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Quantentransport in Spindichtesystemen mit dem Memory-Matrix-Formalismus

Masterthesis
von
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Karlsruhe, den 14. Mai 2018

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

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Contents

1 Motivation

2 Spin-Fermion-Model

- explain the quantum critical point theory
- introduced the spin fermion model in detail used by Sachdev and me
- difference two other spin fermion models and why these changes are important
- show that the momentum is conserved and the current dosen't
- introduced the pertubation Hamiltonian which included umklapp scattering
- show that the current doesn't change and the momentum isn't anymore conserved

3 The damped propagator of spin density waves

In the present chapter the propagator of spin density waves should be computed up to the first order in pertubation theory. The main goal of this masterthesis is the determination of the conductivity for the spin fermion model pertubated via umklapp scattering. These processes are determined by spin density waves, see section . . . , why the propagator of them is needed in the calculation of the conductivity. link to umklapp scattering

Firstly the free spin density wave propagtor is computed. Therefore the equation of motion of Green functions is used. An good introduction of this method can be find in every textbook about quantum field theory in many body physics, but the book by Elk and Gasser [EG79] is recommended. Afterwards the damped propagator is calculated using pertubation theory up the first order. Finally the obtained propagator is transformed into the Matsubara frequency space. An easy way to do this is using the Kramer-Kronig relations (**??**).

3.1 The free propagator of spin density waves

In 4.2 the linear response theory is established and the retarded susceptibility is introduced this way. A susceptibility describes the dynamical behaviour of an operator dependent on an external pertubation. This quantity is close related with the Green function of particles which is called propagator. The only difference is that the operators and the expectation value of the Green function are represented in the Heisenberg picture comparing to the susceptibility, where they are represented with respect to the unpertubated system.

The Green function's equation of motion is easy to get. Therefore the Green function has only to be derivated with respect to the time. The amazing result is that the equation of motion is equally for all typs (retarded, advanced and causal) of Green functions. Only the boundary conditions are different. The obtained equation of motion and the boundary conditions are transformed in Fourier space.

$$\omega\big\langle\big\langle \mathrm{A};\mathrm{B}\big\rangle\big\rangle^{j}_{\omega} = \langle[\mathrm{A},\mathrm{B}]_{\eta}\rangle + \big\langle\big\langle[\mathrm{A},\mathrm{H}]_{-};\mathrm{B}\big\rangle\big\rangle^{j}_{\omega} \tag{3.1}$$

where j labels the typ of the Green function (retarded, advanced and causal) and ω represented that the Green function is in frequency space. The double angle brackets symbolized the Green function of the operators A and B. This equation is an algebraic equation or more precisely an infinite algebraic equation chain for the green function. On the right hand side in general a new more complicated Green function appears.

For this one exists a new equation chain with a more complicted Green function on the right hand side and so on. In the case of free propagators we are mostly lucky. The appearing Green function isn't really complicated, so that the initial Green function appears after one or two interativ steps. Naturally the same procedure can be done for the Green function in Matsubara time representation. The result is similar to the one above, only the frequency ω is replaced with the Matsubara frequancy $i\omega_n$. The simplicity and advantage of this method instead of other ones is that only commutator relations of the (field) operators are needed. Equation (3.1) is all we need to compute the free propagator of spin density waves.
The dynamic of free spin density waves is described by the Hamiltonian H_Φ, introduced in chapter 2. Inserting H_Φ and bosonic field operators Φ_μ for A and B in equation (3.1) is the starting point of the following calculation. Therefore the abbreviation $\langle\langle\Phi_\mu;\Phi_\mu\rangle\rangle_\omega$ is introduced, where the first operator is readed with the momentum argument $\mathbf{k}+\mathbf{G}$ and in comparison the second operator is readed with the opposite one, $-\mathbf{k}-\mathbf{G}$. The time argument is equal in both cases, why it is dropped.

$$\omega\langle\langle\Phi_\mu;\Phi_\mu\rangle\rangle_\omega = \langle[\Phi_\mu(\mathbf{k}+\mathbf{G}),\Phi_\mu(-\mathbf{k}-\mathbf{G})]\rangle + \langle\langle[\Phi_\mu(\mathbf{k}+\mathbf{G}),\mathrm{H}_\Phi];\Phi_\mu\rangle\rangle_\omega \tag{3.2}$$

link zu bosonischen Vertauschungsrelationen

The bosonic commutator relations are given in equation (...). The only non-vanishing commutator relation is that between the bosonic field operator and the corresponding canonical momentum operator. Therefore on the right hand side of (3.2) the inhomogeneity is vanished. Computing the Green function on the same side the Hamiltonian H_Φ in equation ... is used. The commutator is given by

link zu H_Φ

$$\begin{aligned}
[\Phi_\mu(\mathbf{k}+\mathbf{G},t),\mathrm{H}_\Phi] &= -\frac{1}{2\epsilon}\sum_{\mathbf{P}}\int_{\mathbf{p}}[\Phi_\mu(\mathbf{k}+\mathbf{G},t),\pi_\lambda(\mathbf{p}+\mathbf{P},t)\pi_\lambda(-\mathbf{p}-\mathbf{P},t)]\\
\Leftrightarrow\ [\Phi_\mu(\mathbf{k}+\mathbf{G},t),\mathrm{H}_\Phi] &= -\frac{1}{2\epsilon}\sum_{\mathbf{P}}\int_{\mathbf{p}}\Big[\pi_\lambda(\mathbf{p}+\mathbf{P},t)[\Phi_\mu(\mathbf{k}+\mathbf{G},t),\pi_\lambda(-\mathbf{p}-\mathbf{P},t)]\\
&\qquad + [\Phi_\mu(\mathbf{k}+\mathbf{G},t),\pi_\lambda(\mathbf{p}+\mathbf{P},t)]\pi_\lambda(-\mathbf{p}-\mathbf{P},t)\Big]\\
\Leftrightarrow\ [\Phi_\mu(\mathbf{k}+\mathbf{G},t),\mathrm{H}_\Phi] &= -\frac{i}{\epsilon}\pi_\mu(\mathbf{k}+\mathbf{G},t)
\end{aligned} \tag{3.3}$$

where the sum over λ is implied at the beginning. Inserting the obtained result of the commutator in equation (3.2) yields the relationship between the initial and the new Green function.

$$\omega\langle\langle\Phi_\mu;\Phi_\mu\rangle\rangle_\omega = -\frac{i}{\epsilon}\langle\langle\pi_\mu;\Phi_\mu\rangle\rangle_\omega \tag{3.4}$$

Equally to the initial Green function an algebraic equation chain is established for the new Green function.

$$\omega\langle\langle\pi_\mu;\Phi_\mu\rangle\rangle_\omega = \langle[\pi_\mu(\mathbf{k}+\mathbf{G},t),\Phi_\lambda(-\mathbf{k}-\mathbf{G},t)]\rangle + \langle\langle[\pi_\mu(\mathbf{k}+\mathbf{G},t),\mathrm{H}_\Phi];\Phi_\mu\rangle\rangle_\omega \tag{3.5}$$

link to commutator relations

Like above the same things are to do. The inhomogeneity is given by the commutator relations .... In comparison to the case above the commutator dosen't vanish this time but it yields $-i$. For the Green function on the right hand side the commutator has to be calculated again, which yields $[\pi_\mu(\mathbf{k}+\mathbf{G},t),\mathrm{H}_\Phi] = i\big((\mathbf{k}+\mathbf{G})^2+r_0\big)\Phi_\mu(\mathbf{k}+\mathbf{G},t)$. In total we obtain the relation

$$\omega\big\langle\big\langle\pi_\mu;\Phi_\mu\big\rangle\big\rangle_\omega = -i + i\Big((\mathbf{k}+\mathbf{G})^2+r_0\Big)\big\langle\big\langle\Phi_\mu;\Phi_\mu\big\rangle\big\rangle_\omega. \tag{3.6}$$

Again on the right hand side a new Green function appears. This time the new Green function is well known, it's the initial one. Both equations (3.4) and (3.6) are an equation system, where the Green function $\big\langle\big\langle\pi_\mu;\Phi_\mu\big\rangle\big\rangle$ can be eliminated. The easiest way doing this is to multiply equation (3.4) with ω and inserting (3.6) in the obtained relation.

$$\mathcal{D}_\mu^{(0)}(\mathbf{k},\omega) := \big\langle\big\langle\Phi_\mu;\Phi_\mu\big\rangle\big\rangle_\omega = \sum_{\mathbf{G}}\frac{1}{(\mathbf{k}+\mathbf{G})^2+r_0-\xi^{-2}} \tag{3.7}$$

where the inverse squared correlation length $\xi^{-2}=\epsilon\omega^2$ is introduced. The free propagator exhibits a periodicity with respect to the first Brillouin zone. This condition is used in the calculation of the static conductivity in chapter 5.

say a little bit more about that

3.2 The damped spin density wave propagator

In the previous section the free propagator of spin density waves is computed. Beside the free dynamics the spin fermion model considers an interaction between electrons living on different Fermi surfaces, where the interaction is originated by spin density waves. On that reason the propagation of the spin density waves is damped. The damping should be considered in the propagator via doing pertubation theory.
Because the damping is originated by the interaction between electrons the free electron propagator is also needed in the following calculation. The propagator can be calculated in the same way as the one for free spin density waves. This handwork shouldn't be done here explicitly. The free electron propagator is given by

$$\mathcal{G}_\alpha^{(0)}(\mathbf{k},\omega) := \big\langle\big\langle\Psi_\alpha;\Psi_\alpha^\dagger\big\rangle\big\rangle_\omega = \sum_{\mathbf{G}}\frac{1}{\omega-\epsilon_\alpha(\mathbf{k}+\mathbf{G})}, \tag{3.8}$$

where $\alpha=\mathrm{a},\mathrm{b}$ denotes the Fermi surface of the respective electrons. The damped spin density wave propagator is computed using the usually method of pertubation theory in quantum field theory. The full spin density wave propagator is given by

$$\mathcal{D}_\mu(\mathbf{k},t-t') = -i\,\big\langle\mathcal{T}_t\mathrm{U}(\infty,-\infty)\Phi_\mu(\mathbf{k}+\mathbf{G},t)\Phi_\mu(-\mathbf{k}-\mathbf{G},t')\big\rangle_0^{\mathrm{con}} \tag{3.9}$$

where $\mathcal{T}_t$ is the time ordering operator, which orders all contained operators of there right time order. The index 0 denotes that the expectation value is performed with respect to the unpertubated Hamiltonian. The interaction is only incorporated through the time evolution operator U which is given by

$$\mathrm{U}(t,t') = \exp\bigg(-i\int_{t'}^{t}\mathrm{d}t_1\,\mathrm{H}_{\mathrm{int}}(t_1)\bigg). \tag{3.10}$$

The second index "con" at the expectation value denotes that only connected diagrams are considered. In the so called link cluster theorem it is proven that all disconnected diagrams are canceled with the vacuum diagrams, see [Nol09] for it. All these connected diagrams can be simplified a little bit more. There exist diagrams which are contained only diagrams of a lower order in a specific way. It is possible to build these diagrams by multipling diagrams of lower orders. Therefore a new object Π is introduced, called self energy, which contains all irreducible connected diagrams. The self energy offers the oppertunity to write the full Green function as a Dyson equation.

$$\mathcal{D}_\mu = \mathcal{D}_\mu^{(0)} + \mathcal{D}_\mu^{(0)} \Pi_\mu \mathcal{D}_\mu \qquad \Rightarrow \qquad \mathcal{D}_\mu = \frac{1}{\left(\mathcal{D}_\mu^{(0)}\right)^{-1} - \Pi_\mu} \tag{3.11}$$

In general the self energy is a complex quantity. Splitting her in a real and imaginary part the real part of its is a correction to the energy and the imaginary part is interpreted as a life time. A finite life time correspondes to a damped particle. The goal of the following calculation is to compute the imaginary part of the self energy. Getting a feeling how the self energy looks in diagrammatic language the full propagator in (3.9) is investigated.
The time evolution operator is expanded up to the second order. The zeroth order yields the free propagator which is calculated in the previous section. Further the first order vanishes. The interaction Hamiltonian $H_{\Psi\Phi}$ contains one bosonic field operator and therefore combining with the two other bosonic operators this yields an expectation value of three bosonic operators. Wick's theorem says that the expectation value of an odd number of operators is always zero. The reason is that it's impossible to get an term where only contractions are contained. Having an odd number of operators a normal product exist in every term. Taking the equillibrium expectation value of a normal product, it's zero by definition.
The first not vanishing contribution appears at the second order, because the interaction Hamiltonian $H_{\Psi\Phi}$ contributes twice, thus the number of operators is even in both cases, fermionic and bosonic. In the fermonic case four expectation values appear, where those ones have a little bit different structure like the usually known ones of fermionic operators. The feature of them is that two fermionic operators are connected by a Pauli matrix, which prohibit the use of Wick's theorem or any rearrange of the operators. The expectation values has the special form

$$\left\langle \mathcal{T}_t \; \Psi_\alpha^\dagger(\mathbf{p}_4, t_2) \cdot \sigma_{\lambda'} \cdot \Psi_\beta(\mathbf{p}_3, t_2) \cdot \Psi_\gamma^\dagger(\mathbf{p}_2, t_1) \cdot \sigma_\lambda \cdot \Psi_\beta(\mathbf{p}_1, t_1) \right\rangle_0 , \tag{3.12}$$

where $\alpha, \beta, \gamma, \delta \in \{\mathrm{a}, \mathrm{b}\}$ with the property that always two greek letters have to be an "a" and the other two ones a "b". Fierz identity offers the oppertunity to eliminate the Pauli matricies. With the aid of Fierz identity a product of the components of two Pauli matricies can be rewriten as a relation of Kronecker symbols.

$$\sum_{\mu=1}^{3} \sigma_{ij}^\mu \sigma_{kl}^\mu = 2\delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl} \tag{3.13}$$

Acting Fierz identity the product of field operators and Pauli matrix has to be writen in component representation. Then the identity can be use without any doubt and the Kronecker symbols allows us to rewrite the operators without component representation. Doing this we have to rivet on the first term in (3.13), because the order of the operators is rearranged. Therefore the operators has to be commuted with yields a δ-distribution with respect to the momentum, see (C.5). The exact calculation is done in the appendix C.

Each obtained expectation values contains two operators of a-electrons[1] and two operators of b-electrons, so that the expectation value can be seperated. One half of these is constructed in a way that both annihiliation operators are acting with respect to a-electrons, for example. These kinds of expectation values are surely zero. The other half is "normaly" constructed so that one annihiliation and creation operator is acting with respect to a-electrons. The same is surely valid for b-electrons.

writing this argument in a better way

Bringing the remained operators in the order that all annihilaition operators stands on the left side of the creation operators yields a δ-distribution for each commutation, so that in total each term contains two δ-distributions. The obtained expectation value is shown in equation (C.6) in the appendix C.

Inserting equation (C.6) for each of the four expectation values two of the four momentum integrals and sums can be performed. The remaining expression for $\mathcal{D}$ in second order pertubation theory have the form

$$\begin{aligned}\mathcal{D}_{\mu}^{(2)}(\mathbf{k},\omega) = (-i)^3\lambda^2 &\int_{-\infty}^{\infty} \mathrm{d}t_1\,\mathrm{d}t_2 \sum_{\mathbf{P}_1\mathbf{P}_2} \int_{\mathbf{p}_1}\int_{\mathbf{p}_2} \\ &\times \Big\langle \mathcal{T}_t \Phi_{\lambda'}(\tilde{\mathbf{p}}_2-\tilde{\mathbf{p}}_1,t_2)\Phi_{\lambda}(\tilde{\mathbf{p}}_1-\tilde{\mathbf{p}}_2,t_1)\Phi_{\mu}(\tilde{\mathbf{k}},t)\Phi_{\mu}(-\tilde{\mathbf{k}},t')\Big\rangle_0 \\ &\times \Big(\Big\langle \mathcal{T}_t \Psi_{\mathrm{a}}(\tilde{\mathbf{p}}_2,t_1)\Psi_{\mathrm{a}}^{\dagger}(\tilde{\mathbf{p}}_2,t_2)\Big\rangle_0 \Big\langle \mathcal{T}_t \Psi_{\mathrm{b}}(\tilde{\mathbf{p}}_1,t_2)\Psi_{\mathrm{b}}^{\dagger}(\tilde{\mathbf{p}}_1,t_1)\Big\rangle_0 \\ &+ \Big\langle \mathcal{T}_t \Psi_{\mathrm{b}}(\tilde{\mathbf{p}}_2,t_1)\Psi_{\mathrm{b}}^{\dagger}(\tilde{\mathbf{p}}_2,t_2)\Big\rangle_0 \Big\langle \mathcal{T}_t \Psi_{\mathrm{a}}(\tilde{\mathbf{p}}_1,t_2)\Psi_{\mathrm{a}}^{\dagger}(\tilde{\mathbf{p}}_1,t_1)\Big\rangle_0 \Big)\end{aligned} \tag{3.14}$$

where the abbreviation $\tilde{\mathbf{k}} = \mathbf{k}+\mathbf{G}$ and $\tilde{\mathbf{p}}_i = \mathbf{p}_i + \mathbf{P}_i$ with $i = 1,2$ is introduced. In the case of the bosonic expectation value the usually used Wick theorem is utilized. Wick's theorem yields three possibile contractions in the corresponding case, where one of these isn't contributed, because it's yielded disconnected diagrams. The remaining two contractions generate four diagrams in total, which are depicted in figure 3.1. These diagrams differentiate only in two points.

On the one hand the acting point of the bosonic lines is changed comparing the first two and last two diagrams. On the other hand the direction of the electronic lines is interchanged between the first two diagrams and in equal measure for the last two diagrams. For example, in the first diagram an a-electron is annihiliated and a b-electron is created at t_1. Comparing the second diagram, where an a-electron is created

[1] a-electrons denotes electrons living on the Fermi surface labeled with a. In comparison b-electrons are electrons on the Fermi surface labeled with b. Both Fermi surfaces are rotated by $\pi/2$ and shifted by $(\pm\pi,\pm\pi)$ to each other.

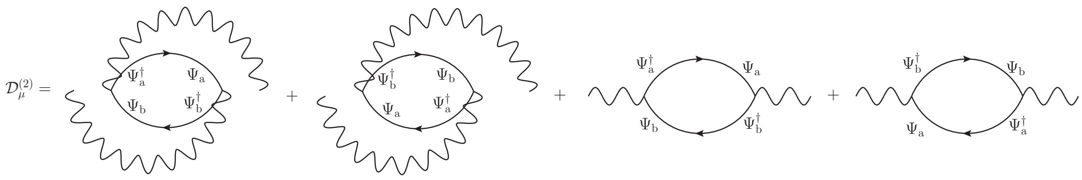

Figure 3.1: caption

and a b-electron is annihilated at t_1. All four diagrams are closly connected with each other, because all diagrams can be generated out of one diagram by interchanging the acting point of the bosonic lines or the direction of the fermionic lines. Therefore all four diagrams yield the same contribution, where it is enough to compute one of them and multiply by four.

$$\begin{aligned}\mathcal{D}_\mu^{(2)}(\mathbf{k}, t-t') = 4i\lambda^2 \int\limits_{-\infty}^{\infty} \mathrm{d}t_1\,\mathrm{d}t_2 \sum_{\mathbf{P}} \int_{\mathbf{p}} \\ \times \left\langle \mathcal{T}_t \Phi_\mu(\tilde{\mathbf{k}}, t_2)\Phi_\mu(-\tilde{\mathbf{k}}, t')\right\rangle_0 \left\langle \mathcal{T}_t \Phi_\mu(-\tilde{\mathbf{k}}, t_1)\Phi_\mu(\tilde{\mathbf{k}}, t)\right\rangle_0 \\ \times \left\langle \mathcal{T}_t \Psi_{\rm a}(\tilde{\mathbf{p}}-\tilde{\mathbf{k}}, t_1)\Psi_{\rm a}^\dagger(\tilde{\mathbf{p}}-\tilde{\mathbf{k}}, t_2)\right\rangle_0 \left\langle \mathcal{T}_t \Psi_{\rm b}(\tilde{\mathbf{p}}, t_2)\Psi_{\rm b}^\dagger(\tilde{\mathbf{p}}, t_1)\right\rangle_0 \qquad (3.15)\end{aligned}$$

where the momentums $\mathbf{p}_1$ and $\mathbf{P}_1$ are relabeled with $\mathbf{p}$ and $\mathbf{P}$, respectivily. Accordingly we write $\tilde{\mathbf{p}}$ instead of $\tilde{\mathbf{p}}_1$. In comparison to the Dyson equation (3.11) the fermionic bubble is identified with the self energy Π_μ, where the bubble diagram surely only represented the zeroth order of the self energy. The self energy in zeroth order is therefore given by

$$\Pi_\mu^{(0)}(\mathbf{k}, \omega) = i \sum_{\mathbf{P}} \int\limits_{|p|\leq|p_{\rm F}} \frac{\mathrm{d}^2\mathbf{p}}{(2\pi)^2} \int\limits_{-\infty}^{\infty} \frac{\mathrm{d}\epsilon}{2\pi}\, \mathcal{G}_{\rm a}^{(0)}(\mathbf{p}+\frac{\mathbf{k}}{2}, \epsilon+\frac{\omega}{2})\mathcal{G}_{\rm b}^{(0)}(\mathbf{p}-\frac{\mathbf{k}}{2}, \epsilon-\frac{\omega}{2}). \qquad (3.16)$$

In comparison to equation (3.15) the self energy is represented in frequency space. Further the outer momentum and frequency is shifted by the half of itself, so that both arguments of the fermionic propagators are symmetricly, which is depicted in figure 3.2. How we see in equation (3.8) the free electron propagator contains the dispersion relation $\epsilon_\alpha(\mathbf{p}+\mathbf{P})$ of the respective electrons. In our considered spin fermion model only electrons near the Fermi surface interacte with each other interfered by spin density waves, which means that the momentum and energy transfer is small. Under this condition the dispersion relation can be expanded near the Fermi surface.

$$\begin{aligned}\epsilon_{\rm a}(\mathbf{p}+\mathbf{P}+\frac{\mathbf{k}+\mathbf{G}}{2}) &= \frac{\left(p_x+P_x+\frac{k_x+G_x}{2}\right)^2}{2m_1} + \frac{\left(p_y+P_y+\frac{k_y+G_y}{2}\right)^2}{2m_2} \\ \Leftrightarrow\ \epsilon_{\rm a}(\mathbf{p}+\mathbf{P}+\frac{\mathbf{k}+\mathbf{G}}{2}) &= \frac{(p_x+P_x)^2}{2m_1} + \frac{1}{2}\frac{p_x+P_x}{m_1}(k_x+G_x) + \frac{(k_x+G_x)^2}{8m_1}\end{aligned}$$

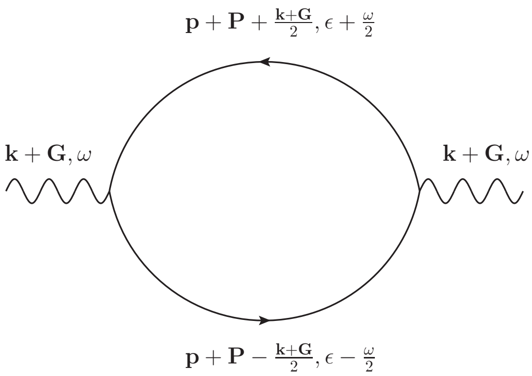

Figure 3.2: caption

$$
\begin{aligned}
&+\frac{(p_y+P_y)^2}{2m_2}+\frac{1}{2}\frac{p_y+P_y}{m_2}(k_y+G_y)+\frac{(k_y+G_y)^2}{8m_2} \\
\Leftrightarrow \quad & \epsilon_{\mathrm{a}}(\mathbf{p}+\mathbf{P}+\frac{\mathbf{k}+\mathbf{G}}{2}) \approx \xi_{\mathrm{a}}+\frac{1}{2}\mathbf{v}_{\mathrm{a,F}}(\mathbf{k}+\mathbf{G})+\mu \qquad (3.17)
\end{aligned}
$$

where the quadratic term with respect to $\mathbf{k}$ is neglectable, because the bosonic transfered momentum is assumed as small. Further the velocity $\mathbf{v}_a$ of the a-electrons is introduced, where the elelctron velocity can be approximated with the Fermi velocity of the corresponding Fermi surface, because only electrons near the Fermi surface are considered. Besides the dispersion relation ξ_{a} of the a-electrons is used, which is given by .... The same procedure is done for the b-electrons. Finally the normalized momentum vector $\mathbf{n}=\frac{\mathbf{p}+\mathbf{P}}{|\mathbf{p}+\mathbf{P}|}$ is introduced. The Fermi velocity of the a-electrons is then given by $\mathbf{v}_{\mathrm{a,F}}=v_{\mathrm{a,F}}\mathbf{n}$ for example. The scalar product between the normalized momentum vector $\mathbf{n}$ and the bosonic spin density wave vector $\mathbf{k}+\mathbf{G}$ is rewriten as his magnitude multiplied with $\cos(\vartheta)$, where ϑ is the angle between both.

link zur dispersion im spin fermion model

In the investigated spin fermion model the electrons on different Fermi surfaces only interacte on so called hot spots like we have it introduced in chapter 2. The energy and the magnitudes of the Fermi velocities are equal on the hot spots.

$$
\xi := \xi_{\mathrm{a}} = \xi_{\mathrm{b}} \qquad v_{\mathrm{F}} := v_{\mathrm{a,F}} = v_{\mathrm{b,F}} \qquad (3.18)
$$

Consider that the direction of the velocities haven't been equal, otherwise the angle ϑ is 0 or π and the imaginary part of Π_μ is zero. Using these assumptions the self energy is given by

$$
\begin{aligned}
\Pi_\mu^{(0)}(\mathbf{k},\omega) = i\nu_{\mathrm{F}} \int_0^\pi \mathrm{d}\vartheta \int_{\xi\leq\xi_{\mathrm{F}}} \mathrm{d}\xi \int_{-\infty}^{\infty} \frac{\mathrm{d}\epsilon}{2\pi} \\
\times \frac{1}{\epsilon+\frac{\omega}{2}-\xi-\frac{1}{2}v_{\mathrm{F}}|\mathbf{k}+\mathbf{G}|\cos(\vartheta)+i\eta\,\mathrm{sign}(\epsilon+\frac{\omega}{2})} \\
\times \frac{1}{\epsilon-\frac{\omega}{2}-\xi+\frac{1}{2}v_{\mathrm{F}}|\mathbf{k}+\mathbf{G}|\cos(\vartheta)+i\eta\,\mathrm{sign}(\epsilon-\frac{\omega}{2})}, \qquad (3.19)
\end{aligned}
$$

where the two dimensional momentum integral is firstly transformed in plane polar coordinates and then the k-integral is transformed into an energy integral over the density of states. Because only electrons near the Fermi surface are considered the density of states can be approximated with the constant one $\nu_\mathrm{F} := \nu(\xi_\mathrm{F})$ at the Fermi surface. The energy integral is certainly limited by the Fermi energy ξ_F.
The further investigation is been starting with the computation of the frequency integral. Therefore the integral over ϵ is transformed into a complex contour integral, where the contour Γ is chosen in two different ways. In both case the contour starts along the real axis. According to the singularities of the integrand the countour is closed in the upper or lower half plane via a semicircle with radius infinity. In both cases the contribution of the semicircle is zero because the integrand is proportional to $1/\epsilon$. The non-contributing of the semicircle ensures the equality between the integral along the real axis and the complex contour integral. The investigated integrand occupies two singularities at

$$\epsilon_1 := \xi - \frac{1}{2}\big(\omega - v_\mathrm{F}|\mathbf{k}+\mathbf{G}|\cos(\vartheta)\big) \quad \text{and} \quad \epsilon_2 := \xi + \frac{1}{2}\big(\omega - v_\mathrm{F}|\mathbf{k}+\mathbf{G}|\cos(\vartheta)\big), \tag{3.20}$$

where both singularities are of first order which allows using Cauchy's integral formula. According to the signum function in both denominators the poles are located in the upper or lower plane. So in total there are four different possible constitutions. On the one hand both singularities can be located in the lower or upper complex plane, which yield in both cases zero. On the other hand one pole can be in the upper plane and the other one can be in the lower plane, or vice versa. Equally both constitutions yields the same contribution.

1. case: $\mathrm{sign}(\epsilon + \frac{\omega}{2}) = \mathrm{sign}(\epsilon - \frac{\omega}{2})$
Both singularities are located in the upper or in the lower complex half plane. The contour is therefore closed in the upper or lower plane, respectivily, so that both poles are enclosed. In the first case the winding number is 1, because the pole is enclosed counterclockwise. Accordingly the winding number is -1 in the second case.

$$\begin{aligned} \mathrm{I}^\mathrm{e}_\omega &:= i \oint_\Gamma \frac{\mathrm{d}\omega}{2\pi i} \frac{1}{\omega - \omega_1 \mp i\eta} \cdot \frac{1}{\omega - \omega_2 \mp i\eta} \\ \Leftrightarrow \mathrm{I}^\mathrm{e}_\omega &= \pm i \left[\frac{1}{\omega_2 - \omega_1} + \frac{1}{\omega_1 - \omega_2} \right] = 0, \end{aligned} \tag{3.21}$$

where the index "e" stands for even and should mean that both poles are located at the same half planes.

2. case: $\mathrm{sign}(\epsilon + \frac{\omega}{2}) \neq \mathrm{sign}(\epsilon - \frac{\omega}{2})$
The singularities are located in different complex half planes, one in the upper and accordingly the other in the lower half plane. In both cases it's arbitrary how the contour is closed. It's only important that one of the two poles is located inside the

contour. In the following computation the contour is closed in the upper half plane, so the winding number is always 1.

$$
\begin{aligned}
\mathrm{I}^{\mathrm{o}}_{\omega} &:= i \oint_{\Gamma} \frac{\mathrm{d}\omega}{2\pi i} \frac{1}{\omega - \omega_1 \mp i\eta} \cdot \frac{1}{\omega - \omega_2 \pm i\eta} \\
\Leftrightarrow \mathrm{I}^{\mathrm{o}}_{\omega} &= \frac{\pm i}{\omega_2 - \omega_1 \pm i\eta}
\end{aligned} \tag{3.22}
$$

where the index "o" stands accordingly for odd and should mean that both poles are located in different half planes.
Inserting both singularities ω_1 and ω_2 causes that the integrand is independent with respect to the energy ξ. The frequency depending signum functions in (3.19) is aquivalent to the signum functions $\mathrm{sign}(\xi \pm \frac{1}{2}v_{\mathrm{F}}|\mathbf{k}+\mathbf{G}|\cos(\vartheta))$ in energy representation. The energy ξ is neglectable because the integrand is independent of ξ. Further the constant factors are also neglectable because them are always positive. The case of sign in the integand depends therefore only on the sign of $|\mathbf{k}+\mathbf{G}|\cos(\vartheta)$. Finally the integrals limits has to be set to $\pm\frac{1}{2}v_{\mathrm{F}}|\mathbf{k}+\mathbf{G}|\cos(\vartheta)$. This follows directly from the location of the poles. For example if ω_1 is in the lower and ω_2 is in the upper half plane than $\epsilon+\frac{\omega}{2} > 0$ and $\epsilon-\frac{\omega}{2} < 0$, respectivily. Transforming both into energy representation the corresponding expressions are $\xi - \frac{1}{2}v_{\mathrm{F}}|\mathbf{k}+\mathbf{G}|\cos(\vartheta) < 0$ and $\xi + \frac{1}{2}v_{\mathrm{F}}|\mathbf{k}+\mathbf{G}|\cos(\vartheta) > 0$, which yields directly the definition interval of ξ. Therefore we obtained

$$
\Pi^{(0)}_{\mu}(\mathbf{k},\omega) = i\nu_{\mathrm{F}} \int_0^{\pi} \mathrm{d}\vartheta \int_{-\xi_0}^{\xi_0} \mathrm{d}\xi \, \frac{i\,\mathrm{sign}(|\mathbf{k}+\mathbf{G}|\cos(\vartheta))}{\omega - v_{\mathrm{F}}|\mathbf{k}+\mathbf{G}|\cos(\vartheta) + i\eta\,\mathrm{sign}(|\mathbf{k}+\mathbf{G}|\cos(\vartheta))} \tag{3.23}
$$

for the self energy, where the abbreviation $\xi_0 = v_{\mathrm{F}}|\mathbf{k}+\mathbf{G}|\cos(\vartheta)/2$ is introduced. The integration over ξ yields the factor $v_{\mathrm{F}}|\mathbf{k}+\mathbf{G}|\cos(\vartheta)$. Subsequently the signum function is reexpressed in frequency representation which corresponds to $\mathrm{sign}(\omega)$.
Like it is shown above the damping of the spin density wave occurs of the imaginary part of the self energy, which is the reason why we take the imaginary part of the above expression in the further computation. The imaginary part of the serlf energy is given by

$$
\mathrm{Im}\left\{\Pi^{(0)}_{\mu}(\mathbf{k},\omega)\right\} = \nu_{\mathrm{F}}\pi \int_0^{\pi} \mathrm{d}\vartheta \, v_{\mathrm{F}}|\mathbf{k}+\mathbf{G}|\cos(\vartheta)\delta(\omega - v_{\mathrm{F}}|\mathbf{k}+\mathbf{G}|\cos(\vartheta)), \tag{3.24}
$$

where the formula $\frac{1}{x \pm i\eta} = \mathrm{P.V.}\frac{1}{x} \mp i\pi\delta(x)$ is used. To perform the last remaining intgeral over ϑ the δ-distribution has to be rewriten. The argument is a ϑ depending function with in general infinite zeros. But in the integrating area, between 0 and π, the cosine only have one zero. The formula

$$
\delta(g(x)) = \sum_{i=1} \frac{\delta(x - x_{0,i})}{|g'(x_{0,i})|} \tag{3.25}
$$

states how a δ-distribution with a functional argument can be writen as a sum over δ-distributions with zeros of $g(x)$ as arguments. The prime denotes the derivative with respect to x which has to be evaluated at the corresponding zero $x_{0,i}$. The argument of the δ-distribution in (3.24) has a single zero at $\vartheta_0 = \cos^{-1}(\omega/(v_\mathrm{F}|\mathbf{k}+\mathbf{G}|))$. Thereby the δ-distribution is rewriten as

$$\begin{aligned} \delta(\omega - v_\mathrm{F}|\mathbf{k}+\mathbf{G}|\cos(\vartheta)) &= \Big(v_\mathrm{F}|\mathbf{k}+\mathbf{G}| \cdot |\sin(\vartheta_0)|\Big)^{-1} \delta(\vartheta - \vartheta_0) \\ \Rightarrow \delta(\omega - v_\mathrm{F}|\mathbf{k}+\mathbf{G}|\cos(\vartheta)) &\approx \Big(v_\mathrm{F}|\mathbf{k}+\mathbf{G}|\Big)^{-1} \delta(\vartheta - \vartheta_0) \end{aligned} \tag{3.26}$$

where in the second line the limit of small frequancies ω is performed. This is valid because of our investigated low energy theory. In other words the interaction is assumed as small and thereby the frequency and momentum transfer is small too. Now the integration over ϑ can be performed easily. The imaginary part of the self energy is given by

$$\mathrm{Im}\Big\{\Pi_\mu^{(0)}(\mathbf{k},\omega)\Big\} = \frac{\nu_\mathrm{F}\pi}{v_\mathrm{F}|\mathbf{k}+\mathbf{G}|} \cdot \omega = \gamma\omega \tag{3.27}$$

where in the last step the damping constant γ is introduced. In equation (3.11) we see that the full propagator is given by the free propagator and the self energy. In general the self energy is a complex quantity why they is splitted into real and imaginary part. With the free propagator in equation (3.7) the damped spin fermion propagator is given by

$$\mathcal{D}_\mu(\mathbf{k},\omega) = \sum_\mathbf{G} \frac{1}{(\mathbf{k}+\mathbf{G})^2 + r - \xi^{-2} - i\gamma\omega} \tag{3.28}$$

where the abbreviation $r = r_0 - \mathrm{Re}\{\Pi_\mu(\mathbf{k},\omega)\}$ is used. Remember that ξ represents the correlation length in this formula instead of the energy like it's used in the previous computation. At the quantum critical point the even introduced quantity r is zero. The real part of self energy is canceled with r_0. Further the investigated model is a low energy theory, why the correlation length ξ, which is proportional to ω^2 is neglectable.

3.3 Transformation of the propagator on the imaginary axis

The spin density wave propagator obtained in the previous section is a complex function of the real quantity ω. In the following the quantity ω should be transformed into an imaginary quantity $i\omega_n$, which we know as Matsubara frequancies. In this representation the computations in chapter 5 are much more convienent. The aim is now to find the real and imaginary part of the propagator with respect to the imaginary quantity $i\omega_n$. The Kramers-Kronig relations yield a relationship between the real part of a function and the imaginary part of the same function, or vice versa, where the argument of both parts is rotated by an arbitrary angle. In section 4.2.3 these relations are established, see (??) for the explicite form. The propagator in (3.28) can be easily seperated into real and imaginary part

$$\mathcal{D}_\mu(\mathbf{k},\omega) = \sum_{\mathbf{G}} \left[\frac{(\mathbf{k}+\mathbf{G})^2}{(\mathbf{k}+\mathbf{G})^4 + (\gamma\omega)^2} + i \frac{\gamma\omega}{(\mathbf{k}+\mathbf{G})^4 + (\gamma\omega)^2} \right], \tag{3.29}$$

where $r = \xi = 0$ is set. It is trivially seen that the real part is a symmetric function and the imaginary part is an antiysmmetric funtion with respect to ω. Similiar to (3.28) the propagator $\mathcal{D}_\mu(\mathbf{k}, i\omega_n)$ can be seperated into a real and imaginary part. The imaginary part is zero, because the integrand in (??) is an antisymmetric function with respect to ω. So the propagator with respect to Matsubara frequencies is given by

$$\mathcal{D}_\mu(\mathbf{k}, i\omega_n) = \frac{1}{\pi} \mathrm{P.V.} \int_{-\infty}^{\infty} \mathrm{d}\omega \, \frac{\mathrm{Im}\{\mathcal{D}_\mu(\mathbf{k},\omega)\}}{\omega - i\omega_n} \tag{3.30}$$

The integral is splitted into two parts and in the first term we substitute with $\omega = -\omega$ and the antismmetry of $\mathrm{Im}\{\mathcal{D}_\mu(\mathbf{k},\omega)\}$ is utilizied.

$$\begin{aligned}
\mathcal{D}_\mu(\mathbf{k}, i\omega_n) &= \frac{1}{\pi} \int_0^{\infty} \mathrm{d}\omega \, \mathrm{Im}\{\mathcal{D}_\mu(\mathbf{k},\omega)\} \left[\frac{1}{\omega + i\omega_n} + \frac{1}{\omega - i\omega_n} \right] \\
\Leftrightarrow \mathcal{D}_\mu(\mathbf{k}, i\omega_n) &= \frac{2}{\pi} \sum_{\mathbf{G}} \int_0^{\infty} \mathrm{d}\omega \, \frac{\gamma\omega}{(\mathbf{k}+\mathbf{G})^4 + (\gamma\omega)^2} \cdot \frac{\omega}{\omega^2 + \omega_n^2} \\
\Leftrightarrow \mathcal{D}_\mu(\mathbf{k}, i\omega_n) &= \sum_{\mathbf{G}} \frac{1}{(\mathbf{k}+\mathbf{G})^2 + \gamma|\omega_n|}
\end{aligned} \tag{3.31}$$

In the last step the integral formula

$$\int_0^{\infty} \mathrm{d}x \, \frac{x}{a^2 + x^2} \cdot \frac{x}{y^2 + x^2} = \frac{\pi}{2} \frac{1}{a + |y|} \tag{3.32}$$

is used, which can be shown by transforming into a complex contour integral.

4 Memory-Matrix-Formalism

write a short introduction

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. One 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 arbitrary dynamical observable and $f(t)$ is a random force like white noise for example. The he second term on the left hand side is originated from some external force, which is coupled to the dynamical observalbe $\mathrm{A}(t)$. The third term is a damping or friction term. Now let us assume 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 of the system. 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

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

where $\mathcal{C}$ denotes 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 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

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

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

$$\mathrm{A}(t) = \Xi(t) \cdot \mathrm{A}(0) + \mathrm{A}'(t) \qquad \text{with} \qquad \mathrm{A}'(t) = \int_0^t \mathrm{d}t'\, \Xi(t-t')F(t'), \tag{4.4}$$

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 that the dynamical observable $\mathrm{A}(t)$ can be splitted into two parts.
For the first term on the right hand side the only time-dependence is adverted from the correlation function $\mathcal{C}$, which is clear considing 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 and 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 her and the retarded susceptibility χ are derivated. In the last section finally the splitting of χ in a real and an imaginary part is 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 $\mathrm{H}_1 = -\mathrm{B} \cdot F(t)$, so that $\mathrm{H}(t) = \mathrm{H}_0 + \mathrm{H}_1$ is the full Hamiltonian. Thereby B is an operator by which the pertubation is coupled to 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 depends 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 integral equation.

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

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 an iterativ solution procedure. Starting with the zeroth order the density operator is trivially the density operator at thermal equilibrium. Inserting the zeroth order on the right hand side of equation (4.7) yields the first order of the density operator, a. s.ø. In linear response theory the iteration is cut 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 $F(t)$.

4.2.2 Kubo relaxation function

After a general equation for the deviation of an observable A from the equilibrium value is 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

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

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

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

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

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 commutator-independent form. Doing this two identities are needed, where the first one is

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

where the invariance of the trace 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 [1] of an operator.

$$\begin{aligned} i[\rho, \mathrm{A}(t)] &= i \Big[\rho \mathrm{A}(t) - \mathrm{A}(t) \rho \Big] \\ \Leftrightarrow \; i[\rho, \mathrm{A}(t)] &= i \Big[\rho \mathrm{A}(t) - e^{-\beta H} e^{\beta \mathrm{H}} \mathrm{A}(t) e^{-\beta \mathrm{H}} \Big] \end{aligned}$$

---

[1] The time evolution of an operator is given by

$$\mathrm{A_H}(t) = e^{\,i\mathrm{H}t/\hbar} \, \mathrm{A_S}(0) e^{\,-i\mathrm{H}t/\hbar}, \tag{4.15}$$

where H and S stands for the Heisenberg and Schrödinger representation, respectivily.

$$\Leftrightarrow \; i[\rho, \mathrm{A}(t)] = -i\rho \int_0^\beta \mathrm{d}\lambda \, \frac{\mathrm{d}}{\mathrm{d}\lambda} e^{\lambda \mathrm{H}} \mathrm{A}(t) e^{-\lambda \mathrm{H}}$$

$$\Leftrightarrow \; i[\rho, \mathrm{A}(t)] = -i\rho \int_0^\beta \mathrm{d}\lambda \left[\mathrm{H} e^{i\tilde{\lambda}\mathrm{H}/\hbar} \mathrm{A}(t) e^{-i\tilde{\lambda}\mathrm{H}/\hbar} - e^{i\tilde{\lambda}\mathrm{H}/\hbar} \mathrm{A}(t) e^{-i\tilde{\lambda}\mathrm{H}/\hbar} \mathrm{H} \right]$$

$$\Leftrightarrow \; i[\rho, \mathrm{A}(t)] = -i\rho \int_0^\beta \mathrm{d}\lambda \left[\mathrm{H}, \mathrm{A}(t + \tilde{\lambda}) \right]$$

$$\Leftrightarrow \; \frac{i}{\hbar}[\rho, \mathrm{A}(t)] = -\rho \int_0^\beta \mathrm{d}\lambda \, \dot{\mathrm{A}}(t + \tilde{\lambda}) = -\rho \int_0^\beta \mathrm{d}\lambda \, \dot{\mathrm{A}}(t - i\lambda\hbar), \tag{4.16}$$

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

Inserting equation (4.14) and (4.16) in the Kubo relaxation function yield the wanted form of the Kubo relaxation function, where on the right hand side of the following compuation is integrated by parts, dedicated with PI.

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

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

$$\overset{(4.16)}{\Leftrightarrow} \Phi_{\mathrm{AB}}(t) = -\lim_{s \to 0} \int_0^\beta \mathrm{d}\lambda \int_t^\infty \mathrm{d}\tau \left\langle \dot{\mathrm{A}}_\mathrm{I}(\tau - i\lambda\hbar) \mathrm{B_I}(0) \right\rangle_0 e^{-s\tau}$$

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

$$\Leftrightarrow \Phi_{\mathrm{AB}}(t) = \int_0^\beta \mathrm{d}\lambda \, \langle \mathrm{A_I}(t - i\lambda\hbar) \mathrm{B_I}(0) \rangle_0 = \int_0^\beta \mathrm{d}\lambda \, \langle \mathrm{A_I}(t) \mathrm{B_I}(i\lambda\hbar) \rangle_0 \tag{4.17}$$

Later we will see that the scalar product defining at the memory-matrix-formalsim has a similar structure. 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.

4.2.3 Kramer-Kronig-relation

All experiences of a human life demonstating that an incident is always bevor the reaction of a system, which 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 which is 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'.

$$\chi_{\mathrm{AB}}(\omega) = \int\limits_{-\infty}^{\infty} \mathrm{d}t\, e^{i(\omega'+i\omega'')t}\chi_{\mathrm{AB}}(t) \tag{4.18}$$

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.

$$\chi_{\mathrm{AB}}(\omega) = \frac{1}{2\pi i}\oint\limits_{\Gamma} \mathrm{d}\zeta\, \frac{\chi_{\mathrm{AB}}(\zeta)}{\zeta - \omega} \tag{4.19}$$

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. For reason of convergency the contour along the real part axis is moved infinitesimal in the upper half plane, indicated with $i\eta$, where $\eta \to 0$ is implicated.
The contribution of the semi-circle vanishs because it is assumed that $\chi_{\mathrm{AB}}(\omega)$ decrease very fast for large values of ω. Only a integral along the real part axis survives which can be evaluated by formally writing $\frac{1}{x+i\eta} = \mathrm{P.V.}\frac{1}{x} - i\pi\delta(x)$ where P.V. stands for taking the principal value.

$$\chi_{\mathrm{AB}}(\omega) = \frac{1}{2\pi i}\int\limits_{-\infty}^{\infty} \mathrm{d}\omega'\, \frac{\chi_{\mathrm{AB}}(\omega')}{\omega' - \omega - i\eta}$$

$$\Leftrightarrow\ \chi_{\mathrm{AB}}(\omega) = \frac{1}{2\pi i}\left[\mathrm{P.V.}\int\limits_{-\infty}^{\infty} \mathrm{d}\omega'\, \frac{\chi_{\mathrm{AB}}(\omega')}{\omega' - \omega} + i\pi \int\limits_{-\infty}^{\infty} \mathrm{d}\omega'\, \chi_{\mathrm{AB}}(\omega')\delta(\omega' - \omega)\right]$$

$$\Leftrightarrow\ \chi_{\mathrm{AB}}(\omega) = -\frac{i}{\pi}\mathrm{P.V.}\int\limits_{-\infty}^{\infty} \mathrm{d}\omega'\, \frac{\mathrm{Re}\{\chi_{\mathrm{AB}}(\omega')\}}{+} i\,\mathrm{Im}\{\chi_{\mathrm{AB}}(\omega')\}\omega' - \omega$$

$$\Leftrightarrow\ \chi_{\mathrm{AB}}(\omega) = \frac{1}{\pi}\mathrm{P.V.}\int\limits_{-\infty}^{\infty} \mathrm{d}\omega' \left[\frac{\mathrm{Im}\{\chi_{\mathrm{AB}}(\omega')\}}{\omega' - \omega} - i\frac{\mathrm{Re}\{\chi_{\mathrm{AB}}(\omega')\}}{\omega' - \omega}\right] \tag{4.20}$$

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.

$$\mathrm{Re}\{\chi_{\mathrm{AB}}(\omega)\} = \frac{1}{\pi}\mathrm{P.V.}\int\limits_{-\infty}^{\infty} \mathrm{d}\omega' \, \frac{\mathrm{Im}\{\chi_{\mathrm{AB}}(\omega')\}}{\omega' - \omega} \tag{4.21}$$

$$\mathrm{Im}\{\chi_{\mathrm{AB}}(\omega)\} = -\frac{1}{\pi}\mathrm{P.V.}\int\limits_{-\infty}^{\infty} \mathrm{d}\omega' \, \frac{\mathrm{Re}\{\chi_{\mathrm{AB}}(\omega')\}}{\omega' - \omega} \tag{4.22}$$

These two relations are called Kramers-Kronig-relation. They take the real and imaginary part of the a function, here the susceptibility, in a very usefull relation.

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, where a pertubation is switched on, is described by this function. Now the processes starting because of the pertubation can be classified into two types. On the one hand in dissipative prozesses and on the other hand in non-dissipative prozesses. In the following dissipative processes are investigated. The dissipative susceptibility of the form

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

$$\chi''_{\mathrm{AB}}(t-t') = \frac{1}{2\hbar}\left\langle [\mathrm{A}(t), \mathrm{B}(t')] \right\rangle \tag{4.23}$$

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

$$\left(\chi''_{\mathrm{AB}}(t-t')\right)^* = -\chi''_{\mathrm{AB}}(t-t') \tag{4.24}$$

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 (4.18). Notice that in the following computation the frequency ω isn't splitted into real and imaginary parts. Our calculation is started by multipling equation (4.8) with $e^{i\omega t}$ and integrating over time t.

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

$$\Leftrightarrow\ \chi_{\mathrm{AB}}(\omega) = \frac{1}{\pi}\mathrm{PV}\int_{-\infty}^{\infty} \mathrm{d}\omega'\,\frac{\chi''_{\mathrm{AB}}(\omega')}{\omega'-\omega} + i\int_{-\infty}^{\infty} \mathrm{d}\omega'\,\delta(\omega'-\omega)\chi''_{\mathrm{AB}}(\omega')$$

$$\Leftrightarrow\ \chi_{\mathrm{AB}}(\omega) = \chi'_{\mathrm{AB}}(\omega) + i\chi''_{\mathrm{AB}}(\omega) \tag{4.25}$$

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

$$\Theta_\eta(t) = i\lim_{\eta\to 0}\int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi}\,\frac{e^{-i\omega' t}}{\omega'+i\eta} \tag{4.26}$$

In equation (4.25) 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 (4.23). Equation (4.25) 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

$$\mathrm{A} = \sum_{i,j} |i\rangle\langle i|\,\mathrm{A}\,|j\rangle\langle j| = \sum_{i,j} \mathrm{A}_{ij}\,|i\rangle\,\langle j|\,, \tag{4.27}$$

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

$$\big|\mathrm{A}\big) := \sum_{ij}^{d} \mathrm{A}_{ij}\big||i\rangle\langle j|\big) \tag{4.28}$$

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 (4.28) 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 (4.28) 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 conditions

1. $\big(\mathrm{A}_i\big|\mathrm{A}_j\big) = \big(\mathrm{A}_j\big|\mathrm{A}_i\big)^*$ (4.29)
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 $c_1, c_2 \in \mathbb{C}$ (4.30)
3. $\big(\mathrm{A}_i\big|\mathrm{A}_i\big) \geq 0$ where equallity is fulfilled if $\mathrm{A}_i = 0.$ (4.31)

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

$$\big(\mathrm{A}_i(t)\big|\mathrm{A}_j(t')\big) = \frac{1}{\beta}\int_0^\beta \mathrm{d}\lambda \left\langle \mathrm{A}_i^\dagger(t)\mathrm{A}_j(t' + i\lambda\hbar)\right\rangle \tag{4.32}$$

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 conditions 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

$$
\begin{aligned}
\big(\mathrm{A}_i(t)\big|\mathrm{B}(t')\big) &= \frac{1}{\beta}\int\limits_0^\beta \mathrm{d}\lambda\,\frac{1}{Z}\,\mathrm{Tr}\Big\{\rho\mathrm{A}_i^\dagger(t)\Big[c_1\mathrm{A}_j(t'+i\lambda\hbar)+c_2\mathrm{A}_k(t'+i\lambda\hbar)\Big]\Big\} \\
\Leftrightarrow\ \big(\mathrm{A}_i(t)\big|\mathrm{B}(t')\big) &= c_1\big(\mathrm{A}_i(t)\big|\mathrm{A}_j(t')\big)+c_2\big(\mathrm{A}_i(t)\big|\mathrm{A}_k(t')\big)
\end{aligned}
\tag{4.33}
$$

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.

$$
\begin{aligned}
\big(\mathrm{A}_i(t)\big|\mathrm{A}_j(t')\big) &= \frac{1}{\beta\cdot Z}\int\limits_0^\beta \mathrm{d}\lambda\sum_{n,m}\langle n|\,e^{-\beta\mathrm{H}}\mathrm{A}_i^\dagger(t)\,|m\rangle\,\langle m|\,e^{-\lambda\mathrm{H}}\mathrm{A}_j(t')e^{\lambda\mathrm{H}}\,|n\rangle \\
\Leftrightarrow\ \big(\mathrm{A}_i(t)\big|\mathrm{A}_j(t')\big) &= \frac{1}{\beta\cdot Z}\sum_{n,m}\langle n|\mathrm{A}_i^\dagger(t)|m\rangle\,\langle m|\mathrm{A}_j(t')|n\rangle\,e^{-\beta E_n}\int\limits_0^\beta \mathrm{d}\lambda\,e^{\lambda(E_n-E_m)} \\
\Leftrightarrow\ \big(\mathrm{A}_i(t)\big|\mathrm{A}_j(t')\big) &= \frac{1}{\beta\cdot Z}\sum_{n,m}\langle n|\mathrm{A}_i^\dagger(t)|m\rangle\,\langle m|\mathrm{A}_j(t')|n\rangle\,\frac{e^{-\beta E_m}-e^{-\beta E_n}}{E_n-E_m}
\end{aligned}
\tag{4.34}
$$

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 (4.34) only the expactation values are complex numbers. For them the complex conjugation yields

$$
\Big(\,\langle n|\mathrm{A}_i^\dagger(t)|m\rangle\,\langle m|\mathrm{A}_j(t')|n\rangle\,\Big)^* = \langle n|\mathrm{A}_j^\dagger(t')|m\rangle\,\langle m|\mathrm{A}_i(t)|n\rangle \tag{4.35}
$$

and inserting back $(\mathrm{A}_i(t)|\mathrm{A}_j(t'))^*$ is exactly the same as (4.34). Proofing the third condition it has to be set $\mathrm{A}_j(t') = \mathrm{A}_i(t)$ in equation (4.34), which one the right hand side results in

$$
\big(\mathrm{A}_i(t)\big|\mathrm{A}_i(t)\big) = \frac{1}{\beta\cdot Z}\sum_{n,m}\big|\,\langle m|\mathrm{A}_i(t)|n\rangle\,\big|^2\frac{e^{-\beta E_m}-e^{-\beta E_n}}{E_n-E_m}. \tag{4.36}
$$

It's clear that the squared expectation 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

$$
\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A}_i(t) = \dot{\mathrm{A}}_i(t) = \frac{i}{\hbar}[\mathrm{H},\mathrm{A}_i(t)] = i\mathrm{L}\mathrm{A}_i(t) \tag{4.37}
$$

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 (4.37) is

$$\mathrm{A}_i(t) = e^{it\mathrm{L}}\mathrm{A}_i(0) = e^{it\mathrm{H}/\hbar}\mathrm{A}_i(0)e^{-it\mathrm{H}/\hbar}. \tag{4.38}$$

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 (4.37), which results in

Have to convince me that it is really so easy.

$$\big|\dot{\mathrm{A}}_i(t)\big) = \frac{i}{\hbar}\big|[\mathrm{H}, \mathrm{A}_i(t)]\big) = i\mathrm{L}\big|\mathrm{A}_i(t)\big) \tag{4.39}$$

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

$$\big|\mathrm{A}_i(t)\big) = e^{it\mathrm{L}}\big|\mathrm{A}_i(0)\big). \tag{4.40}$$

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

$$\mathrm{P} = \sum_{i,j} \big|\mathrm{C}_i(0)\big)\big(\mathrm{C}_i(0)\big|\mathrm{C}_j(0)\big)^{-1}\big(\mathrm{C}_j(0)\big|. \tag{4.41}$$

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

$$\mathcal{C}_{ij}(t) = \big(\mathrm{A}_i(t)\big|\mathrm{A}_j(0)\big) \overset{(4.32)}{=} \frac{1}{\beta}\int_0^\beta \mathrm{d}\lambda \left\langle \mathrm{A}_i^\dagger(t)\mathrm{A}_j(i\lambda\hbar)\right\rangle \tag{4.42}$$

where in the last step the definition of the scalar product is only inserted. Comparing equation (4.42) with (4.17) 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 the goal of t memory ma formalsim

$$\mathcal{C}_{ij}(t=0) = \frac{1}{\beta}\Phi_{ij}(t=0) = \frac{1}{\beta}\chi_{ij}(\omega=0), \tag{4.43}$$

which directly results from equation (4.12). Equation (4.40) is used to bring the time evolution of the correlation function in more suitable expression

$$\mathcal{C}_{ij}(t) = \big(\mathrm{A}_i(0)\big|\mathrm{A}_j(-t)\big) = \big(\mathrm{A}_i(0)\big|e^{-it\mathrm{L}}\big|\mathrm{A}_j(0)\big), \tag{4.44}$$

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

$$\mathcal{C}_{ij}(\omega) = \big(\mathrm{A}_i\big|\int\limits_0^\infty \mathrm{d}t\, e^{i(\omega-\mathrm{L})t}\big|\mathrm{A}_j\big) = \big(\mathrm{A}_i\big|\frac{i}{\omega-\mathrm{L}}\big|\mathrm{A}_j\big), \tag{4.45}$$

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 $\mathrm{Y} = -\mathrm{LP}$.

$$\begin{aligned} \mathcal{C}_{ij}(\omega) &= \big(\mathrm{A}_i\big|\frac{i}{\omega-\mathrm{LQ}-\mathrm{LP}}\big|\mathrm{A}_j\big) \\ \Leftrightarrow\ \mathcal{C}_{ij}(\omega) &= \big(\mathrm{A}_i\big|\frac{i}{\omega-\mathrm{LQ}}\big|\mathrm{A}_j\big) + \big(\mathrm{A}_i\big|\frac{1}{\omega-\mathrm{LQ}}\mathrm{LP}\frac{i}{\omega-\mathrm{L}}\big|\mathrm{A}_j\big) \end{aligned} \tag{4.46}$$

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

$$\frac{i}{\omega-\mathrm{LQ}} = \frac{i}{\omega}\left[1 + \frac{\mathrm{LQ}}{\omega} + \left(\frac{\mathrm{LQ}}{\omega}\right)^2 + \dots\right] \tag{4.47}$$

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

$$\big(\mathrm{A}_i\big|\frac{i}{\omega-\mathrm{LQ}}\big|\mathrm{A}_j\big) = \frac{i}{\omega}\big(\mathrm{A}_i\big|\mathrm{A}_j\big) = \frac{i}{\omega}\mathcal{C}_{ij}(0). \tag{4.48}$$

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.

$$\mathrm{P}\frac{i}{\omega-\mathrm{L}}\big|\mathrm{A}_j\big) = \sum_{k,l}\big|\mathrm{C}_k\big)\big(\mathrm{C}_k\big|\mathrm{C}_l\big)^{-1}\big(\mathrm{C}_l\big|\frac{i}{\omega-\mathrm{L}}\big|\mathrm{A}_j\big) = \sum_{k,l}\big|\mathrm{C}_k\big)\mathcal{C}^{-1}_{kl}(0)\mathcal{C}_{lj}(\omega) \tag{4.49}$$

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

$$\mathcal{C}_{ij}(\omega) = \frac{i}{\omega}\mathcal{C}_{ij}(0) + \sum_{k,l}\big(\mathrm{A}_i\big|\frac{1}{\omega-\mathrm{LQ}}\mathrm{L}\big|\mathrm{C}_k\big)\mathcal{C}^{-1}_{kl}(0)\mathcal{C}_{lj}(\omega). \tag{4.50}$$

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.

$$\frac{\omega}{\omega-\mathrm{LQ}} = \frac{\omega-\mathrm{LQ}+\mathrm{LQ}}{\omega-\mathrm{LQ}} = 1+\frac{\mathrm{LQ}}{\omega-\mathrm{LQ}} \tag{4.51}$$

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

$$\begin{aligned}
&\omega\mathcal{C}_{ij}(\omega) = i\mathcal{C}_{ij}(0) + \sum_{k,l}\big(\mathrm{A}_i\big|\frac{\omega}{\omega-\mathrm{LQ}}\mathrm{L}\big|\mathrm{C}_k\big)\mathcal{C}^{-1}_{kl}(0)\mathcal{C}_{lj}(\omega)\\
\Leftrightarrow\ &\omega\mathcal{C}_{ij}(\omega) = i\mathcal{C}_{ij}(0) + \sum_{k,l}\big(\mathrm{A}_i\big|1+\frac{\mathrm{LQ}}{\omega-\mathrm{LQ}}\mathrm{L}\big|\mathrm{C}_k\big)\mathcal{C}^{-1}_{kl}(0)\mathcal{C}_{lj}(\omega)\\
\Leftrightarrow\ &\omega\sum_l\delta_{il}\mathcal{C}_{lj}(\omega) = i\frac{1}{\beta}\chi_{ij}(0) + \sum_l\Big[\Omega_{il} - i\Sigma_{il}(\omega)\Big]\mathcal{C}_{lj}(\omega)\\
\Leftrightarrow\ &\sum_l\Big[\omega\delta_{il} - \Omega_{il} + i\Sigma_{il}(\omega)\Big]\mathcal{C}_{lj}(\omega) = i\frac{1}{\beta}\chi_{ij}(0)
\end{aligned} \tag{4.52}$$

where equation (4.12) is used and the abbreviations

$$\Omega_{il} := \beta\sum_k\big(\mathrm{A}_i\big|\mathrm{L}\big|\mathrm{C}_k\big)\chi^{-1}_{kl}(0) \quad \text{and} \quad \Sigma_{il}(\omega) := i\beta\sum_k\big(\mathrm{A}_i\big|\frac{\mathrm{LQ}}{\omega-\mathrm{LQ}}\mathrm{L}\big|\mathrm{C}_k\big)\chi^{-1}_{kl}(0) \tag{4.53}$$

are inserted. Equation (4.52) 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 (4.52) 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 (4.39), so that

$$\Omega_{il} = i\beta\sum_k\big(\dot{\mathrm{A}}_i\big|\mathrm{C}_k\big)\chi^{-1}_{kl}(0). \tag{4.54}$$

For the rearrangement of the second abbreviation in a first step equation (4.39) 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.

$$\begin{aligned}
\Sigma_{il}(\omega) &= \frac{i\beta}{\omega}\sum_k \big(\dot{\mathrm{A}}_i\big|\mathrm{Q}\Big[1+\frac{\mathrm{LQ}}{\omega}+\Big(\frac{\mathrm{LQ}}{\omega}\Big)^2+\dots\Big]\big|\dot{\mathrm{C}}_k\big)\chi^{-1}_{kl}(0)\\
\Leftrightarrow \Sigma_{il}(\omega) &= \frac{i\beta}{\omega}\sum_k \big(\dot{\mathrm{A}}_i\big|\mathrm{Q}^2+\frac{\mathrm{Q}^2\mathrm{LQ}^2}{\omega}+\frac{\mathrm{Q}^2\mathrm{LQ}^2\mathrm{LQ}^2}{\omega^2}+\dots\big|\dot{\mathrm{C}}_k\big)\chi^{-1}_{kl}(0)\\
\Leftrightarrow \Sigma_{il}(\omega) &= \frac{i\beta}{\omega}\sum_k \big(\dot{\mathrm{A}}_i\big|\mathrm{Q}\Big[1+\frac{\mathrm{QLQ}}{\omega}+\Big(\frac{\mathrm{QLQ}}{\omega}\Big)^2+\dots\Big]\mathrm{Q}\big|\dot{\mathrm{C}}_k\big)\chi^{-1}_{kl}(0)\\
\Leftrightarrow \Sigma_{il}(\omega) &= i\beta\sum_k \big(\dot{\mathrm{A}}_i\big|\mathrm{Q}\frac{1}{\omega-\mathrm{QLQ}}\mathrm{Q}\big|\dot{\mathrm{C}}_k\big)\chi^{-1}_{kl}(0) \qquad (4.55)
\end{aligned}$$

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 (4.52) 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 $\big(\dot{\mathrm{A}}_i\big|\mathrm{A}_k\big) = 0$. 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 (4.55) with the definition (4.42) of correlation functions exhibits $\Sigma(\omega)$ has the structur of a correlation function but $\Sigma(\omega)$ occupies to differences. On the one hand only $\mathrm{Q}\big|\dot{\mathrm{A}}\big)$ which is perpendicular to $\big|\mathrm{A}\big)$ 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 $\mathrm{Q}\big|\dot{\mathrm{A}}\big)$ 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?

$$\mathrm{A}(t) \to \mathrm{A}'(t) = \mathrm{T}\mathrm{A}(t)\mathrm{T}^{-1} = \epsilon_{\mathrm{A}}\mathrm{A}(-t) \tag{4.56}$$

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.

$$\mathrm{T}e^{i\mathrm{Ht}/\hbar}\mathrm{T}^{-1} = e^{-i\mathrm{Ht}/\hbar} \tag{4.57}$$

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

$$\mathrm{T}\frac{\partial}{\partial t}e^{i\mathrm{Ht}/\hbar}\mathrm{T}^{-1} = \frac{i}{\hbar}\mathrm{T}\mathrm{H}e^{i\mathrm{Ht}/\hbar}\mathrm{T}^{-1} = \frac{i}{\hbar}\mathrm{T}\mathrm{H}\mathrm{T}^{-1}\mathrm{T}e^{i\mathrm{Ht}/\hbar}\mathrm{T}^{-1} = \frac{i}{\hbar}\mathrm{H}e^{-i\mathrm{Ht}/\hbar} \tag{4.58}$$

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

$$\mathrm{T}\mathrm{H} = \mathrm{H}\mathrm{T} \qquad \Leftrightarrow \qquad [\mathrm{H}, \mathrm{T}] = 0 \tag{4.59}$$

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.

$$\langle \mathrm{B} \rangle = \frac{1}{Z}\,\mathrm{Tr}\Big\{e^{-\beta\mathrm{H}}\mathrm{T}\mathrm{B}\mathrm{T}^{-1}\Big\} = \Big\langle \big(\mathrm{T}\mathrm{B}\mathrm{T}^{-1}\big)^{\dagger} \Big\rangle \tag{4.60}$$

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.

$$\Big(\mathrm{T}\big[\mathrm{A}(t), \mathrm{B}(t')\big]\mathrm{T}^{-1}\Big)^{\dagger} = \epsilon_{\mathrm{A}}\epsilon_{\mathrm{B}}\Big(\big[\mathrm{A}(-t), \mathrm{B}(-t')\big]\Big)^{\dagger} = -\epsilon_{\mathrm{A}}\epsilon_{\mathrm{B}}\big[\mathrm{A}(-t), \mathrm{B}(-t')\big] \tag{4.61}$$

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 (4.54). Using equation (4.25) yields

$$i\beta\big(\dot{\mathrm{A}}_i\big|\mathrm{A}_k\big) = i\chi_{\dot{\mathrm{A}}_i\mathrm{A}_k}(\omega = 0) = i\,\mathrm{PV}\int\limits_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{\pi}\frac{\chi''_{\dot{\mathrm{A}}_i\mathrm{A}_k}(\omega')}{\omega'} - \lim_{\omega\to 0}\chi''_{\dot{\mathrm{A}}_i\mathrm{A}_k}(\omega), \tag{4.62}$$

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 (4.23) is formed.

$$\frac{\mathrm{d}}{\mathrm{d}t}\chi''_{\mathrm{A}_i\mathrm{A}_k}(t) = \frac{1}{2\hbar}\left\langle\left[\dot{\mathrm{A}}_i(t),\mathrm{A}_k(0)\right]\right\rangle = \chi''_{\dot{\mathrm{A}}_i\mathrm{A}_k}(t) \tag{4.63}$$

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

$$\chi''_{\dot{\mathrm{A}}_i\mathrm{A}_k}(\omega) = -i\omega\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega) \tag{4.64}$$

Inserting this in (4.65) yields

$$i\beta\big(\dot{\mathrm{A}}_i\big|\mathrm{A}_k\big) = \mathrm{PV}\int\limits_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{\pi}\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega') \tag{4.65}$$

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.

$$\chi''_{\mathrm{A}_i\mathrm{A}_k}(t-t') = \frac{1}{2\hbar}\left\langle\left[\mathrm{A}_i(t),\mathrm{A}_k(t')\right]\right\rangle \tag{4.66}$$

The expectation value is rewriten using equation (4.60) which establishes the oppertunity to use (4.61).

$$\chi''_{\mathrm{A}_i\mathrm{A}_k}(t-t') = -\epsilon_{\mathrm{A}_i}\epsilon_{\mathrm{A}_k}\chi''_{\mathrm{A}_i\mathrm{A}_k}(t'-t), \tag{4.67}$$

where the relation (4.24) is used. The Laplace transformation of this equation yields

$$\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega) = -\epsilon_{\mathrm{A}_i}\epsilon_{\mathrm{A}_k}\chi''_{\mathrm{A}_i\mathrm{A}_k}(-\omega) = \epsilon_{\mathrm{A}_i}\epsilon_{\mathrm{A}_k}\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega), \tag{4.68}$$

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.

$$\Big(\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega)\Big)^* = -\int\limits_{-\infty}^{\infty}\mathrm{d}t\, e^{-i\omega(t-t')}\chi''_{\mathrm{A}_i\mathrm{A}_k}(t-t') = -\chi_{\mathrm{A}_i\mathrm{A}_k}(-\omega) = \chi_{\mathrm{A}_i\mathrm{A}_k}(\omega) \tag{4.69}$$

where equation (4.24) is used.

2. case: $\epsilon_{\mathrm{A}_i} \neq \epsilon_{\mathrm{A}_k}$
If the signature of A_i and A_k is different 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.

$$\Big(\chi''_{\mathrm{A}_i\mathrm{A}_k}(\omega)\Big)^* = -\int\limits_{-\infty}^{\infty} \mathrm{d}t\, e^{-i\omega(t-t')}\chi''_{\mathrm{A}_i\mathrm{A}_k}(t-t') = -\chi_{\mathrm{A}_i\mathrm{A}_k}(-\omega) = -\chi_{\mathrm{A}_i\mathrm{A}_k}(\omega) \quad (4.70)$$

Back to equation (4.65). 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 (4.52) 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 bessere Formulierung finden

besser formulieren

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 (4.52) 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 (4.52) yields

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

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 (4.43). The correlation function at $t = 0$ is given by the scalar product $(\mathrm{J}(0)|\mathrm{J}(0))$, see equation (4.42). 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

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

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 $|\mathrm{P})$.

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

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 $(\mathrm{P}|\mathrm{P})$.

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

Using (4.43) 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

link zu umklapp hamiltonian

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

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

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

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

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

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

vllt noch etwas ausführlicher schreiben

link zum ungestörten Hamiltonian

link zum umklapp Hamiltonian

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.
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 different 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 (4.52) 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 (4.52) 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

Warum ist der erste Term vernachlässigbar. Begründung?

Warum darf QLQ mit L_0 approximiert werden?

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

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

The memory function $\Sigma_{\mathrm{PP}}(\omega)$ is definied in equation (4.55). 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

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

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 equilibrium 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.

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

The norm of the Jacobi determinate is $-i$ and the upper integral limit changes from infinity to β. Further each time derivative yields an i. Totally the factor i is multiplied to the integral. The direction of the momentum is denoted with the index j and to symbolisied clearly that the frequency is an arbitrary number in the complex plane 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 Hamiltonian $\mathrm{H}_0 = \mathrm{H}_\Psi + \mathrm{H}_\Phi$ and the interation $\mathrm{H}_{\Psi\Phi}$ is only entered in the time evolution operator $\mathrm{U}(\beta, 0)$. A series expansion of this one up to the first non-disappearing order yields

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

where it has to be remarked that in quantum field pertubation theory only connected diagrams are considered, which is indicated with "con" at the expectation value. All disconnected diagrams can be factorizied in the numerator. These diagrams are exactly the same one as in the denominator, so both cancel each other.

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 any-more 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

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

where j indicated the direction of the momentum like above. The sum over μ is implied. Inserting the time derivative of the momentum in $\mathrm{I}_{jj}(z)$ yields

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

The expectation value is evaluated by using Wick's theorem, where the expectation value is related to the ground state of the system. Therefore all normal products are zero and only the sum survives, where all operators are contracted. The sum yields three different possible contraction of the operators, where one of them is a disconnected diagram. The diagram is originated by contracting the operators with the same time argument. This diagram is canceled with the vacuum diagrams like discussed above, why it must not considered in the following computation. In total Wick's theorem yields two contributing diagrams, which are depicted in figure . . . .

Bild mit bubble diagram und link

Link zu kommutator relationen

Because the used operators are in momentum space each expectation value of two operators becomes a δ-distribution, originated from the commutator relations in momentum space. The δ-distributions signify the conservation of momentum. In the investigated case the commutator relations ... have to be used. Then one momentum integral and one sum over reziprocal lattive vectors is performed. The remaining momentum and reziprocal lattice vector is renamed into $\mathbf{k}$ and $\mathbf{K}$ respectivily. Further one sum over the spactial direction of Φ, denoted with the greek letter, is performed.

$$\mathcal{G}_{jj}(z) = -\frac{2}{\hbar^2}\sum_{\mathbf{K}} |\mathrm{J}_{\mathbf{K}}|^2 \int\limits_0^\beta \mathrm{d}\tau\, e^{z\tau} \int_{\mathbf{k}} K_j^2 \\ \times \left\langle \mathcal{T}_\tau \Phi_\mu(\mathbf{k},\tau)\Phi_\mu(-\mathbf{k},0)\right\rangle_{\mathrm{H}_0} \left\langle \mathcal{T}_\tau \Phi_\mu(-\mathbf{k}-\mathbf{K},\tau)\Phi_\mu(\mathbf{k}+\mathbf{K},0)\right\rangle_{\mathrm{H}_0} \tag{5.24}$$

where $\mathrm{J}_{-\mathbf{K}} = \mathrm{J}^*_{\mathbf{K}}$ is used. The asterisk denotes the complex conjugated. Every single expectation value correspond to thr free propagator of spin density waves. The free propagator is defined by $\mathcal{D}^{(0)}_\mu(\mathbf{k},\tau) := \left\langle \mathcal{T}_\tau \Phi_\mu(\mathbf{k},\tau)\Phi_\mu(-\mathbf{k},0)\right\rangle_{\mathrm{H}_0}$. Both are speratly transformed into Matsubara frequency space via

$$\mathcal{D}^{(0)}_\mu(\mathbf{k},\tau) = \frac{1}{\beta}\sum_{\omega_n} e^{-i\omega_n\tau}\mathcal{D}^{(0)}_\mu(\mathbf{k},\omega_n) \tag{5.25}$$

where the summation runs over all Matsubara frequencies. Because the transformation rotates our investigated function onto the imaginary frequency axis, the complex frequency z has to be set to $i\omega_l$. After transforming the propagators into Matsubara frequency space the imaginary time dependence is solely originated from the exponential functions. This offers us to perform the τ-integral easily, where relation

$$\int_0^\beta \mathrm{d}\tau\, e^{-i(\omega_m+\omega_n-\omega_l)\tau} = \beta\delta_{\omega_m,\omega_l-\omega_n} \tag{5.26}$$

is used and then one of the two sums over Matsubara frequencies can be performed as well. After all these steps the integral has the form

$$\mathcal{G}_{jj}(i\omega_l) = -\frac{2}{\hbar^2}\sum_{\mathbf{K}} |\mathrm{J}_{\mathbf{K}}|^2 \int_{\mathbf{k}} K_j^2 \frac{1}{\beta}\sum_{\omega_n} \mathcal{D}_\mu(\mathbf{k},\omega_n)\,\mathcal{D}_\mu(-\mathbf{k}-\mathbf{K},\omega_l-\omega_n) \tag{5.27}$$

Link zum freien Propagator in expliziter Form

In the following the Matsubara sum is evaluated. Therefore we have to check the singularities of both propgators. Regarding equation ..., illustrates that the propagator has a discontinuity if the absoulte value of the Matsubara frequency is zero. This kind of singularity is called branch cut, because the whole horizontal line at the singularity is forbidden in the complex plane. Branch cuts are the reason why the Matsubara sum isn't so easily transformed into a contour integral in the complex plane like it is done usually, if the propagators have simple poles. In the investigated case the propagators have to singularity of this kind, one at $\omega_n = 0$ and one at $\omega_n = \omega_l$, which correspond to $n = 0$ and $n = l$. The strategy to evaluate those Matsubara sums is to seperate the singularities from the sum. For reasons of simplizity the momentum argument of the second propagator is abbreviatied as $\mathbf{k}' = -\mathbf{k} - \mathbf{K}$.

$$
\begin{aligned}
S(i\omega_l) :&= \frac{1}{\beta} \sum_{\omega_n} \mathcal{D}_{\mu,\mathbf{k}}(i\omega_n)\, \mathcal{D}_{\mu,\mathbf{k}'}(i\omega_l - i\omega_n) \\
\Leftrightarrow \quad S(i\omega_l) :&= \frac{1}{\beta} \mathcal{D}_{\mu,\mathbf{k}}(0)\, \mathcal{D}_{\mu,\mathbf{k}'}(i\omega_l) + \frac{1}{\beta} \mathcal{D}_{\mu,\mathbf{k}}(i\omega_l)\, \mathcal{D}_{\mu,\mathbf{k}'}(0) \\
&\quad + \frac{1}{\beta} \sum_{\substack{n\neq 0 \\ n\neq l}} \mathcal{D}_{\mu,\mathbf{k}}(i\omega_n)\, \mathcal{D}_{\mu,\mathbf{k}'}(i\omega_l - i\omega_n)
\end{aligned} \tag{5.28}
$$

where the momentum argument is writen as an index until the Matsubara sum is evaluated. Now the remaining sum can be transformed into a complex contour integral. Thereby the contour Γ includes all Matsubara frequencies ω_n on the inaginary axis, beside the two splitted off, and is taken counterclockwise. The contour Γ is depicted in figure . . . .

Link zum Bild der Kontour

$$
\mathrm{I}_{MS}(\omega_l) := \frac{1}{\beta} \sum_{\substack{n\neq 0 \\ n\neq l}} \mathcal{D}_{\mu,\mathbf{k}}(i\omega_n)\, \mathcal{D}_{\mu,\mathbf{k}'}(i\omega_l - i\omega_n) = \oint_{\Gamma} \frac{\mathrm{d}z}{2\pi i} n_{\mathrm{B}}(z) \mathcal{D}_{\mu,\mathbf{k}}(z)\, \mathcal{D}_{\mu,\mathbf{k}'}(i\omega_l - z) \tag{5.29}
$$

where $n_{\mathrm{B}}(z)$ is the Bose distribution. Like it is shown in . . . Γ consists of three single contours which are denoted as Γ_1, Γ_2 and Γ_3. These three contours are expanded to infity where the contour line is never allow to cross the horizontal line at ω_l and 0, see figure .

Link zum Kontourbild

link to figure

The contour Γ_1 is taken along the real axis in negative direction and is closed by a semicircle with infinite radius in the lower complex plane. Γ_2 is the contour between both branch cuts. Starting the contour along the real axis in positive direction. At infinity the contour is going up to the branch cut at ω_n, along this axis back to minus infinity and finally back down to the starting point. The last contour Γ_3 is going along the ω_n-axis in positive direction and is closed by a semicircle with infinite radius in the upper complex plane. The contour along the real and ω_n-axis has to be set infinitesimal beside the axis, which is indicated with the term $\pm i\eta$. The sign has to be chosen according to the contour.

Each one of these three contour integrals can be splitted in parts. Γ_1 and Γ_3 the contour is seperated into the path along the real and ω_n-axis, respectivily, and the semicircle. In both cases the contribution of the semicircles vanish, because the integrand decreases faster than $1/z$. In total Γ_2 is seperated into four parts. Two parts are the paths along the real and ω_n-axis. The other both paths are the connecting path between them. Equally to the case of the semicircles these two path vanish. In summary only the paths along the two branch cuts survive.

$$
\mathrm{I}_{MS}(\omega_l) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\epsilon}{2\pi i} \mathcal{D}_{\mu,\mathbf{k}'}(i\omega_l - \epsilon) \Big[n_{\mathrm{B}}(\epsilon - i\eta) \mathcal{D}_{\mu,\mathbf{k}}(\epsilon - i\eta) - n_{\mathrm{B}}(\epsilon + i\eta) \mathcal{D}_{\mu,\mathbf{k}}(\epsilon + i\eta) \Big]
$$

$$+\int_{-\infty}^{\infty}\frac{\mathrm{d}\epsilon}{2\pi i}\mathcal{D}_{\mu,\mathbf{k}}(i\omega_l+\epsilon)\Big[n_{\mathrm{B}}(i\omega_l+\epsilon-i\eta)\mathcal{D}_{\mu,\mathbf{k}'}(\epsilon-i\eta)$$
$$-\,n_{\mathrm{B}}(i\omega_l+\epsilon+i\eta)\mathcal{D}_{\mu,\mathbf{k}'}(\epsilon+i\eta)\Big] \tag{5.30}$$

where the limit $\eta \to 0^+$ is implied and we used that the propagator $\mathcal{D}$ is symmetric with respect to the frequency argument. It is easy to prove that $n_{\mathrm{B}}(z+i\omega_l) = n_{\mathrm{B}}(z)$, which means that the Bose distribution is invariant with respect to Matsubara frequencies. Thereby is $z \in \mathbb{C}$ and $\omega_l = 2\pi l/\beta$ with $l \in \mathbb{Z}$ is a bosonic Matsubara frequency and therefore $\exp(i\omega_l) = 1$. Now we set $z = \epsilon \pm i\eta$ and investigate the Bose distribution with respect to the limit $\epsilon \to 0$. We expand the exponential function up to the second non disappearing order, because of the singularity of the Bose distribution at $\epsilon = 0$.

$$n_{\mathrm{B}}(\epsilon \pm i\eta) \approx \frac{\beta^{-1}}{\epsilon \pm i\eta} = \beta^{-1}\Big(\mathrm{P.V.}\frac{1}{\epsilon} \mp i\pi\delta(\epsilon)\Big) = n_{\mathrm{B}}(\epsilon) \mp i\pi\beta^{-1}\delta(\epsilon), \tag{5.31}$$

where the last equality is only valid for small frequencies. Going back to equation (5.30). The Bose distributions in both squared brackets become equally, because the Bose distribution is invariant with respect to Matsubara frequencies. Thus the only difference between the terms in the brackets exist in the momentum argument of the propagators. Writing the Bose distribution and the propagators by real and imaginary parts, using that the real parts of n_{B} and $\mathcal{D}$ are symmetric and that the imaginary parts are antisymmetric under changing $\eta \to -\eta$, yield

nachvollziehen, dass die Symmetrieaussage stimmt

$$2i\Big[\,\mathrm{Re}\{n_{\mathrm{B}}(\epsilon+i\eta)\}\,\mathrm{Im}\{\mathcal{D}_{\mu,\mathbf{k}}(\epsilon+i\eta)\}+\mathrm{Im}\{n_{\mathrm{B}}(\epsilon+i\eta)\}\,\mathrm{Re}\{\mathcal{D}_{\mu,\mathbf{k}}(\epsilon+i\eta)\}\Big] \tag{5.32}$$

for the squared brackets in the first line of equation (5.30) and the analogical expression for the squared brackets in the second line, changing $\mathbf{k} \to \mathbf{k}'$. Firstly the second term of (5.32) should be investigated. The imaginary part of the Bose distribution is given by equation (5.31), where the δ-distribution makes life easy for us. Evaluating both integrals over the second terms in (5.32) yield

$$-\frac{1}{\beta}\mathcal{D}_{\mu,\mathbf{k}'}(i\omega_l)\,\mathrm{Re}\{\mathcal{D}_{\mu,\mathbf{k}}(0)\}-\frac{1}{\beta}\mathcal{D}_{\mu,,\mathbf{k}}(i\omega_l)\,\mathrm{Re}\big\{\mathcal{D}_{\mu,\mathbf{k}'}(0)\big\} \tag{5.33}$$

where the obviously relation $\mathrm{Re}\{\mathcal{D}_{\mu,\mathbf{k}}(0)\} = \mathcal{D}_{\mu,\mathbf{k}}(0)$ is used, which is independently of the momentum. Comparing this result with the both first terms in (5.28) we see that both expressions are equally beside a global sign and thus both cancel each other. Therefore the only contribution of the Matsubara sum is originated by the first term of the squared brackets in (5.32). The real part of $n_{\mathrm{B}}(\epsilon+i\eta)$ is $n_{\mathrm{B}}(\epsilon)$, see equation (5.31). Further the imaginary part of the propagator is independent of the additional part $i\eta$.

$$S(i\omega_l) = \int_{-\infty}^{\infty}\frac{\mathrm{d}\epsilon}{\pi}n_{\mathrm{B}}(\epsilon)\Big[\mathcal{D}_{\mu,\mathbf{k}'}(i\omega_l-\epsilon)\,\mathrm{Im}\{\mathcal{D}_{\mu,\mathbf{k}}(\epsilon)\}+\mathcal{D}_{\mu,\mathbf{k}}(i\omega_l+\epsilon)\,\mathrm{Im}\big\{\mathcal{D}_{\mu,\mathbf{k}'}(\epsilon)\big\}\Big] \tag{5.34}$$

Now we are at the point that $S(i\omega_l)$ can be analytical continuated on the real axis of ω, which is a physical quantity beside $i\omega_l$. Therefore we have to set $i\omega_l = \omega + i\eta =: \tilde{\omega}$, where the limit $\eta \to 0^+$ is implied. Regarding equation … we see that $\mathcal{D}_{\mu,\mathbf{k}'}(\epsilon - \omega) = \mathcal{D}^*_{\mu,\mathbf{k}'}(\omega - \epsilon)$, where the asterisk means the complex conjugated.

link to propagator function on real axis

$$S(\omega) = \int\limits_{-\infty}^{\infty} \frac{\mathrm{d}\epsilon}{\pi} n_{\mathrm{B}}(\epsilon) \Big[\mathcal{D}^*_{\mu,\mathbf{k}'}(\epsilon - \omega)\, \mathrm{Im}\{\mathcal{D}_{\mu,\mathbf{k}}(\epsilon)\} + \mathcal{D}_{\mu,\mathbf{k}}(\epsilon + \omega)\, \mathrm{Im}\{\mathcal{D}_{\mu,\mathbf{k}'}(\epsilon)\} \Big] \tag{5.35}$$

In the first term the frequency argument is shifted from $\epsilon - \omega \to \epsilon$, so that the propagators with the same momentum argument have the same frequency argument. The last step is to take the imaginary part of $S(\omega)$. This approach is valid, because the resitivity is defined by the imaginary part of the retarted Green function which corresponds to (5.27). The only possible complex quantity in (5.27) is the Matsubara sum, defined in (5.28). Thus the imaginary part of the Matsubara sum is given by

$$\mathrm{Im}\{S(\omega)\} = \int\limits_{-\infty}^{\infty} \frac{\mathrm{d}\epsilon}{\pi} \Big[n_{\mathrm{B}}(\epsilon) - n_{\mathrm{B}}(\epsilon + \omega) \Big]\, \mathrm{Im}\{\mathcal{D}_{\mu}(-\mathbf{k} - \mathbf{K}, \epsilon)\}\, \mathrm{Im}\{\mathcal{D}_{\mu}(\mathbf{k}, \epsilon + \omega)\} \tag{5.36}$$

where we used that the imaginary part of the propagator $\mathcal{D}$ and his complex conjugated one $\mathcal{D}^*$ are equal beside a minus. $\mathrm{Im}\{S(\omega)\}$ is inserted in equation (5.27), where the analytical continuation, which was done for the Matsubara sum, have similarly to do for the Green function.

$$\begin{aligned} \mathrm{G}^{\mathrm{ret}}_{jj}(\omega) = &-\frac{2}{\hbar^2} \sum_{\mathbf{K}} |\mathrm{J}_{\mathbf{K}}|^2 \int\limits_{-\infty}^{\infty} \frac{\mathrm{d}\epsilon}{\pi} \Big[n_{\mathrm{B}}(\epsilon) - n_{\mathrm{B}}(\epsilon + \omega) \Big] \\ &\times \int_{\mathbf{k}} K_j^2\, \mathrm{Im}\{\mathcal{D}_{\mu}(-\mathbf{k} - \mathbf{K}, \epsilon)\}\, \mathrm{Im}\{\mathcal{D}_{\mu}(\mathbf{k}, \epsilon + \omega)\}, \end{aligned} \tag{5.37}$$

The spin density wave propagator is given by equation … and the imaginary part is obtained by expanding with the complex conjugated denominator. Further the limit of small frequncies ω is considered. On that account the Bose distribution has to be approximated up to the second order, otherwise the expression would be zero. The expression of the propagators is friendly in the limit of small frequencies thus ω can be set to zero. Additional the integrand is an even function with respect to ϵ, which is easy to see. Beside the exponential functions the expression is only depended on ϵ^2-terms, which are obviously even. The eponential expression is even as well, which is easily shown by factorizied the exponential function in the denominator. Therefore the lower limit of the integral is set to zero and the complete expression is multiplied with two.

link to spin fermion propagator for real omega

$$\mathrm{G}^{\mathrm{ret}}_{jj}(\omega) = -\frac{4\gamma^2 \beta \omega}{\pi \hbar^2} \sum_{\mathbf{Q}_1, \mathbf{Q}_2} \sum_{\mathbf{K}} |\mathrm{J}_{\mathbf{K}}|^2 \int\limits_0^{\infty} \mathrm{d}\epsilon\, \frac{\epsilon^2 e^{\beta\epsilon}}{(e^{\beta\epsilon} - 1)^2}$$

$$
\times \int_{\mathbf{k}} K_j^2 \cdot \frac{1}{(\mathbf{k}+\mathbf{K}-\mathbf{Q}_1)^4+\gamma^2\epsilon^2} \cdot \frac{1}{(\mathbf{k}+\mathbf{Q}_2)^4+\gamma^2\epsilon^2} \tag{5.38}
$$

The Green function has to be investigated in different cases to prove the convergence. For large values of the mometum vector the function is clearly convergent because of two reasons. Firstly the function is proportional to $1/\mathbf{k}^4$ which is a fastly decreasing function with respect to large values of $\mathbf{k}$. Secondly the momentum vector is restricted to the first Brillouin zone, so even if there would be a divergence for large $\mathbf{k}$ the values didn't reach these values. Nevertheless there can be a divergence if the reciprocal lattice vector component K_j is large. It's imaginable that K_j is compensated by the respective component of $\mathbf{Q}_1$ and thus the denominater is small compared to the numerator. The convergence of the Green function is ensured by the coupling constant $\mathrm{J}_{\mathbf{K}}$, which is decreasing fast to zero how longer the coupling distance is. This assumption isn't contradicted to any physical observation.
In the case of small values of the momentum vector the situation is slightly different. Consider the case $\mathbf{K}-\mathbf{Q}_1=0$ and $\mathbf{Q}_2=0$, which is the most divergent and hence the most dangerous case.

$$
\mathrm{G}_{jj}^{\mathrm{ret}}(\omega) = -\frac{4\gamma^2\beta\omega}{\pi\hbar^2}|\mathrm{J}_{\mathbf{K}}|^2 \cdot K_j^2 \int_0^\infty \mathrm{d}\epsilon\, \frac{\epsilon^2 e^{\beta\epsilon}}{(e^{\beta\epsilon}-1)^2} \int_{\mathbf{k}} \frac{1}{\left(\mathbf{k}^4+\gamma^2\epsilon^2\right)^2} \tag{5.39}
$$

It's more convenient for the further computation to transform the variables into dimensionless ones. The transformation instruction for the frequancy and momentum is $x=\beta\epsilon$ and $\mathbf{y}=\sqrt{\beta/\gamma}\,\mathbf{k}$, respectivily. The limits of the $\mathbf{y}$-integral are changed to $\pm\pi\sqrt{\beta/\gamma}$. Further the Jacobi determinate yields in total γ/β^2. For reasons of simplicity the constant parameters are combined to the constant C.

$$
\mathrm{G}_{jj}^{\mathrm{ret}}(\omega) = C\cdot\beta\omega|\mathrm{J}_{\mathbf{K}}|^2 \cdot K_j^2 \int_0^\infty \mathrm{d}x\, \frac{x^2 e^{x}}{(e^{x}-1)^2} \int_{\mathbf{y}} \frac{1}{\left(\mathbf{y}^4+x^2\right)^2} \tag{5.40}
$$

The following strategy is the transform the two dimensional $\mathbf{y}$-integral into plane polar coordinates. Considering the integrand decrease very fast to zero with respect to large values of $\mathbf{y}$, thus the upper boundary of the integral can be set to infinity. Further the angle integral yields the value 2π, because the integrand is angular independent.

picture of the function which shows the decreasing condition

$$
\mathrm{G}_{jj}^{\mathrm{ret}}(\omega) = \frac{C}{2\pi}\cdot\beta\omega|\mathrm{J}_{\mathbf{K}}|^2 \cdot K_j^2 \int_0^\infty \mathrm{d}x\, \frac{x^2 e^{x}}{(e^{x}-1)^2} \int_0^\infty \mathrm{d}y\, \frac{y}{\left(y^4+x^2\right)^2} \tag{5.41}
$$

Factorizing x^2 in the fraction and again substituting $z=y^2/x$. The limits of the integral dosen't changed during this transformation. Besides the new differential is given by $x\,\mathrm{d}z = 2y\,\mathrm{d}y$. The resulting z-integral is exactly solvable and yields

$$
\int_0^\infty \mathrm{d}z\, \frac{1}{\left(z^2+1\right)^2} = \frac{1}{2}\left[\frac{z}{z^2+1}+\arctan(z)\right]\Bigg|_0^\infty = \frac{\pi}{4} \tag{5.42}
$$

Thus only one last integral is left. The integrand is decreasing very fast to zero for large values of x, so that we haven't to consider all these values and the upper limit is set to 1. In this integration area the exponential functions can be expanded for small values of x.

$$\mathrm{G}^{\mathrm{ret}}_{jj}(\omega) = \frac{C}{16} \cdot \beta\omega |\mathrm{J}_{\mathbf{K}}|^2 \cdot K_j^2 \int_0^1 \mathrm{d}x \, \frac{1}{x^3} \tag{5.43}$$

In the lower limit the integrand is highly divergent, which is an unphysical solution. Hence the Green function has an infinite value which correspond to an infinite resistance, because of umklapp scattering. Let us consider our problem with an additional renormalization factor r. The renormaliziation factor is connected with the temperature through the relation $r \sim T^{2/z}$ where z is some factor which has to be chosen depending on the problem and temperature regime. Our new starting point is equation (5.39) with the difference that we add r to $\mathbf{k}^2$.

Übergang schreiben

$$\mathrm{G}^{\mathrm{ret}}_{jj}(\omega) = -\frac{4\gamma^2\beta\omega}{\pi\hbar^2} |\mathrm{J}_{\mathbf{K}}|^2 \cdot K_j^2 \int_0^\infty \mathrm{d}\epsilon \, \frac{\epsilon^2 e^{\beta\epsilon}}{(e^{\beta\epsilon}-1)^2} \int_{\mathbf{k}} \frac{1}{\left((\mathbf{k}^2+r)^2+\gamma^2\epsilon^2\right)^2} \tag{5.44}$$

The computing procedure for the integrals are similar to the previous case. In comparison to the computation above the integral isn't transformed into dimensionless variables at this point, it's done later. Firstly the momentum integral is transformed into plane polar coordinates via the transformation $\mathbf{k} = (y\cos\phi, y\sin\phi)$. Again the integrand is angular independent, why the ϕ-integral yields the factor 2π. Furthermore the integrand is proportional to $1/k^4$ and decrease therefor very fast to zero in the limit $k \to \infty$, because of the upper limit of the k-integral is set to infinity.
Subsequently the factor $\gamma^2\epsilon^2$ is factorizied in the denominator. After that the integral is substituted again, this time with $z = (r+k^2)/\gamma\epsilon$. Now it is obvious why the renormaliziation factor is introduced at this place. Bacause of the factor r the lower limit of the integral is now $r/\gamma\epsilon$ instead of zero, which makes sure that the integral is convergent.

$$\mathrm{G}^{\mathrm{ret}}_{jj}(\omega) = -\frac{\beta\omega}{\gamma\pi^2\hbar^2} |\mathrm{J}_{\mathbf{K}}|^2 \cdot K_j^2 \int_0^\infty \mathrm{d}\epsilon \, \frac{\epsilon^{-1} e^{\beta\epsilon}}{(e^{\beta\epsilon}-1)^2} \int_{r/\gamma\epsilon}^\infty \mathrm{d}z \, \frac{1}{\left(z^2+1\right)^2} \tag{5.45}$$

The antiderivative of the z-integral is given by equation (5.42) and the expression of the Green function is

$$\mathrm{G}^{\mathrm{ret}}_{jj}(\omega) = -\frac{\beta\omega}{4\gamma\pi^2\hbar^2} |\mathrm{J}_{\mathbf{K}}|^2 \cdot K_j^2 \int_0^\infty \mathrm{d}\epsilon \, \frac{\epsilon^{-1} e^{\beta\epsilon}}{(e^{\beta\epsilon}-1)^2} \left[\pi - \frac{2\, r/\gamma\epsilon}{1+(r/\gamma\epsilon)^2} - 2\tan^{-1}\left(\frac{r}{\gamma\epsilon}\right)\right] \tag{5.46}$$

Now the time is come, where the integral is tansformed with $x = \beta\epsilon$ into dimensionless variables. The integrand is a function which decrease fast to zero for large values of x, Grafik die den Unterschied der Nherung zum Original zeigt

Grafik die z dass der Int grand schne gegen Null strebt fr gro Werte

which is depicted in figure .... In good approximation the upper limit can be set to an arbitrary value Λ. So the important contribution is originated in the small values of x why the expression in squared brackets is expanded up to leading order. The difference of the original and the approximated function are exhibited in figure .... Furter the fraction of the exponential functions can be approximated. In total the intgerand is independent of the variable x so the integral yields the factor Λ

$$\mathrm{G}^{\mathrm{ret}}_{jj}(\omega) \approx -\frac{\gamma^2\Lambda}{3\pi^2\hbar^2} \cdot |\mathrm{J}_{\mathbf{K}}|^2 \cdot K_j^2 \cdot \frac{1}{\beta^2 r^3} \cdot \omega \tag{5.47}$$

The single tempurature depending factors are β and r. The renormaliziation factor is derelated to the tempurature on $r = T^{2/z}$. Thus the temperature dependence of the Green function is given by

$$\mathrm{G}^{\mathrm{ret}}_{jj}(\omega) \sim \frac{1}{\beta^2 r^3} \sim T^{2-6/z}, \tag{5.48}$$

which means that z has to be three that the Green function and therefor the resistance is a constant function. For $z = 6$ the the Green function or resistance are proportional to T. These values are two much to large. Normally z takes on values of $z = 1$ or $z = 2$. Figure ... shows that the agreement of the original and approximated function are only in a small regime valid. If the variable x increases the value of 1 the agreement is miserable. Therefore we want to find another much better approximation for the expression in the squared brackets in equation (5.46).

Link zum Bild der die Nherung zeigt

For a better approximation again equation (5.44) and let's do the treatment of power counting for the momentum integral. The denominator yields k^8 and the numerator yields k^2, because of the differential $\mathrm{d}^2\mathbf{k}$. In total the power of k^{-6}. Beside that the integrand has two possible divergencies $\gamma\epsilon$ and r, where both of them are proportional to k^2. Because of the structur of the integrand we determine the following expression for the Green function. The function is multiplied by π to get the same upper bound.

$$\mathrm{G}^{\mathrm{ret}}_{jj}(\omega) = -\frac{4\gamma^2\beta\omega}{\pi\hbar^2} |\mathrm{J}_{\mathbf{K}}|^2 \cdot K_j^2 \int_0^\infty \mathrm{d}\epsilon \, \frac{\epsilon^2 e^{\beta\epsilon}}{(e^{\beta\epsilon}-1)^2} \frac{\pi}{(r^2+\gamma^2\epsilon^2)^{3/2}} \tag{5.49}$$

Graph für power counting function

In figure ... the exact solution of the momentum integral and the approximation given by power counting are contrasted. Comparing with our previous approximation this new approximation is much better. Similar to the exact function our approximation is convergent vor large values of ϵ. Nevertheless let us factrizing $\gamma^2\epsilon^2$ in the denominator and transform into dimensionless variables with $x = \beta\epsilon$. Further the dimensionless integral is cupped by an arbitrary value Λ again. Then the exponential functions can be expanded with respect to small x. The resulting integral is exactly solvable.

$$\mathrm{G}^{\mathrm{ret}}_{jj}(\omega) = -\frac{4\beta\omega}{\gamma\hbar^2} |\mathrm{J}_{\mathbf{K}}|^2 \cdot K_j^2 \int_0^\Lambda \mathrm{d}x \, \frac{1}{\left(\left(\frac{\beta r}{\gamma}\right)^2 + x^2\right)^{\frac{3}{2}}} \sim \frac{\Lambda}{\left(\frac{\beta r}{\gamma}\right)^2 \sqrt{\left(\frac{\beta r}{\gamma}\right)^2 + \Lambda^2}} \tag{5.50}$$

These expression can be expanded for small values of $\beta r/\gamma\Lambda$. Now we can insert the tempurature depended renormalization factor $r = T^{2/z}$. Therefore the Green function is given by

$$\mathrm{G}^{\mathrm{ret}}_{jj}(\omega) = -\frac{4\gamma\Lambda^{-1}}{\hbar^2}|\mathrm{J}_{\mathbf{K}}|^2 \cdot K_j^2 \frac{1}{\beta r^2} \cdot \omega \sim T^{1-4/z} \tag{5.51}$$

In comparison to the first investigation of the Green function above, once the term in the squared brackets was expanded in (5.46), this result is a little bit better. Nevertheless the value of z has to be $z = 4$ that the Green function and therefor the resitance is proportional T^0. Normaly the value of z is 1 or 2. If we consider this the resitance would be proportional to T^{-3} and T^{-1}. These results for the temprature dependence are highly divengent.

5.2.2 Computation of the static susceptibility

Equation (5.19) contains two possibile temperature dependent quantities. Beside the integral, which is calculated in the section above, the static susceptibility is the second one. Our expectation is that the static susceptibility dosen't depend on temperature in leading order, but we have to prove it. With the aid of equation (4.43) the static susceptibility is obviously connected with the Kubo relaxation function (4.10) at $t = 0$.

$$\chi_{\mathrm{PJ}}(\omega = 0) = \Phi_{\mathrm{PJ}}(t = 0) = \frac{i}{\hbar}\int\limits_0^\infty \mathrm{d}t' \left\langle \left[\mathrm{P}_j(t'), \mathrm{J}_j(0)\right]\right\rangle \tag{5.52}$$

In the formula above the limit $s \to 0$ is tropped, because we will see that the integral is convegent. The index j signifies the spatial direction of P and J. Like allways the integral is transformed into Matsubara time $\tau = it$. The Jacobi determinate is $-i$ and the integral's limits have to be set to 0 and β. In Matsubara interaction representation the normal treatment of pertubation theory is done, where in the case at hand only the leading order of pertubation series is observed.

$$\chi_{\mathrm{PJ}}(\omega = 0) = \frac{1}{\hbar}\int\limits_0^\beta \mathrm{d}\tau \left\langle \mathcal{T}_\tau \mathrm{P}_j(\tau)\mathrm{J}_j(0)\right\rangle_0 \tag{5.53}$$

The momentum and current operator are given by equation ... and ..., respetivily. Before the operators are inserted into the expectation value let us think about the possible combinations in diagrammatic language. Firstly remember that the numerator and denominator have to be expand in a series. Doing this completly general the appearing diagrams in the denominator can be factorized in the numerator and thus their cancel each other. Making a long story short only connected diagrams have to be taken into account.

link zu impuls im k-raum

link zum strom im k-raum

In the investigated order only one pair of bosonic operators, i. e. one propagator, and no interaction between the spin density waves and the electrons are observed.

Bild von den Bubblediagrammen

Therefore the bosonic propagator yields always a disconnected diagram. Furthermore pairing electrons of different Fermi sufaces isn't allowed, which means that the expactation value of mixed fermionic operators also yields disconnected diagrams. Thus many diagrams of the investigated ones are disconnected, beside of two one. These two bubble diagrams are depicted in figure . . . .

$$\chi_{\mathrm{PJ}}(\omega=0) = -\frac{1}{\hbar}\int_0^\beta \mathrm{d}\tau \int_{\mathbf{k}} \left[\frac{k_j^2}{m_1}\left\langle \mathcal{T}_\tau \Psi_{\mathrm{a}}^\dagger(\mathbf{k},\tau)\Psi_{\mathrm{a}}(\mathbf{k},\tau)\Psi_{\mathrm{a}}^\dagger(\mathbf{k},0)\Psi_{\mathrm{a}}(\mathbf{k},0)\right\rangle_0 + \frac{k_j^2}{m_2}\left\langle \mathcal{T}_\tau \Psi_{\mathrm{b}}^\dagger(\mathbf{k},\tau)\Psi_{\mathrm{b}}(\mathbf{k},\tau)\Psi_{\mathrm{b}}^\dagger(\mathbf{k},0)\Psi_{\mathrm{b}}(\mathbf{k},0)\right\rangle_0\right] \tag{5.54}$$

Vielleicht noch etwas zu der delta-Distribution und so schreiben, damit klar is warum die Operatoren alle beim gleichen Impuls sind.

The two expectation value of four fermionic operators can't be solved directly. Wick's theorem offers the oppertunity to write these expectation values into a product of expectation values contained only two operators, which are nothing else free propagators. Two contraction are possible for each expectation value in the investigated case above, where one of them vanishes, because the time argument of the contracted operator is the same.

$$\chi_{\mathrm{PJ}}(\omega=0) = \frac{1}{\hbar}\int_0^\beta \mathrm{d}\tau \int_{\mathbf{k}} k_j^2 \left[\frac{1}{m_1}\mathcal{G}_{\mathrm{a}}^{(0)}(\mathbf{k},-\tau)\mathcal{G}_{\mathrm{a}}^{(0)}(\mathbf{k},\tau) + \frac{1}{m_2}\mathcal{G}_{\mathrm{b}}^{(0)}(\mathbf{k},-\tau)\mathcal{G}_{\mathrm{b}}^{(0)}(\mathbf{k},\tau)\right] \tag{5.55}$$

where the free fermionic propagator $\mathcal{G}_\alpha^{(0)}(\mathbf{k},\tau) = -\langle \mathcal{T}_\tau \Psi_\alpha(\mathbf{k},\tau)\Psi_\alpha^\dagger(\mathbf{k},0)\rangle$ with $\alpha \in \{\mathrm{a},\mathrm{b}\}$ is introduced. The Green functions of electrons are transformed into the Matsubara frequency space, thus the only time dependence is at the exponential functions. The τ-integral yields a δ-distrubution $\delta(\omega_m - \omega_n)$ and then one sum over the Matsubara frequencies can be taken.

$$\chi_{\mathrm{PJ}}(\omega=0) = \frac{1}{\hbar}\int_{\mathbf{k}} k_j^2 \left[\frac{1}{m_1}S_{\mathrm{a}}(\omega_n) + \frac{1}{m_2}S_{\mathrm{b}}(\omega_n)\right] \tag{5.56}$$

where the Matsubara sum $S_\alpha(\omega_n) = \beta^{-1}\sum_{\omega_n}\mathcal{G}_\alpha^{(0)}(\mathbf{k},\omega_n)\mathcal{G}_\alpha^{(0)}(\mathbf{k},\omega_n)$ is introduced. The Matsubara theory exhibits that these kinds of sums can be evaluated by rewriting the sum as a contour integral in the complex plane, integrating over the Green function multiplied with the Fermi or Bose distribution caused by the nature of the Green function. This transformation yields

$$S = \frac{1}{\beta}\sum_{\omega_n}\mathcal{G}(\omega_n) = -\frac{1}{2\pi i}\oint_\Gamma \mathrm{d}z\, n_{\mathrm{F}}(z)\mathcal{G}(z) \tag{5.57}$$

Bild mit Kontour und verlinken

in the case of a fermionic Green function Thereby the contour is arbitrary. The only important fact is that all singularities of the Green function has to be included in the contour. The singularity of the distribution function isn't included in the contour. In figure . . . a examplar contour is given. The electronic Green function

$$\mathcal{G}_\alpha(\mathbf{k}, \omega_n) = \frac{1}{i\omega_n - \epsilon_\alpha(\mathbf{k})}, \tag{5.58}$$

where $\epsilon_\alpha(\mathbf{k})$ is the electron's dispersion relation with respect to the corresponding Fermi suface denoted with a and b (see equation …), has only simple poles in the complex plane, which means the function is continously in the whole complex plane. Therefore the well known residuum theorem can be used to evaluate the contour integral.

Link zu den Dispersionsrelationen

$$\chi_{\mathrm{PJ}}(\omega = 0) = -\frac{1}{\hbar}\int_{\mathbf{k}} k_j^2 \left[\frac{1}{m_1}\frac{\mathrm{d}n_{\mathrm{F}}(\epsilon_{\mathrm{a}}(\mathbf{k}))}{\mathrm{d}\epsilon_{\mathrm{a}}(\mathbf{k})} + \frac{1}{m_2}\frac{\mathrm{d}n_{\mathrm{F}}(\epsilon_{\mathrm{b}}(\mathbf{k}))}{\mathrm{d}\epsilon_{\mathrm{b}}(\mathbf{k})}\right] \tag{5.59}$$

The derivatives of the distribution function with respect to the dispersion relation appears because the singularity of the Green function at $z_0 = \epsilon_\alpha(\mathbf{k})$ is a singularity of second order. These two integrals are exactly solvable. Therefore them are transformed into polar coordinates $(k_x, k_y) = (q\sqrt{2m_{1,2}}\cos(\phi), q\sqrt{2m_{2,1}}\sin(\phi))$, where two forms are used, because of the different dispersion relation. The k_j^2 is originated the only angular dependence, which yields $\cos^2(\phi)$ or $\sin^2(\phi)$ for the x- or y-direction, respectivily. Because the limits of the integral are 0 and 2π the integral yields the same result in both cases. The upper limit of the q-integral can be set to infity, because the integrand is decreased very fast to zero for large values of q.

$$\chi_{\mathrm{PJ}}(\omega = 0) = \frac{8\beta\pi}{(2\pi)^2\hbar}\sqrt{m_1 m_2}\int_0^\infty \mathrm{d}q\, q^3 \frac{e^{\beta(q^2-\mu)}}{(e^{\beta(q^2-\mu)}+1)^2} \tag{5.60}$$

The resulted integral can be solved by substituting $x = \beta(q^2 - \mu)$. Thereby the first of the two integrals is evaluated with integration by parts and the integrand of second one is equally to the derivative of Fermi distributation. All in one the static susceptibility between P and J is given by

$$\chi_{\mathrm{PJ}}(\omega = 0) = \frac{\sqrt{m_1 m_2}}{\pi\beta\hbar}\ln\left(e^{\beta\mu} + 1\right) \tag{5.61}$$

in first order of pertubation theory. The chemical potential μ is much much larger than β in the limit of small temperature T. Therefore the argument of the exponential function is large and $\ln(e^{\beta\mu} + 1) = \beta\mu$ in the limit of $\mu \ll k_{\mathrm{B}}T$.

Heisst es nullte oder erste Ordnung Störungstheorie?

$$\chi_{\mathrm{PJ}}(\omega = 0) \to \frac{\mu\sqrt{m_1 m_2}}{\pi\hbar} \tag{5.62}$$

The static susceptibility between P and J is temperature independent in the limit of $\mu \ll k_{\mathrm{B}}T$, like exactly we have expected.

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. $\chi_{\mathrm{AB}}(t) = -\Theta(t) \frac{\mathrm{d}}{\mathrm{d}t} \Phi_{\mathrm{AB}}(t)$ (A.2)

2. $\Phi_{\mathrm{AB}}(t = 0) = \chi_{\mathrm{AB}}(\omega = 0)$ (A.3)

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

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

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

$$
\begin{aligned}
&\Leftrightarrow\ \Phi_{\mathrm{AB}}(t=0) = \lim_{\omega\to 0} \int\limits_{-\infty}^{\infty} \mathrm{d}\tau\, \chi_{\mathrm{AB}}(\tau) e^{i\omega\tau} \\
&\Leftrightarrow\ \Phi_{\mathrm{AB}}(t=0) = \chi_{\mathrm{AB}}(\omega=0),
\end{aligned}
\tag{A.7}
$$

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.

$$
\begin{aligned}
\int\limits_{0}^{\infty} \mathrm{d}t\, e^{i\omega t} \chi_{\mathrm{AB}}(t) &= -\int\limits_{0}^{\infty} \mathrm{d}t\, e^{i\omega t} \frac{\mathrm{d}}{\mathrm{d}t} \Phi_{\mathrm{AB}}(t) \\
\overset{\mathrm{PI}}{\Leftrightarrow}\ \chi_{\mathrm{AB}}(\omega) &= -e^{i\omega t}\Phi_{\mathrm{AB}}(t)\Big|_{0}^{\infty} + i\omega \int\limits_{0}^{\infty} \mathrm{d}t\, e^{i\omega t} \Phi_{\mathrm{AB}}(t) \\
\Leftrightarrow\ \chi_{\mathrm{AB}}(\omega) &= \Phi_{\mathrm{AB}}(t=0) + i\omega \Phi_{\mathrm{AB}}(\omega) \\
\Leftrightarrow\ \Phi_{\mathrm{AB}}(\omega) &= \frac{1}{i\omega}\big[\chi_{\mathrm{AB}}(\omega) - \chi_{\mathrm{AB}}(\omega=0)\big]
\end{aligned}
\tag{A.8}
$$

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 $\big(\dot{\mathrm{P}}\big|\big(\omega - \mathrm{L}_0\big)^{-1}\big|\dot{\mathrm{P}}\big)$

In this appendix the short conversion of the expectation value $\big(\dot{\mathrm{P}}\big|\big(\omega - \mathrm{L}_0\big)^{-1}\big|\dot{\mathrm{P}}\big)$ 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 (4.45).

$$\begin{aligned}
&\big(\dot{\mathrm{P}}\big|\big(\omega - \mathrm{L}_0\big)^{-1}\big|\dot{\mathrm{P}}\big) = -i\mathcal{C}_{\dot{\mathrm{P}}\dot{\mathrm{P}}}(\omega) \\
\overset{(A.6)}{\Leftrightarrow}\ &\big(\dot{\mathrm{P}}\big|\big(\omega - \mathrm{L}_0\big)^{-1}\big|\dot{\mathrm{P}}\big) = -i\int\limits_0^\infty \mathrm{d}t\, e^{i\omega t}\mathcal{C}_{\dot{\mathrm{P}}\dot{\mathrm{P}}}(t) \\
\overset{(4.42)}{\Leftrightarrow}\ &\big(\dot{\mathrm{P}}\big|\big(\omega - \mathrm{L}_0\big)^{-1}\big|\dot{\mathrm{P}}\big) = -\frac{i}{\beta}\int\limits_0^\infty \mathrm{d}t\, e^{i\omega t}\int\limits_0^\beta \mathrm{d}\lambda \left\langle \dot{\mathrm{P}}^\dagger(t)\dot{\mathrm{P}}(0)\right\rangle \\
\overset{(4.17)}{\Leftrightarrow}\ &\big(\dot{\mathrm{P}}\big|\big(\omega - \mathrm{L}_0\big)^{-1}\big|\dot{\mathrm{P}}\big) = -\frac{i}{\beta}\Phi_{\dot{\mathrm{P}}\dot{\mathrm{P}}}(\omega) \\
\overset{(4.12)}{\Leftrightarrow}\ &\big(\dot{\mathrm{P}}\big|\big(\omega - \mathrm{L}_0\big)^{-1}\big|\dot{\mathrm{P}}\big) = -\frac{\omega^{-1}}{\beta}\Big[\chi_{\dot{\mathrm{P}}\dot{\mathrm{P}}}(\omega) - \underbrace{\chi_{\dot{\mathrm{P}}\dot{\mathrm{P}}}(\omega = 0)}_{=0}\Big] \\
\Leftrightarrow\ &\big(\dot{\mathrm{P}}\big|\big(\omega - \mathrm{L}_0\big)^{-1}\big|\dot{\mathrm{P}}\big) = -\frac{\omega^{-1}}{\beta}\int\limits_{-\infty}^\infty \mathrm{d}t\, e^{i\omega t}\chi_{\dot{\mathrm{P}}\dot{\mathrm{P}}}(t) \\
\overset{(4.8)}{\Leftrightarrow}\ &\big(\dot{\mathrm{P}}\big|\big(\omega - \mathrm{L}_0\big)^{-1}\big|\dot{\mathrm{P}}\big) = -\frac{i\omega^{-1}}{\hbar\beta}\int\limits_0^\infty \mathrm{d}t\, e^{i\omega t}\left\langle\Big[\dot{\mathrm{P}}(t), \dot{\mathrm{P}}(0)\Big]\right\rangle_0 \qquad \text{(B.1)}
\end{aligned}$$

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 Fierz identity

This appendix shows the use of the Fierz identity in realation to computing products of field operators connected via Pauli matricies. Lets signify the generators of the fundamental representation SU(N) as T^a, where those have the form

$$T^a_{ij} \quad \text{mit} \quad a = 1, 2, 3, \ldots, N^2 - 1 \quad \text{and} \quad i, j = 1, 2, 3, \ldots, N \tag{C.1}$$

The Fierz identity yields the connection between the product of two generators and the Kronecker symbols. In general the Fierz identity is given by

$$\sum_{a=1}^{N^2-1} T^a_{ij} T^a_{kl} = \frac{1}{2}\Big[\delta_{il}\delta_{jk} - \frac{1}{N}\delta_{ij}\delta_{kl}\Big] \tag{C.2}$$

In the case of Pauli matricies the fundamental representation is SU(2) and the generator of SU(2) are connected with the Pauli matricies with the realation $T^a = \frac{1}{2}\sigma^a$. Therefore the Fierz identity for the fundamental representation is given by

$$4\sum_{a=1}^{3} T^a_{ij} T^a_{kl} = \sum_{a=1}^{3} \sigma^a_{ij}\sigma^a_{kl} = 2\delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl} \tag{C.3}$$

Now this identity can be used for computing the fermionic expectation value obtained in section 3.2. In equation (**??**) the product of fermionic operators yields four terms of the structure

$$\mathrm{EV_F} := \Big\langle \Psi^\dagger_\alpha(\nu_1) \cdot \sigma^\mu \cdot \Psi_\beta(\nu_2) \cdot \Psi^\dagger_\gamma(\nu_3) \cdot \sigma^\mu \cdot \Psi_\delta(\nu_4) \Big\rangle\,, \tag{C.4}$$

where $\alpha, \beta, \gamma, \delta \in \{a, b\}$ and has to be chosen with respect to the Fermi surface of the electrons. The explicite quantum numbers of the respected operators aren't important for the use of the Fierz identity, why the dummy quantity ν_i with $i = 1, 2, 3, 4$ is introduced. Firstly the product is writen in component representation, which allows us to use the Fierz identity. In the expectation value above the sum over μ should be implied.

$$\begin{aligned}
&\mathrm{EV_F} = \Big\langle \Big(\Psi^\dagger_\alpha(\nu_1)\Big)_i \cdot \sigma^\mu_{ij} \cdot \Big(\Psi_\beta(\nu_2)\Big)_j \cdot \Big(\Psi^\dagger_\gamma(\nu_3)\Big)_k \cdot \sigma^\mu_{kl} \cdot \Big(\Psi_\delta(\nu_4)\Big)_l \Big\rangle \\
\Leftrightarrow\;& \mathrm{EV_F} = \sigma^\mu_{ij}\sigma^\mu_{kl} \Big\langle \Big(\Psi^\dagger_\alpha(\nu_1)\Big)_i \Big(\Psi_\beta(\nu_2)\Big)_j \Big(\Psi^\dagger_\gamma(\nu_3)\Big)_k \Big(\Psi_\delta(\nu_4)\Big)_l \Big\rangle \\
\Leftrightarrow\;& \mathrm{EV_F} = \big(2\delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl}\big) \Big\langle \Big(\Psi^\dagger_\alpha(\nu_1)\Big)_i \Big(\Psi_\beta(\nu_2)\Big)_j \Big(\Psi^\dagger_\gamma(\nu_3)\Big)_k \Big(\Psi_\delta(\nu_4)\Big)_l \Big\rangle
\end{aligned}$$

$$
\begin{aligned}
\Leftrightarrow\ \mathrm{EV_F} &= 2\left\langle \left(\Psi^\dagger_\alpha(\nu_1)\right)_i \delta_{il}\left(\Psi_\delta(\nu_4)\right)_l \left(\Psi_\beta(\nu_2)\right)_j \delta_{jk}\left(\Psi^\dagger_\gamma(\nu_3)\right)_k \right\rangle \delta_{\nu_3,\nu_4} \\
&\quad - \left\langle \left(\Psi^\dagger_\alpha(\nu_1)\right)_i \delta_{ij}\left(\Psi_\beta(\nu_2)\right)_j \left(\Psi^\dagger_\gamma(\nu_3)\right)_k \delta_{kl}\left(\Psi_\delta(\nu_4)\right)_l \right\rangle \\
\Leftrightarrow\ \mathrm{EV_F} &= 2\left\langle \Psi^\dagger_\alpha(\nu_1)\Psi_\delta(\nu_4)\Psi_\beta(\nu_2)\Psi^\dagger_\gamma(\nu_3)\right\rangle \delta_{\nu_3,\nu_4} - \left\langle \Psi^\dagger_\alpha(\nu_1)\Psi_\beta(\nu_2)\Psi^\dagger_\gamma(\nu_3)\Psi_\delta(\nu_4)\right\rangle
\end{aligned}
\tag{C.5}
$$

The use of the Fierz identity has eliminated the Pauli matrizies in our expression of the expectation value. Instead we get two expectation values with a different order of the field operators. Now let us investigate what happens with the fermionic expectation values in the second order of pertubation theory. In the corresponding expectation values are always two fermionic operators of the same electron family a or b. This means that always two greek letters have to be set to a and the other two ones to b in equation (C.5). The expectation values of different electron families can be seperated without any doubt, because them Hilbert spaces are disconnected. For this reason many combinations of chosing the greek letters are zero. Let us demonstrate this with an example. If we choose $\alpha = \gamma = a$ and the other two ones respectively to b, than an expectation value emerge with two fermionic creation operators and another one emerge with two fermionic annihilation operators, which is always zero. For the fermionic expectation value $\mathrm{EV}(\mathcal{D})$ in equation (**??**) this procedure yields

$$
\begin{aligned}
\mathrm{EV}(\mathcal{D}) &= \left\langle \mathcal{T}_t \Psi_\mathrm{a}(\tilde{\mathbf{p}}_2, t_1)\Psi^\dagger_\mathrm{a}(\tilde{\mathbf{p}}_3, t_2)\right\rangle \left\langle \mathcal{T}_t \Psi_\mathrm{b}(\tilde{\mathbf{p}}_4, t_2)\Psi^\dagger_\mathrm{b}(\tilde{\mathbf{p}}_1, t_1)\right\rangle \delta_{\tilde{\mathbf{p}}_2-\tilde{\mathbf{p}}_3}\delta_{\tilde{\mathbf{p}}_4-\tilde{\mathbf{p}}_1} \\
&\quad + \left\langle \mathcal{T}_t \Psi_\mathrm{b}(\tilde{\mathbf{p}}_2, t_1)\Psi^\dagger_\mathrm{b}(\tilde{\mathbf{p}}_3, t_2)\right\rangle \left\langle \mathcal{T}_t \Psi_\mathrm{a}(\tilde{\mathbf{p}}_4, t_2)\Psi^\dagger_\mathrm{a}(\tilde{\mathbf{p}}_1, t_1)\right\rangle \delta_{\tilde{\mathbf{p}}_2-\tilde{\mathbf{p}}_3}\delta_{\tilde{\mathbf{p}}_4-\tilde{\mathbf{p}}_1}
\end{aligned}
\tag{C.6}
$$

Todo list

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