3.103}$$

For large negative values of t the particle sits in the state $|\sigma_z = -1\rangle$. We assume an adiabatic time dependency. The adiabatic energies are

$$\epsilon_\pm = \pm\frac{1}{2}\sqrt{v^2t^2 + \Delta^2} \tag{3.104}$$

3 Time dependent quantum phenomena

The adiabatic time dependence transports the tunnel system from the state $|\sigma_z = -1\rangle$ at large negative values of t to the state $|\sigma_z = +1\rangle$ at large positive values of t. If, during this process, the system tunnels, it ends up in the state $|\sigma_z = -1\rangle$ at large positive t. Let

$$U(t_i, t_f) = T \exp(i \int_{t_i}^{t_f} H(t)dt) \tag{3.105}$$

be the time evolution operator from the initial time t_i to the final time t_f. The tunneling probability for the system is

$$P = |\langle \sigma_z = -1|U(-\infty, \infty)|\sigma_z = -1\rangle|^2 \tag{3.106}$$

We can explicitly calculate this probability by expanding the time-ordered potential. One obtains

$$\langle \sigma_z = -1|U(-\infty, \infty)|\sigma_z = -1\rangle = \sum_{n=0}^{\infty}(-i)^n \Delta^n \int_{-\infty}^{\infty} dt_n \int_{-\infty}^{t_n} dt_{n-1} \ldots \int_{-\infty}^{t_2} dt_1$$

$$\langle \sigma_z = -1|U_0(t_n, \infty)\sigma_x U_0(t_{n-1}, t_n)\sigma_x \ldots \sigma_x U_0(t_1, -\infty)|\sigma_z = -1\rangle \tag{3.107}$$

where U_0 is the time evolution for Δ_0. In the basis where σ_z is dialonal, U_0 is diagonal. σ_x switches between the two states $|\sigma_z = \pm\rangle$. Only an even number of spin flips contribute. We obtain

$$\langle \sigma_z = -1|U(-\infty, \infty)|\sigma_z = -1\rangle = \sum_{n=0}^{\infty}(-\Delta)^n \int_{-\infty}^{\infty} dt_{2n} \int_{-\infty}^{t_{2n}} dt_{2n-1} \ldots \int_{-\infty}^{t_2} dt_1$$

$$\exp(-\frac{i}{2}v \sum_{j=1}^{2n}(-1)^j t_j^2) \tag{3.108}$$

The integrals can be calculated and one finally obtains

$$\langle \sigma_z = -1|U(-\infty, \infty)|\sigma_z = -1\rangle = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(\frac{\pi\Delta^2}{2v}\right)^n = \exp(-\pi\gamma) \tag{3.109}$$

where $\gamma = \Delta^2/(2v) = \tau_c/\tau_t$. $\tau_c = \Delta/v$ is the time the system stays in the crossover region and $\tau_t = 2/\Delta$ is the tunneling time. The probability is therefore $P = \exp(-2\pi\gamma)$. The adiabatic approach is valid if the variation in time is slow. This is the case if v is small. Since the only other scale in the Hamiltonian is Δ, we need $v \ll \Delta^2$. Therefore, τ_c is large compared to τ_t and γ is large. P is therefore small.

4 Open quantum systems II

4.1 The spin-boson model revisited

We start this chapter with a seemingly simple model, namely the spin-boson model from section 2.3.2 but now with an additional time-dependent field

$$H = -\frac{\Delta}{2}\sigma_x + \frac{1}{2}\sigma_z \sum_k \lambda_k(b_k + b_k^\dagger) + \sum_k \omega_k : b_k^\dagger b_k : + h(t)\sigma_z \tag{4.1}$$

4.1.1 First example: a field quench

We let

$$h(t) = h_0\theta(-t) \tag{4.2}$$

i.e. the external field is h_0 for $t \leq 0$ and is switched off at $t = 0$. We assume that at $t = 0$ the system is in the ground state with field h_0. Denote this field as ψ_0. We then ask how the expectation value of σ_z evolves in time for $t > 0$. This means we need to calculate the expectation value

$$P(t) = \langle\psi_0|\sigma_z(t)|\psi_0\rangle \tag{4.3}$$

All elements to calculate this expectation value are already present in section 2.3.2. We apply the same unitary transformation to the Hamiltonian as before and obtain (see (2.86), (2.99))

$$H(\ell = \infty) = -\frac{\Delta(\infty)}{2}\sigma_x + \sum_k \omega_k : b_k^\dagger b_k : + h(t)\sigma_x \sum_k \chi_k(\infty)(b_k + b_k^\dagger) \tag{4.4}$$

We evaluate (4.3) at $\ell = \infty$. $H(\ell = \infty)$ commutes with σ_x, both have common eigenstates. For $h_0 > \Delta(\infty)$ the ground state has $\langle\sigma_x\rangle = 1$. In that subspace, the Hamiltonian has the form

$$H(\ell = \infty, \sigma_z = 1, t < 0) = \sum_k \omega_k(b_k^\dagger + \frac{h_0\chi_k(\infty)}{\omega_k})(b_k + \frac{h_0\chi_k(\infty)}{\omega_k}) + \text{const.} \tag{4.5}$$

For the ground state we obtain

$$b_k\psi_0 = -\frac{h_0\chi_k(\infty)}{\omega_k}\psi_0 \tag{4.6}$$

Using the expression for $\sigma_z(\infty)$ from (2.99) we get

$$P(t) = \langle\psi_0|\sigma_x \sum_k \chi_k(\infty)(\exp(i\omega_k t)b_k^\dagger + \exp(-i\omega_k t)b_k)|\psi_0\rangle \tag{4.7}$$

which yields

$$P(t) = -2h_0 \sum_k \frac{\chi_k(\infty)^2}{\omega_k}\cos(\omega_k t) \tag{4.8}$$

The Fourier transform $\tilde{P}(\omega)$ of $P(t)$ is therefore related to the Fourier transform $\tilde{C}(\omega)$ of the equilibrium correlation function $C(t)$ through $\tilde{P}(\omega) = -2h_0\tilde{C}(\omega)/\omega$. We got $\tilde{C}(\omega) \sim J(\omega)$ for small ω which means that for the Ohmic bath $J(\omega) \sim \omega$ the Fourier transform $\tilde{P}(\omega)$ approaches a

constant for small ω which means that the correlation function $P(t)$ falls of exponentially for large t.

Let us note that the calculations we needed to obtain these result are not complicated. This shows the strength of the flow equations approach. Other methods to calculate $P(t)$ and $C(t)$ like a field theoretic approach or a Keldysh-type formalism are much more evolved and sometimes even fail to give the correct long time behaviour.

4.1.2 Adiabatic time evolution and the Landau-Zener-Stückelberg problem

The Landau-Zener-Stückelberg problem has applications e.g. in the area of superconducting quantum bits, see e.g. [20]. For such an application, the coupling of the two-level system to an environment is essential. For a general discussion of the dissipative case, see also section 11.5 and 12.5 of [10].

The Hamiltonian (3.103) can be diagonalized via the unitary transformation

$$U(t) = \exp(-\frac{i}{2}\theta(t)\sigma_y) \tag{4.9}$$

with

$$\theta(t) = -\tan^{-1}(\frac{vt}{\Delta}) \tag{4.10}$$

If we add a bath to the Hamiltonian, i.e. (4.1) with $h(t) = -vt/2$, and transform this Hamiltonian with the same unitary transformation, we obtain

$$
\begin{aligned}
H_{ad}(t) &= U(t)H(t)U^\dagger(t) \\
&= -\epsilon_+(t)\sigma_x + \frac{1}{4}(\frac{\Delta}{\epsilon_\pm}\sigma_z + \frac{vt}{\epsilon_+}\sigma_x)\sum_k \lambda_k(b_k + b_k^\dagger) + \sum_k \omega_k b_k^\dagger b_k
\end{aligned} \tag{4.11}
$$

This is only the adiabatic Hamiltonian. Since the full transformed Hamiltonian contains the additional term

$$-iU(t)\frac{dU^\dagger}{dt} = \frac{1}{2}\frac{d\theta}{dt}\sigma_y = \frac{1}{2}\frac{v/\Delta}{(v/\Delta)^2 t^2 + 1}\sigma_y \tag{4.12}$$

which is small compared to $\epsilon_+(t)\sigma_z$ if $v \ll \Delta^2$, the adiabatic treatment is valid if $v \ll \Delta^2$.

There have been several attempts to deal with the adiabatic problem described by H_{ad}. In addition to the two time scales $\tau_c = \Delta/v$ (crossover time) and $\tau_t = 2/\Delta$ (tunneling time) the correlation time $1/\omega_c$ occurs. Grifoni and Hänggi [10] argue that for a fast crossover, $\gamma \ll 1$, when τ_c is the shortest time scale, neither the system nor the bath are fast enough to react so that the result $P = \exp(-2\pi\gamma) = 1 - 2\pi\gamma$ is still valid. This argument is problematic because the adiabatic limit means $\gamma \gg 1$, see 3.3.3. In the limit of slow crossover, which is the adiabatic limit, one idea could be to set approximately

$$\frac{1}{4}(\frac{\Delta}{\epsilon_\pm}\sigma_z + \frac{vt}{\epsilon_+}\sigma_x) = \begin{cases} \frac{1}{2}\sigma_z & \text{for } |t| < \tilde{\tau}_c \\ \frac{1}{2}\sigma_x & \text{for } |t| > \tilde{\tau}_c \end{cases} \tag{4.13}$$

For $|t| > \tilde{\tau}_c$, the spin is in one of the eigenstates of σ_x. For $|t| < \tilde{\tau}_c$, the approximate H_{ad} looks like the usual spin-boson model and the coupling of the bath yields a renormalized tunneling frequency Δ_∞.

4.2 Quantum bits in an environment

From sections (3.1.2) and (3.2.2), where the effect of coherent destruction of tunneling and the reversal of the sign of the kinetic energy in lattice modes are treated, we learn that the properties of a quantum system can be controlled and changed by applying a suitable time-dependent field. In this section, we discuss another model in which this possibility is used.

For the kicked rotator, section (3.2.3), we saw that a time dependence that is given by a series of kicks is much easier to deal with than a continuous time dependence. In this section we will apply this insight to a concrete system which is of importance in current research.

This section is mainly based on a paper by Götz Uhrig [22, 23]. The model, he proposes for a quantum bit in an environment is similar to the spin-boson model

$$H = \frac{1}{2}\sigma_z \sum_k \lambda_k(b_k + b_k^\dagger) + \sum_k \omega_k : b_k^\dagger b_k : -\frac{1}{2}h_z(t)\sigma_z - \frac{1}{2}h_x(t)\sigma_x - \frac{1}{2}h_y(t)\sigma_y \qquad (4.14)$$

where for $J(\omega) = \sum_k \lambda_k^2 \delta(\omega - \omega_k)$ we take an Ohmic bath $J(\omega) = 2\alpha\omega f_c(\omega/\omega_c)$ where ω_c is a high energy (ultra-violet) cutoff and $f_c(x)$ is a cutoff function. e.g. $f_c(x) = \exp(-x)$ or $f_c(x) = \theta(1-x)$.

Let us first take $h_{x,y}(t) = 0$. The Hamiltonian 4.14 can be easily diagonalized by the unitary transformation

$$S = \exp(i\sigma_z K), \quad K = i\sum_k \frac{\lambda_k}{2\omega_k}(b_k - b_k^\dagger) \qquad (4.15)$$

and one gets $H = \sum_k \omega_k : b_k^\dagger b_k : -\frac{1}{2}h_z(t)\sigma_z$ up to an unimportant additive constant. We let $h_z(t) = h_0 > 0$ for $t < 0$ and $h_z(t) = 0$ for $t \geq 0$. σ_z commutes with the Hamiltonian and is therefore a good quantum number. For $t < 0$ the system is in the ground state with $\sigma_z = 1$.

Let us now take as $h_x(t) = h_{x0}\delta(t)$, $h_y(t) = 0$. This means that a state at $t = 0_-$ is transformed to a state $t = 0_+$ by $U_0 = \exp(ih_{x0}\sigma_x/2) = \cos(h_{x0}/2) + i\sigma_x \sin(h_{x0}/2)$, which corresponds to a rotation of the quantum bit around the x-axis. We obtain

$$U_0\sigma_z U_0^\dagger = (\cos(h_{x0}/2) + i\sigma_x \sin(h_{x0}/2))\sigma_z(\cos(h_{x0}/2) - i\sigma_x \sin(h_{x0}/2)) \qquad (4.16)$$

$$= (\cos^2(h_{x0}/2) - \sin^2(h_{x0}/2))\sigma_z + 2\cos(h_{x0}/2)\sin(h_{x0}/2)\sigma_y \qquad (4.17)$$

$$= \cos(h_{x0})\sigma_z + \sin(h_{x0})\sigma_y \qquad (4.18)$$

Let us choose $h_{x0} = \frac{\pi}{2}$ which means that σ_z is rotated to σ_y. This means that the ground state with $\sigma_z = 1$ at $t < 0$ is transformed to the state with $\sigma_y = 1$ and $t = 0_+$.

$$U_0|\sigma_z = 1\rangle = \frac{1}{\sqrt{2}}(|\sigma_z = 1\rangle + i|\sigma_z = -1\rangle) = |\sigma_y = 1\rangle \qquad (4.19)$$

We now want to measure σ_y at time t with $h(t) = 0$ for $t > 0$. Since H does not depend on time, this can be done by calculating

$$\sigma_y(t) = \exp(iHt)\sigma_y \exp(-iHt) \qquad (4.20)$$

. We get

$$\langle\sigma_y(t)\rangle = \langle\langle\sigma_y = 1|\sigma_y(t)|\sigma_y = 1\rangle\rangle_T \qquad (4.21)$$

The outer $\langle.\rangle_T$ is the thermal expectation value for the bosonic bath. We calculate the right hand side by transforming everything using S in (4.15) to have a simple representation for H.

$$\langle\sigma_y(t)\rangle = \langle\langle\sigma_y = 1|SS^\dagger\sigma_y(t)SS^\dagger|\sigma_y = 1\rangle\rangle_T$$

Using

$$S^\dagger\sigma_y S = \cos(2K)\sigma_y - \sin(2K)\sigma_x \qquad (4.22)$$

we obtain

$$S^\dagger \sigma_y(t)S = \cos(2K(t))\sigma_y - \sin(2K(t))\sigma_x \tag{4.23}$$

with

$$K(t) = i\sum_k \frac{\lambda_k}{2\omega_k}(\exp(-i\omega_k t)b_k - \exp(i\omega_k t)b_k^\dagger) \tag{4.24}$$

Further, we have

$$S^\dagger|\sigma_y = 1\rangle = \frac{1}{\sqrt{2}}(\exp(-iK)|\sigma_z = 1\rangle + i\exp(iK)|\sigma_z = -1\rangle \tag{4.25}$$

so that we finally obtain

$$\langle\sigma_y(t)\rangle = \frac{1}{2}\langle(\exp(iK)\exp(-2iK(t))\exp(iK) + \exp(-iK)\exp(2iK(t))\exp(-iK)\rangle_T \tag{4.26}$$

K and $K(t)$ are operators which are linear in the bosonic operators. Therefore, the commutator is a number and we can apply the formular $\exp(A)\exp(B) = \exp(A + B)\exp([A, B])$ which holds if $[A, B]$ is a number. Further, for an operator C that is linear in the bosonic operators one has $\langle\exp(C)\rangle = \exp(\langle C^2\rangle/2)$. This finally yields

$$\langle\sigma_y(t)\rangle = \cos(\varphi(t))\exp(-2\chi(t)) \tag{4.27}$$

with

$$\varphi(t) = \int_0^\infty d\omega\, J(\omega)\frac{\sin(\omega t)}{\omega^2} \tag{4.28}$$

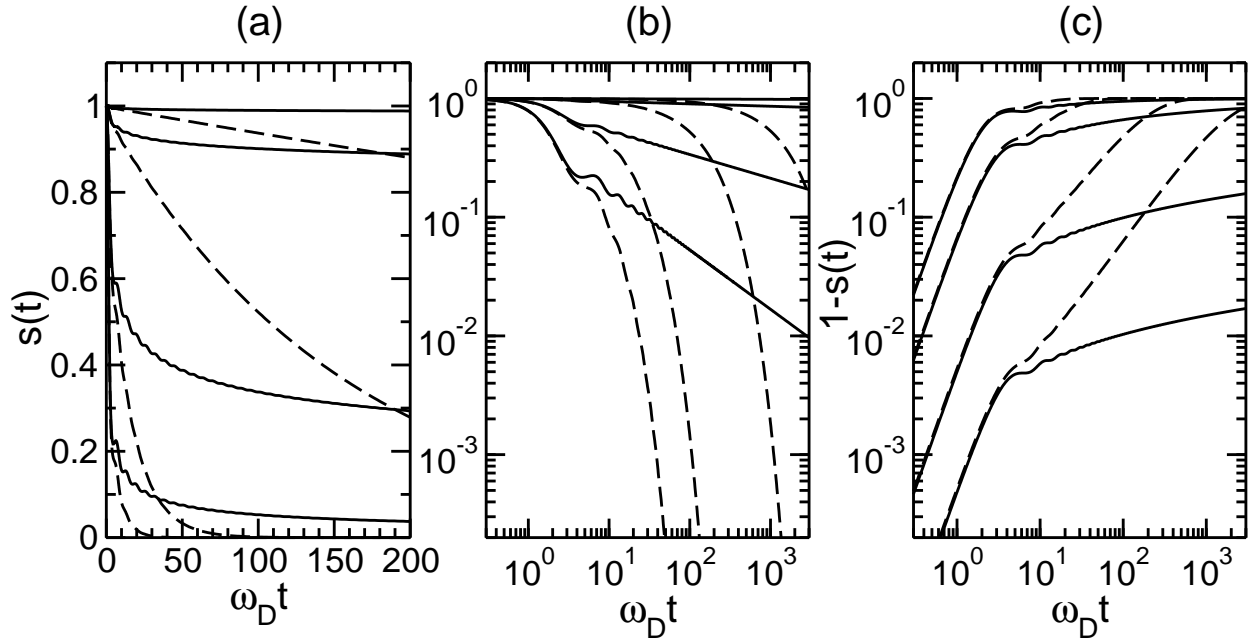$$\chi(t) = \int_0^\infty d\omega\, J(\omega)\frac{\sin^2(\omega t)}{\omega^2}\coth(\beta\omega/2) \tag{4.29}$$

Figure 4.1: Signal vs. time (4.27). Solid lines for $T = 0$; dashed ones for $T = 0.1\omega_D$. Panels (a) (linear) and (b) (double logarithmic) from bottom to top for $\alpha = 0.25, 0.1, 0.01, 0.001$. Panel (c) (double logarithmic) displays $1 - s(t)$ for the same values from top to bottom.

Figure 4.1 shows $s(t) = \langle \sigma_y(t) \rangle$ from (4.27) in different representations for an Ohmic bath

$$J(\omega) = 2\alpha f_c(\omega/\omega_D) \text{ with } f_c(x) = \theta(1-x) \tag{4.30}$$

with the cutoff frequency ω_D. One clearly sees the loss of coherence, $s(t) = \langle \sigma_y(t) \rangle$ falls down as a function of t. As discussed in [22], an experimentally acceptable level for $1 - s(t)$ lies between 10^{-4} and 10^{-2}. The figure shows that for weak couplings $\alpha \lesssim 0.01$, values $\omega_D t \approx 1$ can be reached which corresponds in experimental situation to times of the order of 1ps. For more realistic couplings $\alpha \gtrsim 0.1$ only very small values $\omega_D t$ are possible, thus coherence gets lost already after very tiny fractions of 1ps.

The main idea proposed in [22] is to stabilize the Q-bit by applying a sequence of pulses in y-direction, i.e. to apply a field $h_y(t) = \sum_n h_{yn}\delta(t-t_n)$. This was not a totally new idea, it was known before that one or two pulses can stabilize the Q-bit to a certain extend. Actually, Uhrig proposes to look at $s(t_f)$ at some final time t_f and to take $t_n = \delta_n t_f$ with $0 < \delta_1 < \delta_2 < \ldots < 1$. A pulse in y-direction corresponds to a rotation and he chooses π-pulses, i.e. rotations around the y-axis by an angle π. This effectively changes the sign of σ_z and thus the sign of the spin-bath-coupling in the Hamiltonian (4.14).

Mathematically, the calculation is similar to what we did so far, only more complicated. The rotation at time t_n corresponds to a unitary transformation $U_n = \exp(ih_{yn}\sigma_y) = \cos(h_{yn}) + i\sigma_y \sin(h_{yn})$, which for the π-pulse that corresponds to $h_{yn} = \pi$ yields $U_n = i\sigma_y$. Since the algebra of the Pauli matrices is closed and since in the unitary time evolution between two subsequent pulses is trivial after the application of the unitary transformation S, the entire calculation is just a matter of doing the algebra, but it can be done exactly. This allows to calculate $s(t)$ for this case as well and to derive and optimal sequence δ_n. The outcome is that by using 100 pulses, one can achieve times up to $\omega_D t \approx 10^3$.

To summarize this section, we showed that

1. Q-bits loose their coherence after a very short time which limits the calculation time of quantum computers.

2. The coherence time of Q-bits can be significantly enhanced by using suitable pulses. This can be calculated explicitly and exactly in a simple model given by the Hamiltonian (4.14) and is already applied in experimental situations.

3. A time dependent Hamiltonian where the time dependence is a series of pulses or kicks with a unitary time evolution given by a time independent Hamiltonian between those kicks can be calculated much more easily than a for a Hamiltonian with a continuous time dependence.

4.3 Periodically driven systems, quantum stochastic resonance

Periodically driven dissipative quantum systems play an important role in the theory of matter and radiation with many applications from high energy physics to condensed matter physics and quantum chemistry. Many phenomena can again be described by the driven dissipative two-level system. In this section I will only give a very brief qualitative look on these systems. For a more comprehensive discussion, see the book by Ulrich Weiss [26], chapter 22, or the review by Grifoni and Hänggi [10].

One of the important phenomena in driven classical dissipative systems is stochastic resonance. Consider a particle in a symmetric double well potential that is coupled to a bath and is subject to a periodic driving force. The full time-dependent potential is $V(x,t) = -\frac{a}{2}x^2 + \frac{b}{4}x^4 - A_0 x \cos(\omega t)$. For the non-driven system, there are two minima at $x_m = \pm\sqrt{a/b}$ and a potential well of height $\Delta V = a^2/4b$ between them. The system has a characteristic time, scale, the mean first passage

time for transitions between the two minima $\tau \propto \exp(-\Delta V/T)$. If one couples the periodic force $F(t) = A_0 \cos(\omega t)$ to the system, one obtains a periodic change of ΔV. The particle prefers to sit in the deeper minimum. If the driving frequency ω corresponds to the inverse of the mean first passage time, one may get a synchronization between the external driving force $F(t)$ and the motion of the particle. The synchronization can be measured e.g. by the signal to noise ratio. For the simple classical system this ratio can be calculated. For a given frequency ω this means that there is an optimal value for the noise strength, i.e. the temperature, where the signal to noise ratio has a maximum. This effect is called stochastic resonance. It has been observed in many system ranging from biology to laser physics or astronomy. The observed amplification factor in those systems has values up to 10^6.

The question now is whether a similar effect can be observed in the quantum regime. This is indeed the case. At low temperatures one observes the so called quantum stochastic resonance (QSR).

In principle, we have all the material at hand to calculate the correlation functions and the signal to noise ratio. At low temperature one can use the two-level system One needs to know the long-time behaviour. The periodic time dependence can be treated via the Floquet map and the effective operator, the latter can then be dealt with using flow equations. Many other methods have been used to treat that system, see the above references. The main results are:

1. For low temperatures, i.e. $T \ll \omega_c$ and weak coupling to the bath ($\alpha < 1$ for the Ohmic bath), a static asymmetry is needed to observe QSR. The static asymmetry must be larger than the driving strength. For stronger coupling, QSR occurs also in the symmetric case.

2. QSR occurs as an effect of the interplay between coherent and incoherent dynamics. The incoherence must dominate the coherent processes.

3. QSR as the usual stochastic resonance can be well understood within a linear response theory. Non-linear effects occur and can be taken into account but are not necessary to calculate the effect.

5 The (fractional) quantum Hall effect

5.1 Introduction

The quantum Hall effect was found 1980 by von Klitzing and published in a paper by von Klitzing, Dorda, and Pepper [14], Klaus von Klitzing received in 1985 the Nobel prize. For a general introduction I refer to [19]. 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

$$\sigma = \begin{pmatrix} 0 & -n\frac{e^2}{h} \\ n\frac{e^2}{h} & 0 \end{pmatrix} \tag{5.1}$$

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

$$\sigma_0 = \rho e^2\tau_0/m \tag{5.2}$$

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

$$\vec{j} = \sigma_0\vec{E} - \frac{\sigma_0}{\rho e c}\vec{j} \times \vec{B} \tag{5.3}$$

In a two dimensional system we therefore obtain

$$\sigma^{-1} = \begin{pmatrix} \sigma_0^{-1} & \frac{B}{\rho ec} \\ -\frac{B}{\rho ec} & \sigma_0^{-1} \end{pmatrix} \tag{5.4}$$

The conductivity is therefore

$$\sigma_{xx} = \frac{\sigma_0}{1 + \omega_c^2\tau_0^2}, \quad \sigma_{xy} = \frac{\rho ec}{B} + \frac{\sigma_{xx}}{\omega_c\tau_0} \tag{5.5}$$

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 relatively 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 magnetic field. The Hamiltonian is

$$H = \frac{\hbar^2}{2m} \left[\left(\frac{1}{i} \frac{\partial}{\partial x} - \frac{eB}{\hbar c} y \right)^2 - \frac{\partial^2}{\partial y^2} \right] \tag{5.6}$$

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

$$\psi \propto \exp(ikx)\phi(y) \tag{5.7}$$

for the eigenfunctions. This leads to the eigenvalue equation

$$\frac{\hbar\omega_c}{2} \left(-l_B^2 \frac{\partial^2}{\partial y^2} + \left(\frac{y}{l_B} - l_B k \right)^2 \right) \phi = E\phi \tag{5.8}$$

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

$$\phi_{n,k} \propto H_n(y/l_B - l_B k) \exp(-(y - l_B^2 k)/2l_B^2) \tag{5.9}$$

$$E_{nk} = \hbar\omega_c(n + 1/2) \tag{5.10}$$

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

$$n_B = \frac{1}{2\pi l_B^2} = \frac{eB}{hc} \tag{5.11}$$

The single-particle states constructed in that way are localized 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 localized in x-direction and extended in y-direction or that are localized 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

$$\nu = \frac{\rho}{n_B} \tag{5.12}$$

is an even number and for the conductivity tensor one obtains

$$\sigma^{-1} = \begin{pmatrix} \sigma_0^{-1} & \frac{B}{\rho e c} \\ -\frac{B}{\rho e c} & \sigma_0^{-1} \end{pmatrix} = \begin{pmatrix} 0 & \frac{h}{\nu e^2} \\ -\frac{h}{\nu e^2} & 0 \end{pmatrix} \tag{5.13}$$

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

$$\vec{v} = c \frac{\vec{E} \times \vec{B}}{B^2} \tag{5.14}$$

which contains no electric field and therefore no macroscopic current. In the original system, the current density is therefore

$$\vec{j} = -\rho e \vec{v} \tag{5.15}$$

which yields the same conductivity tensor. Therefore, without imperfections, defects or impurities one always obtains

$$\sigma_{xx} = 0, \quad \sigma_{xy} = \frac{\rho e c}{B} = \nu \frac{e^2}{h} \tag{5.16}$$

The question now is, what is the influence of disorder.

## 5.2 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.

5.2.1 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 localization, this is the so called Anderson localization, see section 3.2.3. P. W. Anderson received the Nobel prize (together with Mott and van Fleck) in 1977 for his contribution to the theory of localization. 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 diagonalize the Hamiltonian

$$H_0 = P_0 V(x, y) P_0 \tag{5.17}$$

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 realized as a random potential. Such a potential lifts the degeneracy of the Landau level and tends to localize the electrons. Electrons close to deep minima or maxima of the potential will be stronger localized and will have an energy far away from the original energy of the Landau level. On the other hand, we know that the

Figure 5.1: The cylinder geometry
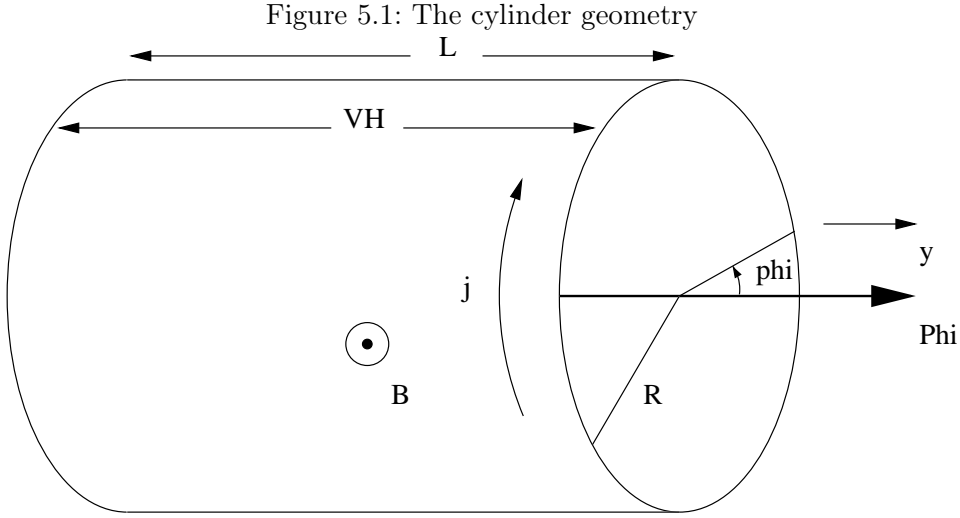
complete Landau level must still yield a contribution $\frac{e^2}{h}$ to the Hall conductivity. This contribution cannot come from localized states. It must come from extended states which we expect to find in the middle of the broadened Landau level. If we now change the filling factor, e.g. by changing the magnetic field, the Fermi energy will move through the spectrum. There are regions in the spectrum where all states are localized 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 [19].

5.2.2 Laughlins gauge argument

Let us choose the vector potential to be

$$A_x = -By + \frac{\Phi}{2\pi R}, \quad A_y = 0 \tag{5.18}$$

so that the Hamiltonian reads

$$H = \frac{\hbar^2}{2m}\left[\left(\frac{1}{i}\frac{\partial}{\partial x} - \frac{eB}{\hbar c}y + \frac{e\Phi}{2\pi R\hbar c}\right)^2 - \frac{\partial^2}{\partial y^2}\right] + V(x,y) \tag{5.19}$$

Further, we assume periodic boundary conditions in x-direction, i.e.

$$x = \varphi R \tag{5.20}$$

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 characterized by the Landau index n. Within a Landau level one introduces a second index. The eigenfunctions are

$$\psi_{n,k} \propto \exp(ikx)H_n(y/l_B - l_B(k + \frac{e\Phi}{2\pi R\hbar c}))\exp(-(y - l_B^2(k + \frac{e\Phi}{2\pi R\hbar c})/2l_B^2) \tag{5.21}$$

where $k = l/R$, $l \in Z$ because of the periodic boundary conditions. We can write as well

$$\psi_{n,l} \propto \exp(2\pi i l\varphi)H_n\left(\frac{y}{l_B} - \frac{l_B}{R}(l + \frac{e\Phi}{hc})\right)\exp\left(-\frac{1}{2}\left(\frac{y}{l_B} - \frac{l_B}{R}(l + \frac{e\Phi}{hc})\right)^2\right) \tag{5.22}$$

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

$$E_{n,l}(\Phi + \frac{hc}{e}) = E_{n,l+1}(\Phi) \tag{5.23}$$

$V_0(y)$ is only at the boundary different from 0. The states are therefore still localized in y-direction close to $\frac{l_B^2}{R}(l + \frac{e\Phi}{hc})$ and only those states where the localization is close to the boundary will be affected by the potential. Therefore, 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-direction is

$$I_{n,l} = -c\frac{dE_{n,l}(\Phi)}{d\Phi} \tag{5.24}$$

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

$$
\begin{aligned}
I &= \frac{e}{h}\int_0^{hc/e} d\Phi \sum_{n,l} n_{n,l} I_{n,l} \\
&= -\frac{e}{h}\sum_{n,l} n_{n,l}(E_{n,l}(hc/e) - E_{n,l}(0)) \\
&= -\frac{e}{h}\sum_{n=0}^{\nu}(E_{n,l_{max}}(0) - E_{n,l_{min}}(0)) \\
&= \frac{e^2}{h}\nu V_H
\end{aligned}
\tag{5.25}
$$

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 localize 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.

There is one important note to make here: The argument still holds if one adds an arbitrary potential $V(x,y)$ as in the initial Hamiltonian, as long as this potential is small and does not mix states out of different Landau levels.

5.2.3 Topological arguments

There are two types of quantum numbers in quantum physics: Those related to symmetry and those related to topology. An example for a quantum number related to symmetry is the angular momentum. It is a good quantum number if the system is rotationally invariant. The relationship

between symmetry and good quantum numbers is given by Noether's theorem. In systems with disorder and arbitrary boundaries one cannot expect symmetries. Therefore it is natural to assume that the quantization of the Hall current is related to topology. This is indeed the case. For details see chapter 4 by D.J. Thouless in [19]. One can show that the Hall conductivity is determined by a topological invariant, the so called Chern number. The Chern number is related to the Berry phase. It is given by the integral of the Berry curvature over all states in an energy band.

5.3 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 [21]. First theoretical approaches followed immediately, the main theoretical achievement was the work by Laughlins [15] 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.

5.3.1 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

$$H = \sum_j \left[\frac{1}{2m} \left(\frac{\hbar}{i} \nabla_j + \frac{e}{c} \vec{A}_j \right)^2 + V_1(\vec{r}_j) \right] + \frac{1}{2} \sum_{j \neq k} V(|\vec{r}_j - \vec{r}_k|) \tag{5.26}$$

$V_1(\vec{r})$ 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

$$V(|\vec{r}|) = \frac{e^2}{|\vec{r}|} \tag{5.27}$$

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

$$\vec{A} = \frac{B}{2}(y\vec{e}_x - x\vec{e}_y) \tag{5.28}$$

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

$$
\begin{aligned}
H &= \frac{1}{2}\hbar\omega_c \left[\left(-il_B \frac{\partial}{\partial x} - \frac{y}{2l_B} \right)^2 + \left(-il_B \frac{\partial}{\partial y} + \frac{x}{2l_B} \right)^2 \right] \\
&= \frac{1}{2}\hbar\omega_c [z^* z + z^* \partial_{z^*} - z\partial_z - \partial_z \partial_{z^*}]
\end{aligned}
\tag{5.29}
$$

where

$$z = \frac{1}{2l_B}(x - iy), \quad z^* = \frac{1}{2l_B}(x + iy) \tag{5.30}$$

$$\partial_z = l_B \left(\frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right), \quad \partial_{z^*} = l_B \left(\frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right) \tag{5.31}$$

We define

$$a^\dagger = \frac{1}{\sqrt{2}} (z^* - \partial_z) \tag{5.32}$$

$$a = \frac{1}{\sqrt{2}} (z + \partial_{z^*}) \tag{5.33}$$

where $[a, a^\dagger] = 1$, and obtain

$$H = \hbar \omega_c (a^\dagger a + \frac{1}{2}) \tag{5.34}$$

A wave function in the lowest Landau level obeys the condition

$$a\psi = 0 \tag{5.35}$$

$$z\psi + \partial_{z^*} \psi = 0 \tag{5.36}$$

with the general solution

$$\psi = f(z) \exp(-z^* z) \tag{5.37}$$

$f(z)$ 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

$$\Psi = f(z_1, \ldots, z_{N_e}) \exp(- \sum_i z_i^* z_i) \tag{5.38}$$

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

$$\begin{aligned} L_z &= ix \frac{\partial}{\partial y} - iy \frac{\partial}{\partial x} \\ &= z\partial_z - z^* \partial_{z^*} \end{aligned} \tag{5.39}$$

$$L_z f(z) \exp(-z^* z) = z f'(z) \exp(-z^* z) \tag{5.40}$$

The eigenstates of L_z are therefore

$$\psi_m = z^m \exp(-z^* z) \tag{5.41}$$

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 normalization 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

$$\Psi = f(z_1, \ldots, z_{N_e}) \exp(- \sum_i z_i^* z_i) \tag{5.42}$$

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

$$\prod_{j<k} f(\vec{r}_j - \vec{r}_k) \tag{5.43}$$

In our case this means

$$\Psi = \prod_{j<k} f(z_j - z_k) \exp(-\sum_i z_i^* z_i) \tag{5.44}$$

This wave function must have the following properties

- It should be an eigenfunction of L_z. Therefore $f(z) \propto z^m$.

- It should be antisymmetric with respect to permutations of two particles. Therefore, m must be odd.

This means that the Jastrow ansatz yields

$$\Psi = \Psi_m = \prod_{j<k}(z_j - z_k)^m \exp(-\sum_i z_i^* z_i) \tag{5.45}$$

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 diagonalization of the Hamiltonian for small numbers of particles. An exact diagonalization 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 [4]. 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 diagonalizations 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

$$V(r) = V_2 \nabla^2 \delta(r) \tag{5.46}$$

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 $m = 1$.

$$\Psi_1 = \prod_{j<k}(z_j - z_k)\exp(-\sum_i z_i^* z_i) \tag{5.47}$$

The factor $\prod_{j<k}(z_j - z_k)$ is a so called Vandermonde determinant. One has

$$\prod_{j<k}(z_j - z_k) = (-1)^{N_e(N_e-1)/2}\sum_P(-1)^P\prod_i z_{P(i)}^i \tag{5.48}$$

Up to a normalization 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

$$|\Psi_m|^2 = \exp(-\beta\phi_m(z_1, \ldots, z_{N_e})) \tag{5.49}$$

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

$$\phi_m(z_1, \ldots, z_{N_e}) = -m^2\sum_{j<k}\ln|z_j - z_k| + m\sum_{l=1}^{N_e}|z_l|^2 \tag{5.50}$$

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

$$\phi_m(z_1, \ldots, z_{N_e}) = -e^2\sum_{j<k}\ln|z_j - z_k| + \frac{\pi}{2}\rho_0 e\sum_{l=1}^{N_e}|z_l|^2 \tag{5.51}$$

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

$$\rho_0 = \frac{2}{\pi} \tag{5.52}$$

The plasma is neutral, the particle density is

$$\rho = \frac{2}{\pi m} \tag{5.53}$$

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

$$g(z_1, z_2) = \frac{N_e(N_e - 1)}{\rho^2}\frac{\int d^2z_3 \ldots d^2z_{N_e}|\Psi_m|^2}{\int d^2z_1 \ldots d^2z_{N_e}|\Psi_m|^2} \tag{5.54}$$

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

$$E_{WW} = \frac{1}{2}\int d^2z\,g(|z|)V(|z|) \tag{5.55}$$

Taking into account the homogeneous background, the total energy is

$$E = \frac{1}{2} \int d^2 z (g(|z|) - 1) V(|z|) \tag{5.56}$$

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

$$g(r) = 1 - \exp(-r^2) \tag{5.57}$$

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.

5.3.2 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, $\epsilon = \epsilon_p + \epsilon_h$ 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

$$\Psi_m^{(-)} = S_{z_0} \Psi_m \tag{5.58}$$

$$S_{z_0} = \prod_{j=1}^{N_e} (z_j - z_0) \tag{5.59}$$

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 diagonalizing 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 $0.025 e^2 / l_B$. 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

$$\Psi_m^{(+)} = \exp(-\sum_j |z_j|^2) \prod_{j=1}^{N_e} \frac{\partial}{\partial z_j} \prod_{k<l} (z_k - z_l)^m \tag{5.60}$$

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.

5.3.3 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 localized and thereby on can explain the existence of a plateau in the Hall conductivity.

5.4 Universality

In a seminal paper, Fröhlich and Kerler [7] 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.

5.4.1 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

$$\sigma = \begin{pmatrix} 0 & -\sigma_H \\ \sigma_H & 0 \end{pmatrix} = \sigma_H \epsilon \tag{5.61}$$

where $\epsilon = (\epsilon_{\alpha\beta})_{\alpha,\beta=1,2}$ with $\epsilon_{12} = -\epsilon_{21} = 1$, $\epsilon_{11} = \epsilon_{22} = 0$. 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

$$\partial_\alpha = \frac{\partial}{\partial x^\alpha} \tag{5.62}$$

The current density is given by

$$j^\alpha(x) = \sigma_H \epsilon^{\alpha\beta} E_\beta(x) \tag{5.63}$$

The continuity condition is

$$\partial_\alpha j^\alpha = 0 \tag{5.64}$$

and Faradays law has the form

$$\frac{\partial B}{\partial x^0}(x) + \nabla \times \vec{E}(x) = 0 \tag{5.65}$$

or

$$\epsilon^{\alpha\beta\gamma}\partial_\alpha F_{\beta\gamma}(x) = 0 \tag{5.66}$$

Taking the continuity condition and Faradays law, we obtain

$$\sigma_H\partial_0 B = -\sigma_H\nabla \times \vec{E} = -\nabla \cdot \vec{j} = \partial_0 j^0 \tag{5.67}$$

and therefore

$$j^0(x) = \sigma_H B(x) \tag{5.68}$$

Taking this equation together with the material equations for $\vec{j}$ we may put everything together in the compact form

$$J_{\alpha\beta}(x) = \sigma_H F_{\alpha\beta}(x) \tag{5.69}$$

where

$$J_{\alpha\beta}(x) = \epsilon_{\alpha\beta\gamma}j^\gamma(x) \tag{5.70}$$

$\epsilon_{\alpha\beta\gamma}$ is the complete anti-symmetric tensor. The continuity equation now takes the form

$$\epsilon^{\alpha\beta\gamma}\partial_\alpha J_{\beta\gamma}(x) = 0 \tag{5.71}$$

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

$$F_{\alpha\beta} = \partial_\alpha A_\beta - \partial_\beta A_\alpha \tag{5.72}$$

$$J_{\alpha\beta} = \partial_\alpha a_\beta - \partial_\beta a_\alpha \tag{5.73}$$

and we obtain

$$\partial_\alpha(a_\beta - \sigma_H A_\beta) - \partial_\beta(a_\alpha - \sigma_H A_\alpha) = 0 \tag{5.74}$$

This relation can be derived from the action

$$S_{CS}(a - \sigma_H A) = \int_{R\times\Omega} d^3x \epsilon^{\alpha\beta\gamma}(a_\alpha - \sigma_H A_\alpha)\partial_\beta(a_\gamma - \sigma_H A_\gamma) \tag{5.75}$$

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

$$S(a, A) = S_{CS}(a - \sigma_H A) + S_I(a, A) \tag{5.76}$$

where the behaviour on long time and length scales is determined by S_{CS}.

5.4.2 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 quantize the action $S(a, A)$ where A will be treated as an external, classical field. The quantization can be performed using a path integral. We use Euclidean path integrals and introduce the coordinates

$$a_0 \rightarrow -ia_0, \quad A_0 \rightarrow -iA_0, \quad \partial_0 \rightarrow -i\partial_0, \quad dx^0 \rightarrow idx^0 \tag{5.77}$$

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

$$dP_A(a) := Z(A_c + A)^{-1} \exp(-\frac{1}{\hbar} S^E(a, A)) D[a] \tag{5.78}$$

where

$$S^E(a, A) = -i\kappa S_{CS}(a - \sigma_H A) + S_I(a, A) \tag{5.79}$$

$$D[a] = \prod_x \prod_{\alpha=0}^{2} da_\alpha(x) \tag{5.80}$$

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 [19] 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

$$\sigma_H = \pm\frac{1}{2l + 1}\frac{e^2}{h} \tag{5.81}$$

This was shown by Fröhlich and Kerler [7]. 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

$$J^{(i)} = \sigma_H^{(i)} F \tag{5.82}$$

must hold. This then explains the experimentally observed values of σ_H.

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