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Quantentransport in Spindichtesystemen mit dem Memory-Matrix-Formalismus

Masterthesis

von

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Karlsruhe, den 23. Mai 2018

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(**Martin Lietz**)

Acknowledgment

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1 Introduction

2 Infinite Conductivity in Translation Invariant Systems

Ever since Drude published his theory about the electrical conductivity in metals [Dru00] at the beginning of the last century, it is well known that non-conservation of electron momentum in a system is required for finite electrical conductivity. In Drude's model, the electrons possess a mean scattering time τ_{el} representing the mean time between two scattering events of an electron and a lattice atom. At each scattering event, the electrons transfer momentum to the lattice atoms, which is the reason electron momentum is not a conserved quantity. In the case of conserved momentum, if an electrical field is exemplarily applied, it accelerates electrons up to an infinite velocity, causing infinite conductivity.

In the following section, a momentum conserving system is considered and the electrical conductivity is computed using the memory-matrix-formalism, where an infinite conductivity is expected. Beforehand, a short overview over the memory-matrix-formalism is given, followed by detailed and explicit deviations in chapter 5.

overview oder
review?

2.1 An Overview over the Memory-Matrix-Formalism

Let us assume a physical dynamical variable $A(t)$ in an arbitrary system and an arbitrary perturbation too. Our interest is now the time evolution of $A(t)$ depending on the perturbation. Completely general, a physical dynamical variable can be splitted into two parts, a secular one and a non-secular one, which is shown in [Mor65]. The latter represent processes like fluctuations or initial transient processes, which have in common a short lifetime comparing to the secular processes. The dynamic and time evolution of $A(t)$ is therefore dominated by secular processes.

This separation enables a simple but clever geometrical interpretation, where dynamical variables are considered to be vectors in a vector space. The variables of the unperturbed system represent the basis vectors of this vector space, denoting in the case of the variable $A(t)$ as A-axis. Due to perturbation the direction of the variable $A(t)$ changes with respect to the A-axis. The projection of $A(t)$ onto the A-axis corresponds to the secular part, whereas the perpendicular component represents the non-secular parts.

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First of all, the mathematical framework for this vector space has to be established. In quantum mechanics, the Liouville space, also called as operator space, is the respective vector space of the memory-matrix-formalism. As indicated by the name *operator space*, the vectors of the Liouville space are operators, all of which being Hermitian. The basis of the Liouville space is signified as $\{|A_i\rangle\}$, where $i = 1, 2, 3, \dots, n$, and the

corresponding dual space basis is denoted as $\{(A_i|\}$. To complete the definition of any vector space, a scalar product is required. The following one is chosen:

$$(A_i(t)|A_j(t')) = \frac{1}{\beta} \int_0^\beta d\lambda \left\langle A_i^\dagger(t) A_j(t' + i\lambda) \right\rangle. \quad (2.1)$$

The normal time evolution $A_i(t) = e^{iHt/\hbar} A_i(0) e^{-iHt/\hbar}$ of an operator should be valid so that $A_i(i\lambda) = e^{-\lambda H} A_i(0) e^{\lambda H}$ can be used. If secular processes are neglected, the choice of the scalar product is determined under the aspect that as a consequence the time evolution of $A(t)$ given the most probably path, see [Mor65]. In quantum mechanics, the dynamic of an operator is ususally described by the Heisenberg equation of motion, which is transformed using the dyad product into the Liouville space

$$|\dot{A}_i(t)\rangle = \frac{i}{\hbar} [H, A_i(t)] = iL|A_i(t)\rangle. \quad (2.2)$$

Here the Hermitian Liouville operator, $L = \hbar^{-1}[H, \bullet]$, is introduced, which is defined by acting onto an arbitrary operator. The formal solution of this equation is given by $|A_i(t)\rangle = \exp(itL) \cdot |A_i(0)\rangle$, where the time evolution of an operator is therefore given by the Liouville operator. For our approach a further operator is required in the Liouville space, namely the projection operator. A set of arbitrary operators $\{C_i\}$ is therefore defined. The choice of them is different for each observed problem and unimportant at the moment. The definition of the projection operator in Liouville space follows directly from the projection operator defined in the commonly used Hilbert space in quantum mechanics.

zweiter Hauptsatz verbessern

$$P = \sum_{i,j} \frac{|C_i(0)\rangle \langle C_j(0)|}{\langle C_i(0)|C_j(0)\rangle} \quad (2.3)$$

The projection operator acting on some vector in Liouville space yields the projection onto the subspace spanned by the operator C_i . Thus, the operator $Q = 1 - P$ yields the corresponding part projected out of the subspace. Furthermore, the projection operator is Hermitian and fullfills the two properties $P^2 = P$ and $PQ = QP = 0$. This completes the required mathematical basis of the memory-matrix formalism.

Correlation functions are the natural approach to describe the reaction of a dynamic variable on a perturbation. In quantum mechanics, the correlation function is defined in Kubo's linear response theory as an integral over an expectation value of two operators, one of them being the investigated operator, and the other one being the coupling operator from the perturbation Hamiltonian. In the Liouville space, the correlation function is defined as

$$c_{ij}(t) := (A_i(t)|A_j(0)) = \frac{1}{\beta} \int_0^\beta d\lambda \left\langle A_i^\dagger(t) A_j(i\lambda\hbar) \right\rangle, \quad (2.4)$$

using the definition of the scalar product (2.1) in the second step. Expressing the time evolution of $A_i(t)$ with the Liouville operator, using the Laplace transformation and a few conversions yields an algebraic matrix equation of the correlation function, which has the form

$$\sum_l \left[\omega \delta_{il} - \Omega_{il} + i \Sigma_{il}(\omega) \right] C_{lj}(\omega) = \frac{i}{\beta} \chi_{ij}(0), \quad (2.5)$$

where the abbreviations

$$\Omega_{il} := i\beta \sum_k (\dot{A}_i | C_k) \chi_{kl}^{-1}(0) \quad \text{and} \quad \Sigma_{il}(\omega) := i\beta \sum_k (\dot{A}_i | Q \frac{1}{\omega - QLQ} Q | \dot{C}_k) \chi_{kl}^{-1}(0) \quad (2.6)$$

are introduced. Both sums over l and k run over the set of operators, defined by the projection operator. Similarly, the indices i and j have to be chosen from this set of operators so that (2.5) yields n^2 equations, if n is the number of operators in the set. Both abbreviations can be combined to a function $M_{il}(\omega) := \Sigma_{il}(\omega) + i\Omega_{il}$, called the memory function. In this function, $\Sigma_{il}(\omega)$ takes the role of the quantum mechanical self energy, while Ω_{il} represents dissipative effects. Ω_{il} vanishes under to conditions. The model Hamiltonian has to be invariant under time reversal symmetry. Furthermore, both operators, A_i and C_k , have to be the same sign with respect to time reversal symmetry. This assertion is proven in great detail in 5.3.1. It folloes that the memory function is solely determined by $\Sigma_{il}(\omega)$.

The structur of $\Sigma_{il}(\omega)$ resembles the one of the Laplace transformed correlation function, comparing equation (??), with two differences. The expectation value is performed with respect to the operators like $Q|\dot{A}_i)$ instead of $|A_i)$, while only the reduced Liouville operator QLQ is considered. The latter projects at the part of the full Liouville operator, which causes the intrinsic fluctuations of the operator A . In other words, the operator QLQ describes the internal dynamics of all other degrees of freedom of the system, called the *bath*, excluded A . The coupling to the bath is characterized by the vector $Q|\dot{A}_i)$ and is clearly changing the dynamic behaviour of A .

2.2 Electrical Conductivity in a Momentum Conserving System

In the following section, the electrical conductivity is computed for a system, where momentum is conserved, using the memory-matrix-formalism. An infinite conductivity is expected due to the fact that electrons do not transfer any momentum to other degrees of freedom. Besides conserving momentum, the observed system has to satisfy some additional requirements. Firstly, the current has to be an unconserved quantity. Furthermore, the scalar product $(J|P)$ of current and momentum has to be non-zero. In other words, both quantities possess a finite overlap. These two quantities should also generate the subspace into the projection operator projects. The sum in (2.3)

summerizes over all operators C_i , where the choice has now to be done with respect to the electrical conductivity. As electrical conductivity is determined by momentum and current, these are chosen as operators. The last requirement is for the Hamiltonian to be invariant under time reversal symmetry, which is our last requirement.

Nevertheless, one remark has to be made for computing the conductivity. Due to the fact that the Hamiltonian is invariant under time reversal symmetry and the subspace is generated by J and P , which have same signature under time reversal symmetry, no dissipative effects exist. The quantity Ω , defined in (2.6), is therefore zero.

In the strictly general sense, the electrical conductivity is given by the current-current correlation function $\mathcal{C}_{JJ}(\omega)$ (see [Czy17]). The static case is obtained by taking the small frequency limit, $\omega \rightarrow 0$, of the conductivity.

$$\sigma_{\text{dc}} = \lim_{\omega \rightarrow 0} \sigma(\omega) = \lim_{\omega \rightarrow 0} \beta \mathcal{C}_{JJ}(\omega) \quad (2.7)$$

The current-current correlation function is given by equation (2.5), which is in the case of the J-P subspace a 2×2 matrix equation. The quantity Σ is simplified by two aspects. Firstly, the momentum is conserved, which means the time derivative of P is zero and therefore all expectation values are trivially zero where \dot{P} is a taken vector. The remaining expectation values of Σ contains only the current J , but these ones are vanishing as well. The operator QLQ describes the intrinsic fluctuation of $|J\rangle$, which are assumed to be zero. Furthermore, the operator Q acting on $|J\rangle$ yields the coupling to these intrinsic fluctuation and, leading to $Q|J\rangle = 0$. The obtained matrix equation has a very simple form and the current-current correlation function can be directly read out as

$$\mathcal{C}_{JJ}(z) = \frac{i}{\omega} \beta^{-1} \chi_{JJ}(\omega = 0) = \frac{i}{\omega} \mathcal{C}_{JJ}(t = 0), \quad (2.8)$$

where relation (5.43) is being used. The correlation function at time $t = 0$ is given by the scalar product $\langle J(0)|J(0) \rangle$ (see (2.4)). Due to the fact that current and momentum are two closely connected quantities, this is also valid for their correlation functions. For this reason, the current-current correlation function is expressed with respect to the momentum-momentum correlation function.

The vector operator $|J(0)\rangle$ is separated into two pieces, one parallel and one perpendicular part, which are labeled as $|J_{\parallel}\rangle$ and $|J_{\perp}\rangle$, respectively. As discussed above, every variable generally consists of a secular and non-secular part, which does not mean that both parts need to exist in the observing model. The non-secular part is represented by the perpendicular component of $|J\rangle$. In the experiment, these processes are observed as a constant slowly fluctuating background, known as noise. The secular part is represented by the parallel component of $|J\rangle$, which is responsible for the electrical conductivity and is visible as a peak in the measurement, depicted in figure 2.1.

Drude's theory of conductivity yields a direct proportionality between J and P (see for example [GM14]). Since momentum is conserved and current is unconserved, in the investigated system this proportionality can't be valid. Nevertheless, both quantities possess a finite overlap, which means that a part of the current is conserved and

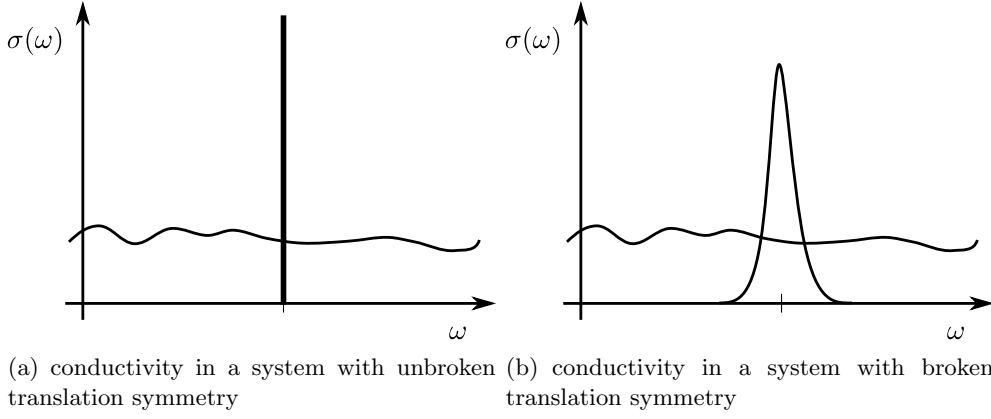


Figure 2.1: caption

therefore parallel to the momentum. This part is the parallel component of \mathbf{J} and given by the projection von $|\mathbf{J}\rangle$ onto $|\mathbf{P}\rangle$.

$$|\mathbf{J}_{\parallel}\rangle = \mathcal{P}|\mathbf{J}\rangle = \frac{|\mathbf{P}\rangle\langle\mathbf{P}|}{\langle\mathbf{P}|\mathbf{P}\rangle}|\mathbf{J}\rangle = \frac{\chi_{\mathbf{P}\mathbf{J}}}{\chi_{\mathbf{P}\mathbf{P}}}|\mathbf{P}\rangle \quad (2.9)$$

Separating both current operator in $(\mathbf{J}(0)|\mathbf{J}(0))$ yields four new correlation functions, where the mixed ones are zero, since $|\mathbf{J}_{\parallel}\rangle$ and $|\mathbf{J}_{\perp}\rangle$ are perpendicular to each other by construction. For the operators in the parallel correlation function, $(\mathbf{J}_{\parallel}(0)|\mathbf{J}_{\parallel}(0))$ equation (2.9) is used. In this equation, the correlation function of the parallel components is represented as a momentum-momentum correlation function. Inserting the obtained expression for the current-current correlation function in (2.8) the conductivity is given by

$$\sigma(\omega) = \frac{|\chi_{\mathbf{P}\mathbf{J}}|^2}{|\chi_{\mathbf{P}\mathbf{P}}|} \frac{i}{\omega} + \sigma_{\text{reg}}(\omega), \quad (2.10)$$

where the momentum-momentum correlation function is expressed as static susceptibility (see (5.43)), and the regular conductivity $\sigma_{\text{reg}}(\omega) = i(\omega\beta)^{-1}(\mathbf{J}_{\perp}|\mathbf{J}_{\perp})$ is introduced, which represents the noise (see figure 2.1).

In the above equation the quantity ω is a complex number. Since ω has to be a real number for a physical interpretation, it is transformed on the real axis using analytical continuation. The conductivity is then given by

$$\sigma(\omega) = \frac{|\chi_{\mathbf{P}\mathbf{J}}|^2}{|\chi_{\mathbf{P}\mathbf{P}}|} \left(\text{P.V.} \frac{i}{\omega} + \pi\delta(\omega) \right) + \sigma_{\text{reg}}(\omega) \quad (2.11)$$

where $\frac{1}{\omega+i\eta} = \text{P.V.} \frac{1}{\omega} - i\pi\delta(\omega)$ is used and P.V. symbolizes the prinzipel value. Taking now the small frequency limit $\omega \rightarrow 0$ the δ -distribution is the dominant term and the static conductivity becomes infinite, which is the exactly expected result. The static

electrical conductivity is infinite in a momentum conserving system, thus conductivity is getting finite if the momentum is not a conserved quantity any more. The respective underlying symmetry is translation symmetry. For breaking this symmetry, many possibilities are available, but in the following computation only one of them, namely umklapp scattering, is considered.

In the next chapter, the observed spin-fermion model is introduced. Beforehand, quantum phase transitions are reviewed. The conservation of momentum and non-conservation of current is further constituted. Finally, umklapp scattering is introduced for breaking translation symmetry and unconserving momentum.

3 Spin-Fermion-Model

In the following chapter, the spin-fermion-model is introduced for a metal exhibiting an antiferromagnetic quantum phase transition, as presented in [ACS03]. Bosonic spin fluctuations arise in the vicinity of the quantum critical point due to fermionic particle-hole-excitations, enabling an attractive interaction between electrons. This chapter is not displaying a detailed mathematical and microscopic derivation of the spin-fermion-model, but rather it is based on a qualitative description to justify its form. A short overview over quantum phase transitions is established as suggested in [Sac11]. In particular, we focus one's attention on the arising spin fluctuations, argue they carry large momentum \mathbf{Q} and introduce the damped spin density propagator and their periodicity. Further, we present the basic concepts of hot-spot theory, emerging as points on the Fermi surface in 2D since the magnetic Brillouin zone is cutting it. Besides, the conservation of momentum and non-conservation of current is reviewed for the observed model Hamiltonian. Umklapp scattering is introduced for breaking translation symmetry and the consequently non-conservation of momentum is constituted.

3.1 The Spin-Fermion-Model at the Onset of the Antiferromagnetic Quantum Phase Transition

An antiferromagnetic phase transition is exhibited in many metals at a characteristic temperature T_N , called Néel-temperature. The random ordered spins of lattice atoms are ordered along one axis in consequence of thermal fluctuations, where the nearest neighbors are always aligned in opposite direction. This temperature is changed by tuning a certain parameter as pressure or doping. A schematic and simplified phase diagram is depicted in figure 3.1. A certain value g_c is reached for the tuning parameter g at $T = 0$, decreasing temperature and following the phase line between both magnetic phases. This point is called quantum critical point and quantum fluctuations are the origin of this phase transition in comparison with phase transitions at finite temperature.

A short and rudimentary description of quantum phase transition is given, before starting with a qualitative derivation of the spin-fermion-model. This overview is required for the analytical discussion of our computation later. However, the reason for phase transitions is always level crossing between the ground and an excited state. A band gap Δ is arising, due to the fact that level crossing is forbidden. This band gap is therefore a characteristic energy scale for the quantum phase transition. The

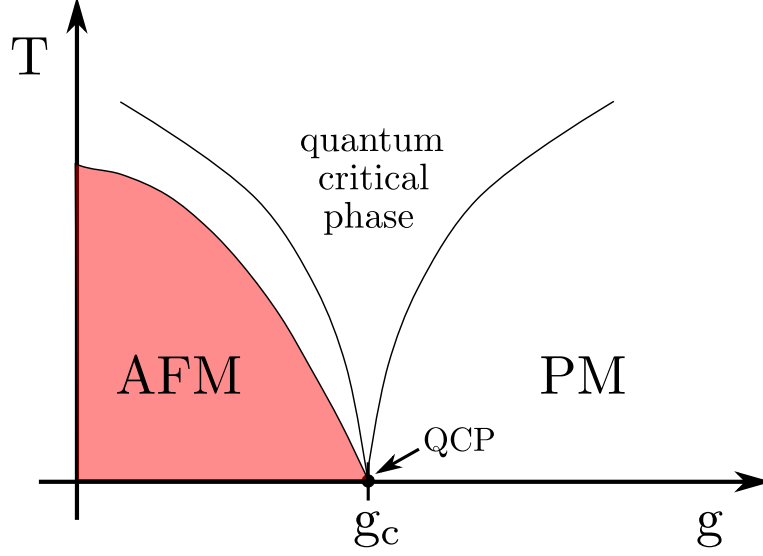


Figure 3.1: A schematic and simplified phase diagram is shown for metals transition from a paramagnetic (PM) into an antiferromagnetic (AFM) phase depending on a tuning parameter g . The phase line of the AFM phase ends in a quantum critical point (QCP) at $g = g_c$, decreasing temperature down to $T = 0$. At this point, the phase transition is only caused by quantum fluctuations. At $T > 0$, thermal fluctuations more and more dominates the phase transition. Nevertheless, the physical behaviour is influenced due to quantum fluctuations in a large regime, labeled as quantum critical phase.

characteristic energy scale Δ is proportional to the tuning parameter as

$$\Delta \sim J|g - g_c|^{z\nu}, \quad (3.1)$$

considering only phase transitions of second order. Here, $z\nu$ is a critical exponent and J an energy scale of a microscopic coupling [Sac11]. A characteristic length scale ξ is also required for quantum phase transitions. This length scale is called correlation length, which diverges right at the quantum critical point.

$$\xi^{-1} \sim \Lambda|g - g_c|^\nu, \quad (3.2)$$

where ν is again a critical exponent and Λ an arbitrary inverse length scale as a momentum cut-off. A directly relation between both characteristic quantities is yielded, inserting (3.2) in (3.1). For finite temperatures, $T > 0$, a second energy scale is given by $k_B T$, where k_B is the Boltzmann constant. A proportionality between temperature and correlation length is yielded, comparing both energy scales

$$T \sim \xi^{-z}. \quad (3.3)$$

The curved conical boundary phase lines of the quantum critical phase is explained with this relation, as depicted in figure 3.1. In the case of small temperatures, the critical exponent z attains the value $z = 2$, so that the phase lines are shaped like a square root. Increasing temperature the phase boundary lines are linear, since the critical exponent is changed to $z = 1$ [PS14]. Inside this regime the physical behaviour of the metals is determined by quantum fluctuations.

The spin-fermion-model is now introduced, knowing the physical origin of quantum phase transitions. Instead of an microscopic and detailed mathematical description, our focus is based on an introduction with qualitative arguments motivating the model. Metals in the vicinity of a magnetic quantum critical point are described with the spin-fermion-model, considering fermionic quasi-particles and bosonic spin density waves. Thereby, the fermionic propagator is determined by the usual free fermionic Green function. Spin fluctuations are constituted as collective modes and their propagator is characterized by the dynamical magnetic susceptibility.

$$\mathcal{D}_\mu(\mathbf{q}, \omega) = \sum_{\mathbf{Q}} \frac{1}{(\mathbf{q} + \mathbf{Q})^2 + \xi^{-2} - (\omega/v_S)^2}, \quad (3.4)$$

where μ is the spatial direction of the spin density wave, ξ is the magnetic correlation length and v_S is the spin wave velocity. The latter is of the same order as the Fermi velocity since spin fluctuations are originated due to fermions in the vicinity of the Fermi surface. Furthermore, a peak at the momentum vector $\mathbf{Q} = (\pi, \pi)$ is exhibit in the magnetic susceptibility. A strong coupling interaction is therefore implicated between momentum vectors \mathbf{k} and $\mathbf{k} + \mathbf{Q}$.

Phase transitions are always associated by an order parameter, equally the investigated antiferromagnetic phase transition. In this case, the local magnetization is the corresponding order parameter measured by the spin expectation value $\langle \mathbf{S}(\mathbf{r}_i) \rangle$. Naturally, it is summerarized over all spins located at a certain position \mathbf{r}_i . The order parameter is finite in the antiferromagnetic ordered phase and vanishes in the paramagnetic disordered phase. Furthermore, the expectation value of the spin operator is spatially modulated according to $\langle \mathbf{S}_\mu \rangle \sim \exp(i\mathbf{Q}\mathbf{R})$, where \mathbf{R} is some lattice vector [Wei15]. The order parameter and equally the propagator are therefore periodic quantities. In reciprocal space this is reflected in the periodicity of the magnetic Brillouin zone spanned by the vector \mathbf{Q} .

Our description of the antiferromagnetic quantum phase transition in the spin-fermion-model is based on a few fundamental assumptions, comparatively to [ACS03]. It is assumed, spin fluctuations are generated over a large range of the tuning parameter g and other low-energy collective degrees of freedom, independent of spin excitations, are neglected. Starting by large values of the tuning parameter g in the paramagnetic phase, the physical behaviour is described by Landau's Fermi liquid theory. Decreasing the tuning parameter and getting closer to the quantum critical point the behaviour is changed to a Non-Fermi liquid behaviour. Only one type of fermions is assumed and the arising collective modes are originated due to permanent interaction between particles and holes. The physics in the vicinity of the quantum critical point is determined by spin excitations, turning into smooth modes. One dominant channel is only

assumed containing fermion-fermion interaction with energies smaller than a certain energy cut-off Λ .

In the vicinity of the quantum critical point the (magnetic) correlation length ξ and the coupling constant λ is divergent. Therefore, the correlation length is much larger than the lattice constant, $\xi \gg a$, and the coupling constant is much larger than the band gap, $\lambda g \Delta$. The band gap is associated with the energy of spin excitations. In the limit of large distance and small energies or temperatures a microscopic consideration of the lattice Hamiltonian is unnecessary. In this low-energy theory, spin fluctuations are described as a three component bosonic field $\Phi_\mu(\mathbf{x}, \tau)$. The field is defined as a sum over all spin operators analysed in the neighbourhood of the spin's position i and is formally written as $\Phi_\mu(\mathbf{x}, \tau) \sim \sum_{i \in \Gamma(\mathbf{r}_i)} S_\mu(\mathbf{r}_i)$, where μ is the spatial direction of the field and $\Gamma(\mathbf{r}_i)$ represented the neighbourhood around the spin position \mathbf{r}_i [Sac11]. The magnitude of the bosonic field is chosen arbitrary and the field itself is considered as a real field. In the low-energy theory, the obtained effective Hamiltonian for spin fluctuations is then given by

$$H_\Phi = \sum_\mu \int_{\mathbf{k}} \left[-\frac{\mathbf{k}^2}{2} - \frac{r}{2} \right] \Phi_\mu(\mathbf{k}, \tau) \Phi_\mu(-\mathbf{k}, \tau) + \frac{v_S^2}{2} \pi_\mu(\mathbf{k}, \tau) \pi_\mu(-\mathbf{k}, \tau), \quad (3.5)$$

where r is a control parameter and corresponds to the squared inverse correlation length, $r = \xi^{-2}$. The integral is extended over the first Brillouin zone and the sum runs over the spatial direction of the bosonic field.

It has to take into account that the spin density waves are damped in consequence of the interaction with fermions. The spin itself does not possess an own damping source. The whole damping is governed by decaying of particle-holes-pairs and the full renormalized particle-hole bubble corresponds to the inverse lifetime of spin fluctuations. The interaction Hamiltonian between spin density waves and fermions is given by

$$H_{\Psi\Phi} = -\lambda \sum_\mu \int_{\mathbf{k}} \int_{\mathbf{q}} \Phi_\mu(\mathbf{k} - \mathbf{q}, \tau) \left[\Psi_a^\dagger(\mathbf{k}, \tau) \cdot \sigma_\mu \cdot \Psi_b(\mathbf{q}, \tau) + \Psi_b^\dagger(\mathbf{k}, \tau) \cdot \sigma_\mu \cdot \Psi_a(\mathbf{q}, \tau) \right], \quad (3.6)$$

where λ is the coupling constant. Both integrals are extended over the first Brillouin zone and the sum runs over all spatial directions of the bosonic field. σ_μ is the Pauli matrix with respect to the spatial direction. The two different Fermi surfaces in the obtained model are represented by the indices a and b at the fermionic fields Ψ . A detailed explanation is presently given below. The imaginary part of the susceptibility has to be computed in the low-energy limit with tools of the quantum field perturbation theory. An explicit calculation is presented in the appendix ???. Furthermore, the dynamic of the spin fluctuations is assumed to be governed by the low-energy fermions. The ω^2 -term in the susceptibility (3.4) is neglected [ACS03] and at the vicinity of the quantum critical point the correlation length diverges, implying $\xi^{-2} \rightarrow 0$. The damped magnetic susceptibility is then given by

$$\mathcal{D}_\mu(\mathbf{q}, i\omega_n) = \sum_{\mathbf{Q}} \frac{1}{(\mathbf{q} + \mathbf{Q})^2 + \gamma|\omega_n|}, \quad (3.7)$$

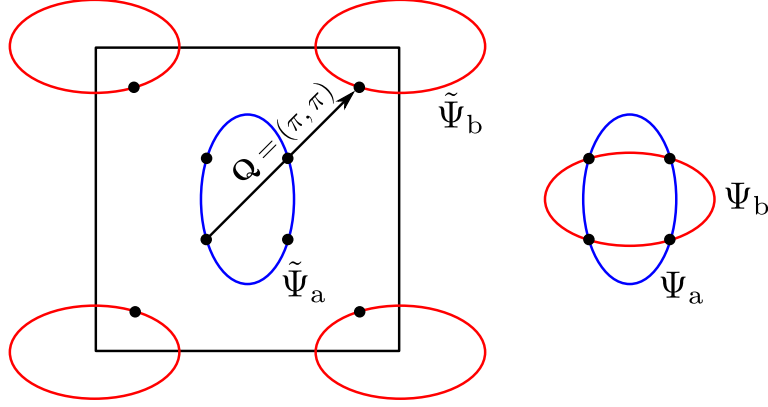


Figure 3.2: On the left hand side the Brillouin zone is depicted containing the Fermi surface of both species of fermions, $\tilde{\Psi}_a$ and $\tilde{\Psi}_b$. While the fermions $\tilde{\Psi}_a$ are located with an anisotropic parapolical dispersion at the origin $(0,0)$, the fermions $\tilde{\Psi}_b$ are located with a $\pi/2$ -rotated anisotropic parapolical dispersion at the corners of the Brillouin zone, (π, π) for example. The vector \mathbf{Q} connects certain points on the Fermi surface, called hotspots and represented with dots. As a result of this an attraction between these fermions occurs. On the right hand side the fermions $\tilde{\Psi}_a$ are shifted to the corner at (π, π) . The convenience of this representation is that the coupling between fermions and spin fluctuations is local and independent of the position.

where ω_n represent the bosonic Matsubara frequency. Spin fluctuations are no independent degrees of freedom due to the fact that their damping is strongly connected to fermions. The interaction between fermions on the Fermi surface separated by the large vector \mathbf{Q} is constituted in the damped susceptibility. These points separated by \mathbf{Q} on the Fermi surface are called hot-spots in two dimensions and their theory is discussed next. In comparison to a normal metals, the new interaction of spin fluctuations are separated the Fermi surface in *hot* and *cold* manifolds. A point \mathbf{k} is considered on the Fermi surface of a d -dimensional system and there, the fermion is assumed to has zero energy. This point is connected to another point $\mathbf{k} + \mathbf{Q}$, via the spin density wave, and is required to be also on the Fermi surface. A $d - 2$ -dimension manifold is yielded for a d -dimensional system due to both constraints. In the case of $d = 2$ the *hot* manifold is therefore called a hot-spot. Another visualization of *hot* manifolds is offered by the magnetic Brillouin zone spanned by the vector \mathbf{Q} . The intersections of the magnetic Brillouin zone and the Fermi surface are equivalent to the *hot* manifolds. In our investigated model the fermions are considered as free, up to the interaction with the spin fluctuations. Two species of fermions are assumed, $\tilde{\Psi}_a$ and $\tilde{\Psi}_b$. Their dispersion is anisotropic and parabolic, as suggested in [PS14]. The anisotropic parabolic Fermi surfaces are depicted on the left hand side in figure 3.2. This is not a discrepancy to our previous constraint, assuming one fermion, since both species of fermions

are electrons and differ only in their dispersion. The fermions $\tilde{\Psi}_a$ and $\tilde{\Psi}_b$ are located on an ellipse around the origin $(0,0)$ and (π,π) , respectively. Both ellipses are separated by the vector $\mathbf{Q} = (\pi,\pi)$ and rotated by $\pi/2$ to each other. For achieving a continuum theory the ellipse centered around (π,π) is shifted by the vector \mathbf{Q} to the origin. Therefore new fermionic fields, $\tilde{\Psi}_a(\mathbf{r}) = \Psi_a(\mathbf{r})$ and $\tilde{\Psi}_b(\mathbf{r}) = \Psi_b(\mathbf{r}) \exp(i\mathbf{Q}\mathbf{r})$, are introduced. The new Fermi surfaces of the fermions $\Psi_a(\mathbf{r})$ and $\Psi_b(\mathbf{r})$ are depicted on the right hand side in figure 3.2. The enormous advantage is that the coupling between the fermions, caused by spin density waves, is now local and independent of the position. In reciprocal space, the free continuum Hamiltonian of the fermions $\Psi_a(\mathbf{r})$ and $\Psi_b(\mathbf{r})$ is given by

$$H_\Psi = \int_{\mathbf{k}} \left[\epsilon_a(\mathbf{k}) \psi_a^\dagger(\mathbf{k}, \tau) \psi_a(\mathbf{k}, \tau) + \epsilon_b(\mathbf{k}) \psi_b^\dagger(\mathbf{k}, \tau) \psi_b(\mathbf{k}, \tau) \right], \quad (3.8)$$

where the integral is extended over the first Brillouin zone. $\epsilon_a(\mathbf{k})$ and $\epsilon_b(\mathbf{k})$ are the anisotropic parabolical dispersions, corresponding to the fermion species a and b, and are given by

$$\epsilon_a(\mathbf{k}) = \frac{k_x^2}{2m_1} + \frac{k_y^2}{2m_2} - \mu_0 \quad \text{and} \quad \epsilon_b(\mathbf{k}) = \frac{p_x^2}{2m_2} + \frac{p_y^2}{2m_1} - \mu_0, \quad (3.9)$$

where μ_0 is the chemical potential.

3.2 Momentum Conservation in the Spin-Fermion-Model and the Consequence of Umklapp Scattering

In the low-energy theory, our investigated 2D-model is described by the continuum Hamiltonian H_Ψ for free fermions on the Fermi surface, the effective Hamiltonian H_Φ for spin fluctuations and by the interaction Hamiltonian $H_{\Psi\Phi}$ between both. Directly at the quantum critical point the control parameter r in (3.5) is zero, due to $r = \xi^{-2}$ and the correlation length ξ is divergent. r is thus set to zero in the Hamiltonian H_Φ . The obtained model Hamiltonian is given by $H = H_\Psi + H_\Phi + H_{\Psi\Phi}$. Our further approach is to prove the conservation of momentum and current for this model Hamiltonian. After that, a perturbation Hamiltonian is introduced for considering umklapp scattering since translation symmetry is broken by this perturbation and momentum is not a conserved quantity any more.

A physical quantity is conserved, if its time derivative vanishes. In quantum mechanics the time derivative is given by Heisenberg equation of motion, $\dot{A}(t) = i[H, A(t)]_-$, where $A(t)$ is an arbitrary operator and its partial time derivative is assumed to be zero. The momentum operator is given by

$$P_j = \int_{\mathbf{k}} k_j \left[\Psi_a^\dagger(\mathbf{k}, \tau) \Psi_a(\mathbf{k}, \tau) + \Psi_b^\dagger(\mathbf{k}, \tau) \Psi_b(\mathbf{k}, \tau) - \pi_\mu(\mathbf{k}, \tau) \Phi_\mu(-\mathbf{k}, \tau) \right], \quad (3.10)$$

where the spatial direction is indicated by j . The integral is extended over the first Brillouin zone and the sum over μ is implied in the last term. The energy-momentum-tensor, as suggested in [Ili02], is used for the computation, shown in appendix ?? . Further the x-component of current operator is given by

$$J_x = - \int_{\mathbf{k}} \left[\frac{k_x}{m_1} \Psi_a^\dagger(\mathbf{k}, \tau) \Psi_a(\mathbf{k}, \tau) + \frac{k_x}{m_2} \Psi_b^\dagger(\mathbf{k}, \tau) \Psi_b(\mathbf{k}, \tau) \right], \quad (3.11)$$

where the integral is also extended over the first Brillouin zone. The y-component of the current operator is yielded changing the index x to y and interchanging the index a and b of the fermionic field operators. Now, the time derivative of both quantities is computed by using the basic bosonic and fermionic commutator relations. An explicite calculation is represented in the appendix ?? . This yields a vanishing time derivative for the the momentum,

$$\dot{P}_j = 0, \quad (3.12)$$

and the following expression for the time derivative of the x-component of the current

$$\begin{aligned} \dot{J}_x = \lambda \sum_{\mu} \int_{\mathbf{k}} \int_{\mathbf{q}} \Phi_{\mu}(\mathbf{k} - \mathbf{q}, \tau) & \left[\left(\frac{q_x}{m_1} - \frac{k_x}{m_2} \right) \Psi_b^\dagger(\mathbf{k}, \tau) \cdot \sigma_{\mu} \cdot \Psi_a(\mathbf{q}, \tau) \right. \\ & \left. + \left(\frac{q_x}{m_2} - \frac{k_x}{m_1} \right) \Psi_a^\dagger(\mathbf{k}, \tau) \cdot \sigma_{\mu} \cdot \Psi_b(\mathbf{q}, \tau) \right]. \end{aligned} \quad (3.13)$$

The y-component of the current is obtained by changing again the index x to y and interchanging the index a and b of the fermionic field operators. Therefore, momentum is a conserved quantity and the current is an unconserved quantity in the spin-fermion-model, described by the Hamiltonian H . The Hamiltonian is further invariant with respect to time reversal symmetry and a finite overlap is possessed between both quantities. Infinity is obtained for the static electrical conductivity in comparsion to the discussion of the previous chapter. A finite conductivity is only obtained breaking translation symmetry. This is equivalent to an unconserved momentum. Therefore, the model Hamiltonian H is pertubated by umklapp scattering via the Hamiltonian

$$H_{\text{umklapp}} = \sum_{\mu, \mathbf{G}} J_{\mathbf{G}} \int_{\mathbf{k}} \Phi_{\mu}(\mathbf{k}, \tau) \Phi_{\mu}(-\mathbf{k} + \mathbf{G}, \tau), \quad (3.14)$$

where the integral extends over the first Brillouin zone and the sum over \mathbf{G} included all reciprocal lattice vectors. The quantity $J_{\mathbf{G}}$ is a coupling constant depending on reciprocal lattice vectors. It is assumed that the coupling is decreasing fast to zero in the limit of large reciprocal lattice vectors ($|\mathbf{G}| \rightarrow \infty$). The time derivative of the momentum is given by

$$\dot{P}_j(\tau) = i \sum_{\mathbf{G}} J_{\mathbf{G}} \int_{\mathbf{k}} G_j \Phi_{\mu}(\mathbf{k}, \tau) \Phi_{\mu}(-\mathbf{k} - \mathbf{G}, \tau) \quad (3.15)$$

with respect to the new model Hamiltonian $H' = H + H_{\text{umklapp}}$. The time derivative of the current is persisted, since the current and perturbation Hamiltonian depends on different field operators and the commutator is therefore trivially zero. The static electrical conductivity is become finite due to the unconserved momentum. In the next chapter, the static electrical conductivity is computed using diagrammatic perturbation theory and the results are analysed.

4 The Static Conductivity in the Spin Fermion Model including Umklapp Scattering

The static electrical conductivity σ_{dc} is computed in this chapter, using the memory-matrix-formalism. The underlying model is the spin-fermion-model (see chapter 3), including umklapp scattering as a translation symmetry breaking perturbation. In this chapter, our attention is focused on the physical analysis of the obtained expression for the conductivity. An explicit computation is demonstrated in appendix ?? Two physical objects, fermions near the Fermi surface and spin fluctuations, are considered in the spin-fermion-model, introduced in the previous chapter. Spin fluctuations are generated at the vicinity of an antiferromagnetic quantum critical point due to particle-holes-excitations. Fermions, located at the point \mathbf{k} and $\mathbf{k} + \mathbf{Q}$ on the Fermi surface, are connected to each other because of these fluctuations. In the previous chapter, it is shown that the model Hamiltonian of the spin-fermion-model is conserved the momentum. The static electrical conductivity is thus infinite as it is proven in chapter 2. Considering umklapp scattering, the translation symmetry is broken and the momentum is unconserved. As a consequence the static conductivity becomes finite, which is computed in the following.

In chapter ?? over the memory-matrix-formalism, the following formula is derived for the static electrical conductivity, considering the spin-fermion-model and umklapp scattering.

$$\sigma_{\text{dc}} = - \lim_{z \rightarrow 0} \frac{z \cdot |\chi_{\text{JP}}(\omega = 0)|^2}{\mathcal{G}_{\dot{\mathbf{P}}\dot{\mathbf{P}}}(\mathbf{k}, z)} \quad (4.1)$$

Here, z is a complex frequency and $\chi_{\text{JP}}(\omega = 0)$ is the static susceptibility between current and momentum. In the denominator the Green function is given by

$$\mathcal{G}_{\dot{\mathbf{P}}\dot{\mathbf{P}}}(\mathbf{k}, z) = \int_0^\infty dt e^{izt} \left\langle \left[\dot{\mathbf{P}}(t), \dot{\mathbf{P}}(0) \right]_- \right\rangle_0, \quad (4.2)$$

where the usual quantum mechanical commutator is used, indicated with the minus sign at the squared brackets. The expectation value is generated with respect to the unperturbative Hamiltonian H , illustrated with the index 0. Here, the interaction between fermions and spin fluctuations is included. The time derivative of momentum is given by equation (3.15).

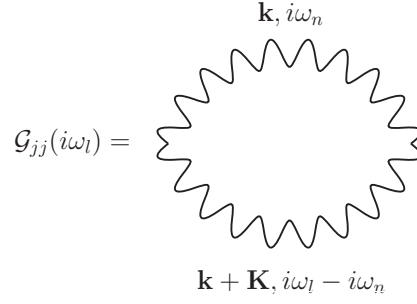


Figure 4.1: caption

Why? -i P and J are explicitly time independent

The Green function $\mathcal{G}_{\hat{P}\hat{P}}(\mathbf{k}, z)$ and the static susceptibility $\chi_{JP}(\omega = 0)$ are investigated, due to their possible temperature dependence. The latter is expected to be temperature independent. This is computed in detail in the appendix ??, using the diagrammatic perturbation technique. The considered diagrams are the electron-pair bubble for each species of fermions, depicted in figure ??. Therefore, the obtained expression of the susceptibility is given by

$$\chi_{PJ}(\omega = 0) = \frac{\sqrt{m_1 m_2}}{\pi} T \cdot \ln(e^{\mu/T} + 1), \quad (4.3)$$

where the chemical potential is denoted as μ . The logarithm is approximated in the limit of small temperatures ($\mu \gg T$) to $\ln(e^{\mu/T} + 1) \rightarrow \mu/T$. Inserting this expression, the temperature is canceled and the static susceptibility is given by constant parameters, $\chi_{PJ}(\omega = 0) = \mu \sqrt{m_1 m_2} / \pi$. The chemical potential is assumed as temperature independent in the observed regime.

The only temperature dependence of the static electrical conductivity is hence emerged by the Green function $\mathcal{G}_{\hat{P}\hat{P}}(\mathbf{k}, z)$. Only the free bubble diagram is considered computing the Green function with diagrammatic perturbation theory, which is depicted in figure 4.1. Higher order terms in the diagrammatic treatment are corrections of the bubble diagram and since spin fluctuations are the observing objects only bubble diagrams occur. Therefore the conductivity or resistance is only determined by spin fluctuations. Resistance is a consequence of fermionic coupling to other degrees of freedom, obtained as finite fermionic lifetime. The resistance is thus proportional to the imaginary part of the retarded Green function $\mathcal{G}_{\hat{P}\hat{P}}^{\text{ret}}(\mathbf{k}, z)$. Appendix ?? is shown the detailed computation of the expression of the retarded Green function.

$$\begin{aligned} \text{Im}\{\mathcal{G}_{\hat{P}\hat{P}}^{\text{ret}}(\mathbf{k}, z)\} &= -\frac{4\gamma^2\beta\omega}{\pi} \sum_{\mathbf{Q}_1, \mathbf{Q}_2} \sum_{\mathbf{G}} |\mathbf{J}_{\mathbf{G}}|^2 \int_0^\infty d\epsilon \frac{\epsilon^2 e^{\beta\epsilon}}{(e^{\beta\epsilon} - 1)^2} \\ &\times \int_{\mathbf{k}} G_j^2 \cdot \frac{1}{(\mathbf{k} + \mathbf{G} - \mathbf{Q}_1)^4 + \gamma^2\epsilon^2} \cdot \frac{1}{(\mathbf{k} + \mathbf{Q}_2)^4 + \gamma^2\epsilon^2} \end{aligned} \quad (4.4)$$

Here the term under the momentum integral is given by the imaginary part of the damped spin density propagator, denoted in (??). The integral itself is extended over

the first Brillouin zone. The periodicity of the spin susceptibility and perturbation is considered by the sums over \mathbf{Q}_i ($i = 1, 2$) and \mathbf{G} , respectively. In both cases these are reciprocal lattice vectors. Spatial direction of the momentum is represented by the index j and $\beta^{-1} = T$.

The obtained integrals is now investigated with respect to different cases since their are not exactly solvable. A detailed discussion of the single cases and an approximated computation of the integral is demonstrated in the following.

Convergence of the integral is surely given, if one of the momentum terms, $\mathbf{k} + \mathbf{G} - \mathbf{Q}_1$ or $\mathbf{k} + \mathbf{Q}_2$, is large according to amount. Since both terms are of the power of four, the integral is a fast decreasing function in the large momentum limit. Nevertheless, divergences of the integral are reached, if these terms are zero and this happens in many cases. One of the most divergent cases is assumed in the following approach. The vector \mathbf{k} is limited on the first Brillouin zone and the reciprocal lattice vectors are set to $\mathbf{G} = \mathbf{Q}_1$ and $\mathbf{Q}_2 = 0$. The choice of the reciprocal lattice vectors is arbitrary and it is therefore possible that the j -component of \mathbf{G} is large. This divergence is canceled by the coupling parameter $J_{\mathbf{G}}$ assumed as fast decreasing for large $|\mathbf{G}|$.

The remaining momentum integral is now exactly integrable. First of all, the momentum and frequency variables are transformed into dimensionless variables, using the transformation rules $\mathbf{k} = \mathbf{y} \cdot \sqrt{\gamma T}$ and $\epsilon = x \cdot T$, respectively. The new variable \mathbf{y} is further transformed into plane polar coordinates. The upper limit of the radius $|\mathbf{y}|$ is set to infinity, since the integrand is decreasing fast to zero for $|\mathbf{y}| \rightarrow \infty$. As a consequence the angular integral is easily evaluated, yielding the factor 2π . The remaining integral is given by the following expression.

$$\text{Im}\left\{\mathcal{G}_{\text{PP}}^{\text{ret}}(\mathbf{k}, z)\right\} = -\frac{2 \cdot G_j^2 \cdot |J_{\mathbf{K}}|^2}{\gamma \cdot \pi^2} \cdot \frac{\omega}{T} \int_0^\infty dx \frac{x^2 e^x}{(e^x - 1)^2} \int_0^\infty dy \frac{y}{(y^4 + x^2)^2} \quad (4.5)$$

The y -integral is substituted one last time, using the transformation rule $y^2 = z \cdot x$. The obtained integral is evaluated to $\pi/4$, using the integral formula (??). Both limits, $x \rightarrow 0$ and $x \rightarrow \infty$, of the integral over x are investigated. In the case of large x , the integral is decreasing fast to zero due to the ratio of the exponential functions. The upper limit is thus set to one and the integrand is expanded for small values of x . In first order the integrand is approximated to $1/x^3$. This is a highly divergent function in the limit $x \rightarrow 0$ and as a consequence the static conductivity is divergent as well.

The result of a divergent conductivity is clearly incorrect in a system with broken translation symmetry. In chapter 2, it is shown that translation symmetry and the consequent conserved momentum is caused an infinite conductivity in the static limit. As showing in chapter 3, momentum is conserved in the unpertubated spin-fermion-model (equation (3.12)) and it is thus a system with unbroken translation symmetry. Momentum is unconserved (equation (3.15)), introducing umklapp scattering as an observing perturbation. A finite conductivity is now expected, instead of a divergent one.

Our supposed correct choice of the control parameter r is the origin of this discrepancy. The paramter r is assumed to be zero, since its proportional to ξ^{-2} and the correlation

length ξ is divergent at the quantum critical point. This assumption is incorrect in the sense that the system is not directly at the quantum critical point, but rather in the vicinity of it. The system is supposed to be in the quantum critical phase, depicted in the phase diagram 3.1, at a point with tuning parameter $g = g_c$ and temperature $T > 0$. While the temperature is decreased to get closer to the quantum critical point, the tuning parameter is fixed. Considering the finite value of the control parameter r , the imaginary part of the retarded Green function is given by

$$\begin{aligned} \text{Im}\left\{\mathcal{G}_{\text{PP}}^{\text{ret}}(\mathbf{k}, z)\right\} &= -\frac{4\gamma^2\beta\omega}{\pi} \sum_{\mathbf{Q}_1, \mathbf{Q}_2} \sum_{\mathbf{G}} |\mathbf{J}_{\mathbf{G}}|^2 \int_0^\infty d\epsilon \frac{\epsilon^2 e^{\beta\epsilon}}{(e^{\beta\epsilon} - 1)^2} \\ &\quad \times \int_{\mathbf{k}} G_j^2 \cdot \frac{1}{((\mathbf{k} + \mathbf{G} - \mathbf{Q}_1)^2 + r)^2 + \gamma^2\epsilon^2} \cdot \frac{1}{((\mathbf{k} + \mathbf{Q}_2)^2 + r)^2 + \gamma^2\epsilon^2} \end{aligned} \quad (4.6)$$

The approach is nearly the same for solving the integrals as previously. Firstly, the convergence of large values of momenta is not changed, because of considering r . One of the most divergent cases is still $\mathbf{G} = \mathbf{Q}_1$ and $\mathbf{Q}_2 = 0$. Furthermore, the divergence, generated by large values of G_j , is still canceled since the coupling parameter $\mathbf{J}_{\mathbf{G}}$ is decreased fast in the limit $|\mathbf{G}| \rightarrow \infty$. The remaining momentum integral is of the same structure as above and exactly solvable. Therefore, the momentum integral is firstly transformed into plane polar coordinates, $\mathbf{k} = (k \cos \phi, k \sin \phi)$. The upper limit of k is again set to infinity, since the integrand is fast decreasing to zero for $k \rightarrow \infty$ and the contributions are neglectable.

$$\text{Im}\left\{\mathcal{G}_{\text{PP}}^{\text{ret}}(\mathbf{k}, z)\right\} = -\frac{|\mathbf{J}_{\mathbf{G}}|^2 \cdot G_j^2}{\gamma\pi^2} \cdot \frac{\omega}{T} \int_0^\infty d\epsilon \frac{\epsilon^2 e^{\beta\epsilon}}{(e^{\beta\epsilon} - 1)^2} \int_0^\infty dk \frac{k}{((r + k^2)^2 + \gamma^2\epsilon^2)^2} \quad (4.7)$$

where the angular integral is performed. The obtained momentum integral is substituted using $z = (r + k^2)/\gamma\epsilon$. In comparison to the case above, the lower limit is changed to $r/\gamma\epsilon$. Both cases are equivalent in the limit $r \rightarrow 0$. The finite lower boundary guarantees the convergence of the remaining integral over ϵ . The integral over z is performed, utilizing the integral formula (??) again. Dimensionless variables are introduced, using $x = \beta\epsilon$. The obtained expression is given by

$$\begin{aligned} \text{Im}\left\{\mathcal{G}_{\text{PP}}^{\text{ret}}(\mathbf{k}, z)\right\} &= -\frac{|\mathbf{J}_{\mathbf{G}}|^2 \cdot G_j^2}{4\gamma\pi^2} \cdot \frac{\omega}{T} \\ &\quad \times \int_0^\infty dx \frac{1}{x} \frac{e^x}{(e^x - 1)^2} \cdot \left[\pi - \frac{2\tilde{r}/x}{(\tilde{r}/x)^2 + 1} - 2 \arctan(\tilde{r}/x) \right], \end{aligned} \quad (4.8)$$

where the abbreviation $\tilde{r} = r/\gamma T$ is introduced. The integral over x is not analytical exactly solvable. However, the integral is finite in both limits, $x \rightarrow 0$ and $x \rightarrow \infty$. The latter is surely satisfied. The ratio of exponential functions is fast decreasing to zero and no other term is divergent. In the limit $x \rightarrow 0$, the integrand is limited by

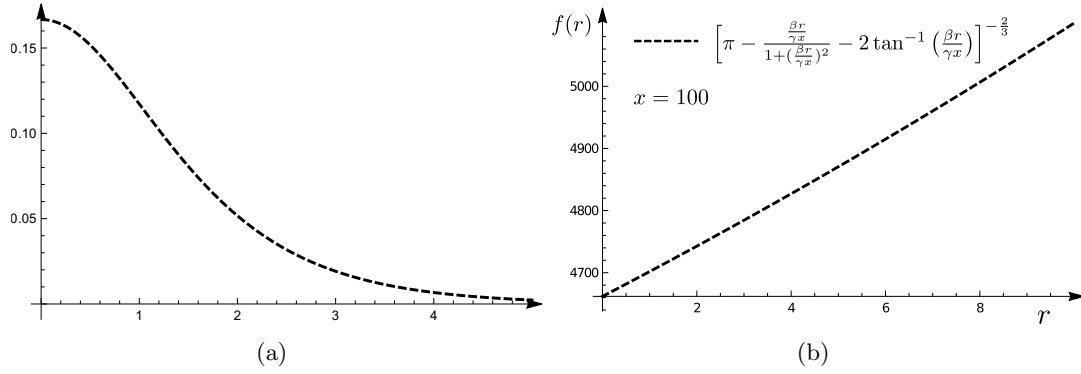


Figure 4.2: caption

$4/3r^3$, which is only divergent for $r \rightarrow 0$. The behaviour of the integrand is depicted on left hand side in figure 4.2, setting $\tilde{r} = 2$. A solution of the integral is evaluated determining the behaviour of the expression in squared brackets. For large values of x , a linear r -dependence is given by the power of $-2/3$. This is depicted in the right hand side of figure 4.2, where x is set to 100. An approximated expression is generated for the interand using the method of power counting. The initial point of this approach is the momentum integral in euqtion (4.7). Numerator and differatial yield in total the power of two, while the denominator generates the power of eight. Combining both, the integrand is a function proportional to k^{-6} . The further approach is now to investigate singularities of the integrand. The limit $r \rightarrow 0$ or $\epsilon \rightarrow 0$ is seperately generated singularities in the function. Both are considered with the power of three, since the power of them is half in comparison to the power of k in equation (4.7). The integrand is therefore approximated by the following expression.

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$$\text{Im}\left\{\mathcal{G}_{\text{PP}}^{\text{ret}}(\mathbf{k}, z)\right\} \approx -\frac{2|\mathbf{J}_{\mathbf{G}}|^2 \cdot G_j^2}{\gamma\pi^2} \cdot \frac{\omega}{T} \int_0^\infty dx \frac{x^2 e^x}{(e^x - 1)^2} \frac{1}{(\tilde{r}^2 + x^2)^{3/2}} \quad (4.9)$$

In figure 4.3, the approximated expression is confronted with the exact one. The behaviour of both are nearly identical and the estimation is inspected as valid. The integrand is still decreasing fast to zero for $x \rightarrow \infty$, while the upper limit is set to some arbitrary cut-off Λ . The ratio of the exponential functions are then expanded for small values of x up to the first non-vanishing order. The remained integral is exactly solvable and expanding the solution for small \tilde{r}/Λ the solution of the integral is given by

$$\text{Im}\left\{\mathcal{G}_{\text{PP}}^{\text{ret}}(\mathbf{k}, z)\right\} \approx -\frac{2\gamma|\mathbf{J}_{\mathbf{G}}|^2 \cdot G_j^2}{\pi^2\Lambda} \cdot \frac{\omega T}{r^2} \quad (4.10)$$

Inserting this expression and the approximated static susceptibility of (4.3) into equa-

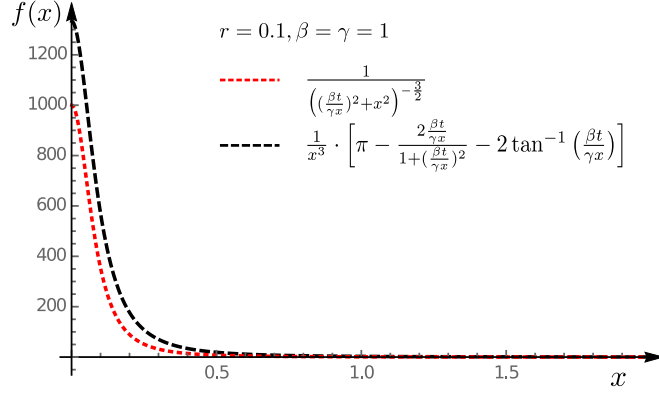


Figure 4.3: caption

tion (4.1), the static electrical conductivity is given by

$$\sigma_{\text{dc}}(T) = \frac{\mu}{2} \frac{m_1}{\gamma} \frac{m_2}{|\mathbf{J}_{\mathbf{G}}|^2} \frac{\Lambda}{G_j^2} \cdot \frac{r^2}{T} \quad (4.11)$$

Beside the temperature itself, the only temperature dependent parameter is the control parameter r , which is proportional to the squard inverse correlation length, $r = \xi^{-2}$. The correlation length is originated due to the fact that the system possesses a quantum phase transition and is temperature dependent is given by $\xi = T^{-1/z}$, as shown in chapter 3. z is a critical exponent and it is chosen in dependence of the distance to the quantum critical point. The corresponding temperature dependence of the control parameter is therefore provided to $r = T^{2/z}$. The resistance is determined by the inverse of the conductivity. Considering only the temperature dependent parameter, the static resistance is given by

$$\rho_{\text{dc}}(T) \sim T^{1-4/z} \quad (4.12)$$

Two possible choices are mentioned for the critical exponent z in chapter 3. In the vicinity of the quantum critical point at higher temperatures, z is chosen to be one. The T -dependence of the resistance is then given by T^{-3} . In the limit $T \rightarrow 0$, this is highly divergent. z is chosen to be two for lower temperatures. Nevertheless, the T -dependence is evaluated to T^{-1} , which is still divergent in the limit $T \rightarrow 0$.

Our physical expectation is not confirmed with this divergent behaviour of the resistance. Experiments of the investigated metals [Löh+07] are shown a linear temperature dependence of the resistance, $\rho(T) = \rho_0 + A T$. The behaviour of the resistance is described incorrect with our obtained solution (4.12). A possible origin of this discrepancy between experiment and theory is maybe the diagrammatic perturbation theory. In equation (4.2), the time evolution operator is expanded up to the first non-vanishing order. This yields the free bubble diagram, while correction to the bubble are considered expanding the time evolution operator up to the next order.

5 Memory-Matrix-Formalism

write a short
introduction

5.1 Motivation

A physicist is always interested in the behaviour and time evolution of the observables of the investigated 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 stochastic theory of these certain physical process is based on the Langevin equation

$$\frac{\partial}{\partial t}A(t) - F_{\text{ex}}(x, t) + \gamma \cdot A(t) = f(t), \quad (5.1)$$

where $A(t)$ is some arbitrary dynamical observable and $f(t)$ is a random force like white noise for example. The second term on the left hand side is originated from some external force, which is coupled to the dynamical observable $A(t)$. The third term is a damping or friction term. Now let us assume to separate equation (5.1) into two parts. The first part, called f_1 , is a functional of the dynamical observable $A(t')$, 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 summarized to the quantity $F(t)$. The result is a linearized form of the Langevin equation

$$\frac{\partial}{\partial t}A(t) = \int_{t_0}^t dt' \mathcal{C}(t - t')A(t') + F(t), \quad (5.2)$$

where \mathcal{C} denotes a correlation function and $A(t')$ is the deviation of the invariant part of the Hamiltonian. For large time scales the deviation should be vanish, so the time-integral over $A(t')$ 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

$$\mathcal{L}\{A(t)\} = A(s) = \int_0^{\infty} dt A(t)e^{-st}. \quad (5.3)$$

Using the Laplace transformation equation (5.2) becomes a algebraic equation of motion. The solution of this equation is given by

$$A(t) = \Xi(t) \cdot A(0) + A'(t) \quad \text{with} \quad A'(t) = \int_0^t dt' \Xi(t-t') F(t'), \quad (5.4)$$

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 transformation of the correlation function $\mathcal{C}(t)$. The main result of equation (5.4) and the motivation for the following introduced memory-matrix-formalism is that the dynamical observable $A(t)$ 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 considering the definition of Ξ . This term included the linear contributions of $A(t)$ by construction. These ones are the mostly important contributions to the time evolution 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 $F(t')$. 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 (5.4) and put it in a general and exact form, so that it can be used classically and quantum mechanically.

figure to visualize to splitting of A(t)

5.2 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.

5.2.1 Kubo formula

Consider a system in equilibrium represented by the Hamiltonian H_0 . At an arbitrary time t' a pertubation is switched on, where the pertubation is given by the Hamiltonian $H_1 = -B \cdot F(t)$, so that $H(t) = H_0 + H_1$ is the full Hamiltonian. Thereby B is an operator by which the pertubation is coupled 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 perturbation switched on at t' . The answer is given by the thermodynamical expectation value of the operator corresponding to the observable A

$$\langle A \rangle(t) := \text{Tr}\{\rho_S(t)A_S\} = \text{Tr}\{\rho_I(t)A_I\}, \quad (5.5)$$

where the label S and I stand for the Schrödinger and Interaction picture, respectively. The equality of the expectation value in the different representations is shown by the invariance of the trace with respect to cycle permutation. The transformation into the interaction picture is very usefull what we will see after the next step below. In quantum mechanics the time evolution of the density operator is determined by the von Neumann-equation.

$$\frac{d}{dt}\rho_S(t) = -\frac{i}{\hbar}[H(t), \rho_S(t)] \quad \Leftrightarrow \quad \frac{d}{dt}\rho_I(t) = -\frac{i}{\hbar}[H_I, \rho_I(t)] \quad (5.6)$$

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_I now. Integrating and using the boundary condition that the system is in thermal equilibrium at $t \rightarrow -\infty$ equation (5.6) is resulted in a integral equation.

$$\rho_I(t) = \rho_0 + \frac{i}{\hbar} \int_{-\infty}^t dt' [B_I(t'), \rho_I(t')] F(t') \quad (5.7)$$

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 (5.7) 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 (5.5) and defining the dynamical susceptibility

$$\chi_{AB}(t-t') = \frac{i}{\hbar} \Theta(t-t') \langle [A_I(t-t'), B_I(0)] \rangle_{H_0} \quad (5.8)$$

yield the Kubo formula

$$\delta \langle A(t) \rangle := \langle A \rangle(t) - \langle A(t) \rangle_{H_0} \approx \int_{-\infty}^{\infty} dt' \chi_{AB}(t-t') F(t'), \quad (5.9)$$

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 $\chi_{AB}(t-t')$ and the time evolution function $F(t)$.

5.2.2 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 perturbation. Let us assume $F(t) = \Theta(-t) \cdot F \cdot e^{-s\tau}$ the time evolution function of a perturbation, which is switched on adiabatically at $t = -\infty$ and switched off at t . Inserting this in equation (5.9) and substituting $\tau = t - t'$ yield $\delta \langle A(t) \rangle = \Phi_{AB}(t) \cdot F e^{st}$ with the Kubo relaxation function

$$\Phi_{AB}(t) = \frac{i}{\hbar} \lim_{s \rightarrow 0} \int_t^\infty d\tau \langle [A_I(\tau), B_I(0)] \rangle_0 e^{-s\tau}. \quad (5.10)$$

The arising Θ -distributions determine the lower limit of the integral 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

$$1. \quad \chi_{AB}(t) = -\Theta(t) \frac{d}{dt} \Phi_{AB}(t) \quad (5.11)$$

$$2. \quad \Phi_{AB}(t = 0) = \chi_{AB}(\omega = 0) \quad (5.12)$$

$$3. \quad \Phi_{AB}(\omega) = \frac{1}{i\omega} [\chi_{AB}(\omega) - \chi_{AB}(\omega = 0)]. \quad (5.13)$$

The evidence of these three relations are shown in the appendix ???. 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

$$\langle [A(t), B(t')] \rangle = \frac{1}{Z} \text{Tr} \{ [\rho, A(t)] B(t') \}, \quad (5.14)$$

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 use the analogy of the exponential functions to the time evolution¹ of an operator.

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

¹ The time evolution of an operator is given by

$$A_H(t) = e^{iHt/\hbar} A_S(0) e^{-iHt/\hbar}, \quad (5.15)$$

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

$$\begin{aligned}
&\Leftrightarrow i[\rho, A(t)] = -i\rho \int_0^\beta d\lambda \frac{d}{d\lambda} e^{\lambda H} A(t) e^{-\lambda H} \\
&\Leftrightarrow i[\rho, A(t)] = -i\rho \int_0^\beta d\lambda \left[H e^{i\tilde{\lambda}H/\hbar} A(t) e^{-i\tilde{\lambda}H/\hbar} - e^{i\tilde{\lambda}H/\hbar} A(t) e^{-i\tilde{\lambda}H/\hbar} H \right] \\
&\Leftrightarrow i[\rho, A(t)] = -i\rho \int_0^\beta d\lambda \left[H, A(t + \tilde{\lambda}) \right] \\
&\Leftrightarrow \frac{i}{\hbar} [\rho, A(t)] = -\rho \int_0^\beta d\lambda \dot{A}(t + \tilde{\lambda}) = -\rho \int_0^\beta d\lambda \dot{A}(t - i\lambda\hbar), \tag{5.16}
\end{aligned}$$

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 (5.14) and (5.16) in the Kubo relaxation function yield the wanted form of the Kubo relaxation function, where on the right hand side of the following computation is integrated by parts, dedicated with PI.

$$\begin{aligned}
\Phi_{AB}(t) &= \frac{i}{\hbar} \lim_{s \rightarrow 0} \int_t^\infty d\tau \langle [A_I(\tau), B_I(0)] \rangle_0 e^{-s\tau} \\
\stackrel{(5.14)}{\Leftrightarrow} \Phi_{AB}(t) &= \frac{i}{\hbar} \lim_{s \rightarrow 0} \int_t^\infty d\tau \frac{1}{Z_0} \text{Tr}\{[\rho_0, A_I(\tau)] B_I(0)\} e^{-s\tau} \\
\stackrel{(5.16)}{\Leftrightarrow} \Phi_{AB}(t) &= -\lim_{s \rightarrow 0} \int_0^\beta d\lambda \int_t^\infty d\tau \langle \dot{A}_I(\tau - i\lambda\hbar) B_I(0) \rangle_0 e^{-s\tau} \\
\stackrel{\text{PI}}{\Leftrightarrow} \Phi_{AB}(t) &= -\lim_{s \rightarrow 0} \int_0^\beta d\lambda \left\langle \left[A_I(\tau - i\lambda\hbar) e^{-s\tau} \right]_t^\infty + s \int_t^\infty d\tau \dot{A}_I(\tau - i\lambda\hbar) e^{-s\tau} \right\rangle B_I(0) \Big|_0 \\
\Leftrightarrow \Phi_{AB}(t) &= \int_0^\beta d\lambda \langle A_I(t - i\lambda\hbar) B_I(0) \rangle_0 = \int_0^\beta d\lambda \langle A_I(t) B_I(i\lambda\hbar) \rangle_0 \tag{5.17}
\end{aligned}$$

Later we will see that the scalar product defining at the memory-matrix-formalism has a similar structure. This provide the opportunity to transform the correlation function out of the language of the memory-matrix-formalism into the Kubo relaxation function, which in turn provide the opportunity to compute the correlation function perturbatively.

5.2.3 Kramer-Kronig-relation

All experiences of a human life demonstrating that an incident is always before the reaction of a system, which is called causality. Causality and the condition that the dynamical susceptibility $\chi_{AB}(t - t')$ is zero for times t smaller than t' are equivalent assertions. It's often useful to work in the frequency space which is why we want to investigate what causality means in Fourier space. Consider the Fourier transformation $\chi_{AB}(\omega)$, 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' .

$$\chi_{AB}(\omega) = \int_{-\infty}^{\infty} dt e^{i(\omega' + i\omega'')t} \chi_{AB}(t) \quad (5.18)$$

The integral converges if the exponential functions decrease to zero. Causality in time space yields $t > 0$ 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 ($\text{Im}\{\omega\} = \omega'' > 0$).

Cauchy's integral theorem offers us the opportunity 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 precisely in the regime where $\chi_{AB}(\omega)$ is holomorphic.

$$\chi_{AB}(\omega) = \frac{1}{2\pi i} \oint_{\Gamma} d\zeta \frac{\chi_{AB}(\zeta)}{\zeta - \omega} \quad (5.19)$$

Our choice of the contour is some which goes from minus infinity 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 $\eta \rightarrow 0$ is implicated.

The contribution of the semi-circle vanishes because it is assumed that $\chi_{AB}(\omega)$ decrease very fast for large values of ω . Only an integral along the real part axis survives which can be evaluated by formally writing $\frac{1}{x+i\eta} = \text{P.V.} \frac{1}{x} - i\pi\delta(x)$ where P.V. stands for taking the principal value.

$$\begin{aligned} \chi_{AB}(\omega) &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega' \frac{\chi_{AB}(\omega')}{\omega' - \omega - i\eta} \\ \Leftrightarrow \chi_{AB}(\omega) &= \frac{1}{2\pi i} \left[\text{P.V.} \int_{-\infty}^{\infty} d\omega' \frac{\chi_{AB}(\omega')}{\omega' - \omega} + i\pi \int_{-\infty}^{\infty} d\omega' \chi_{AB}(\omega') \delta(\omega' - \omega) \right] \\ \Leftrightarrow \chi_{AB}(\omega) &= -\frac{i}{\pi} \text{P.V.} \int_{-\infty}^{\infty} d\omega' \frac{\text{Re}\{\chi_{AB}(\omega')\}}{\omega' - \omega} + i \text{Im}\{\chi_{AB}(\omega')\} \omega' - \omega \\ \Leftrightarrow \chi_{AB}(\omega) &= \frac{1}{\pi} \text{P.V.} \int_{-\infty}^{\infty} d\omega' \left[\frac{\text{Im}\{\chi_{AB}(\omega')\}}{\omega' - \omega} - i \frac{\text{Re}\{\chi_{AB}(\omega')\}}{\omega' - \omega} \right] \end{aligned} \quad (5.20)$$

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.

$$\operatorname{Re}\{\chi_{AB}(\omega)\} = \frac{1}{\pi} \text{P.V.} \int_{-\infty}^{\infty} d\omega' \frac{\operatorname{Im}\{\chi_{AB}(\omega')\}}{\omega' - \omega} \quad (5.21)$$

$$\operatorname{Im}\{\chi_{AB}(\omega)\} = -\frac{1}{\pi} \text{P.V.} \int_{-\infty}^{\infty} d\omega' \frac{\operatorname{Re}\{\chi_{AB}(\omega')\}}{\omega' - \omega} \quad (5.22)$$

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.

5.2.4 Spectral representation

In section 5.2.1 the dynamical susceptibility χ_{AB} is introduced by deviated the Kubo-formula (5.9). 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

$$\chi''_{AB}(t - t') = \frac{1}{2\hbar} \langle [A(t), B(t')] \rangle \quad (5.23)$$

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

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

$$(\chi''_{AB}(t - t'))^* = -\chi''_{AB}(t - t') \quad (5.24)$$

is trivially shown because the commutator of two Hermitian operators is anti-Hermitian. The Fourier transformation of $\chi''_{AB}(t - t')$ is given by equation (5.18). Notice that in the following computation the frequency ω isn't splitted into real and imaginary parts. Our calculation is started by multipling equation (5.8) with $e^{i\omega t}$ and integrating over time t .

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

$$\begin{aligned}
\Leftrightarrow \chi_{AB}(\omega) &= \frac{1}{\pi} \text{PV} \int_{-\infty}^{\infty} d\omega' \frac{\chi''_{AB}(\omega')}{\omega' - \omega} + i \int_{-\infty}^{\infty} d\omega' \delta(\omega' - \omega) \chi''_{AB}(\omega') \\
\Leftrightarrow \chi_{AB}(\omega) &= \chi'_{AB}(\omega) + i\chi''_{AB}(\omega)
\end{aligned} \tag{5.25}$$

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

$$\Theta_{\eta}(t) = i \lim_{\eta \rightarrow 0} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{e^{-i\omega't}}{\omega' + i\eta} \tag{5.26}$$

In equation (5.25) we see that the dynamical susceptibility $\chi_{AB}(\omega)$ is separated into two functions $\chi'_{AB}(\omega)$ and $\chi''_{AB}(\omega)$, where the latter is the dissipative susceptibility defined at the beginning of this section in (5.23). Equation (5.25) is general and for any susceptibility valid. Assuming the dissipative susceptibility is a real number, then this is also valid for $\chi'_{AB}(\omega)$ and the both functions $\chi'_{AB}(\omega)$ and $\chi''_{AB}(\omega)$ are real and imaginary part of $\chi_{AB}(\omega)$, respectively.

5.3 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. This chapter started splitting an arbitrary 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 a system after a perturbation is switched off for a long time the secular part depending the evolution. Furthermore all processes with a short lifetime or small magnitudes compared with the linear term in perturbation 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 a 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

$$A = \sum_{i,j} |i\rangle\langle i| A |j\rangle\langle j| = \sum_{i,j} A_{ij} |i\rangle\langle j|, \tag{5.27}$$

where $A_{ij} := \langle i| A |j\rangle$ 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 also operator space.

The Liouville-space is a 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 A, B, \dots 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

$$|A\rangle := \sum_{ij}^d A_{ij} |i\rangle\langle j|. \quad (5.28)$$

Similiarly to the quantum mechanic the Dirac notation is used with the difference that round brackets are used instead of angle brackets to distinguish both spaces. Out of the definition (5.28) 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 opportunities to choose the basis in the Liouville space \mathbb{L} , but the definition in (5.28) should be the one we are working with.

In the following the basis of our Liouville space is denoted with $\{|A_i\rangle\}$ where $i = 1, 2, 3, \dots, n$ and A_i is an operator. The corresponding basis of the dual space is given by $\{\langle A_i|\}$, similarly to the Hilbert space. The last needed element of our Liouville space is a scalar product which has to fulfill the following three conditions.

$$1. \quad (A_i|A_j) = (A_j|A_i)^* \quad (5.29)$$

$$2. \quad (A_i|B) = c_1(A_i|A_j) + c_2(A_i|A_k),$$

$$\text{where } B = c_1 A_j + c_2 A_k \quad \text{and} \quad c_1, c_2 \in \mathbb{C} \quad (5.30)$$

$$3. \quad (A_i|A_i) \geq 0, \quad \text{where equality is fulfilled if } A_i = 0. \quad (5.31)$$

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

$$(A_i(t)|A_j(t')) = \frac{1}{\beta} \int_0^\beta d\lambda \langle A_i^\dagger(t) A_j(t' + i\lambda\hbar) \rangle \quad (5.32)$$

as our scalar product, where the normal time evolution of an operator $A_i(t) = e^{iHt/\hbar} A_i(0) e^{-iHt/\hbar}$ is valid, so that $A_i(i\lambda\hbar) = e^{-\lambda H} A_i(0) e^{\lambda H}$ can be used. Now we have to proof if the conditions are fulfilled by the choice of our scalar product. Let's get started with the second one because it's easily shown transforming the expectation value into the trace representation and then using the properties of the trace.

Motivation why we choose this kind of a scalar product

$$(A_i(t)|B(t')) = \frac{1}{\beta} \int_0^\beta d\lambda \frac{1}{Z} \text{Tr} \left\{ \rho A_i^\dagger(t) [c_1 A_j(t' + i\lambda\hbar) + c_2 A_k(t' + i\lambda\hbar)] \right\}$$

maybe the computation isn't needed here

$$\Leftrightarrow (A_i(t)|B(t')) = c_1(A_i(t)|A_j(t')) + c_2(A_i(t)|A_k(t')) \quad (5.33)$$

The first and third condition can be shown by transforming the scalar product in the spectral representation. Therefore the trace is written 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 .

$$\begin{aligned} (A_i(t)|A_j(t')) &= \frac{1}{\beta \cdot Z} \int_0^\beta d\lambda \sum_{n,m} \langle n| e^{-\beta H} A_i^\dagger(t) |m\rangle \langle m| e^{-\lambda H} A_j(t') e^{\lambda H} |n\rangle \\ \Leftrightarrow (A_i(t)|A_j(t')) &= \frac{1}{\beta \cdot Z} \sum_{n,m} \langle n| A_i^\dagger(t) |m\rangle \langle m| A_j(t') |n\rangle e^{-\beta E_n} \int_0^\beta d\lambda e^{\lambda(E_n - E_m)} \\ \Leftrightarrow (A_i(t)|A_j(t')) &= \frac{1}{\beta \cdot Z} \sum_{n,m} \langle n| A_i^\dagger(t) |m\rangle \langle m| A_j(t') |n\rangle \frac{e^{-\beta E_m} - e^{-\beta E_n}}{E_n - E_m} \end{aligned} \quad (5.34)$$

The complex conjugated of the expectation value is considered in the Liouville space and using $\langle n| A_j^\dagger(t) |m\rangle^* = \langle m| A_j(t) |n\rangle$ let us find instantly the first condition. Notice that on the right hand side of equation (5.34) only the expectation values are complex quantities. For them the complex conjugation yields

$$\left(\langle n| A_i^\dagger(t) |m\rangle \langle m| A_j(t') |n\rangle \right)^* = \langle n| A_j^\dagger(t') |m\rangle \langle m| A_i(t) |n\rangle \quad (5.35)$$

and inserting back $(A_i(t)|A_j(t'))^*$ is exactly the same as (5.34). Proofing the third condition it has to be set $A_j(t') = A_i(t)$ in equation (5.34), which on the right hand side yields

$$\frac{1}{\beta \cdot Z} \sum_{n,m} \left| \langle m| A_i(t) |n\rangle \right|^2 \frac{e^{-\beta E_m} - e^{-\beta E_n}}{E_n - E_m}. \quad (5.36)$$

It's clear that the squared expectation value is always non-negative. The fraction is positive too, which is easily seen by proofing the two cases $E_n > E_m$ and $E_n < E_m$. Therefore the expectation value $(A_i(t)|A_i(t)) \geq 0$ and equality is only possible if $A_i = 0$. All three conditions are well proven and the chosen scalar product is really one's. At this point all the mathematical ground work is done, we know how the vectors look in the Liouville space and we have a well defined scalar product.

The goal of every physical theory is to describe the measurement results. Typically in statistical or quantum mechanics this is done via correlation functions. So our goal is 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

$$\frac{d}{dt} A_i(t) = \dot{A}_i(t) = \frac{i}{\hbar} [H, A_i(t)] = iL A_i(t) \quad (5.37)$$

where the operators are in the Heisenberg representation and the Hermitian Liouville operator $L = \hbar^{-1}[H, \bullet]$ is introduced, defined by his action on an arbitrary operator. The formal solution of equation (5.37) is given by

$$A_i(t) = e^{itL}A_i(0) = e^{itH/\hbar}A_i(0)e^{-itH/\hbar}. \quad (5.38)$$

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 (5.37), which results in

Have to convince me that it is really so easy.

$$|\dot{A}_i(t)\rangle = \frac{i}{\hbar}|[H, A_i(t)]\rangle = iL|A_i(t)\rangle \quad (5.39)$$

for the equation of motion in the Liouville space and there formal solution is given by

$$|A_i(t)\rangle = e^{itL}|A_i(0)\rangle. \quad (5.40)$$

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 $\{C_i\}$, where the choice of these operators are differently 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

$$P = \sum_{i,j} |C_i(0)\rangle (C_i(0)|C_j(0)\rangle)^{-1} (C_j(0)|. \quad (5.41)$$

The action of P on some vector $|A(t)\rangle$ in the Liouville space yields the parallel components to the chosen operators C_i , which is the projection from $|A(t)\rangle$ at the vector subspace spanned by C_i . The corresponding vertical component of $|A(t)\rangle$ with respect to the operators C_i is given by $Q = 1 - P$, which is the projection out of the vector subspace. Naturally the projection operator is fullfilled the two properties $P^2 = P$ and $PQ = QP = 0$ of a projection operator, which follows immediately from the definition of P.

figure of the projector's acting

After the deviation of the time evolution of an operator and the projection operator in Liouville space the correlation function can be defined as

$$C_{ij}(t) = (A_i(t)|A_j(0)) \stackrel{(5.32)}{=} \frac{1}{\beta} \int_0^\beta d\lambda \langle A_i^\dagger(t) A_j(i\lambda\hbar) \rangle, \quad (5.42)$$

where in the last step the definition of the scalar product is only inserted. Comparing equation (5.42) with (5.17) our choice of the correlation function is more clear. The

defined correlation function is proportional to the Kubo relaxation function, which describes the system's reaction on a switched off perturbation, how we learned in section 5.2.2. For $t = 0$ the correlation function is also proportional to the Fourier transformed susceptibility

$$C_{ij}(t=0) = \frac{1}{\beta} \Phi_{ij}(t=0) = \frac{1}{\beta} \chi_{ij}(\omega=0), \quad (5.43)$$

which directly results from equation (5.12). Equation (5.40) is used to bring the time evolution of the correlation function in more suitable expression

$$C_{ij}(t) = (A_i(0)|A_j(-t)) = (A_i(0)|e^{-itL}|A_j(0)), \quad (5.44)$$

which opens the possibility for using the Laplace transformation. Instead of the definition in equation (5.3) here a form of the Laplace transformation is used where s is substituted by $-i\omega$ which is nothing else as a rotation of the definition area by $\pi/2$. Multiplying the last equation with $e^{i\omega t}$ and integrate from zero to infinity with respect to t yields

$$C_{ij}(\omega) = (A_i|\int_0^\infty dt e^{i(\omega-L)t}|A_j) = (A_i|\frac{i}{\omega-L}|A_j), \quad (5.45)$$

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 $L = LQ + LP$ which follows immediately by using the definition of P and Q and the identity $(X+Y)^{-1} = X^{-1} - X^{-1}Y(X+Y)^{-1}$ is used to simplify the correlation function, where $X = \omega - LQ$ and $Y = -LP$.

$$\begin{aligned} C_{ij}(\omega) &= (A_i|\frac{i}{\omega-LQ-LP}|A_j) \\ \Leftrightarrow C_{ij}(\omega) &= (A_i|\frac{i}{\omega-LQ}|A_j) + (A_i|\frac{1}{\omega-LQ}LP\frac{i}{\omega-L}|A_j) \end{aligned} \quad (5.46)$$

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

$$\frac{i}{\omega-LQ} = \frac{i}{\omega} \left[1 + \frac{LQ}{\omega} + \left(\frac{LQ}{\omega}\right)^2 + \dots \right] \quad (5.47)$$

Each term of the series in the square brackets acting on the operator $|A_j\rangle$. Remember this is the operator at time $t=0$, which means that no vertical component exists and therefore $Q|A_j\rangle = 0$. Every term except the first one contains an operator Q , so the first term of the correlation function yields

$$(A_i|\frac{i}{\omega-LQ}|A_j) = \frac{i}{\omega} (A_i|A_j) = \frac{i}{\omega} C_{ij}(0). \quad (5.48)$$

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Ask Jörg if this
explanation is
correct

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

$$P \frac{i}{\omega - L} |A_j\rangle = \sum_{k,l} |C_k\rangle (C_k | C_l)^{-1} (C_l | \frac{i}{\omega - L} |A_j\rangle = \sum_{k,l} |C_k\rangle C_{kl}^{-1}(0) C_{lj}(\omega) \quad (5.49)$$

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

$$C_{ij}(\omega) = \frac{i}{\omega} C_{ij}(0) + \sum_{k,l} (A_i | \frac{1}{\omega - LQ} L | C_k) C_{kl}^{-1}(0) C_{lj}(\omega). \quad (5.50)$$

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 a null $LQ - LQ$ is added in the nominator.

$$\frac{\omega}{\omega - LQ} = \frac{\omega - LQ + LQ}{\omega - LQ} = 1 + \frac{LQ}{\omega - LQ} \quad (5.51)$$

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

$$\begin{aligned} \omega C_{ij}(\omega) &= i C_{ij}(0) + \sum_{k,l} (A_i | \frac{\omega}{\omega - LQ} L | C_k) C_{kl}^{-1}(0) C_{lj}(\omega) \\ \Leftrightarrow \omega C_{ij}(\omega) &= i C_{ij}(0) + \sum_{k,l} (A_i | 1 + \frac{LQ}{\omega - LQ} L | C_k) C_{kl}^{-1}(0) C_{lj}(\omega) \\ \Leftrightarrow \omega \sum_l \delta_{il} C_{lj}(\omega) &= i \frac{1}{\beta} \chi_{ij}(0) + \sum_l [\Omega_{il} - i \Sigma_{il}(\omega)] C_{lj}(\omega) \\ \Leftrightarrow \sum_l [\omega \delta_{il} - \Omega_{il} + i \Sigma_{il}(\omega)] C_{lj}(\omega) &= i \frac{1}{\beta} \chi_{ij}(0) \end{aligned} \quad (5.52)$$

where equation (5.12) is used and the abbreviations

$$\Omega_{il} := \beta \sum_k (A_i | L | C_k) \chi_{kl}^{-1}(0) \quad \text{and} \quad \Sigma_{il}(\omega) := i \beta \sum_k (A_i | \frac{LQ}{\omega - LQ} L | C_k) \chi_{kl}^{-1}(0) \quad (5.53)$$

are inserted. Equation (5.52) 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 summarized over all operators included in the set $\{C_i\}$ of selected operators. The indicies i and j have to be chosen out of this set too, so that equation (5.52) yields n^2 algebraic equations if n is the number of operators in $\{C_i\}$.

write that the founded expression is an exact one

It's useful for later computations to write the even defined abbreviations in another form. For Ω_{il} not much work is to do, because we use only equation (5.39), so that

$$\Omega_{il} = i\beta \sum_k (\dot{A}_i | C_k) \chi_{kl}^{-1}(0). \quad (5.54)$$

For the rearrangement of the second abbreviation equation (5.39) is used at the first step too and the fraction is written as the geometric series at the second step. Then in every term the relation $Q = Q^2$ is inserted, where the proof is an easy finger exercise. After factorizing one Q to each vector operator the geometric series is written back as a fraction.

$$\begin{aligned} \Sigma_{il}(\omega) &= \frac{i\beta}{\omega} \sum_k (\dot{A}_i | Q \left[1 + \frac{LQ}{\omega} + \left(\frac{LQ}{\omega} \right)^2 + \dots \right] | \dot{C}_k) \chi_{kl}^{-1}(0) \\ \Leftrightarrow \Sigma_{il}(\omega) &= \frac{i\beta}{\omega} \sum_k (\dot{A}_i | Q^2 + \frac{Q^2 L Q^2}{\omega} + \frac{Q^2 L Q^2 L Q^2}{\omega^2} + \dots | \dot{C}_k) \chi_{kl}^{-1}(0) \\ \Leftrightarrow \Sigma_{il}(\omega) &= \frac{i\beta}{\omega} \sum_k (\dot{A}_i | Q \left[1 + \frac{QLQ}{\omega} + \left(\frac{QLQ}{\omega} \right)^2 + \dots \right] Q | \dot{C}_k) \chi_{kl}^{-1}(0) \\ \Leftrightarrow \Sigma_{il}(\omega) &= i\beta \sum_k (\dot{A}_i | Q \frac{1}{\omega - QLQ} Q | \dot{C}_k) \chi_{kl}^{-1}(0) \end{aligned} \quad (5.55)$$

After all this exhausting mathematical and algebraical conversions the correlation function in the memory matrix formalism is in a useful and workable form. In equation (5.52) the abbreviations can be combined to one function $M_{il}(\omega) := \Sigma_{il}(\omega) + i\Omega_{il}$. The symbol Σ is selected in dependence on the quantum mechanical self energy. The function $M(\omega)$ 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 vanishes 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 $(\dot{A}_i | A_k) = 0$. This assertion is immediately proven extensively in the section below. In this case the memory function is solely given by the function $\Sigma(\omega)$. Comparising (5.55) with the definition (5.42) of correlation functions exhibits $\Sigma(\omega)$ has the structure of a correlation function but $\Sigma(\omega)$ occupies to differences. On the one hand only $Q | \dot{A}$ which is perpendicular to $|A\rangle$ 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 that the function $\Sigma(\omega)$ describes the dynamic of the operators, which 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 the "bath". Then $Q | \dot{A}$ characterizes the coupling to the bath and it's clear, that the dynamic of the bath changes the behaviour of A .

5.3.1 Time Reversal Symmetry

Even above the assertion was postulated that the quantity Ω_{il} vanishes if the considered Hamiltonian is symmetric and if the operators \dot{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 transformation rule

$$A(t) \rightarrow A'(t) = TA(t)T^{-1} = \epsilon_A A(-t), \quad (5.56)$$

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

$$Te^{iHt/\hbar}T^{-1} = e^{-iHt/\hbar} \quad (5.57)$$

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

$$T \frac{\partial}{\partial t} e^{iHt/\hbar} T^{-1} = \frac{i}{\hbar} T H e^{iHt/\hbar} T^{-1} = \frac{i}{\hbar} T H T^{-1} T e^{iHt/\hbar} T^{-1} = \frac{i}{\hbar} H e^{-iHt/\hbar}, \quad (5.58)$$

where in the second step the unit element $\mathbb{1} = TT^{-1}$ is inserted. 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 by

$$TH = HT \quad \Leftrightarrow \quad [H, T] = 0. \quad (5.59)$$

This is equivalent to the assumption that the Hamiltonian is invariant with respect to time reversal symmetry. This is all we need to know about the time reversal operator to prove the assertion. The expectation value of a Hermitian operator can be easily manipulated with the aim of the time reversal operator T .

$$\langle B \rangle = \frac{1}{Z} \text{Tr} \left\{ e^{-\beta H} T B T^{-1} \right\} = \left\langle (T B T^{-1})^\dagger \right\rangle \quad (5.60)$$

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.

$$\left(T [A(t), B(t')] T^{-1} \right)^\dagger = \epsilon_A \epsilon_B \left([A(-t), B(-t')] \right)^\dagger = -\epsilon_A \epsilon_B [A(-t), B(-t')] \quad (5.61)$$

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

(5.54). Using equation (5.25) yields

$$i\beta(\dot{A}_i|A_k) = i\chi_{\dot{A}_i A_k}(\omega = 0) = i \text{P.V.} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''_{\dot{A}_i A_k}(\omega')}{\omega'} - \lim_{\omega \rightarrow 0} \chi''_{\dot{A}_i A_k}(\omega), \quad (5.62)$$

where the dissipative susceptibility $\chi''_{\dot{A}_i A_k}(\omega)$ occurs, which differs a little but significant from the dissipative susceptibility $\chi''_{A_i A_k}(\omega)$ defined in section 5.2.4. To find the relation between both the derivative of (5.23) is formed.

$$\frac{d}{dt} \chi''_{A_i A_k}(t) = \frac{1}{2\hbar} \left\langle \left[\dot{A}_i(t), A_k(0) \right] \right\rangle = \chi''_{\dot{A}_i A_k}(t) \quad (5.63)$$

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

$$\chi''_{\dot{A}_i A_k}(\omega) = -i\omega \chi''_{A_i A_k}(\omega) \quad (5.64)$$

Inserting this in (5.65) yields

$$i\beta(\dot{A}_i|A_k) = \text{P.V.} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \chi''_{A_i A_k}(\omega') \quad (5.65)$$

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 $\chi''_{A_i A_k}(\omega')$. On the other hand the founded expression establishes the possibility to analyse the behaviour of Ω_{il} under time reversal symmetry.

$$\chi''_{A_i A_k}(t - t') = \frac{1}{2\hbar} \left\langle [A_i(t), A_k(t')] \right\rangle \quad (5.66)$$

The expectation value is rewritten using equation (5.60) which establishes the opportunity to use (5.61).

$$\chi''_{A_i A_k}(t - t') = -\epsilon_{A_i} \epsilon_{A_k} \chi''_{A_i A_k}(t' - t), \quad (5.67)$$

where the relation (5.24) is used. The Laplace transformation of this equation yields

$$\chi''_{A_i A_k}(\omega) = -\epsilon_{A_i} \epsilon_{A_k} \chi''_{A_i A_k}(-\omega) = \epsilon_{A_i} \epsilon_{A_k} \chi''_{A_i A_k}(\omega), \quad (5.68)$$

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 $\chi''_{A_i A_k}(\omega)$, which are $\epsilon_{A_i} = \epsilon_{A_k}$ and $\epsilon_{A_i} \neq \epsilon_{A_k}$. The analysis gives us the required properties to compute the integral over the dissipative susceptibility.

1. case: $\epsilon_{A_i} = \epsilon_{A_k}$

This yields $\chi''_{A_i A_k}(\omega) = \chi''_{A_k A_i}(\omega)$ which means that the dissipative susceptibility is symmetrical under interchanging A_i and A_k . Further the dissipative susceptibility is an antisymmetrical function, because $\chi''_{A_i A_k}(\omega) = -\chi''_{A_i A_k}(-\omega)$. Consider the complex conjugated of $\chi''_{A_i A_k}(\omega)$ yields that the dynamical susceptibility is a real number.

$$\left(\chi''_{A_i A_k}(\omega)\right)^* = - \int_{-\infty}^{\infty} dt e^{-i\omega(t-t')} \chi''_{A_i A_k}(t-t') = -\chi_{A_i A_k}(-\omega) = \chi_{A_i A_k}(\omega) \quad (5.69)$$

where equation (5.24) is used.

2. case: $\epsilon_{A_i} \neq \epsilon_{A_k}$

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

$$\left(\chi''_{A_i A_k}(\omega)\right)^* = - \int_{-\infty}^{\infty} dt e^{-i\omega(t-t')} \chi''_{A_i A_k}(t-t') = -\chi_{A_i A_k}(-\omega) = -\chi_{A_i A_k}(\omega) \quad (5.70)$$

Back to equation (5.65). We see that the integral vanishes in the first case because the susceptibility is an odd function. This means that $i\beta(\dot{A}_i|A_k)$ 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 assertion is equivalent to the one that \dot{A}_i and A_k have opposite signature with respect to time reversal symmetry. This is exactly the assertion which we want to prove.

6 Conclusion

A Computation of the Damped Spin Density Propagator

In the present appendix, the propagator of damped spin density fluctuations is computed, considering the first order in perturbation theory. Our approach is separated in two parts. Firstly, the free spin density propagator is determined, using the equation of motion for Green functions, as suggested in [EG79] or many other textbooks. The damped propagator is then calculated, using the diagrammatic perturbation theory. The obtained propagator is transformed into Matsubara frequency space, since the computation of the conductivity is treated into there.

A.1 Computation of the Free Propagator

Free propagators are easily computed, using the equation of motion of Green functions. The equation of motion is obtained, derivating the Green function with respect to the time t . In Fourier space the equation of motion is given by

$$\omega \langle\langle A; B \rangle\rangle_{\omega}^j = \langle[A, B]_{\eta}\rangle + \langle\langle[A, H]_{-}; B\rangle\rangle_{\omega}^j, \quad (\text{A.1})$$

where the typ of the Green function (retarded, advanced and causal) is denoted with j and the frequency dependence of the Green function is represented with an index ω . The Green function itself is symbolized by double angle brackets. This equation is an algebraic equation or more precisely an infinite algebraic equation chain for Green functions. A new more complicated Green function appears on the right hand side. For this one exists a new equation chain with a more complicated Green function, and so on. Nevertheless, the equation chain is not infinity in the case of free propagators. The dynamic of free spin density waves is described by the Hamiltonian H_{Φ} , introduced in chapter ?? . Inserting H_{Φ} and bosonic field operators Φ_{μ} for A and B in equation (A.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.

$$\omega \langle\langle\Phi_{\mu}; \Phi_{\mu}\rangle\rangle_{\omega} = \langle[\Phi_{\mu}(\mathbf{k} + \mathbf{G}), \Phi_{\mu}(-\mathbf{k} - \mathbf{G})]\rangle + \langle\langle[\Phi_{\mu}(\mathbf{k} + \mathbf{G}), H_{\Phi}]; \Phi_{\mu}\rangle\rangle_{\omega} \quad (\text{A.2})$$

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 (A.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 bosonischen Vertauschungsrelationen

link zu H_{Φ}

$$\begin{aligned}
[\Phi_\mu(\mathbf{k} + \mathbf{G}, t), H_\Phi] &= -\frac{1}{2\epsilon} \sum_{\mathbf{P}} \int_{\mathbf{p}} [\Phi_\mu(\mathbf{k} + \mathbf{G}, t), \pi_\lambda(\mathbf{p} + \mathbf{P}, t) \pi_\lambda(-\mathbf{p} - \mathbf{P}, t)] \\
\Leftrightarrow [\Phi_\mu(\mathbf{k} + \mathbf{G}, t), H_\Phi] &= -\frac{1}{2\epsilon} \sum_{\mathbf{P}} \int_{\mathbf{p}} \left[\pi_\lambda(\mathbf{p} + \mathbf{P}, t) [\Phi_\mu(\mathbf{k} + \mathbf{G}, t), \pi_\lambda(-\mathbf{p} - \mathbf{P}, t)] \right. \\
&\quad \left. + [\Phi_\mu(\mathbf{k} + \mathbf{G}, t), \pi_\lambda(\mathbf{p} + \mathbf{P}, t)] \pi_\lambda(-\mathbf{p} - \mathbf{P}, t) \right] \\
\Leftrightarrow [\Phi_\mu(\mathbf{k} + \mathbf{G}, t), H_\Phi] &= -\frac{i}{\epsilon} \pi_\mu(\mathbf{k} + \mathbf{G}, t)
\end{aligned} \tag{A.3}$$

where the sum over λ is implied at the beginning. Inserting the obtained result of the commutator in equation (A.2) yields the relationship between the initial and the new Green function.

$$\omega \langle \langle \Phi_\mu; \Phi_\mu \rangle \rangle_\omega = -\frac{i}{\epsilon} \langle \langle \pi_\mu; \Phi_\mu \rangle \rangle_\omega \tag{A.4}$$

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

$$\omega \langle \langle \pi_\mu; \Phi_\mu \rangle \rangle_\omega = \langle [\pi_\mu(\mathbf{k} + \mathbf{G}, t), \Phi_\lambda(-\mathbf{k} - \mathbf{G}, t)] \rangle + \langle \langle [\pi_\mu(\mathbf{k} + \mathbf{G}, t), H_\Phi]; \Phi_\mu \rangle \rangle_\omega \tag{A.5}$$

Like above the same things are to do. The inhomogeneity is given by the commutator relations In comparison to the case above the commutator doesn'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 $[\pi_\mu(\mathbf{k} + \mathbf{G}, t), H_\Phi] = i((\mathbf{k} + \mathbf{G})^2 + r_0) \Phi_\mu(\mathbf{k} + \mathbf{G}, t)$. In total we obtain the relation

$$\omega \langle \langle \pi_\mu; \Phi_\mu \rangle \rangle_\omega = -i + i((\mathbf{k} + \mathbf{G})^2 + r_0) \langle \langle \Phi_\mu; \Phi_\mu \rangle \rangle_\omega. \tag{A.6}$$

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 (A.4) and (A.6) are an equation system, where the Green function $\langle \langle \pi_\mu; \Phi_\mu \rangle \rangle$ can be eliminated. The easiest way doing this is to multiply equation (A.4) with ω and inserting (A.6) in the obtained relation.

$$\mathcal{D}_\mu^{(0)}(\mathbf{k}, \omega) := \langle \langle \Phi_\mu; \Phi_\mu \rangle \rangle_\omega = \sum_{\mathbf{G}} \frac{1}{(\mathbf{k} + \mathbf{G})^2 + r_0 - \xi^{-2}} \tag{A.7}$$

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 ??.

A.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

link to commutator relations

say a little bit more about that

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 perturbation 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

$$\mathcal{G}_\alpha^{(0)}(\mathbf{k}, \omega) := \langle \langle \Psi_\alpha; \Psi_\alpha^\dagger \rangle \rangle_\omega = \sum_{\mathbf{G}} \frac{1}{\omega - \epsilon_\alpha(\mathbf{k} + \mathbf{G})}, \quad (\text{A.8})$$

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

$$\mathcal{D}_\mu(\mathbf{k}, t - t') = -i \langle \mathcal{T}_t U(\infty, -\infty) \Phi_\mu(\mathbf{k} + \mathbf{G}, t) \Phi_\mu(-\mathbf{k} - \mathbf{G}, t') \rangle_0^{\text{con}} \quad (\text{A.9})$$

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

$$U(t, t') = \exp \left(-i \int_{t'}^t dt_1 H_{\text{int}}(t_1) \right). \quad (\text{A.10})$$

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.

$$\mathcal{D}_\mu = \mathcal{D}_\mu^{(0)} + \mathcal{D}_\mu^{(0)} \Pi_\mu \mathcal{D}_\mu \quad \Rightarrow \quad \mathcal{D}_\mu = \frac{1}{(\mathcal{D}_\mu^{(0)})^{-1} - \Pi_\mu} \quad (\text{A.11})$$

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 (A.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 a term where only contractions are contained. Having an odd number of operators a normal product exist in every term. Taking the equilibrium 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 fermionic 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 prohibits the use of Wick's theorem or any rearrange of the operators. The expectation values has the special form

$$\left\langle \mathcal{T}_t \Psi_{\alpha}^{\dagger}(\mathbf{p}_4, t_2) \cdot \sigma_{\lambda'} \cdot \Psi_{\beta}(\mathbf{p}_3, t_2) \cdot \Psi_{\gamma}^{\dagger}(\mathbf{p}_2, t_1) \cdot \sigma_{\lambda} \cdot \Psi_{\delta}(\mathbf{p}_1, t_1) \right\rangle_0, \quad (\text{A.12})$$

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

$$\sum_{\mu=1}^3 \sigma_{ij}^{\mu} \sigma_{kl}^{\mu} = 2\delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl} \quad (\text{A.13})$$

Acting Fierz identity the product of field operators and Pauli matrix has to be written in component representation. Then the identity can be used without any doubt and the Kronecker symbols allows us to rewrite the operators without component representation. Doing this we have to be careful with the first term in (A.13), because the order of the operators is rearranged. Therefore the operators have to be commuted with yields a δ -distribution with respect to the momentum, see (D.5). The exact calculation is done in the appendix D.

Each obtained expectation value contains two operators of a-electrons¹ and two operators of b-electrons, so that the expectation value can be separated. One half of these is constructed in a way that both annihilation operators are acting with respect to a-electrons, for example. These kinds of expectation values are surely zero. The other half is "normal" constructed so that one annihilation and creation operator is acting with respect to a-electrons. The same is surely valid for b-electrons.

Bringing the remained operators in the order that all annihilation operators stand 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 (D.6) in the appendix D.

writing this argument in a better way

¹a-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.

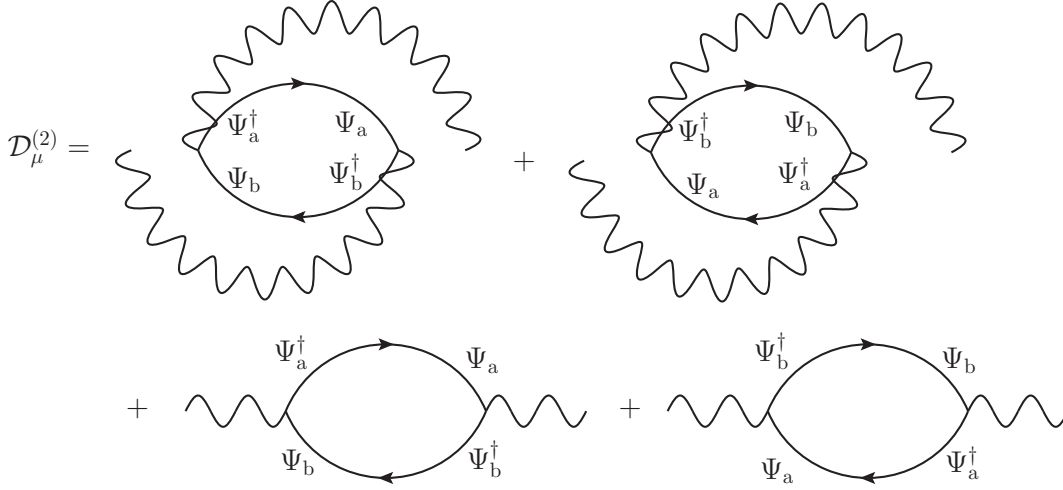


Figure A.1: caption

Inserting equation (D.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 perturbation theory have the form

$$\begin{aligned}
\mathcal{D}_\mu^{(2)}(\mathbf{k}, \omega) = & (-i)^3 \lambda^2 \int_{-\infty}^{\infty} dt_1 dt_2 \sum_{\mathbf{P}_1 \mathbf{P}_2} \int_{\mathbf{P}_1} \int_{\mathbf{P}_2} \\
& \times \left\langle \mathcal{T}_t \Phi_{\lambda'}(\tilde{\mathbf{p}}_2 - \tilde{\mathbf{p}}_1, t_2) \Phi_\lambda(\tilde{\mathbf{p}}_1 - \tilde{\mathbf{p}}_2, t_1) \Phi_\mu(\tilde{\mathbf{k}}, t) \Phi_\mu(-\tilde{\mathbf{k}}, t') \right\rangle_0 \\
& \times \left(\left\langle \mathcal{T}_t \Psi_a(\tilde{\mathbf{p}}_2, t_1) \Psi_a^\dagger(\tilde{\mathbf{p}}_2, t_2) \right\rangle_0 \left\langle \mathcal{T}_t \Psi_b(\tilde{\mathbf{p}}_1, t_2) \Psi_b^\dagger(\tilde{\mathbf{p}}_1, t_1) \right\rangle_0 \right. \\
& \left. + \left\langle \mathcal{T}_t \Psi_b(\tilde{\mathbf{p}}_2, t_1) \Psi_b^\dagger(\tilde{\mathbf{p}}_2, t_2) \right\rangle_0 \left\langle \mathcal{T}_t \Psi_a(\tilde{\mathbf{p}}_1, t_2) \Psi_a^\dagger(\tilde{\mathbf{p}}_1, t_1) \right\rangle_0 \right) \quad (\text{A.14})
\end{aligned}$$

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 possible 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 A.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 annihilated and a b-electron is created at t_1 . Comparing the second diagram, where an a-electron is created and a b-electron is annihilated at t_1 . All four diagrams are closely connected with each other, because all diagrams can be generated out of one diagram by interchanging the

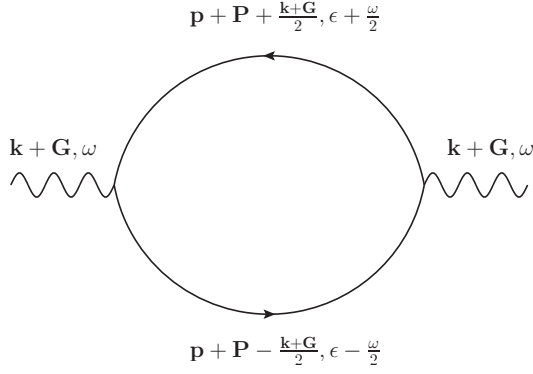


Figure A.2: caption

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.

$$\begin{aligned}
\mathcal{D}_\mu^{(2)}(\mathbf{k}, t - t') &= 4i\lambda^2 \int_{-\infty}^{\infty} dt_1 dt_2 \sum_{\mathbf{P}} \int_{\mathbf{p}} \\
&\times \left\langle \mathcal{T}_t \Phi_\mu(\tilde{\mathbf{k}}, t_2) \Phi_\mu(-\tilde{\mathbf{k}}, t') \right\rangle_0 \left\langle \mathcal{T}_t \Phi_\mu(-\tilde{\mathbf{k}}, t_1) \Phi_\mu(\tilde{\mathbf{k}}, t) \right\rangle_0 \\
&\times \left\langle \mathcal{T}_t \Psi_a(\tilde{\mathbf{p}} - \tilde{\mathbf{k}}, t_1) \Psi_a^\dagger(\tilde{\mathbf{p}} - \tilde{\mathbf{k}}, t_2) \right\rangle_0 \left\langle \mathcal{T}_t \Psi_b(\tilde{\mathbf{p}}, t_2) \Psi_b^\dagger(\tilde{\mathbf{p}}, t_1) \right\rangle_0 \quad (\text{A.15})
\end{aligned}$$

where the momentums \mathbf{p}_1 and \mathbf{P}_1 are relabeled with \mathbf{p} and \mathbf{P} , respectively. Accordingly we write $\tilde{\mathbf{p}}$ instead of $\tilde{\mathbf{p}}_1$. In comparison to the Dyson equation (A.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

$$\Pi_\mu^{(0)}(\mathbf{k}, \omega) = i \sum_{\mathbf{P}} \int_{|p| \leq p_F} \frac{d^2 \mathbf{p}}{(2\pi)^2} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \mathcal{G}_a^{(0)}(\mathbf{p} + \frac{\mathbf{k}}{2}, \epsilon + \frac{\omega}{2}) \mathcal{G}_b^{(0)}(\mathbf{p} - \frac{\mathbf{k}}{2}, \epsilon - \frac{\omega}{2}). \quad (\text{A.16})$$

In comparison to equation (A.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 A.2. How we see in equation (A.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 interact 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.

$$\epsilon_a(\mathbf{p} + \mathbf{P} + \frac{\mathbf{k} + \mathbf{G}}{2}) = \frac{(p_x + P_x + \frac{k_x + G_x}{2})^2}{2m_1} + \frac{(p_y + P_y + \frac{k_y + G_y}{2})^2}{2m_2}$$

$$\begin{aligned}
\Leftrightarrow \epsilon_a(\mathbf{p} + \mathbf{P} + \frac{\mathbf{k} + \mathbf{G}}{2}) &= \frac{(p_x + P_x)^2}{2m_1} + \frac{1}{2} \frac{p_x + P_x}{m_1} (k_x + G_x) + \frac{(k_x + G_x)^2}{8m_1} \\
&\quad + \frac{(p_y + P_y)^2}{2m_2} + \frac{1}{2} \frac{p_y + P_y}{m_2} (k_y + G_y) + \frac{(k_y + G_y)^2}{8m_2} \\
\Leftrightarrow \epsilon_a(\mathbf{p} + \mathbf{P} + \frac{\mathbf{k} + \mathbf{G}}{2}) &\approx \xi_a + \frac{1}{2} \mathbf{v}_{a,F}(\mathbf{k} + \mathbf{G}) + \mu
\end{aligned} \tag{A.17}$$

where the quadratic term with respect to \mathbf{k} is neglectable, because the bosonic transferred momentum is assumed as small. Further the velocity \mathbf{v}_a of the a-electrons is introduced, where the electron 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 $\mathbf{v}_{a,F} = v_{a,F} \mathbf{n}$ for example. The scalar product between the normalized momentum vector \mathbf{n} and the bosonic spin density wave vector $\mathbf{k} + \mathbf{G}$ is rewritten as his magnitude multiplied with $\cos(\vartheta)$, where ϑ is the angle between both.

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

link zur dispersion im spin fermion model

$$\xi := \xi_a = \xi_b \quad v_F := v_{a,F} = v_{b,F} \tag{A.18}$$

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

$$\begin{aligned}
\Pi_\mu^{(0)}(\mathbf{k}, \omega) &= i\nu_F \int_0^\pi d\vartheta \int_{\xi \leq \xi_F} d\xi \int_{-\infty}^\infty \frac{d\epsilon}{2\pi} \\
&\quad \times \frac{1}{\epsilon + \frac{\omega}{2} - \xi - \frac{1}{2}v_F |\mathbf{k} + \mathbf{G}| \cos(\vartheta) + i\eta \text{sign}(\epsilon + \frac{\omega}{2})} \\
&\quad \times \frac{1}{\epsilon - \frac{\omega}{2} - \xi + \frac{1}{2}v_F |\mathbf{k} + \mathbf{G}| \cos(\vartheta) + i\eta \text{sign}(\epsilon - \frac{\omega}{2})},
\end{aligned} \tag{A.19}$$

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 $\nu_F := \nu(\xi_F)$ 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

$$\epsilon_1 := \xi - \frac{1}{2}(\omega - v_F|\mathbf{k} + \mathbf{G}|\cos(\vartheta)) \quad \text{and} \quad \epsilon_2 := \xi + \frac{1}{2}(\omega - v_F|\mathbf{k} + \mathbf{G}|\cos(\vartheta)), \quad (\text{A.20})$$

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: $\text{sign}(\epsilon + \frac{\omega}{2}) = \text{sign}(\epsilon - \frac{\omega}{2})$

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, respectively, 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.

$$\begin{aligned} I_\omega^e &:= i \oint_\Gamma \frac{d\omega}{2\pi i} \frac{1}{\omega - \omega_1 \mp i\eta} \cdot \frac{1}{\omega - \omega_2 \mp i\eta} \\ \Leftrightarrow I_\omega^e &= \pm i \left[\frac{1}{\omega_2 - \omega_1} + \frac{1}{\omega_1 - \omega_2} \right] = 0, \end{aligned} \quad (\text{A.21})$$

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

2. case: $\text{sign}(\epsilon + \frac{\omega}{2}) \neq \text{sign}(\epsilon - \frac{\omega}{2})$

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.

$$\begin{aligned} I_\omega^o &:= i \oint_\Gamma \frac{d\omega}{2\pi i} \frac{1}{\omega - \omega_1 \mp i\eta} \cdot \frac{1}{\omega - \omega_2 \pm i\eta} \\ \Leftrightarrow I_\omega^o &= \frac{\pm i}{\omega_2 - \omega_1 \pm i\eta} \end{aligned} \quad (\text{A.22})$$

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 (A.19) is equivalent to the signum functions $\text{sign}(\xi \pm \frac{1}{2}v_F|\mathbf{k} + \mathbf{G}|\cos(\vartheta))$ in energy representation. The energy ξ is neglectable because the integrand is independent of ξ . Further the constant factors are also neglectable because they are always positive. The case of sign in the integrand depends therefore only on the sign of $|\mathbf{k} + \mathbf{G}|\cos(\vartheta)$. Finally the integrals limits has to be set to $\pm \frac{1}{2}v_F|\mathbf{k} + \mathbf{G}|\cos(\vartheta)$. 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 $\epsilon - \frac{\omega}{2} < 0$, respectively. Transforming both into energy representation the corresponding expressions are $\xi - \frac{1}{2}v_F|\mathbf{k} + \mathbf{G}|\cos(\vartheta) < 0$ and $\xi + \frac{1}{2}v_F|\mathbf{k} + \mathbf{G}|\cos(\vartheta) > 0$, which yields directly the definition interval of ξ . Therefore we obtained

$$\Pi_{\mu}^{(0)}(\mathbf{k}, \omega) = i\nu_F \int_0^{\pi} d\vartheta \int_{-\xi_0}^{\xi_0} d\xi \frac{i \text{sign}(|\mathbf{k} + \mathbf{G}|\cos(\vartheta))}{\omega - v_F|\mathbf{k} + \mathbf{G}|\cos(\vartheta) + i\eta \text{sign}(|\mathbf{k} + \mathbf{G}|\cos(\vartheta))} \quad (\text{A.23})$$

for the self energy, where the abbreviation $\xi_0 = v_F|\mathbf{k} + \mathbf{G}|\cos(\vartheta)/2$ is introduced. The integration over ξ yields the factor $v_F|\mathbf{k} + \mathbf{G}|\cos(\vartheta)$. Subsequently the signum function is reexpressed in frequency representation which corresponds to $\text{sign}(\omega)$.

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 self energy is given by

$$\text{Im}\left\{\Pi_{\mu}^{(0)}(\mathbf{k}, \omega)\right\} = \nu_F \pi \int_0^{\pi} d\vartheta v_F|\mathbf{k} + \mathbf{G}|\cos(\vartheta) \delta(\omega - v_F|\mathbf{k} + \mathbf{G}|\cos(\vartheta)), \quad (\text{A.24})$$

where the formula $\frac{1}{x \pm i\eta} = \text{P.V.} \frac{1}{x} \mp i\pi\delta(x)$ is used. To perform the last remaining integral over ϑ the δ -distribution has to be rewritten. 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

$$\delta(g(x)) = \sum_{i=1} \frac{\delta(x - x_{0,i})}{|g'(x_{0,i})|} \quad (\text{A.25})$$

states how a δ -distribution with a functional argument can be written 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 (A.24) has a single zero at $\vartheta_0 = \cos^{-1}(\omega/(v_F|\mathbf{k} + \mathbf{G}|))$. Thereby the δ -distribution is rewritten as

$$\begin{aligned} \delta(\omega - v_F|\mathbf{k} + \mathbf{G}|\cos(\vartheta)) &= \left(v_F|\mathbf{k} + \mathbf{G}| \cdot |\sin(\vartheta_0)|\right)^{-1} \delta(\vartheta - \vartheta_0) \\ \Rightarrow \delta(\omega - v_F|\mathbf{k} + \mathbf{G}|\cos(\vartheta)) &\approx \left(v_F|\mathbf{k} + \mathbf{G}|\right)^{-1} \delta(\vartheta - \vartheta_0) \end{aligned} \quad (\text{A.26})$$

where in the second line the limit of small frequencies 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

$$\text{Im}\left\{\Pi_{\mu}^{(0)}(\mathbf{k}, \omega)\right\} = \frac{\nu_F \pi}{v_F |\mathbf{k} + \mathbf{G}|} \cdot \omega = \gamma \omega \quad (\text{A.27})$$

where in the last step the damping constant γ is introduced. In equation (A.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 (A.7) the damped spin fermion propagator is given by

$$\mathcal{D}_{\mu}(\mathbf{k}, \omega) = \sum_{\mathbf{G}} \frac{1}{(\mathbf{k} + \mathbf{G})^2 + r - \xi^{-2} - i\gamma\omega} \quad (\text{A.28})$$

where the abbreviation $r = r_0 - \text{Re}\{\Pi_{\mu}(\mathbf{k}, \omega)\}$ 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.

A.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 frequencies. In this representation the computations in chapter ?? are much more convenient. 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 5.2.3 these relations are established, see (??) for the explicite form. The propagator in (A.28) can be easily separated into real and imaginary part

$$\mathcal{D}_{\mu}(\mathbf{k}, \omega) = \sum_{\mathbf{G}} \left[\frac{(\mathbf{k} + \mathbf{G})^2}{(\mathbf{k} + \mathbf{G})^4 + (\gamma\omega)^2} + i \frac{\gamma\omega}{(\mathbf{k} + \mathbf{G})^4 + (\gamma\omega)^2} \right], \quad (\text{A.29})$$

where $r = \xi = 0$ is set. It is trivially seen that the real part is a symmetric function and the imaginary part is an antisymmetric function with respect to ω . Similiar to (A.28) the propagator $\mathcal{D}_{\mu}(\mathbf{k}, i\omega_n)$ can be separated 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

$$\mathcal{D}_\mu(\mathbf{k}, i\omega_n) = \frac{1}{\pi} \text{P.V.} \int_{-\infty}^{\infty} d\omega \frac{\text{Im}\{\mathcal{D}_\mu(\mathbf{k}, \omega)\}}{\omega - i\omega_n} \quad (\text{A.30})$$

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

$$\begin{aligned} \mathcal{D}_\mu(\mathbf{k}, i\omega_n) &= \frac{1}{\pi} \int_0^\infty d\omega \text{Im}\{\mathcal{D}_\mu(\mathbf{k}, \omega)\} \left[\frac{1}{\omega + i\omega_n} + \frac{1}{\omega - i\omega_n} \right] \\ \Leftrightarrow \mathcal{D}_\mu(\mathbf{k}, i\omega_n) &= \frac{2}{\pi} \sum_{\mathbf{G}} \int_0^\infty d\omega \frac{\gamma\omega}{(\mathbf{k} + \mathbf{G})^4 + (\gamma\omega)^2} \cdot \frac{\omega}{\omega^2 + \omega_n^2} \\ \Leftrightarrow \mathcal{D}_\mu(\mathbf{k}, i\omega_n) &= \sum_{\mathbf{G}} \frac{1}{(\mathbf{k} + \mathbf{G})^2 + \gamma|\omega_n|} \end{aligned} \quad (\text{A.31})$$

In the last step the integral formula

$$\int_0^\infty dx \frac{x}{a^2 + x^2} \cdot \frac{x}{y^2 + x^2} = \frac{\pi}{2} \frac{1}{a + |y|} \quad (\text{A.32})$$

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

B Conversion of $(\dot{P} | (\omega - L_0)^{-1} | \dot{P})$

In this appendix the short conversion of the expectation value $(\dot{P} | (\omega - L_0)^{-1} | \dot{P})$ is done. Therefore only realtions are used which we find in chapter 5. Firstly the expectation value is written as the correlation function in the frequency space using equation (5.45).

$$\begin{aligned}
& (\dot{P} | (\omega - L_0)^{-1} | \dot{P}) = -i \mathcal{C}_{\dot{P}\dot{P}}(\omega) \\
& \stackrel{(C.6)}{\Leftrightarrow} (\dot{P} | (\omega - L_0)^{-1} | \dot{P}) = -i \int_0^\infty dt e^{i\omega t} \mathcal{C}_{\dot{P}\dot{P}}(t) \\
& \stackrel{(5.42)}{\Leftrightarrow} (\dot{P} | (\omega - L_0)^{-1} | \dot{P}) = -\frac{i}{\beta} \int_0^\infty dt e^{i\omega t} \int_0^\beta d\lambda \langle \dot{P}^\dagger(t) \dot{P}(0) \rangle \\
& \stackrel{(5.17)}{\Leftrightarrow} (\dot{P} | (\omega - L_0)^{-1} | \dot{P}) = -\frac{i}{\beta} \Phi_{\dot{P}\dot{P}}(\omega) \\
& \stackrel{(5.12)}{\Leftrightarrow} (\dot{P} | (\omega - L_0)^{-1} | \dot{P}) = -\frac{\omega^{-1}}{\beta} \left[\chi_{\dot{P}\dot{P}}(\omega) - \underbrace{\chi_{\dot{P}\dot{P}}(\omega = 0)}_{=0} \right] \\
& \Leftrightarrow (\dot{P} | (\omega - L_0)^{-1} | \dot{P}) = -\frac{\omega^{-1}}{\beta} \int_{-\infty}^\infty dt e^{i\omega t} \chi_{\dot{P}\dot{P}}(t) \\
& \stackrel{(5.8)}{\Leftrightarrow} (\dot{P} | (\omega - L_0)^{-1} | \dot{P}) = -\frac{i\omega^{-1}}{\hbar\beta} \int_0^\infty dt e^{i\omega t} \langle [\dot{P}(t), \dot{P}(0)] \rangle_0 \tag{B.1}
\end{aligned}$$

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 $\dot{P} = 0$ at $t = 0$.

C Properties of the Kubo Relaxation Function

In section 5.2.2 the Kubo relaxation function

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

and the three relations

$$1. \quad \chi_{AB}(t) = -\Theta(t) \frac{d}{dt} \Phi_{AB}(t) \quad (C.2)$$

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

$$3. \quad \Phi_{AB}(\omega) = \frac{1}{i\omega} [\chi_{AB}(\omega) - \chi_{AB}(\omega=0)]. \quad (C.4)$$

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 easily gotten by derivating the Kubo relaxation function with respect to t and comparing the result with the definition of the dynamical susceptibility (5.8).

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

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

$$\Phi_{AB}(\omega) = \int_0^{\infty} dt \Phi_{AB}(t) e^{i\omega t} \quad (C.6)$$

In this definition of the Laplace transformation compared to (5.3) we set $s = -i\omega$ which correspond to a rotation of $\frac{\pi}{2}$ of the definition space . Using (C.6) after setting $t = 0$ in (C.1) yield

reference to a book of laplace transformation

$$\begin{aligned} \Phi_{AB}(t=0) &= \frac{i}{\hbar} \lim_{s \rightarrow 0} \int_0^{\infty} d\tau \langle [A_I(\tau), B_I(0)] \rangle_0 e^{-s\tau} \\ \Leftrightarrow \Phi_{AB}(t=0) &= \frac{i}{\hbar} \lim_{\substack{s \rightarrow 0 \\ \omega \rightarrow 0}} \int_{-\infty}^{\infty} d\tau \Theta(\tau) \langle [A_I(\tau), B_I(0)] \rangle_0 e^{i\omega\tau} e^{-s\tau} \end{aligned}$$

$$\begin{aligned}
&\Leftrightarrow \Phi_{AB}(t=0) = \lim_{\omega \rightarrow 0} \int_{-\infty}^{\infty} d\tau \chi_{AB}(\tau) e^{i\omega\tau} \\
&\Leftrightarrow \Phi_{AB}(t=0) = \chi_{AB}(\omega=0),
\end{aligned} \tag{C.7}$$

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 computed 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 .

$$\begin{aligned}
&\int_0^{\infty} dt e^{i\omega t} \chi_{AB}(t) = - \int_0^{\infty} dt e^{i\omega t} \frac{d}{dt} \Phi_{AB}(t) \\
&\stackrel{\text{PI}}{\Leftrightarrow} \chi_{AB}(\omega) = -e^{i\omega t} \Phi_{AB}(t) \Big|_0^{\infty} + i\omega \int_0^{\infty} dt e^{i\omega t} \Phi_{AB}(t) \\
&\Leftrightarrow \chi_{AB}(\omega) = \Phi_{AB}(t=0) + i\omega \Phi_{AB}(\omega) \\
&\Leftrightarrow \Phi_{AB}(\omega) = \frac{1}{i\omega} [\chi_{AB}(\omega) - \chi_{AB}(\omega=0)]
\end{aligned} \tag{C.8}$$

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

D Fierz Identity

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

$$T_{ij}^a \quad \text{mit} \quad a = 1, 2, 3, \dots, N^2 - 1 \quad \text{and} \quad i, j = 1, 2, 3, \dots, N \quad (\text{D.1})$$

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

$$\sum_{a=1}^{N^2-1} T_{ij}^a T_{kl}^a = \frac{1}{2} \left[\delta_{il} \delta_{jk} - \frac{1}{N} \delta_{ij} \delta_{kl} \right] \quad (\text{D.2})$$

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

$$4 \sum_{a=1}^3 T_{ij}^a T_{kl}^a = \sum_{a=1}^3 \sigma_{ij}^a \sigma_{kl}^a = 2\delta_{il} \delta_{jk} - \delta_{ij} \delta_{kl} \quad (\text{D.3})$$

Now this identity can be used for computing the fermionic expectation value obtained in section A.2. In equation (??) the product of fermionic operators yields four terms of the structure

$$\text{EV}_F := \left\langle \Psi_\alpha^\dagger(\nu_1) \cdot \sigma^\mu \cdot \Psi_\beta(\nu_2) \cdot \Psi_\gamma^\dagger(\nu_3) \cdot \sigma^\mu \cdot \Psi_\delta(\nu_4) \right\rangle, \quad (\text{D.4})$$

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 written in component representation, which allows us to use the Fierz identity. In the expectation value above the sum over μ should be implied.

$$\begin{aligned} \text{EV}_F &= \left\langle \left(\Psi_\alpha^\dagger(\nu_1) \right)_i \cdot \sigma_{ij}^\mu \cdot \left(\Psi_\beta(\nu_2) \right)_j \cdot \left(\Psi_\gamma^\dagger(\nu_3) \right)_k \cdot \sigma_{kl}^\mu \cdot \left(\Psi_\delta(\nu_4) \right)_l \right\rangle \\ \Leftrightarrow \text{EV}_F &= \sigma_{ij}^\mu \sigma_{kl}^\mu \left\langle \left(\Psi_\alpha^\dagger(\nu_1) \right)_i \left(\Psi_\beta(\nu_2) \right)_j \left(\Psi_\gamma^\dagger(\nu_3) \right)_k \left(\Psi_\delta(\nu_4) \right)_l \right\rangle \\ \Leftrightarrow \text{EV}_F &= (2\delta_{il} \delta_{jk} - \delta_{ij} \delta_{kl}) \left\langle \left(\Psi_\alpha^\dagger(\nu_1) \right)_i \left(\Psi_\beta(\nu_2) \right)_j \left(\Psi_\gamma^\dagger(\nu_3) \right)_k \left(\Psi_\delta(\nu_4) \right)_l \right\rangle \end{aligned}$$

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

The use of the Fierz identity has eliminated the Pauli matrices 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 perturbation 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 (D.5). The expectation values of different electron families can be separated without any doubt, because their Hilbert spaces are disconnected. For this reason many combinations of choosing 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, then an expectation value emerges with two fermionic creation operators and another one emerges with two fermionic annihilation operators, which is always zero. For the fermionic expectation value $\text{EV}(\mathcal{D})$ in equation (??) this procedure yields

$$\begin{aligned}
\text{EV}(\mathcal{D}) &= \left\langle \mathcal{T}_t \Psi_a(\tilde{\mathbf{p}}_2, t_1) \Psi_a^\dagger(\tilde{\mathbf{p}}_3, t_2) \right\rangle \left\langle \mathcal{T}_t \Psi_b(\tilde{\mathbf{p}}_4, t_2) \Psi_b^\dagger(\tilde{\mathbf{p}}_1, t_1) \right\rangle \delta_{\tilde{\mathbf{p}}_2 - \tilde{\mathbf{p}}_3} \delta_{\tilde{\mathbf{p}}_4 - \tilde{\mathbf{p}}_1} \\
&\quad + \left\langle \mathcal{T}_t \Psi_b(\tilde{\mathbf{p}}_2, t_1) \Psi_b^\dagger(\tilde{\mathbf{p}}_3, t_2) \right\rangle \left\langle \mathcal{T}_t \Psi_a(\tilde{\mathbf{p}}_4, t_2) \Psi_a^\dagger(\tilde{\mathbf{p}}_1, t_1) \right\rangle \delta_{\tilde{\mathbf{p}}_2 - \tilde{\mathbf{p}}_3} \delta_{\tilde{\mathbf{p}}_4 - \tilde{\mathbf{p}}_1}
\end{aligned} \tag{D.6}$$

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