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Quantentransport in Spindichtesystemen mit dem Memory-Matrix-Formalismus

Masterthesis

von

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27. Mai 2017 bis 27. Mai 2018

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Ich erkläre hiermit, dass die Arbeit selbstständig angefertigt, alle benutzten Quellen und Hilfsmittel vollständig und genau angegeben und alles kenntlich gemacht wurde, das aus Arbeiten anderer unverändert oder mit Abänderungen entnommen ist.

Karlsruhe, den 4. Mai 2018

.....
(**Martin Lietz**)

Acknowledgments

I would like to express my thanks to my advisor Jörg Schmalian who encouraged and supported me and gave the right hints at the right time during the last year. His essential input lead to the results presented in this work.
Furthermore, I would like to thank Una Karahasanovic for all the discussions and information which became decisive for one topic of this work.
Then, I have to thank especially Jian Kang who crucially contributed to the discussion of bond currents and Rafael Fernandes for the fruitful discussions on the general topic.
Special thanks to all the colleagues of the condensed matter group at the KIT. Especially to Bhilahari Jeevanesan for all the discussions and help with several problems and to Pablo Schad for finalizing this work.
Last but not least, I have to thank my family, my mother and sister and especially Anja for all the support and encouraging words.

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Einleitung zum Kapitel schreiben

3.1 The free propagator of spin density waves

The dynamic of spin density waves without interaction is described by the Hamiltonian H_Φ, introduced in chapter 2. The equation of motion of the Green's functions are one naturally, simple and elegant method to compute a free propagtor of an aribtrary typ of particle. The equation of motion in frequency spce is the first item of an infinte algebraic equation chain. Mostly the initial Green function appears lately in the second item of the chain which is resulting in an solvable algebraic equtaion system. For a detailed deviation the book of Elk and Gasser [EG79] is recommended. In the case of the free spin density waves the first item of the chain is

$$\omega\langle\langle\Phi_\mu(\mathbf{k}+\mathbf{G},t);\Phi_\lambda(\mathbf{k}'+\mathbf{G}',t')\rangle\rangle_\omega = \langle[\Phi_\mu(\mathbf{k}+\mathbf{G},t),\Phi_\lambda(\mathbf{k}'+\mathbf{G}',t')]\rangle + \langle\langle[\Phi_\mu(\mathbf{k}+\mathbf{G},t),\mathrm{H}_\Phi];\Phi_\lambda(\mathbf{k}'+\mathbf{G}',t')\rangle\rangle_\omega, \quad (3.1)$$

where the double angle brackets denotes the Green function of spin density waves and the index ω means that the Green function has to be considered in the frequency space. The simplicity and advantage of the method instead of other ones is that only the commutator relations of the (field) operators are needed. The bosonic commutator relations are given in equation (...) and the Hamiltonian is given by equation (...). The inhomogeneity is trivially zero and the commutator in the second term yields

link zu bosonischen Vertauschungsrelationen

Link zu H_Φ

$$[\Phi_\mu(\mathbf{k}+\mathbf{G},t),\mathrm{H}_\Phi] = -\frac{1}{2\epsilon}\sum_{\mathbf{P}}\int_{\mathbf{p}}[\Phi_\mu(\mathbf{k}+\mathbf{G},t),\pi_\nu(\mathbf{p}+\mathbf{P},t_1)\pi_\nu(-\mathbf{p}-\mathbf{P},t_1)]$$

$$\Leftrightarrow\ [\Phi_\mu(\mathbf{k}+\mathbf{G},t),\mathrm{H}_\Phi] = -\frac{1}{2\epsilon}\sum_{\mathbf{P}}\int_{\mathbf{p}}\Big[\pi_\nu(\mathbf{p}+\mathbf{P},t_1)[\Phi_\mu(\mathbf{k}+\mathbf{G},t),\pi_\nu(-\mathbf{p}-\mathbf{P},t_1)] + [\Phi_\mu(\mathbf{k}+\mathbf{G},t),\pi_\nu(\mathbf{p}+\mathbf{P},t_1)]\pi_\nu(-\mathbf{p}-\mathbf{P},t_1)\Big]$$

$$\Leftrightarrow\ [\Phi_\mu(\mathbf{k}+\mathbf{G},t),\mathrm{H}_\Phi] = -\frac{i}{\epsilon}\pi_\mu(\mathbf{k}+\mathbf{G},t) \quad (3.2)$$

where in the beginning the sum over λ is implied. Equation (3.1) yields

$$\omega\langle\langle\Phi_\mu(\mathbf{k}+\mathbf{G},t);\Phi_\lambda(\mathbf{k}'+\mathbf{G}',t')\rangle\rangle_\omega = -\frac{i}{\epsilon}\langle\langle\pi_\mu(\mathbf{k}+\mathbf{G},t);\Phi_\lambda(\mathbf{k}'+\mathbf{G}',t')\rangle\rangle_\omega \quad (3.3)$$

where on the right hand side a new Green function appears. Nobody bars us doing the exactly same procedure for this one as for the initial Green function.

$$\begin{aligned}\omega\big\langle\big\langle\pi_\mu(\mathbf{k}+\mathbf{G},t);\Phi_\lambda(\mathbf{k}'+\mathbf{G}',t')\big\rangle\big\rangle_\omega &= \big\langle\big[\pi_\mu(\mathbf{k}+\mathbf{G},t),\Phi_\lambda(\mathbf{k}'+\mathbf{G}',t')\big]\big\rangle \\ &\quad+\big\langle\big\langle[\pi_\mu(\mathbf{k}+\mathbf{G},t),\mathrm{H}_\Phi];\Phi_\lambda(\mathbf{k}'+\mathbf{G}',t')\big\rangle\big\rangle_\omega \quad (3.4)\end{aligned}$$

The inhomogeneity of the equations is trivially, too, but in this case yields something differant to zero.

$$\big[\pi_\mu(\mathbf{k}+\mathbf{G},t),\Phi_\lambda(\mathbf{k}'+\mathbf{G}',t')\big] = -i(2\pi)^2\sum_{\mathbf{G}}\delta(\mathbf{k}'+\mathbf{k})\delta_{-\mathbf{G}',\mathbf{G}}\delta_{\mu,\lambda} \quad (3.5)$$

Equally the commutator can be computed with the same method.

$$\begin{aligned}[\pi_\mu(\mathbf{k}+\mathbf{G},t),\mathrm{H}_\Phi] &= -\sum_{\mathbf{P}}\int_{\mathbf{p}}\frac{(\mathbf{p}+\mathbf{P})^2+r}{2} \\ &\quad\times[\pi_\mu(\mathbf{k}+\mathbf{G},t),\Phi_\nu(\mathbf{p}+\mathbf{P},t_1)\Phi_\nu(-\mathbf{p}-\mathbf{P},t_1)] \\ \Leftrightarrow\ [\pi_\mu(\mathbf{k}+\mathbf{G},t),\mathrm{H}_\Phi] &= i(2\pi)^2\sum_{\mathbf{P}}\int_{\mathbf{p}}\frac{(\mathbf{p}+\mathbf{P})^2+r}{2} \\ &\quad\times\Big[\Phi_\mu(\mathbf{p}+\mathbf{P},t)\delta(\mathbf{k}-\mathbf{p})\delta_{\mathbf{G},\mathbf{P}} \\ &\quad+\Phi_\mu(-\mathbf{p}-\mathbf{P},t)\delta(\mathbf{k}+\mathbf{p})\delta_{-\mathbf{G},\mathbf{P}}\Big] \\ \Leftrightarrow\ [\pi_\mu(\mathbf{k}+\mathbf{G},t),\mathrm{H}_\Phi] &= i\Big((\mathbf{k}+\mathbf{G})^2+r\Big)\Phi_\mu(\mathbf{k}+\mathbf{G},t) \quad (3.6)\end{aligned}$$

Inserting both commutator resuls in equation (3.4) yields

$$\begin{aligned}\omega\big\langle\big\langle\pi_\mu(\mathbf{k}+\mathbf{G},t);\Phi_{\mu'}(\mathbf{k}'+\mathbf{G}',t')\big\rangle\big\rangle_\omega &= -i(2\pi)^2\delta(\mathbf{k}'+\mathbf{k})\delta_{-\mathbf{G}',\mathbf{G}}\delta_{\mu,\lambda}\delta_{t,t'} \\ &\quad+i\Big((\mathbf{k}+\mathbf{G})^2+r\Big)\big\langle\big\langle\Phi_\mu(\mathbf{k}+\mathbf{G},t);\Phi_{\mu'}(\mathbf{k}'+\mathbf{G}',t')\big\rangle\big\rangle_\omega \quad (3.7)\end{aligned}$$

where on the right hand side the initial wanted Green function appears. Puting all together we get an algebraic equation for the spin density wave propagator. Solving this equation yields

$$\big\langle\big\langle\Phi_\mu(\mathbf{k}+\mathbf{G},t);\Phi_\lambda(\mathbf{k}'+\mathbf{G}',t')\big\rangle\big\rangle_\omega = (2\pi)^2\delta(\mathbf{k}'+\mathbf{k})\delta_{-\mathbf{G}',\mathbf{G}}\delta_{\mu,\lambda}\mathcal{D}^{(0)}_{\mu\lambda}(\mathbf{k},\omega) \quad (3.8)$$

where for resons of simplicity the free spin density propagator $\mathcal{D}^{(0)}$ is introduced.

$$\mathcal{D}^{(0)}_{\mu\lambda}(\mathbf{k},\omega) := \sum_{\mathbf{G}}\frac{1}{(\mathbf{k}+\mathbf{G})^2+r-\epsilon\omega^2} \quad (3.9)$$

In computation of the conductivity below the free Propagator isn't only needed. The damping of the spin density waves has to be taken into account in the considered

model, which is ususally done via pertubation theory. The pertubation of the spin density waves is caused by the interaction with the electrons living on differant Fermi suffaces. Therefore the free electron propagator is needed. In the same way as the free spin density propagator is calculated the free electron propagator can be calculated. This handwork isn't done here explicitly. The result should be enough for the moment, which is

$$\left\langle\left\langle \Psi_\alpha(\mathbf{k}+\mathbf{G},t);\Psi^\dagger_\beta(\mathbf{k}'+\mathbf{G}',t')\right\rangle\right\rangle_\omega = (2\pi)^2\delta(\mathbf{k}'-\mathbf{k})\delta_{\mathbf{G}',\mathbf{G}}\delta_{\alpha,\beta}\mathcal{G}^{(0)}_{\alpha\beta}(\mathbf{k},\omega) \tag{3.10}$$

with

$$\mathcal{G}^{(0)}_{\alpha\beta}(\mathbf{k},\omega) = \sum_{\mathbf{G}} \frac{1}{\omega-\epsilon_\alpha(\mathbf{k}+\mathbf{G})}, \tag{3.11}$$

where $\alpha,\beta = \mathrm{a},\mathrm{b}$ and denotes the typ of electron with respect to the Fermi surfaces.

3.2 The damped spin density wave propagator

The full Green function of spin density waves is given by

$$\mathcal{D}_{\mu\lambda}(\mathbf{k},\omega) = -i\frac{\langle\mathcal{T}_t \mathrm{U}(\infty,-\infty)\Phi_\mu(\mathbf{k}+\mathbf{G},t)\Phi_\lambda(\mathbf{k}'+\mathbf{G}',t')\rangle_0}{\langle\mathcal{T}_t \mathrm{U}(\infty,-\infty)\rangle_0} \tag{3.12}$$

where the index 0 means that the expectation value is taken with respect to the unpertubated Hamiltonian. Thus the whole pertubation is only going into account throught the time evolution operator U, defined by

$$\mathrm{U}(t,t') = \exp\left(-i\int_{t'}^{t}\mathrm{d}t_1\,\mathrm{H}_{\mathrm{int}}(t_1)\right) \tag{3.13}$$

The time evolution operator is expanded into a series up to the second order. Like it is known from lectures about quantum field theory the denominator denotes the vacuum energy and can be canceled out with terms of the numerator. In quantum field theory language this means that only connected diagrams have to be investigated.

$$\begin{aligned}\mathcal{D}^{(1)}_{\mu\lambda}(\mathbf{k},\omega) = &-i\left\langle\mathcal{T}_t\Phi_\mu(\mathbf{k}+\mathbf{G},t)\Phi_\lambda(\mathbf{k}'+\mathbf{G}',t')\right\rangle_0 \\ &+(-i)^2\int_{-\infty}^{\infty}\mathrm{d}t_1\left\langle\mathcal{T}_t\mathrm{H}_\Phi(t_1)\Phi_\mu(\mathbf{k}+\mathbf{G},t)\Phi_\lambda(\mathbf{k}'+\mathbf{G}',t')\right\rangle_0 \\ &+(-i)^3\int_{-\infty}^{\infty}\mathrm{d}t_1\,\mathrm{d}t_2\left\langle\mathcal{T}_t\mathrm{H}_\Phi(t_2)\mathrm{H}_\Phi(t_1)\Phi_\mu(\mathbf{k}+\mathbf{G},t)\Phi_\lambda(\mathbf{k}'+\mathbf{G}',t')\right\rangle_0\end{aligned} \tag{3.14}$$

The expectation value in the first row correspondes to the free propagator. The term in the second row vanishes, which is easily seen by regarding the Hamiltonian. At first the expectation value of the fermionic and bosonic operators can be seperated.

Doing this an expectation value with three bosonic operators appear, which is zero. The term in the last row is the first non-disapearing contribution. Let us investigate this beast at first seperatly.

$$
\begin{aligned}
E^{(2)} := (-i)^3\lambda^2 \int_{-\infty}^{\infty} \mathrm{d}t_1\,\mathrm{d}t_2 \sum_{\mathbf{P}_1\mathbf{P}_2} \int_{\mathbf{p}_1}\int_{\mathbf{p}_2} \sum_{\mathbf{P}_3\mathbf{P}_4} \int_{\mathbf{p}_3}\int_{\mathbf{p}_4} \\
\times \left\langle \mathcal{T}_t \Phi_{\nu'}(\mathbf{p}_3-\mathbf{p}_4+\mathbf{P}_3-\mathbf{P}_4,t_2)\Phi_{\nu}(\mathbf{p}_1-\mathbf{p}_2+\mathbf{P}_1-\mathbf{P}_2,t_1)\Phi_{\mu}(\mathbf{k}+\mathbf{G},t)\Phi_{\lambda}(\mathbf{k}'+\mathbf{G}',t')\right\rangle_0 \\
\times \left\langle \mathcal{T}_t \Big(\Psi^{\dagger}_{\mathrm{a}}(\mathbf{p}_3+\mathbf{P}_3,t_2)\cdot\sigma_{\nu'}\cdot\Psi_{\mathrm{b}}(\mathbf{p}_4+\mathbf{P}_4,t_2) + \Psi^{\dagger}_{\mathrm{b}}(\mathbf{p}_3+\mathbf{P}_3,t_2)\cdot\sigma_{\nu'}\cdot\Psi_{\mathrm{a}}(\mathbf{p}_4+\mathbf{P}_4,t_2)\Big) \right. \\
\times \left. \Big(\Psi^{\dagger}_{\mathrm{a}}(\mathbf{p}_1+\mathbf{P}_1,t_1)\cdot\sigma_{\nu'}\cdot\Psi_{\mathrm{b}}(\mathbf{p}_2+\mathbf{P}_2,t_1) + \Psi^{\dagger}_{\mathrm{b}}(\mathbf{p}_1+\mathbf{P}_1,t_1)\cdot\sigma_{\nu'}\cdot\Psi_{\mathrm{a}}(\mathbf{p}_2+\mathbf{P}_2,t_1)\Big) \right\rangle_0
\end{aligned}
\tag{3.15}
$$

4 Memory-Matrix-Formalsim

4.1 Motivation

A physicist is always interested in the beaviour and time evolution of the observables of the investigates system. In the middle of the last century many physicists worked on the understanding and mathematical description of one physical process, the Brownian motion. On stochasical theory of these certain physical process is based on the Langevin equation

$$\frac{\partial}{\partial t}\mathrm{A}(t) - \mathrm{F}_{\mathrm{ex}}(x,t) + \gamma \cdot \mathrm{A}(t) = f(t), \tag{4.1}$$

where $\mathrm{A}(t)$ is some dynamical observable and $f(t)$ is a random force like white noise for example. The origin of the second term on the left hand side is some external force result from a coupling between $\mathrm{A}(t)$ and some external potential. The third term on the left hand side is a damping or friction term. Now let us assume it's possible to seperate equation (4.1) into two parts. The first part, called f_1, is a functional of the dynamical observable $\mathrm{A}(t')$, where $t_0 \leq t' \leq t$, so that this part is depending on the history of A. The second part f_2 should be depending on all other degrees of freedom. Now f_1 is expanded up to the linear order and all terms of higher order and the part f_2 are summerized to the quantity $F(t)$. The result is a linearized form of the Langevin equation

$$\frac{\partial}{\partial t}\mathrm{A}(t) = \int_{t_0}^{t} \mathrm{d}t'\, \mathcal{C}(t-t')\mathrm{A}(t') + F(t), \tag{4.2}$$

where $\mathcal{C}$ is a correlation function and $\mathrm{A}(t')$ is the deviation of the invariant part of the Hamiltonian. For large time scales the deviation should be vanish, so the time-integral over $\mathrm{A}(t')$ should be become zero. For simplification the origin of the time axis is moved to t_0. In general the Laplace transformation of a function is given by

$$\mathcal{L}\big\{\mathrm{A}(t)\big\} = \mathrm{A}(s) = \int_{0}^{\infty} \mathrm{d}t\, \mathrm{A}(t)e^{-st}. \tag{4.3}$$

Using the Laplace transformation equation (4.2) becomes a algebratic equation of motion. The solution of this equation is

$$\mathrm{A}(t) = \Xi(t) \cdot \mathrm{A}(0) + \mathrm{A}'(t) \qquad \text{with} \qquad \mathrm{A}'(t) = \int_{0}^{t} \mathrm{d}t'\, \Xi(t-t')F(t'), \tag{4.4}$$

where the function $\Xi(t)$ is defined by the Laplace transformation of $\Xi(s) = [s - \mathcal{C}(s)]^{-1}$ and $\mathcal{C}(s)$ is the Laplace transformtion of the correlation function $\mathcal{C}(t)$. The main result of equation (4.4) and the motivation for the following introduced memory-matrix-formalism is the splitting of the dynamical observable $\mathrm{A}(t)$ into two parts.
For the first term on the right hand side the only time-dependence is adverted through the correlation function $\mathcal{C}$, which is clear consider the definition of Ξ. This term included the linear contributions of $\mathrm{A}(t)$ by construction. These ones are the mostly important contributions to the time evolutaion of an observable, because they are secular. In contrast the second term on the right hand side is the convolution between the function $\Xi(t - t')$ and the function $\mathrm{F}(t')$. The latter summerize all the non-linear effects, fluctuations and intital transient processes, which are all effects with a small lifetimes in contrast with the secular effects. Therefore these effects shouldn't have large influences on the time evolution of an observable, always large time scales in mind.
Beside the physical interpretation a simple geometrical and mathematical one is very usefull. Let us assume a vector space ana the observable should be a vector in this vector space. Then the secular term is a projection on the A-axis and the non-secular term is aquivalent to a vector perpendicular to the A-axis. The memory-matrix-formalism take up this simple interpretation of equation (4.4) and put it in a general and exact form, so that it can be used classicaly and quantum mechanicaly.

4.2 Linear Response Theory

Before the derivation of the memory-matrix-formalism can be started some ground work is to do. This section begins with a short reminder of the kubo formula. After that the Kubo relaxation function are introduced and some important relations between there and the retarded susceptibility χ are derivated. In the last section finally the splitting of χ in a real and an imaginary part are dicussed.

4.2.1 Kubo formula

Consider a system in equilibrium represented by the Hamiltonian H_0. At an arbitrary time t' a pertubation is switched on, where the pertubation is given by the Hamiltonian $H_1 = -B \cdot F(t)$, so that $H(t) = H_0 + H_1$ is the full Hamiltonian. Thereby B is an operator by which the pertubation is coupled on the system and $F(t)$ is a function determining the time evolution of the pertubation. It is assumed that $F(t) = 0$ for $t < t'$ so that the system is in thermal equilibrium for all these times.
The physical interest is existed in the question how does an observable A react on the pertubation switched on at t'. The answer is given by the thermodynamical expectation value of the operator corresponding to the observable A

$$\langle \mathrm{A} \rangle (t) := \mathrm{Tr}\{\rho_{\mathrm{S}}(t)\mathrm{A}_{\mathrm{S}}\} = \mathrm{Tr}\{\rho_{\mathrm{I}}(t)\mathrm{A}_{\mathrm{I}}\}, \tag{4.5}$$

where the label S and I stand for the Schrdinger and Interaction picture, respectivily. The equality of the expectation value in the different representations is shown by the

invariance of the trace with resprect to cycle permutation. The transformation into the interaction picture is very usefull what we will see after the next step below. In quantum mechnics the time evolution of the density operator is determined by the von Neumann-equation.

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}}(t) = -\frac{i}{\hbar}[H(t), \rho_{\mathrm{S}}(t)] \quad \Leftrightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{I}}(t) = -\frac{i}{\hbar}[H_1, \rho_{\mathrm{I}}(t)] \tag{4.6}$$

The equation is also transformed into the interaction picture, which doesn't change the structure itself but the density operator deponds only on the Hamiltonian H_1 now. Integrating and using the boundary condition that the system is in thermal equilibrium at $t \to -\infty$ equation (4.6) is resulted in a integrable equation for the density operator.

$$\rho_{\mathrm{I}}(t) = \rho_0 + \frac{i}{\hbar}\int_{-\infty}^{t} \mathrm{d}t' \left[B_{\mathrm{I}}(t'), \rho_{\mathrm{I}}(t')\right] F(t') \tag{4.7}$$

Jet it is clear why the interection picture is used. The integrand depends on the Hamiltonian of the pertubation only in linear order which is a perfect starting point for a iterativ solution procedure. Starting with the zeroth order the density operator is trivially the density operator at thermical equilibrium. Inserting the zeroth order on the right hand side of equation (4.7) yield the first order of the density operator, a. s.ø. In linear response theory the iteration is cutted off after the first order. Inserting this in equation (4.5) and defining the dynamical susceptibility

$$\chi_{\mathrm{AB}}(t - t') = \frac{i}{\hbar}\Theta(t - t') \left\langle \left[A_{\mathrm{I}}(t - t'), B_{\mathrm{I}}(0)\right] \right\rangle_{H_0} \tag{4.8}$$

yield the Kubo formula

$$\delta \langle \mathrm{A}(t) \rangle := \langle \mathrm{A} \rangle (t) - \langle \mathrm{A}(t) \rangle_{H_0} \approx \int_{-\infty}^{\infty} \mathrm{d}t' \, \chi_{\mathrm{AB}}(t - t') F(t'), \tag{4.9}$$

where the label H_0 means that the expactation value is taken with respect to the unpertubated Hamiltonian. We see that the deviation of the observable A caused by the pertubation is given by the convolution of the dynamical suszeptibilty $\chi_{\mathrm{AB}}(t - t')$ and the time evolution function $F(t)$.

noch schöner schreiben

4.2.2 Kubo relaxation function

After a general equation for the deviation of an observable A from the equilibrium value was established, we want to investigate a certain kind of pertubation. Let us assume $F(t) = \Theta(-t) \cdot F \cdot e^{-s\tau}$ the time evolution function of a pertubation, which is switched on adiabatically at $t = -\infty$ and switched off at t. Inserting this in equation (4.9) and substituting $\tau = t - t'$ yield $\delta \langle \mathrm{A}(t) \rangle = \Phi_{AB}(t) \cdot F e^{st}$ with the Kubo relaxation function

$$\Phi_{\mathrm{AB}}(t) = \frac{i}{\hbar} \lim_{s \to 0} \int_{t}^{\infty} \mathrm{d}\tau \, \langle [\mathrm{A}_{\mathrm{I}}(\tau), \mathrm{B}_{\mathrm{I}}(0)] \rangle_0 \, e^{-s\tau}. \tag{4.10}$$

The arising Θ-distributions determine the lower limit of the intergal to t. For a more detailed derivation of the Kubo relaxation function see [Sch08] or [Sch06]. It's not really surprisingly that the Kubo relaxation function and the dynamical susceptibility are closely connected, because the first is derivated out of the latter one. However there exist three very important relations between them both, which are

1. $\chi_{\mathrm{AB}}(t) = -\Theta(t)\dfrac{\mathrm{d}}{\mathrm{d}t}\Phi_{\mathrm{AB}}(t)$ (4.11)

2. $\Phi_{\mathrm{AB}}(t=0) = \chi_{\mathrm{AB}}(\omega=0)$ (4.12)

3. $\Phi_{\mathrm{AB}}(\omega) = \dfrac{1}{i\omega}\big[\chi_{\mathrm{AB}}(\omega) - \chi_{\mathrm{AB}}(\omega=0)\big].$ (4.13)

The evidence of these tree relations are shown in the appendix A. For the later deviation of the memory-matrix-formalism it's more usefull to write the Kubo relaxation function in another, not so intuitivly form. The goal of the rewriting is to get the expectation value in a form with no commutator and to do this two identities are needed. The first one is

$$\big\langle\big[\mathrm{A}(t),\mathrm{B}(t')\big]\big\rangle = \frac{1}{Z}\,\mathrm{Tr}\big\{[\rho,\mathrm{A}(t)]\mathrm{B}(t')\big\}, \tag{4.14}$$

where the invariance of the expactation value with respect to cycling permutation is used. The second one is the Kubo-identity. Thereby the main idea is to used the analogy of the exponential functions to the time evolution of an operator.

$$\begin{aligned}
& i[\rho,\mathrm{A}(t)] = i\Big[\rho\mathrm{A}(t) - \mathrm{A}(t)\rho\Big] \\
\Leftrightarrow\ & i[\rho,\mathrm{A}(t)] = i\Big[\rho\mathrm{A}(t) - e^{-\beta H}e^{\beta\mathrm{H}}\mathrm{A}(t)e^{-\beta\mathrm{H}}\Big] \\
\Leftrightarrow\ & i[\rho,\mathrm{A}(t)] = -i\rho\int_0^\beta \mathrm{d}\lambda\,\frac{\mathrm{d}}{\mathrm{d}\lambda}e^{\lambda\mathrm{H}}\mathrm{A}(t)e^{-\lambda\mathrm{H}} \\
\Leftrightarrow\ & i[\rho,\mathrm{A}(t)] = -i\rho\int_0^\beta \mathrm{d}\lambda\,\Big[\mathrm{H}e^{i\tilde{\lambda}\mathrm{H}/\hbar}\mathrm{A}(t)e^{-i\tilde{\lambda}\mathrm{H}/\hbar} - e^{i\tilde{\lambda}\mathrm{H}/\hbar}\mathrm{A}(t)e^{-i\tilde{\lambda}\mathrm{H}/\hbar}\mathrm{H}\Big] \\
\Leftrightarrow\ & i[\rho,\mathrm{A}(t)] = -i\rho\int_0^\beta \mathrm{d}\lambda\,\Big[\mathrm{H},\mathrm{A}(t+\tilde{\lambda})\Big] \\
\Leftrightarrow\ & \frac{i}{\hbar}[\rho,\mathrm{A}(t)] = -\rho\int_0^\beta \mathrm{d}\lambda\,\dot{\mathrm{A}}(t+\tilde{\lambda}) = -\rho\int_0^\beta \mathrm{d}\lambda\,\dot{\mathrm{A}}(t-i\lambda\hbar),
\end{aligned} \tag{4.15}$$

where the derivation of A with respect to t is symbolized with the dot above A. For reasons of lucidity $\tilde{\lambda} = -i\lambda\hbar$ is introduced through the computation.

Now inserting equation (4.14) and (4.15) in the Kubo relaxation function (4.10) yield the searching form of the Kubo relaxation function, where the right hand side of the following compuation has to be integrated by parts, dedicated with PI.

$$\Phi_{\mathrm{AB}}(t) = \frac{i}{\hbar}\lim_{s\to 0}\int_t^\infty \mathrm{d}\tau\,\langle[\mathrm{A_I}(\tau),\mathrm{B_I}(0)]\rangle_0\, e^{-s\tau}$$

$$\overset{(4.14)}{\Leftrightarrow}\quad \Phi_{\mathrm{AB}}(t) = \frac{i}{\hbar}\lim_{s\to 0}\int_t^\infty \mathrm{d}\tau\,\frac{1}{Z_0}\,\mathrm{Tr}\{[\rho_0,\mathrm{A_I}(\tau)]\mathrm{B_I}(0)\}e^{-s\tau}$$

$$\overset{(4.15)}{\Leftrightarrow}\quad \Phi_{\mathrm{AB}}(t) = -\lim_{s\to 0}\int_0^\beta \mathrm{d}\lambda\int_t^\infty \mathrm{d}\tau\,\left\langle \dot{\mathrm{A}}_{\mathrm{I}}(\tau-i\lambda\hbar)\mathrm{B_I}(0)\right\rangle_0 e^{-s\tau}$$

$$\overset{\mathrm{PI}}{\Leftrightarrow}\quad \Phi_{\mathrm{AB}}(t) = -\lim_{s\to 0}\int_0^\beta \mathrm{d}\lambda\left\langle\left[\,\mathrm{A_I}(\tau-i\lambda\hbar)e^{-s\tau}\Big|_t^\infty + s\int_t^\infty \mathrm{d}\tau\,\dot{\mathrm{A}}_{\mathrm{I}}(\tau-i\lambda\hbar)e^{-s\tau}\right]\mathrm{B_I}(0)\right\rangle_0$$

$$\Leftrightarrow\quad \Phi_{\mathrm{AB}}(t) = \int_0^\beta \mathrm{d}\lambda\,\langle\mathrm{A_I}(t-i\lambda\hbar)\mathrm{B_I}(0)\rangle_0 = \int_0^\beta \mathrm{d}\lambda\,\langle\mathrm{A_I}(t)\mathrm{B_I}(i\lambda\hbar)\rangle_0 \tag{4.16}$$

Later we will see that the scalar product defining at the memory-matrix-formalsim has a similar structure as this form of the kubo relaxation function. This provide the oppertunity to transform the correlation function out of the language of the memory-matrix-formalism into the Kubo relaxation function, which in turn provide the oppertunity to compute the correlation function pertubativly. However the should be enough for the fist time. Later the transformation is discussed in more detail.

4.2.3 Kramer-Kronig-relation

All experiences of a human life demonstating that an incident is always bevor the reaction of a system to it. In physics this is called causality. Causality and the condition that the dynamical sysceptibilty $\chi_{\mathrm{AB}}(t-t')$ is zero for times t smaller than t' are aquivalent assertions. It's often usefull to work in the frequency space why we want to investigate what causality means in Fourier space. Consider the Fourier transformation $\chi_{\mathrm{AB}}(\omega)$ where ω is replaced by the complex number $\omega' + i\omega''$. For reasons of simplification the origin of the time axis is set to t'.

$$\chi_{\mathrm{AB}}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, e^{i(\omega'+i\omega'')t}\chi_{\mathrm{AB}}(t) \tag{4.17}$$

The integral converge if the exponential functions decrease to zero. Causality in time space yield $t > 0$ and because of that $e^{-\omega'' t}$ decreases only for $\omega'' > 0$ to zero. In summary causality in Fourier space means that the susceptibility is holomorphic in the upper complex plane ($\mathrm{Im}\{\omega\} = \omega'' > 0$).

Cauchy's integral theorem offers us the oppertunity to express the Fourier transformed susceptibility by a contour integral, where the arbitrary contour Γ has to be taken in the upper complex plane or more presicly in the regime where $\chi_{\mathrm{AB}}(\omega)$ is holomorphic.

$$\chi_{\mathrm{AB}}(\omega) = \frac{1}{2\pi i} \oint_{\Gamma} \mathrm{d}\zeta \, \frac{\chi_{\mathrm{AB}}(\zeta)}{\zeta - \omega} \tag{4.18}$$

link to figure of contour

Our choice of the contour is some which goes from minus infity to infinity along the real part axis. Along a semi circle in the upper half plane the contour is closed, see figure . For reason of convergency the contour along the real part axis is moved in the upper half plane infinitesimal indicated with $i\eta$ where $\eta \to 0$ is implicated.
The contribution of the semi circle vanishs because $\chi_{\mathrm{AB}}(\omega)$ decreasing very fast for large values of ω is assumed. Only a integral along the real part axis survives which can be evaluated by formally writing $\frac{1}{x+i\eta} = \mathrm{PV}\frac{1}{x} - i\pi\delta(x)$ where PV stands for taking the principal value.

$$\begin{aligned}
& \chi_{\mathrm{AB}}(\omega) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \mathrm{d}\omega' \, \frac{\chi_{\mathrm{AB}}(\omega')}{\omega' - \omega - i\eta} \\
\Leftrightarrow \quad & \chi_{\mathrm{AB}}(\omega) = \frac{1}{2\pi i} \left[\mathrm{PV} \int_{-\infty}^{\infty} \mathrm{d}\omega' \, \frac{\chi_{\mathrm{AB}}(\omega')}{\omega' - \omega} + i\pi \int_{-\infty}^{\infty} \mathrm{d}\omega' \, \chi_{\mathrm{AB}}(\omega')\delta(\omega' - \omega) \right] \\
\Leftrightarrow \quad & \chi_{\mathrm{AB}}(\omega) = -\frac{i}{\pi} \mathrm{PV} \int_{-\infty}^{\infty} \mathrm{d}\omega' \, \frac{\mathrm{Re}\{\chi_{\mathrm{AB}}(\omega')\} + i\,\mathrm{Im}\{\chi_{\mathrm{AB}}(\omega')\}}{\omega' - \omega} \\
\Leftrightarrow \quad & \chi_{\mathrm{AB}}(\omega) = \frac{1}{\pi} \mathrm{PV} \int_{-\infty}^{\infty} \mathrm{d}\omega' \left[\frac{\mathrm{Im}\{\chi_{\mathrm{AB}}(\omega')\}}{\omega' - \omega} - i \frac{\mathrm{Re}\{\chi_{\mathrm{AB}}(\omega')\}}{\omega' - \omega} \right]
\end{aligned} \tag{4.19}$$

In the second step one right hand side the complex susceptibility is written explicitly by her real and imaginary part. Nothing keep us from doing this on the left side hand too and compare the real and imaginary parts of both sides respectively.

$$\mathrm{Re}\{\chi_{\mathrm{AB}}(\omega)\} = \frac{1}{\pi} \mathrm{PV} \int_{-\infty}^{\infty} \mathrm{d}\omega' \, \frac{\mathrm{Im}\{\chi_{\mathrm{AB}}(\omega')\}}{\omega' - \omega} \tag{4.20}$$

$$\mathrm{Im}\{\chi_{\mathrm{AB}}(\omega)\} = -\frac{1}{\pi} \mathrm{PV} \int_{-\infty}^{\infty} \mathrm{d}\omega' \, \frac{\mathrm{Re}\{\chi_{\mathrm{AB}}(\omega')\}}{\omega' - \omega} \tag{4.21}$$

These two relations are called Kramer-Kronig-relation. They take the real and imaginary part of the a function, here the susceptibility, in a very usefull relation. In the later computation them are used to compute the Green function on the real axis out off the Green function on the imaginary axis and vice versa. This is always needed if analytical continuation isn't possible, which is the case considering damping in the Green function.

4.2.4 Spectral representation

In section 4.2.1 the dynamical susecptibility χ_{AB} is introduced by deviated the Kubo-formula (4.9). The evolution of a system switching on a pertubation is described by this function. Now the processes starting because of the pertubation can be classified into two types one the one hand in dissipative prozesses and on the other hand in non-dissipative prozesses. In the following computation dissipative processes are investigated. The dissipative susceptibility of the form

Why do we chose this typ of $\chi''(t-t')$

$$\chi''_{\mathrm{AB}}(t-t') = \frac{1}{2\hbar}\left\langle\left[\mathrm{A}(t),\mathrm{B}(t')\right]\right\rangle \tag{4.22}$$

is considered, where the operators A and B are two Hermitian operators. The property

$$\left(\chi''_{\mathrm{AB}}(t-t')\right)^* = -\chi''_{\mathrm{AB}}(t-t') \tag{4.23}$$

is trivially shown because the commutator of two Hermitian operators is anti-Hermitian. The Fourier transformation of $\chi''_{\mathrm{AB}}(t-t')$ is given by equation (4.17). Notice that in the following computation the frequency ω isn't splitted into real and imaginary part like it's done in equation (4.17). Starting our calculation multipling equation (4.8) and integrating over time t.

$$\begin{aligned}
&\chi_{\mathrm{AB}}(t) = \frac{i}{\hbar}\Theta(t)\left\langle[\mathrm{A}(t),\mathrm{B}(0)]\right\rangle = 2i\Theta(t)\chi''_{\mathrm{AB}}(t)\\
\Leftrightarrow\ &\chi_{\mathrm{AB}}(\omega) = 2i\int_{-\infty}^{\infty}\mathrm{d}t\, e^{i\omega t}\Theta(t)\chi''_{\mathrm{AB}}(t)\\
\Leftrightarrow\ &\chi_{\mathrm{AB}}(\omega) = -\frac{1}{\pi}\lim_{\eta\to 0}\int_{-\infty}^{\infty}\mathrm{d}\omega'\,\frac{1}{\omega'+i\eta}\int_{-\infty}^{\infty}\mathrm{d}t\, e^{i(\omega-\omega')t}\chi''_{\mathrm{AB}}(t)\\
\Leftrightarrow\ &\chi_{\mathrm{AB}}(\omega) = \frac{1}{\pi}\lim_{\eta\to 0}\int_{-\infty}^{\infty}\mathrm{d}\omega'\,\frac{\chi''_{\mathrm{AB}}(\omega')}{\omega'-\omega-i\eta}\\
\Leftrightarrow\ &\chi_{\mathrm{AB}}(\omega) = \frac{1}{\pi}\mathrm{PV}\int_{-\infty}^{\infty}\mathrm{d}\omega'\,\frac{\chi''_{\mathrm{AB}}(\omega')}{\omega'-\omega} + i\int_{-\infty}^{\infty}\mathrm{d}\omega'\,\delta(\omega'-\omega)\chi''_{\mathrm{AB}}(\omega')\\
\Leftrightarrow\ &\chi_{\mathrm{AB}}(\omega) = \chi'_{\mathrm{AB}}(\omega) + i\chi''_{\mathrm{AB}}(\omega)
\end{aligned} \tag{4.24}$$

where in the second step the following definition of the Θ-function is used.

$$\Theta_\eta(t) = i\lim_{\eta\to 0}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{2\pi}\frac{e^{-i\omega' t}}{\omega'+i\eta} \tag{4.25}$$

In equation (4.24) we see that the dynamical susceptibility $\chi_{\mathrm{AB}}(\omega)$ is seperated into two functions $\chi'_{\mathrm{AB}}(\omega)$ and $\chi''_{\mathrm{AB}}(\omega)$, where the latter is the dissipative susceptibility

defined at the beginning of this section in (4.22). Equation (4.24) is general and for any susceptibility valid. Assuming the dissipative susceptibility is a real number, than this is also valid for $\chi'_{\mathrm{AB}}(\omega)$ and the both functions $\chi'_{\mathrm{AB}}(\omega)$ and $\chi''_{\mathrm{AB}}(\omega)$ are real and imaginary part of $\chi_{\mathrm{AB}}(\omega)$, respectivily.

4.3 Deviation of the Memory-Matrix-Formalism

After this short reminder of the linear response theorie and the investigation of the dynamical susceptibility the groundwork for the deviation of the memory-matrix-formalism is done and we want to go back. This chapter started by splitting a dynamical observable into two parts, a secular and a non-secular one. The systematical evolution of observables is determined by the secular part. Looking at the system after a pertubation is switched off for a long time this secular part is depended the evolution. Furthermore all processes with a short lifetime or small quantity compared with the linear term in pertubation series are summerized in the non-secular part. This result is the starting point to a simple geometrical interpretation in a vector space, which we want define in the following.
Therefore the mathematical framework in quantum mechanics has to be clear, why a short review based on [Aud05] is given in the following. A d-dimensional Hilbert-space is mormaly the mathematical working area in quantum mechanics. This vector space is linear, complex and has a defined scalar product. The vectors $|\phi\rangle$, usually denoted in the Dirac-notation, are identified with all possible states for the system. Because the man is always interested in observables, linear operators are defined in the Hilbert-space where the eigenvalues of them conform to the observables. Defining the dyad product $\sum_i |i\rangle\langle i|$ it's not hard to see that any linear operator occupies a dyad decomposition

$$\mathrm{A} = \sum_{i,j} |i\rangle\langle i| \,\mathrm{A}\, |j\rangle\langle j| = \sum_{i,j} \mathrm{A}_{ij} \,|i\rangle \,\langle j|\,, \tag{4.26}$$

where $\mathrm{A}_{ij} := \langle i| \,\mathrm{A}\, |j\rangle$ is a matrix element of the linear operator. The dyad product of an operator is now used to introduce a new vector space of all linear operators acting on the d-dimensional Hilbert-space which is called the Liouville-space $\mathbb{L}$ or operator space.
The Liouville-space is linear and complex vector space equally to the Hilbert-space. The difference between both are the vectors or elements living in the space. In the Liouville-space the vectors are linear operators $\mathrm{A}, \mathrm{B}, \ldots$ which are acting on some Hilbert-space. In other words this means that the dyad decomposition of an vector in the d-dimensional Hilbert-space is the new vector in the Liouville-space. So some vector in the Liouville-space is notated as

$$\big|\mathrm{A}\big) := \sum_{ij}^{d} \mathrm{A}_{ij} \big||i\rangle\langle j|\big) \tag{4.27}$$

Similiarly to the quantum mechanic the Dirac notation is used with the difference that round brackets are used instead of angle brackets to distinghush both spaces. Out of the definition (4.27) it's clear, that the basis in the Liouville-space is build by the d^2 dyads of the Hilbert-space . The dimension of the Liouville-space is therefore d^2. Equally to a Hilbert-space there are many other oppertunities to choose the basis in the Liouville space $\mathbb{L}$, but the defintion in (4.27) should be the one we are working with.
In the following the basis of our Liouville space is denoted with $\{|\mathrm{A_i})\}$ where $i = 1, 2, 3, \ldots, n$ and A_i is an operator. The corresponding basis of the dual space is given by $\{(\mathrm{A_i}|\}$, similarily to the Hilbert space. The last needed element of our Liouville space is a scalar product which fullfills the three condictions

1. $\big(\mathrm{A}_i\big|\mathrm{A}_j\big) = \big(\mathrm{A}_j\big|\mathrm{A}_i\big)^*$ (4.28)
2. $\big(\mathrm{A}_i\big|\mathrm{B}\big) = c_1\big(\mathrm{A}_i\big|\mathrm{A}_j\big) + c_2\big(\mathrm{A}_i\big|\mathrm{A}_k\big)$

   where $\mathrm{B} = c_1\mathrm{A_j} + c_2\mathrm{A_k}$ and $c_1, c_2 \in \mathbb{C}$ (4.29)
3. $\big(\mathrm{A}_i\big|\mathrm{A}_i\big) \geq 0$ where equallity is fulfilled if $\mathrm{A}_i = 0$. (4.30)

Beside these the choice of the scalar product is arbitrary. For the moment let us choose

$$\big(\mathrm{A}_i(t)\big|\mathrm{A}_j(t')\big) = \frac{1}{\beta}\int_0^\beta \mathrm{d}\lambda \left\langle \mathrm{A}_i^\dagger(t)\mathrm{A}_j(t' + i\lambda\hbar)\right\rangle \tag{4.31}$$

as our scalar product, where the normal time evolution of an operator $\mathrm{A}_i(t) = e^{i\mathrm{H}t/\hbar}\mathrm{A}_i(0)e^{-i\mathrm{H}t/\hbar}$ is valid, so that $\mathrm{A}_i(i\lambda\hbar) = e^{-\lambda\mathrm{H}}\mathrm{A}_i(0)e^{\lambda\mathrm{H}}$ can be used. A more detailed discussion of the choice of the sclar product is given at the end of this chapter in . Now we have to proof if the condictions are fullfilled by the choice of our scalar product.
Let's get started with the second one because it's easily shown transforming the expactation value into the trace representation and then using the properties of the trace.

link to the section where the scalar product is motivated

maybe the computation isn't needed here

$$\begin{aligned}\big(\mathrm{A}_i(t)\big|\mathrm{B}(t')\big) &= \frac{1}{\beta}\int_0^\beta \mathrm{d}\lambda\, \frac{1}{Z}\,\mathrm{Tr}\Big\{\rho\mathrm{A}_i^\dagger(t)\Big[c_1\mathrm{A}_j(t' + i\lambda\hbar) + c_2\mathrm{A}_k(t' + i\lambda\hbar)\Big]\Big\} \\ \Leftrightarrow\ \big(\mathrm{A}_i(t)\big|\mathrm{B}(t')\big) &= c_1\big(\mathrm{A}_i(t)\big|\mathrm{A}_j(t')\big) + c_2\big(\mathrm{A}_i(t)\big|\mathrm{A}_k(t')\big)\end{aligned} \tag{4.32}$$

The first and third condition can be shown by transforming the scalar product in the spectral representation. Therefore the trace is writen explicitly as a sum over all states and the unity operator written as a sum over all projection operators are inserted between both operators A_i and A_j.

$$\big(\mathrm{A}_i(t)\big|\mathrm{A}_j(t')\big) = \frac{1}{\beta\cdot Z}\int_0^\beta \mathrm{d}\lambda \sum_{n,m} \langle n|\, e^{-\beta\mathrm{H}}\mathrm{A}_i^\dagger(t)\,|m\rangle\,\langle m|\, e^{-\lambda\mathrm{H}}\mathrm{A}_j(t')e^{\lambda\mathrm{H}}\,|n\rangle$$

$$\Leftrightarrow \quad \big(\mathrm{A}_i(t)\big|\mathrm{A}_j(t')\big) = \frac{1}{\beta\cdot Z}\sum_{n,m}\langle n|\mathrm{A}_i^\dagger(t)|m\rangle\ \langle m|\mathrm{A}_j(t')|n\rangle\, e^{-\beta E_n}\int_0^\beta \mathrm{d}\lambda\, e^{\lambda(E_n-E_m)}$$

$$\Leftrightarrow \quad \big(\mathrm{A}_i(t)\big|\mathrm{A}_j(t')\big) = \frac{1}{\beta\cdot Z}\sum_{n,m}\langle n|\mathrm{A}_i^\dagger(t)|m\rangle\ \langle m|\mathrm{A}_j(t')|n\rangle\, \frac{e^{-\beta E_m}-e^{-\beta E_n}}{E_n-E_m} \tag{4.33}$$

The complex conjugated of the expectation value in the Liouville space is considered and using $\langle n|\mathrm{A}_j^\dagger(t)|m\rangle^* = \langle m|\mathrm{A}_j(t)|n\rangle$ let us find instantly the first condition. Notice that on the right hand side of equation (4.33) only the expactation values are complex numbers. For them the complex conjugation yields

$$\Big(\ \langle n|\mathrm{A}_i^\dagger(t)|m\rangle\ \langle m|\mathrm{A}_j(t')|n\rangle\ \Big)^* = \langle n|\mathrm{A}_j^\dagger(t')|m\rangle\ \langle m|\mathrm{A}_i(t)|n\rangle \tag{4.34}$$

and inserting back $(\mathrm{A}_i(t)|\mathrm{A}_j(t'))^*$ is exactly the same as (4.33). Proofing the third condition it has to be set $\mathrm{A}_j(t') = \mathrm{A}_i(t)$ in equation (4.33), which one the right hand side results in

$$\big(\mathrm{A}_i(t)\big|\mathrm{A}_i(t)\big) = \frac{1}{\beta\cdot Z}\sum_{n,m}\big|\ \langle m|\mathrm{A}_i(t)|n\rangle\ \big|^2\frac{e^{-\beta E_m}-e^{-\beta E_n}}{E_n-E_m}. \tag{4.35}$$

It's clear that the squared expactation value is always non-negative. The friction is positive too, which is easily seen by proofing the two cases $E_n > E_m$ and $E_n < E_m$. Therefore the expactation value $\big(\mathrm{A}_i(t)\big|\mathrm{A}_i(t)\big) \geq 0$ and equallity is only possible if $\mathrm{A}_i = 0$. All three conditions are well proofed and the chosen scalar product is really one's. At this point all the mathematical ground work is done, we know how the vectors in the Liouville space looks like and we have a well defined scalar product.
The goal of every physical theory is to describe the measurment results. Typically in statistical or quantum mechanics this is done by correlations functions. So our goal is it now to find a useable expression for correlation functions in our new Liouville space. The natural starting point describing the time evolution of an operator A_i is in quantum mechanics the Heisenberg equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A}_i(t) = \dot{\mathrm{A}}_i(t) = \frac{i}{\hbar}[\mathrm{H},\mathrm{A}_i(t)] = i\mathrm{L}\mathrm{A}_i(t) \tag{4.36}$$

where the operators are in the Heisenberg representation and the Hermitian Liouville operator defined by his action on an operator $\mathrm{L} = \hbar^{-1}[\mathrm{H},\bullet]$ is introduced. The formal solution of equation (4.36) is

$$\mathrm{A}_i(t) = e^{it\mathrm{L}}\mathrm{A}_i(0) = e^{it\mathrm{H}/\hbar}\mathrm{A}_i(0)e^{-it\mathrm{H}/\hbar}. \tag{4.37}$$

Have to convince me that it is really so easy.

In the second step only the definition of the Liouville operator and some algebraic transformations are used. In this notation it is more clearly that the time evolution of an operator is given by the Liouville operator. The same result is obtained in the Liouville space if the Liouville operator is acting on the basis vectors. This isn't really

surprisingly because only the dyad product has to be insert in equation (4.36), which results in

$$\big|\dot{\mathrm{A}}_i(t)\big) = \frac{i}{\hbar}\big|[\mathrm{H}, \mathrm{A}_i(t)]\big) = i\mathrm{L}\big|\mathrm{A}_i(t)\big) \tag{4.38}$$

for the equation of motion in the Liouville space and there fromal solution

$$\big|\mathrm{A}_i(t)\big) = e^{it\mathrm{L}}\big|\mathrm{A}_i(0)\big). \tag{4.39}$$

Beside the Liouville operator one more operator has to be introduced for the deviation of the correlation function, called the projection operator. Therefore let us define a set of operators $\{\mathrm{C}_i\}$, where the choice of these operators are different depending on the investigated system and correlation function. In the later computation of a certain problem the choice of the operators is discussed in more detail. For the moment it's sufficient to know that the set of operators exists. Directly follwing out the definition of the projection operator in quantum mechanics the projection operator in the Liouville space looks like

$$\mathrm{P} = \sum_{i,j} \big|\mathrm{C}_i(0)\big)\big(\mathrm{C}_i(0)\big|\mathrm{C}_j(0)\big)^{-1}\big(\mathrm{C}_j(0)\big|. \tag{4.40}$$

The action of P on some vector $\big|\mathrm{A}(t)\big)$ in the Liouville space yields the parallel components to the chosen operators C_i, which is the projection from $\big|\mathrm{A}(t)\big)$ at the vector subspace spanned by C_i. The corresponding vertical component of $\big|\mathrm{A}(t)\big)$ with respect to the operators C_i is given by $\mathrm{Q} = 1 - \mathrm{P}$, which is the projection out of the vector subspace. Naturally the projection operator is fullfilled the two properties $\mathrm{P}^2 = \mathrm{P}$ and $\mathrm{PQ} = \mathrm{QP} = 0$ of a projection operator, which follows immediately from the definition of P.
After the deviation of the time evolution of an operator and the projection operator in Liouville space the correlation function can be defined as

$$\mathcal{C}_{ij}(t) = \big(\mathrm{A}_i(t)\big|\mathrm{A}_j(0)\big) \overset{(4.31)}{=} \frac{1}{\beta}\int_0^\beta \mathrm{d}\lambda \left\langle \mathrm{A}_i^\dagger(t)\mathrm{A}_j(i\lambda\hbar)\right\rangle \tag{4.41}$$

where in the last step the definition of the scalar product is only inserted. Comparing equation (4.41) with (4.16) our choice of the correlation function is more clear. The defined correlation function is proportional to the Kubo relaxation function, which how we learned in section 4.2.2 describes the system's reaction on a switched off pertubation. For $t = 0$ the correlation function is also proportional to the Fourier transformated susebtibility

write more to the goal of the memory matrix formalsim

$$\mathcal{C}_{ij}(t=0) = \frac{1}{\beta}\Phi_{ij}(t=0) = \frac{1}{\beta}\chi_{ij}(\omega = 0), \tag{4.42}$$

which directly results from equation (4.12). Equation (4.39) is used to bring the time evolution of the correlation function in more suitable expression

$$\mathcal{C}_{ij}(t) = \big(\mathrm{A}_i(0)\big|\mathrm{A}_j(-t)\big) = \big(\mathrm{A}_i(0)\big|e^{-it\mathrm{L}}\big|\mathrm{A}_j(0)\big), \tag{4.43}$$

which opens the possibility for using the Laplace transformation. Instead of the definition in equation (4.3) here a form of the Laplace transformation is used where s is substituted by $-i\omega$ which is nothing else a rotation of the definition regime by $\frac{\pi}{2}$. Multipling the last equation with $e^{i\omega t}$ and intgrate from zero to infinty with resprct to t yields

$$\mathcal{C}_{ij}(\omega) = \big(\mathrm{A}_i\big| \int_0^\infty \mathrm{d}t\, e^{i(\omega-\mathrm{L})t} \big|\mathrm{A}_j\big) = \big(\mathrm{A}_i\big| \frac{i}{\omega - \mathrm{L}} \big|\mathrm{A}_j\big), \tag{4.44}$$

where for reasons of clarity and comprehensibility from now on the argument $t = 0$ isn't anymore written at the basis vectors. Now the relation $\mathrm{L} = \mathrm{LQ} + \mathrm{LP}$ which follows immediatly by using the definition of P and Q and the identity $(\mathrm{X}+\mathrm{Y})^{-1} = \mathrm{X}^{-1} - \mathrm{X}^{-1}\mathrm{Y}(\mathrm{X}+\mathrm{Y})^{-1}$ is used to simplify the correlation function, where $\mathrm{X} = \omega - \mathrm{LQ}$ and $\mathrm{Y} = -\mathrm{LP}$.

$$\begin{aligned} & \mathcal{C}_{ij}(\omega) = \big(\mathrm{A}_i\big| \frac{i}{\omega - \mathrm{LQ} - \mathrm{LP}} \big|\mathrm{A}_j\big) \\ \Leftrightarrow\ & \mathcal{C}_{ij}(\omega) = \big(\mathrm{A}_i\big| \frac{i}{\omega - \mathrm{LQ}} \big|\mathrm{A}_j\big) + \big(\mathrm{A}_i\big| \frac{1}{\omega - \mathrm{LQ}} \mathrm{LP} \frac{i}{\omega - \mathrm{L}} \big|\mathrm{A}_j\big) \end{aligned} \tag{4.45}$$

The both terms on the right hand side are considered seperatly starting with the first one. The fraction can be written as the geometric series assuming $\frac{\mathrm{LQ}}{\omega} < 1$, which means that the pertubation is small compared to other quantities in the system.

Ask Jörg if this explanation is correct

$$\frac{i}{\omega - \mathrm{LQ}} = \frac{i}{\omega}\left[1 + \frac{\mathrm{LQ}}{\omega} + \Big(\frac{\mathrm{LQ}}{\omega}\Big)^2 + \ldots\right] \tag{4.46}$$

Each term of the series in the squard brackets acting on the operator $\big|\mathrm{A}_j\big)$. Remember this is the operator at time $t = 0$, which means that no vertical component exists and therefore $\mathrm{Q}\big|\mathrm{A}_j\big) = 0$. Every term except the first one conatins an operator Q, so the first term of the correlation function yields

$$\big(\mathrm{A}_i\big| \frac{i}{\omega - \mathrm{LQ}} \big|\mathrm{A}_j\big) = \frac{i}{\omega}\big(\mathrm{A}_i\big|\mathrm{A}_j\big) = \frac{i}{\omega}\mathcal{C}_{ij}(0). \tag{4.47}$$

At the second term only the back term is considered. Here only the explicit expression of the propagator is inserted, which yields the definition of the Laplace transformed correlation function.

$$\mathrm{P}\frac{i}{\omega - \mathrm{L}}\big|\mathrm{A}_j\big) = \sum_{k,l} \big|\mathrm{C}_k\big)\big(\mathrm{C}_k\big|\mathrm{C}_l\big)^{-1}\big(\mathrm{C}_l\big|\frac{i}{\omega - \mathrm{L}}\big|\mathrm{A}_j\big) = \sum_{k,l} \big|\mathrm{C}_k\big)\mathcal{C}^{-1}_{kl}(0)\mathcal{C}_{lj}(\omega) \tag{4.48}$$

Inserting back both simplifications the correlation function is get the formal expression

$$\mathcal{C}_{ij}(\omega) = \frac{i}{\omega}\mathcal{C}_{ij}(0) + \sum_{k,l} \big(\mathrm{A}_i\big|\frac{1}{\omega - \mathrm{LQ}}\mathrm{L}\big|\mathrm{C}_k\big)\mathcal{C}^{-1}_{kl}(0)\mathcal{C}_{lj}(\omega). \tag{4.49}$$

The form of the resulting correlation function is now much more useable beside the fraction in the expectation value, but this one can be simplified too. Therefore the fraction is multiplied with ω and the Null $\mathrm{LQ} - \mathrm{LQ}$ is added in the numinator.

$$\frac{\omega}{\omega - \mathrm{LQ}} = \frac{\omega - \mathrm{LQ} + \mathrm{LQ}}{\omega - \mathrm{LQ}} = 1 + \frac{\mathrm{LQ}}{\omega - \mathrm{LQ}} \tag{4.50}$$

Multipling with ω and inserting the rearrangement of the fraction yields an algebratic equation for the correlation function.

$$\begin{aligned}
&\omega \mathcal{C}_{ij}(\omega) = i\mathcal{C}_{ij}(0) + \sum_{k,l} \big(\mathrm{A}_i\big|\frac{\omega}{\omega - \mathrm{LQ}}\mathrm{L}\big|\mathrm{C}_k\big)\mathcal{C}^{-1}_{kl}(0)\mathcal{C}_{lj}(\omega) \\
\Leftrightarrow\ &\omega \mathcal{C}_{ij}(\omega) = i\mathcal{C}_{ij}(0) + \sum_{k,l} \big(\mathrm{A}_i\big|1 + \frac{\mathrm{LQ}}{\omega - \mathrm{LQ}}\mathrm{L}\big|\mathrm{C}_k\big)\mathcal{C}^{-1}_{kl}(0)\mathcal{C}_{lj}(\omega) \\
\Leftrightarrow\ &\omega \sum_l \delta_{il}\mathcal{C}_{lj}(\omega) = i\frac{1}{\beta}\chi_{ij}(0) + \sum_l \Big[\Omega_{il} - i\Sigma_{il}(\omega)\Big]\mathcal{C}_{lj}(\omega) \\
\Leftrightarrow\ &\sum_l \Big[\omega\delta_{il} - \Omega_{il} + i\Sigma_{il}(\omega)\Big]\mathcal{C}_{lj}(\omega) = i\frac{1}{\beta}\chi_{ij}(0)
\end{aligned} \tag{4.51}$$

where equation (4.12) is used and the abbreviations

$$\Omega_{il} := \beta \sum_k \big(\mathrm{A}_i\big|\mathrm{L}\big|\mathrm{C}_k\big)\chi^{-1}_{kl}(0) \quad \text{and} \quad \Sigma_{il}(\omega) := i\beta \sum_k \big(\mathrm{A}_i\big|\frac{\mathrm{LQ}}{\omega - \mathrm{LQ}}\mathrm{L}\big|\mathrm{C}_k\big)\chi^{-1}_{kl}(0) \tag{4.52}$$

are inserted. Equation (4.51) is the wanted algebraic equation for the correlation function. The sums over k and l are originated from the utilization of the projection operator. Therefore each sum is a sum over all operators included in the set of operators $\{\mathrm{C}_i\}$. The indicies i and j have to be chosen out of this set too, so that equation (4.51) yields n^2 algebraic equations if n is the number of operators in $\{\mathrm{C}_i\}$.
It's useful for a our later computation to write the even defined abbreviations in another form. For Ω_{il} not much work is to do, because we use only equation (4.38), so that

$$\Omega_{il} = i\beta \sum_k \big(\dot{\mathrm{A}}_i\big|\mathrm{C}_k\big)\chi^{-1}_{kl}(0). \tag{4.53}$$

For the rearrangement of the second abbreviation in a first step equation (4.38) is used too and in a second step the fraction is written as the geometric series. Then in every term the relation $\mathrm{Q} = \mathrm{Q}^2$ is inserted, where the proof is an easy finger excercise. After factorizing one Q to each vector operator the geometric series is written back as a fraction.

$$\Sigma_{il}(\omega) = \frac{i\beta}{\omega} \sum_k \big(\dot{\mathrm{A}}_i\big|\mathrm{Q}\Big[1 + \frac{\mathrm{LQ}}{\omega} + \Big(\frac{\mathrm{LQ}}{\omega}\Big)^2 + \ldots\Big]\big|\dot{\mathrm{C}}_k\big)\chi^{-1}_{kl}(0)$$

$$\Leftrightarrow \Sigma_{il}(\omega) = \frac{i\beta}{\omega}\sum_k \left(\dot{\mathrm{A}}_i\middle|\mathrm{Q}^2 + \frac{\mathrm{Q}^2\mathrm{L}\mathrm{Q}^2}{\omega} + \frac{\mathrm{Q}^2\mathrm{L}\mathrm{Q}^2\mathrm{L}\mathrm{Q}^2}{\omega^2} + \ldots\middle|\dot{\mathrm{C}}_k\right)\chi^{-1}_{kl}(0)$$

$$\Leftrightarrow \Sigma_{il}(\omega) = \frac{i\beta}{\omega}\sum_k \left(\dot{\mathrm{A}}_i\middle|\mathrm{Q}\left[1 + \frac{\mathrm{QLQ}}{\omega} + \left(\frac{\mathrm{QLQ}}{\omega}\right)^2 + \ldots\right]\mathrm{Q}\middle|\dot{\mathrm{C}}_k\right)\chi^{-1}_{kl}(0)$$

$$\Leftrightarrow \Sigma_{il}(\omega) = i\beta\sum_k \left(\dot{\mathrm{A}}_i\middle|\mathrm{Q}\frac{1}{\omega - \mathrm{QLQ}}\mathrm{Q}\middle|\dot{\mathrm{C}}_k\right)\chi^{-1}_{kl}(0) \tag{4.54}$$

After all this exhausting mathematical and algebraical conversions the correlation function in the memory matrix formalsim is in a useful and workable form. In equation (4.51) the abbreviations can be combined to one function $\mathrm{M}_{il}(\omega) := \Sigma_{il}(\omega) + i\Omega_{il}$. The symbol Σ is selected in dependence on the quantum mechanical self energy and the function $\mathrm{M}(\omega)$ is called the mass operator in quantum field theory and the memory function in non-equilibrium physics.
Let us discuss the physical meaning of Ω and $\Sigma(\omega)$ in more detail. The quantity Ω always vanishs in the case if the considered Hamiltonian occupies time reversal symmetry and if the operators A_i and A_k transform with the same signature with respect to time reversal symmetry since then $\left(\dot{\mathrm{A}}_i\middle|\mathrm{A}_k\right) = 0$. This assertion is proven extensivly in the section below immediatly. In this case the memory function is solely given by the function $\Sigma(\omega)$. Comparising (4.54) with the definition (4.41) of correlation functions exhibits $\Sigma(\omega)$ has the structur of a correlation function but $\Sigma(\omega)$ occupies to differences. On the one hand only $\mathrm{Q}\middle|\dot{\mathrm{A}}\right)$ which is perpendicular to $\middle|\mathrm{A}\right)$ forms the basis vectors of the expectation value. On the other hand only the reduced Liouville operator QLQ contribute to the expectation value. Let us understand these two object better.
The latter one projects at the part of L, the full Liouville operator, which causes the intrinsic fluctuations of the operator A. This means the function $\Sigma(\omega)$ describes the dynamic of the operators what is the interesting part for us. In other words the operators QLQ describes the internal dynamics of all other degrees of freedom of the system excluded A, called "bath". Then $\mathrm{Q}\middle|\dot{\mathrm{A}}\right)$ characterizes the coupling to the bath and it's clear, that the dynamic of the bath changes the behaviour of A.

4.3.1 Time Reversal Symmetry

Even above the assertion was postulated that the quantity Ω_{il} vanishs if the considered Hailtonian is symmetric and if the operators $\dot{\mathrm{A}}$ and A have different signature under time reversal symmetry. In the following section the evidence of this statement is proven. Our starting point is the introduction of the time reversal operator T via the following transformation prescription.

or instruction?

$$\mathrm{A}(t) \to \mathrm{A}'(t) = \mathrm{T}\mathrm{A}(t)\mathrm{T}^{-1} = \epsilon_{\mathrm{A}}\mathrm{A}(-t) \tag{4.55}$$

where ϵ_A assumes two different values, $+1$ or -1. The first one takes it if the physical quantity is something like a position or electrical field and the latter takes it if the

physical quantity is a momentum, angular momentum or magnetic field. Now let us firstly investigate the action of T at the time evolution of an operator.

$$\mathrm{T}e^{i\mathrm{H}t/\hbar}\mathrm{T}^{-1} = e^{-i\mathrm{H}t/\hbar} \tag{4.56}$$

Remembering the Hamiltonian is assumed as invariant under time reversal symmetry, so that the only changed quantity is the explicit time argument t. At next the time derivative of the time evolution of an operator is investigated which yields

$$\mathrm{T}\frac{\partial}{\partial t}e^{i\mathrm{H}t/\hbar}\mathrm{T}^{-1} = \frac{i}{\hbar}\mathrm{T}\mathrm{H}e^{i\mathrm{H}t/\hbar}\mathrm{T}^{-1} = \frac{i}{\hbar}\mathrm{T}\mathrm{H}\mathrm{T}^{-1}\mathrm{T}e^{i\mathrm{H}t/\hbar}\mathrm{T}^{-1} = \frac{i}{\hbar}\mathrm{H}e^{-i\mathrm{H}t/\hbar} \tag{4.57}$$

where in the second step the unit elememt $\mathbb{1} = \mathrm{T}\mathrm{T}^{-1}$. Setting $t = 0$ and multipling with T from the right hand side immediatly the commutator relation between the time reversal operator and the Hamiltonian is given

$$\mathrm{T}\mathrm{H} = \mathrm{H}\mathrm{T} \qquad \Leftrightarrow \qquad [\mathrm{H},\mathrm{T}] = 0 \tag{4.58}$$

This is all we need to know about the time reversal operator to prove the assertion. The expectation value of a Hermitain operator can be easily manipulated with the aim of the time reversal operator T.

$$\langle \mathrm{B}\rangle = \frac{1}{Z}\,\mathrm{Tr}\Big\{e^{-\beta\mathrm{H}}\mathrm{T}\mathrm{B}\mathrm{T}^{-1}\Big\} = \Big\langle\big(\mathrm{T}\mathrm{B}\mathrm{T}^{-1}\big)^{\dagger}\Big\rangle \tag{4.59}$$

where the invariance of the trace with respect to cycling permutation and the commutator relation between T and H is used in the first step. The anti-unitarity of the time reversal operator and the hermiticity of B is utilized in the last step. The same stuff is done with the commutator between two Hermitian operators.

$$\Big(\mathrm{T}\big[\mathrm{A}(t),\mathrm{B}(t')\big]\mathrm{T}^{-1}\Big)^{\dagger} = \epsilon_{\mathrm{A}}\epsilon_{\mathrm{B}}\Big(\big[\mathrm{A}(-t),\mathrm{B}(-t')\big]\Big)^{\dagger} = -\epsilon_{\mathrm{A}}\epsilon_{\mathrm{B}}\big[\mathrm{A}(-t),\mathrm{B}(-t')\big] \tag{4.60}$$

Finitely coming to the quantity Ω_{il} which is proportional to the correlation function $\big(\dot{\mathrm{A}}_i\big|\mathrm{A}_k\big)$ between a time derivative quantity $\dot{\mathrm{A}}_i$ and the quantity A_k, as seen in equation (4.53). Using equation (4.24) yields

$$i\beta\big(\dot{\mathrm{A}}_i\big|\mathrm{A}_k\big) = i\chi_{\dot{\mathrm{A}}_i\mathrm{A}_k}(\omega=0) = i\,\mathrm{PV}\int\limits_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{\pi}\frac{\chi''_{\dot{\mathrm{A}}_i\mathrm{A}_k}(\omega')}{\omega'} - \lim_{\omega\to 0}\chi''_{\dot{\mathrm{A}}_i\mathrm{A}_k}(\omega), \tag{4.61}$$

where the dissipative susceptibility $\chi''_{\dot{\mathrm{A}}_i\mathrm{A}_k}(\omega)$ occurs, which differs a little but significant from the dissipative susceptibility $\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega)$ defined in section 4.2.4. To find the relation between both the derivative of (4.22) is formed.

$$\frac{\mathrm{d}}{\mathrm{d}t}\chi''_{\mathrm{A}_i\mathrm{A}_k}(t) = \frac{1}{2\hbar}\Big\langle\Big[\dot{\mathrm{A}}_i(t),\mathrm{A}_k(0)\Big]\Big\rangle = \chi''_{\dot{\mathrm{A}}_i\mathrm{A}_k}(t) \tag{4.62}$$

Express on both sides the susceptibilities by her Fourier transform yields the wanted relation between both.

$$\chi''_{\dot{\mathrm{A}}_i\mathrm{A}_k}(\omega) = -i\omega\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega) \tag{4.63}$$

Inserting this in (4.64) yields

$$i\beta\big(\dot{\mathrm{A}}_i\big|\mathrm{A}_k\big) = \mathrm{PV}\int\limits_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{\pi}\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega') \tag{4.64}$$

where the limit in the second term is taken. This result entails two very important advantages. One the one hand the physical meaning of the quantity Ω_{il} becomes clearer, because Ω_{il} is directly associated with dissipative processes via $\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega')$. On the other hand the founded expression establishs the possibility to analyse the behaviour of Ω_{il} under time reversal symmetry.

$$\chi''_{\mathrm{A}_i\mathrm{A}_k}(t-t') = \frac{1}{2\hbar}\left\langle\left[\mathrm{A}_i(t),\mathrm{A}_k(t')\right]\right\rangle \tag{4.65}$$

The expectation value is rewriten using equation (4.59) which establishes the oppertunity to use (4.60).

$$\chi''_{\mathrm{A}_i\mathrm{A}_k}(t-t') = -\epsilon_{\mathrm{A}_i}\epsilon_{\mathrm{A}_k}\chi''_{\mathrm{A}_i\mathrm{A}_k}(t'-t), \tag{4.66}$$

where the relation (4.23) is used. The Laplace transformation of this equation yields

$$\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega) = -\epsilon_{\mathrm{A}_i}\epsilon_{\mathrm{A}_k}\chi''_{\mathrm{A}_i\mathrm{A}_k}(-\omega) = \epsilon_{\mathrm{A}_i}\epsilon_{\mathrm{A}_k}\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega), \tag{4.67}$$

where the antisymmetry of the commutator with respect of interchanging both operators is utilized. Two cases has to be investigated by analyzing the analytical properties of $\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega)$, which are $\epsilon_{\mathrm{A}_i} = \epsilon_{\mathrm{A}_k}$ and $\epsilon_{\mathrm{A}_i} \neq \epsilon_{\mathrm{A}_k}$. The analysis gives us the required properties to compute the integral over the dissipative susceptibility.

1. case: $\epsilon_{\mathrm{A}_i} = \epsilon_{\mathrm{A}_k}$
This yields $\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega) = \chi''_{\mathrm{A}_k\mathrm{A}_i}(\omega)$ which means that the dissipative susceptibility is symmetrical under interchange of A_i and A_k. Furthermore the dissipative sysceptibility is an antisymmetrical function, because $\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega) = -\chi''_{\mathrm{A}_i\mathrm{A}_k}(-\omega)$. Consider the complex conjugated of $\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega)$ yields that the dynamical susceptibility is a real number.

$$\left(\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega)\right)^* = -\int\limits_{-\infty}^{\infty}\mathrm{d}t\, e^{-i\omega(t-t')}\chi''_{\mathrm{A}_i\mathrm{A}_k}(t-t') = -\chi_{\mathrm{A}_i\mathrm{A}_k}(-\omega) = \chi_{\mathrm{A}_i\mathrm{A}_k}(\omega) \tag{4.68}$$

where equation (4.23) is used.

2. case: $\epsilon_{\mathrm{A}_i} \neq \epsilon_{\mathrm{A}_k}$
If the signature of A_i and A_k is differant under time reversal symmetry than the dissipative susceptibility is antisymmetric under interchange of the both operators so that this yields $\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega) = -\chi''_{\mathrm{A}_k\mathrm{A}_i}(\omega)$. For the same reason $\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega)$ is a symmetrical function because $\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega) = \chi''_{\mathrm{A}_i\mathrm{A}_k}(-\omega)$. Towards the first case the dissipative susceptibility is an imaginary number which ensures by the complex conjugation likewise.

$$\left(\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega)\right)^* = -\int_{-\infty}^{\infty} \mathrm{d}t\, e^{-i\omega(t-t')}\chi''_{\mathrm{A}_i\mathrm{A}_k}(t-t') = -\chi_{\mathrm{A}_i\mathrm{A}_k}(-\omega) = -\chi_{\mathrm{A}_i\mathrm{A}_k}(\omega) \quad (4.69)$$

Back to equation (4.64). We see that the integral vanishs in the first case because the suscebtibility is an odd function. This means that $i\beta\big(\dot{\mathrm{A}}_i\big|\mathrm{A}_k\big)$ is always zero when the operators A_i and A_k have the same signature with respect to time reversal symmetry, assumed the Hamiltonian is invariant under time reversal symmetry. This is exactly the assertion which was to prove.

5 Calculation

In the last chapter the memory-matrix-formalism was introduced, which give us an exact formula to calculate correlation functions. Now this formalism is used to determine the static conductivity of the spin-fermion-model, see chapter (), pertubated by umklapp-scattering.

make link to chapter spin-fermion-model

5.1 Infinite conductivity in systems with unbroken translation symmetry

After Drude published his theory about the electrical transport in metals [Dru00] in the beginning of the last century it is well known that a broken translation symmetry is needed to get a finite static conductivity. Because of Neother's theorem it is also well known that a unbroken symmetry always implies a conserved quantity. In the case of translation symmetry this quantity is the momentum. Phenomenas breaking the translation symmetry are for example impurity scattering, electron-electron scattering and umklapp scattering. Let us firstly investigate the standard spin-fermion-model without a translation symmetry breaking pertubation. In chapter 2 it is showed that the unpertubated Hamiltonian conserves the momentum but dosen't conserves the current. This property is utilized to calculate the static conductivity.
In general the static conductivity is given by taking the small frequency limit of the conductivity and the conductivity itself is given by the current-current correlation function (J-J correlation function). This can be proven by assuming a oscillating electrical field and compute the expactaion value of the current via linear response theory, which is done in [Czy17].

$$\sigma_{\mathrm{dc}} = \lim_{\omega \to 0} \sigma(\omega) = \lim_{\omega \to 0} \beta \, \mathcal{C}_{\mathrm{JJ}}(\omega) \tag{5.1}$$

In chapter 4 above the memory matrix formalism is introduced. Our main goal was to establish equation (4.51) which is an algebraic matrix equation for the correlation function. Before the computation of $\mathcal{C}_{\mathrm{JJ}}(\omega)$ can be started we have to clarify the set of operators over which we sum up. The sums over k and l arise from the projection operator which means we have to discuss the Liouville subspace into the projection operator projects. In general to choice of these operators has to be done for each calculation seperatly depending on the working model and the quantity of interest. In this case the electrical conductivity and the induction of umklapp scattering at its is computated. As it is said above the electrical conductivity is proportional to the current operator, why this should be the first operator of our sought set of operators. If an electrical field is applied the electrons accelareate because of the potential difference

which increase the momentum of the electrons. Thus the momentum is an inevitable quantity speaking about current and electrical conductivity this should be the second operator. Beside these two operators now more operators are necessary.
The current and momentum have the same signature with respect to time reversal symmetry which simplifies the computation a lot. Considering a invariant Hamiltonian under time reversal symmetrie. Than in equation (4.51) Ω_{il} vanishes if both operators have the same signature under time reversal symmetry. This assertion is proven in section 4.3.1 in detail. In addition let do the investigation of Σ_{il}. The expactation value is generated with respect to the derivative of an operator at each side. On the right hand side the sum over k has to be carried out which produces $|\dot{\mathrm{P}})$ and $|\dot{\mathrm{J}})$. The first one is trivially zero, because the momentum is a conserved quantity. The latter has to be investigated under the action of the operator Q, which projected out off the J-P-subspace. $\mathrm{Q}|\dot{\mathrm{J}})$ describes the coupling on all the outher degrees of freedom in the system which is zero in the considered system.With all these simplifications equation (4.51) yields

bessere Formulierung finden

besser formulieren

$$\begin{pmatrix} \mathcal{C}_{\mathrm{JJ}}(\omega) & \mathcal{C}_{\mathrm{JP}}(\omega) \\ \mathcal{C}_{\mathrm{PJ}}(\omega) & \mathcal{C}_{\mathrm{PP}}(\omega) \end{pmatrix} = \frac{i}{\beta} \begin{pmatrix} \omega^{-1} & 0 \\ 0 & \omega^{-1} \end{pmatrix} \cdot \begin{pmatrix} \chi_{\mathrm{JJ}}(\omega) & \chi_{\mathrm{JP}}(\omega) \\ \chi_{\mathrm{PJ}}(\omega) & \chi_{\mathrm{PP}}(\omega) \end{pmatrix} \tag{5.2}$$

where the current current correlation function is given by

$$\mathcal{C}_{\mathrm{JJ}}(z) = \frac{i}{\beta}\omega^{-1}\chi_{\mathrm{JJ}}(\omega = 0) = \frac{i}{\omega}\mathcal{C}_{\mathrm{JJ}}(t = 0), \tag{5.3}$$

using relation (4.42). The correlation function at $t = 0$ is given by the scalar product $(\mathrm{J}(0)|\mathrm{J}(0))$, see equation (4.41). Nothing or nobody bars us from splitting the vector operator $|\mathrm{J}(0))$ into two pieces, one parallel and one vertical part, which corresponds to the secular and non-secular part of the observable, respectivily. Formaly this look like

$$\big|\mathrm{J}\big) = \big|\mathrm{J}_{||}\big) + \big|\mathrm{J}_{\perp}\big). \tag{5.4}$$

In general every observable can be consist a conserved and a non-conserved part, what shouldn't mean that both parts exist in every investigated system. Dissipative prozesses like fluctuations or initial transient processes for example are included in the non-conserved part. These non-secular effects are visible as noise in the experiement and the vertical part of the vector is indetified with these kinds of prozesses. Apart from this the secular conserved part of the observable is represented by the parallel part of $|\mathrm{J})$. In Drude's theory of conductivity the current is proportional to the momentum in the way that $j = -\frac{en}{m}p$. In the spin fermion model, see chapter 2, the momentum is conserved and the current isn't it, which means that the conductivity can't given by Drude's theory at all. Nevertheless because the momentum is conserved the conserved part of the current has to be in the direction of the momentum. In mathematical language the parallel part of the current $|\mathrm{J}_{||})$ is the projection from $|\mathrm{J})$ on $|\mathrm{P})$.

$$\big|\mathrm{J}_{||}\big) = \mathcal{P}\big|\mathrm{J}\big) = \frac{\big|\mathrm{P}\big)\big(\mathrm{P}\big|}{\big(\mathrm{P}\big|\mathrm{P}\big)}\big|\mathrm{J}\big) = \frac{\chi_{\mathrm{PJ}}}{\chi_{\mathrm{PP}}}\big|\mathrm{P}\big) \tag{5.5}$$

This give us the oppertunity to write the J-J correlation function into two parts one parrallel and one perpendicular correlation function using equation (5.4). The mixed correlation functions are zero by construction because $|\mathrm{J}_{||})$ and $|\mathrm{J}_{\perp})$ are orthogonal and therfore the terms vanish.

$$\mathcal{C}_{\mathrm{JJ}}(t=0) = \big(\mathrm{J}(0)\big|\mathrm{J}(0)\big) = \big(\mathrm{J}_{||}\big|\mathrm{J}_{||}\big) + \big(\mathrm{J}_{\perp}\big|\mathrm{J}_{\perp}\big) \tag{5.6}$$

Equation (5.5) is used to express the parallel J-J correlation function as a momentum-momentum correlation function (P-P correlation) formaly given by (P|P).

$$\mathcal{C}_{\mathrm{JJ}}(t=0) = \frac{|\chi_{\mathrm{PJ}}|^2}{|\chi_{\mathrm{PP}}|^2}\mathcal{C}_{\mathrm{PP}}(t=0) + \big(\mathrm{J}_{\perp}\big|\mathrm{J}_{\perp}\big) \tag{5.7}$$

Using (4.42) and insert back this expression into equation (5.3) which give us multipling with β the conductivity

$$\sigma(z) = \frac{|\chi_{\mathrm{PJ}}|^2}{|\chi_{\mathrm{PP}}|}\frac{i}{\omega} + \sigma_{\mathrm{reg}}(\omega) \tag{5.8}$$

where the regular conductivity $\sigma_{\mathrm{reg}}(z) = \frac{i\beta}{\omega}\big(\mathrm{J}_{\perp}\big|\mathrm{J}_{\perp}\big)$ is introduced. The physical meaning of $\sigma_{\mathrm{reg}}(\omega)$ is directly connected to the vertical component of $|\mathrm{J})$. Thus the regular conductivity includes fluctuations and other effects influenced by random forces called noise. Figure shows this continuously over all frequencies never disappearing background.

referenz zu bild mit delta peak und rauschen

In the whole calculation never a condiction on ω is made, so the equation for the conductivity is valid for each ω in the complex plane. In reality the conductivity isn't depending on a complex frequency, because physical quantities are always real. Therefore we have to set $\omega = \omega + i\eta$, where now $\omega \in \mathbb{R}$ and the limit $\eta \to 0$ is implied. Using $\frac{1}{\omega+i\eta} = \mathrm{PV}\frac{1}{\omega} - i\pi\delta(\omega)$ the conductivity is given by

$$\sigma(\omega) = \frac{|\chi_{\mathrm{PJ}}|^2}{|\chi_{\mathrm{PP}}|}\left(\mathrm{PV}\frac{i}{\omega} + \pi\delta(\omega)\right) + \sigma_{\mathrm{reg}}(\omega) \tag{5.9}$$

where PV sympolizied that the prinzipal value is taken. Equation (5.9) yield us exactly the expected result. For small frequencies the main contribution is generated by the δ-distribution, so the conductivity becomes infinity. This isn't really surprising because the translation symmetry isn't broken in the investigated system. If voltage is applied on a system with unbroken translational symmetry the electrons accelerate infinite long. There is nothing they can scatter on and loss momentum. The electrons accelerate more and more and this results in an infinite conductivity. Only in a system with broken translation symmetry it's possible for the electrons to loss some momentum by scattering with the lattice for example. This results in a finite conductivity, thus the δ-peak becomes smaller. The factor in front of the δ-distribution is the so called Drude weight. The Drude peak and the effect of breaking translation symmetry is visualizied in figure too.

link to figure

5.2 Finite conductivity because of breaking the translation symmetry via umklapp scattering

The conservation of momentum connected with an unbroken translation symmetry yields a infinite electrical conductivity, which is computated in the section above. In the next calculation a system with broken translation symmetry is considered. The assumed symmetry breaking pertubation is umklapp scattering, where the Hamiltonian is given by equation (). In ... it is shown that this pertubation is the reason for an unconserved momentum. Thus the above disscusion about the Drude weight and conductivity let us expect that the conductivity is lessened to a finite value. The static electrical conductivity is given by equation (5.1) in general. Again the memory matrix formalsim is now used to compute the current-current correlation function given by the formal equation

link zu umklapp hamiltonian

link zum abschnitt in dem gezeigt wird das P nicht mehr erhalten ist

$$\sum_l \Big[\omega\delta_{il} - \Omega_{il} + i\Sigma_{il}(\omega)\Big]\mathcal{C}_{lj}(\omega) = \frac{i}{\beta}\chi_{ij}(0) \tag{5.10}$$

where Ω_{il} and $\Sigma_{il}(\omega)$ are given by

$$\Omega_{il} = i\beta\sum_k \big(\dot{\mathrm{A}}_i\big|\mathrm{C}_k\big)\chi^{-1}_{kl}(0) \quad \text{and} \tag{5.11}$$

$$\Sigma_{il}(\omega) = i\beta\sum_k \big(\dot{\mathrm{A}}_i\big|\mathrm{Q}\frac{1}{\omega - \mathrm{QLQ}}\mathrm{Q}\big|\dot{\mathrm{C}}_k\big)\chi^{-1}_{kl}(0). \tag{5.12}$$

vllt noch etwas ausführlicher schreiben

Always the first step is to think about the vector subspace, generated by the vectors of the projection operator. Computing the electrical conductivity the current and the momentum operator are usually the operators of interest. Therefore our decision is make and our subspace should be generated by these two operators. What does this choice of operators mean for the quantities Ω_{il} and $\Sigma_{il}(\omega)$? Starting with the first one. Ω_{il} vanishs if two properties are valid. The first one is, that the considered Hamiltonian has to be invariant with respect to time reversal symmetry. The unpertubated Hamiltonian (...) and the pertubation Hamiltonian (...) occupy this condiction which is trivially to prove. The second property is that both operators labeled with A_i and C_k must have the same signature under time reversal symmetry. Both operators can be either J or P, where both have the same signature under time reversal symmetry. Therefore in all cases the quantity Ω_{il} is zero. In $\Sigma_{il}(\omega)$ the expecation value is formed with respect of the derivative of vector operators, which are $|\dot{\mathrm{J}})$ and $|\dot{\mathrm{P}})$. In the discussion above a translation invariant system is assumed why the derivative of the momentum vanishes. Now the momentum isn't conserved anymore and the derivative yields a finite value.

link zum ungestörten Hamiltonian

link zum umklapp Hamiltonian

For further assertions the action of the operator Q on both vector operator has to be investigated. $\mathrm{Q}|\dot{\mathrm{C}}_\mathrm{k})$ describes the coupling to all other degrees of freedom which aren't included in the subspace. Firstly remember that umklapp scattering is the considered pertubation. What does this pertubation change in our system? It breaks translation

symmetry which yields some finite value for $\dot{\mathrm{P}}$ instead of zero in the unpertubated system. This means the complete unconserved part of the momentum is coupled to the crystal lattice which is clearly a degree of freedom out off the J-P subspace. This is the reason why $\mathrm{Q}|\dot{\mathrm{P}}) = |\dot{\mathrm{P}})$. Further the pertubation doesn't change the quantity $|\dot{\mathrm{J}})$. The unconserved current yields from the interaction between the electrons lives on differant Fermi spaces coupeld via spin density waves. This process is included in the J-P subspace and therefore $\mathrm{Q}|\dot{\mathrm{J}}) = 0$. This signifies for the memory function that Σ_{il} doesn't vanish if $i = \mathrm{P}$ and vanish if $i = \mathrm{J}$.
In summary umklapp scattering yields a non-zero contribution to the memory function $\Sigma_{il}(\omega)$ and is therefore a correction of the correlation function instead of the unpertubated case where the memory function is zero. Equation (4.51) yields 4 equations in the J-P subspace, which can be writen as a matrix equation.

$$\begin{pmatrix} \omega & 0 \\ -i\Sigma_{\mathrm{PJ}}(\omega) & \omega - i\Sigma_{\mathrm{PP}}(\omega) \end{pmatrix} \cdot \begin{pmatrix} \mathcal{C}_{\mathrm{JJ}}(\omega) & \mathcal{C}_{\mathrm{JP}}(\omega) \\ \mathcal{C}_{\mathrm{PJ}}(\omega) & \mathcal{C}_{\mathrm{PP}}(\omega) \end{pmatrix} = \frac{i}{\beta} \begin{pmatrix} \chi_{\mathrm{JJ}}(0) & \chi_{\mathrm{JP}}(0) \\ \chi_{\mathrm{PJ}}(0) & \chi_{\mathrm{PP}}(0) \end{pmatrix} \tag{5.13}$$

Before the computation is going on we want to make a short remark. Equation (4.51) is an exact algebraic matrix equation. At the derivation no assumtions are made and up to this point we have also made no assumptions. All the conversion we have done are exact and only depending on the considered model.
The electrical conductivity is given by the J-J correlation function, which has the formal expression

$$\mathcal{C}_{\mathrm{JJ}}(\omega) = \big(\mathrm{J}\big|\frac{i}{\omega - \mathrm{L}}\big|\mathrm{J}\big) \tag{5.14}$$

in frequenzy space. Equally to the case of conserved momentum nothing bars us to split the current into one parallel and one vertical part, where the parallel part is pointed in the direction of the secular component of J. The appearing mixed correlation functions vanishes because $|\mathrm{J}_{||})$ and $|\mathrm{J}_{\perp})$ are orthogonal. How we have seen in the previous section the background or noise originated by fluctuation and other random processes is represented by the correlation function of the vertical component. This term isn't necessary to write it every time down. A theoretical phyisicist would say that the origin is always taken arbitrary. A experimental phyisicist would say that he calibrates the measurement. For a discussion in more detail the work of Jung [Jun07] is suggested. However the only important part for us is the parallel component of the correlation function. On the other hand the parallel componend of the correlation function is given by the projection of J onto P, see equation (5.5). Thus the J-J correlation function is rewriten in a momentum -momentum correlation function mutiplied with a fraction of some susceptibilities.

$$\mathcal{C}_{\mathrm{JJ}}(\omega) = \big(\mathrm{J}_{||}\big|\frac{i}{\omega - \mathrm{L}}\big|\mathrm{J}_{||}\big) = \frac{|\chi_{\mathrm{PJ}}|^2}{|\chi_{\mathrm{PP}}|^2}\mathcal{C}_{\mathrm{PP}}(\omega) \tag{5.15}$$

The P-P correlation function can be readed out of equation (5.13). Therefore the invers of the memory matrix has to be multiplied from the left hand side. The P-P

correlation function is given by

$$\mathcal{C}_{\mathrm{PP}}(\omega) = \frac{i}{\beta} \cdot \frac{i\Sigma_{\mathrm{PJ}}(\omega)\chi_{\mathrm{JP}}(0)}{\omega\big(\omega - i\Sigma_{\mathrm{PP}}(\omega)\big)} + \frac{i}{\beta} \cdot \frac{\chi_{\mathrm{PP}}(0)}{\omega - i\Sigma_{\mathrm{PP}}(\omega)} \approx \frac{i}{\beta} \cdot \frac{i\chi_{\mathrm{PP}}(0)}{\Sigma_{\mathrm{PP}}(\omega)} \tag{5.16}$$

where in the last step the limit of small frequencies is taken. Then on the one hand the first term is neglectable compared to the second term. On the other hand is $\omega \ll \Sigma_{\mathrm{PP}}(\omega)$. Thus in the second term ω is neglectable against $\Sigma_{\mathrm{PP}}(\omega)$. In summary the static conductivity is given by

Warum ist der erste Term vernachlässigbar. Begründung?

$$\sigma_{\mathrm{dc}} = \lim_{\omega\to 0} \beta\mathcal{C}_{\mathrm{JJ}}(\omega) = \frac{i}{\beta} \lim_{\omega\to 0} \frac{|\chi_{\mathrm{PJ}}|^2}{\chi_{\mathrm{PP}}} \frac{i\beta}{\Sigma_{\mathrm{PP}}(\omega)} \tag{5.17}$$

The memory function $\Sigma_{\mathrm{PP}}(\omega)$ is definied in equation (4.54). Because of the considered Hamiltonian only the term included $\dot{P}$ yields a non-zero contribution. Further the operator QLQ can be approximated by L_0 the Liouville operator of the unpertubated system. The final expression for the dc-conductivity is given by

Warum darf QLQ mit L_0 approximiert werden?

$$\sigma_{\mathrm{dc}} \approx \frac{i}{\beta} \lim_{\omega\to 0} |\chi_{\mathrm{PJ}}|^2 \big(\dot{\mathrm{P}}\big| \frac{1}{\omega - \mathrm{L}_0} \big|\dot{\mathrm{P}}\big)^{-1} \tag{5.18}$$

In a short conversion the expectation value can be expressed as a time integral over the $\dot{\mathrm{P}}$-$\dot{\mathrm{P}}$ susceptibility. This expression is more usefull for explicite computations, because its allow us to use the Matsubara formalism. For the detailed conversion see appendix B.

$$\sigma_{\mathrm{dc}} \approx -\hbar \lim_{\omega\to 0} \frac{\omega|\chi_{\mathrm{JP}}(\omega = 0)|^2}{\int_0^\infty \mathrm{d}t\, e^{i\omega t} \left\langle \left[\dot{\mathrm{P}}(t), \dot{\mathrm{P}}(0)\right]\right\rangle_0} \tag{5.19}$$

This formula of the static conductivity is the final expression which is used in the compuation below. The calculation is splitted into two parts. At first the computation of the denominator is perfermed, which gives us the temperature dependence of the conductivity. Further the J-P susceptibility has to be calculated. In first order form this quantity no temperature dependence is expected, but we have to convience us from this.

5.2.1 Temperature dependence of the dc-conductivity

Our starting point is the integral in the denominator of the last equation above. The index 0 at the expectation value means that it has to be computed with respect to the Hamiltonian $\mathrm{H}_1 = \mathrm{H}_\Psi + \mathrm{H}_\Phi + \mathrm{H}_{\Psi\Phi}$. The considered umklapp scattering is only entered in the time derivative of the momentum. Commonly the sort of this calculation is done in the Matsubara time $\tau = it$, see e. g. [BF10] for an introduction or a review.

$$\mathrm{I}(z) := -\int_0^\infty \mathrm{d}t\, e^{izt} \left\langle \left[\dot{\mathrm{P}}(t), \dot{\mathrm{P}}(0)\right]\right\rangle_{\mathrm{H}_1} = \int_0^\beta \mathrm{d}\tau\, e^{z\tau} \left\langle \mathcal{T}_\tau \dot{\mathrm{P}}(\tau)\dot{\mathrm{P}}(0)\right\rangle_{\mathrm{H}_1} \tag{5.20}$$

The norm of the Jacobi determinate is 1. Further each derivative yields an i which gives us in total one minus. To symbolisied clearly that the frequency is an arbitrary complex number the variable z is used instead of ω at this point. Like it is done every time in pertubation theory the operators are transformed into the Matsubara interaction representation. The transformation's aim is that the expectation value is only taken with respect to the free Hamiltonians $\mathrm{H}_0 = \mathrm{H}_\Psi + \mathrm{H}_\Phi$ and the interation $\mathrm{H}_{\Psi\Phi}$ is only entered in the time evolution operator $\mathrm{U}(\beta, 0)$. A series expansion of the time evolution operator up to the first non-disappearing order yields

$$\mathrm{I}(z) = \int_0^\beta \mathrm{d}\tau \, e^{z\tau} \left\langle \mathcal{T}_\tau \dot{\mathrm{P}}(\tau) \dot{\mathrm{P}}(0) \right\rangle_{\mathrm{H}_0} \tag{5.21}$$

In chapter 2 umklapp scattering is introduced as a pertubation of the spin fermion system described by H_1. On the basis of this pertubation the momentum isn't anymore conserved, thus the time derivative of the momentum doesn't vanish. The time derivative of an operator is given via the Heisenberg equation of motion, which yields for the momentum

$$\dot{\mathrm{P}}_x(\tau) = \frac{i}{\hbar} \sum_{\mathbf{K}} \mathrm{J}_{\mathbf{K}} \int_{\mathbf{k}} K_x \Phi_\mu(\mathbf{k}, \tau) \Phi_\mu(-\mathbf{k} - \mathbf{K}, \tau) \tag{5.22}$$

where the direction of the momentum is chosen to the x-direction without loss of generality. The sum over μ should be implied. Inserting the time derivative of the momentum in $\mathrm{I}(z)$ yields

$$\begin{aligned} \mathrm{I}_{xx}(z) = -\frac{1}{\hbar^2} \sum_{\mathbf{K}_1, \mathbf{K}_2} \mathrm{J}_{\mathbf{K}_1} \mathrm{J}_{\mathbf{K}_2} \int_0^\beta \mathrm{d}\tau \, e^{z\tau} \int_{\mathbf{k}_1} \int_{\mathbf{k}_2} K_{1,x} K_{2,x} \\ \times \langle \mathcal{T}_\tau \Phi_\mu(\mathbf{k}_1, \tau) \Phi_\mu(-\mathbf{k}_1 - \mathbf{K}_1, \tau) \Phi_\mu(\mathbf{k}_2, 0) \Phi_\mu(-\mathbf{k}_2 - \mathbf{K}_2, 0) \rangle_{\mathrm{H}_0} \end{aligned} \tag{5.23}$$

6 Conclusion

A Properties of the Kubo relaxation function

In section 4.2.2 the Kubo relaxation function

$$\Phi_{\mathrm{AB}}(t) = \frac{i}{\hbar} \lim_{s\to 0} \int_t^\infty \mathrm{d}\tau \, \langle [\mathrm{A_I}(\tau), \mathrm{B_I}(0)] \rangle_0 \, e^{-s\tau}. \tag{A.1}$$

and the three relations

1. $\chi_{\mathrm{AB}}(t) = -\Theta(t) \dfrac{\mathrm{d}}{\mathrm{d}t} \Phi_{\mathrm{AB}}(t)$ (A.2)
2. $\Phi_{\mathrm{AB}}(t=0) = \chi_{\mathrm{AB}}(\omega = 0)$ (A.3)
3. $\Phi_{\mathrm{AB}}(\omega) = \dfrac{1}{i\omega} \big[\chi_{\mathrm{AB}}(\omega) - \chi_{\mathrm{AB}}(\omega = 0) \big]$. (A.4)

connecting the dynamical susceptibility χ_{AB} with Φ_{AB} are introduced. In the following we want to proof these three relations.
The first one is easly gotten by derivating the Kubo relaxation function with respect to t and comparing the result with the definition of the dynamical susceptibility (4.8).

$$-\Theta(t) \frac{\mathrm{d}}{\mathrm{d}t} \Phi_{\mathrm{AB}}(t) = \frac{i}{\hbar} \Theta(t) \, \langle [\mathrm{A_I}(t), \mathrm{B_I}(0)] \rangle_0 = \chi_{\mathrm{AB}}(t) \tag{A.5}$$

The second relation is found with the aim of the Laplace transformation of the Kubo relaxation function.

$$\Phi_{\mathrm{AB}}(\omega) = \int_0^\infty \mathrm{d}t \, \Phi_{\mathrm{AB}}(t) e^{i\omega t} \tag{A.6}$$

In this definition of the Laplace transformation compared to (4.3) we set $s = -i\omega$ which correspond to a rotation of $\frac{\pi}{2}$ of the definition space . Using (A.6) after setting $t = 0$ in (A.1) yield

reference to a book of laplace transformation

$$\Phi_{\mathrm{AB}}(t=0) = \frac{i}{\hbar} \lim_{s\to 0} \int_0^\infty \mathrm{d}\tau \, \langle [\mathrm{A_I}(\tau), \mathrm{B_I}(0)] \rangle_0 \, e^{-s\tau}$$

$$\Leftrightarrow \quad \Phi_{\mathrm{AB}}(t=0) = \frac{i}{\hbar} \lim_{\substack{s\to 0 \\ \omega\to 0}} \int_{-\infty}^\infty \mathrm{d}\tau \, \Theta(\tau) \, \langle [\mathrm{A_I}(\tau), \mathrm{B_I}(0)] \rangle_0 \, e^{i\omega\tau} e^{-s\tau}$$

$$\Leftrightarrow \ \Phi_{\mathrm{AB}}(t=0) = \lim_{\omega\to 0} \int\limits_{-\infty}^{\infty} \mathrm{d}\tau\, \chi_{\mathrm{AB}}(\tau) e^{i\omega\tau}$$

$$\Leftrightarrow \ \Phi_{\mathrm{AB}}(t=0) = \chi_{\mathrm{AB}}(\omega=0), \tag{A.7}$$

where it is assumed the susceptibility is a good function in the sense they decay fast enough and the convergence generating faktor is negligible. The third relation is computated with the aim of the first and second relation. Therefore relation one is multiplied with $e^{i\omega t}$ and is integrated with respect to t.

$$\int\limits_{0}^{\infty} \mathrm{d}t\, e^{i\omega t} \chi_{\mathrm{AB}}(t) = -\int\limits_{0}^{\infty} \mathrm{d}t\, e^{i\omega t} \frac{\mathrm{d}}{\mathrm{d}t} \Phi_{\mathrm{AB}}(t)$$

$$\overset{\mathrm{PI}}{\Leftrightarrow} \ \chi_{\mathrm{AB}}(\omega) = -e^{i\omega t} \Phi_{\mathrm{AB}}(t)\Big|_{0}^{\infty} + i\omega \int\limits_{0}^{\infty} \mathrm{d}t\, e^{i\omega t} \Phi_{\mathrm{AB}}(t)$$

$$\Leftrightarrow \ \chi_{\mathrm{AB}}(\omega) = \Phi_{\mathrm{AB}}(t=0) + i\omega \Phi_{\mathrm{AB}}(\omega)$$

$$\Leftrightarrow \ \Phi_{\mathrm{AB}}(\omega) = \frac{1}{i\omega} \big[\chi_{\mathrm{AB}}(\omega) - \chi_{\mathrm{AB}}(\omega=0)\big] \tag{A.8}$$

In the first step the right hand side is integrated by parts and in last step the first relation and (A.6) is used. So the third relation gives us the dependence between the Kubo relaxation function and the dynamical susceptibility in frequency space.

B Conversion of $\left(\dot{\mathrm{P}}\middle|\left(\omega-\mathrm{L}_0\right)^{-1}\middle|\dot{\mathrm{P}}\right)$

In this appendix the short conversion of the expectation value $\left(\dot{\mathrm{P}}\middle|\left(\omega-\mathrm{L}_0\right)^{-1}\middle|\dot{\mathrm{P}}\right)$ is done. Therefore only realtions are used which we find in chapter 4. Firstly the expectation value is writen as the correlation function in the frequency space using equation (4.44).

$$
\begin{aligned}
& \left(\dot{\mathrm{P}}\middle|\left(\omega-\mathrm{L}_0\right)^{-1}\middle|\dot{\mathrm{P}}\right) = -i\mathcal{C}_{\dot{\mathrm{P}}\dot{\mathrm{P}}}(\omega) \\
\overset{(A.6)}{\Leftrightarrow}\ & \left(\dot{\mathrm{P}}\middle|\left(\omega-\mathrm{L}_0\right)^{-1}\middle|\dot{\mathrm{P}}\right) = -i\int_0^\infty \mathrm{d}t\, e^{i\omega t}\mathcal{C}_{\dot{\mathrm{P}}\dot{\mathrm{P}}}(t) \\
\overset{(4.41)}{\Leftrightarrow}\ & \left(\dot{\mathrm{P}}\middle|\left(\omega-\mathrm{L}_0\right)^{-1}\middle|\dot{\mathrm{P}}\right) = -\frac{i}{\beta}\int_0^\infty \mathrm{d}t\, e^{i\omega t}\int_0^\beta \mathrm{d}\lambda \left\langle \dot{\mathrm{P}}^\dagger(t)\dot{\mathrm{P}}(0)\right\rangle \\
\overset{(4.16)}{\Leftrightarrow}\ & \left(\dot{\mathrm{P}}\middle|\left(\omega-\mathrm{L}_0\right)^{-1}\middle|\dot{\mathrm{P}}\right) = -\frac{i}{\beta}\Phi_{\dot{\mathrm{P}}\dot{\mathrm{P}}}(\omega) \\
\overset{(4.12)}{\Leftrightarrow}\ & \left(\dot{\mathrm{P}}\middle|\left(\omega-\mathrm{L}_0\right)^{-1}\middle|\dot{\mathrm{P}}\right) = -\frac{\omega^{-1}}{\beta}\left[\chi_{\dot{\mathrm{P}}\dot{\mathrm{P}}}(\omega) - \underbrace{\chi_{\dot{\mathrm{P}}\dot{\mathrm{P}}}(\omega=0)}_{=0}\right] \\
\Leftrightarrow\ & \left(\dot{\mathrm{P}}\middle|\left(\omega-\mathrm{L}_0\right)^{-1}\middle|\dot{\mathrm{P}}\right) = -\frac{\omega^{-1}}{\beta}\int_{-\infty}^\infty \mathrm{d}t\, e^{i\omega t}\chi_{\dot{\mathrm{P}}\dot{\mathrm{P}}}(t) \\
\overset{(4.8)}{\Leftrightarrow}\ & \left(\dot{\mathrm{P}}\middle|\left(\omega-\mathrm{L}_0\right)^{-1}\middle|\dot{\mathrm{P}}\right) = -\frac{i\omega^{-1}}{\hbar\beta}\int_0^\infty \mathrm{d}t\, e^{i\omega t}\left\langle\left[\dot{\mathrm{P}}(t),\dot{\mathrm{P}}(0)\right]\right\rangle_0
\end{aligned}
\tag{B.1}
$$

In line 5 the susceptibility at frequency $\omega = 0$ is set to zero, because at $\omega = 0$ the susceptibility corresponds to the Kubo relaxation function at $t = 0$. This function is zero because $\dot{\mathrm{P}} = 0$ at $t = 0$.

C Analysis of Matsubara-sums

In the following appendix it is shown how to calculate two kinds of Matsubara-sums, where the diffrence is depending on the kind of singularity of thee Green-functions. The first one have simple poles so that the sum can transform without any problems into a contour integral. These Matsubara-sums are easy to calculate by using the residue theorem. The second kind of sum contains one or more Green-functions, which have non-continuity at a arbitary value. Therefore a little bit more work is to do, nevertheless the calculation isn't very complicated. These type of singularities are called branch cuts.

C.1 Simple poles

Let us assume a Matsubara-sum like

$$S(i\omega_n) := \frac{1}{\beta} \sum_{\omega_n} G(k, i\omega_n) e^{i\omega_n \tau}, \tag{C.1}$$

where $G(k, i\omega_n)$ is a product of Green-functions, which are analytical except single poles in the complex plane. Often these kinds of sums appear by using Green-functions of free propagators. The exponential function is only needed for conergent.

Todo list

Bibliography

[EG79] K. Elk and W. Gasser. *Die Methode der Greenschen Funktionen in der Festkörperphysik*. Akademie-Verl., 1979.

[Sch08] F. Schwabl. *Advanced Quantum Mechanics*. 4. ed. 2008.

[Sch06] F. Schwabl. *Statistische Mechanik*. 3., aktualisierte Aufl. 2006.

[Aud05] J. Audretsch. *Verschränkte Systeme: die Quantenphysik auf neuen Wegen*. Wiley-VCH, 2005. ISBN: 3-527-40452-X; 978-3-527-40452-0978-325-40452-0.

[Dru00] P. Drude. „Zur Elektronentheorie der Metalle“. In: *Annalen der Physik* 306.3 (1900), pp. 566–613. DOI: 10.1002/andp.19003060312.

[Czy17] G. Czycholl. *Theoretische Festkörperphysik Band 2 : Anwendungen: Nichtgleichgewicht, Verhalten in äußeren Feldern, kollektive Phänomene*. 4. Aufl. 2017. SpringerLink : Bücher, 2017. ISBN: 978-3-662-53701-5.

[Jun07] P. Jung. „Transport and Approximate Conservation Laws in Low Dimensional Systems“. dissertation. Universität zu Kön, 2007.

[BF10] H. Bruus and K. Flensberg. *Many-body quantum theory in condensed matter physics: an introduction*. Repr. Oxford Univ. Press, 2010. ISBN: 978-0-19-856633-5.