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Quantentransport in Spindichtesystemen mit dem Memory-Matrix-Formalismus

Masterthesis

von

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Karlsruhe, den 25. April 2018

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(**Martin Lietz**)

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3.1 Motivation

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

$$\frac{\partial}{\partial t}\mathrm{A}(t) - \mathrm{F}_{\mathrm{ex}}(x,t) + \gamma \cdot \mathrm{A}(t) = f(t), \tag{3.1}$$

where $\mathrm{A}(t)$ is some dynamical observable and $f(t)$ is a random force like white noise for example. The origin of the second term on the left hand side is some external force result from a coupling between $\mathrm{A}(t)$ and some external potential. The third term on the left hand side is a damping or friction term. Now let us assume it's possible to seperate equation (3.1) into two parts. The first part, called f_1, is a functional of the dynamical observable $\mathrm{A}(t')$, where $t_0 \leq t' \leq t$, so that this part is depending on the history of A. The second part f_2 should be depending on all other degrees of freedom. Now f_1 is expanded up to the linear order and all terms of higher order and the part f_2 are summerized to the quantity $F(t)$. The result is a linearized form of the Langevin equation

$$\frac{\partial}{\partial t}\mathrm{A}(t) = \int_{t_0}^{t} \mathrm{d}t'\, \mathcal{C}(t-t')\mathrm{A}(t') + F(t), \tag{3.2}$$

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

$$\mathcal{L}\big\{\mathrm{A}(t)\big\} = \mathrm{A}(s) = \int_{0}^{\infty} \mathrm{d}t\, \mathrm{A}(t)e^{-st}. \tag{3.3}$$

Using the Laplace transformation equation (3.2) becomes a algebratic equation of motion. The solution of this equation is

$$\mathrm{A}(t) = \Xi(t) \cdot \mathrm{A}(0) + \mathrm{A}'(t) \qquad \text{with} \qquad \mathrm{A}'(t) = \int_{0}^{t} \mathrm{d}t'\, \Xi(t-t')F(t'), \tag{3.4}$$

where the function $\Xi(t)$ is defined by the Laplace transformation of $\Xi(s) = [s - \mathcal{C}(s)]^{-1}$ and $\mathcal{C}(s)$ is the Laplace transformtion of the correlation function $\mathcal{C}(t)$. The main result of equation (3.4) and the motivation for the following introduced memory-matrix-formalism is the splitting of the dynamical observable $\mathrm{A}(t)$ into two parts.
For the first term on the right hand side the only time-dependence is adverted through the correlation function $\mathcal{C}$, which is clear regarding the definition of Ξ. This term included the linear contributions of $\mathrm{A}(t)$ by construction. These ones are the mostly important contributions to the time evolutaion of an observable, because they are secular. In contrast the second term on the right hand side is the convolution between the function $\Xi(t - t')$ and the function $\mathrm{F}(t')$. The latter summerize all the non-linear effects, fluctuations and intital transient processes, which are all effects with a small lifetimes in contrast with the secular effects. Therefore these effects shouldn't have large influences on the time evolution of an observable, always large time scales in mind.
Beside the physical interpretation a simple geometrical and mathematical one is very usefull. Let us assume a vector space ana the observable should be a vector in this vector space. Then the secular term is a projection on the A-axis and the non-secular term is aquivalent to a vector perpendicular to the A-axis. The memory-matrix-formalism take up this simple interpretation of equation (3.4) and put it in a general and exact form, so that it can be used classicaly and quantum mechanicaly.

3.2 Linear Response Theory

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

3.2.1 Kubo formula

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

$$\langle \mathrm{A} \rangle (t) := \mathrm{Tr}\{\rho_{\mathrm{S}}(t)\mathrm{A}_{\mathrm{S}}\} = \mathrm{Tr}\{\rho_{\mathrm{I}}(t)\mathrm{A}_{\mathrm{I}}\}, \tag{3.5}$$

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{S}}(t) = -\frac{i}{\hbar}[H(t), \rho_{\mathrm{S}}(t)] \quad \Leftrightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathrm{I}}(t) = -\frac{i}{\hbar}[H_1, \rho_{\mathrm{I}}(t)] \tag{3.6}$$

The equation is also transformed into the interaction picture, which doesn't change the structure itself but the density operator deponds only on the Hamiltonian H_1 now. Integrating and using the boundary condition that the system is in thermal equilibrium at $t \to -\infty$ equation (3.6) is resulted in a integrable equation for the density operator.

$$\rho_{\mathrm{I}}(t) = \rho_0 + \frac{i}{\hbar}\int_{-\infty}^{t} \mathrm{d}t' \left[B_{\mathrm{I}}(t'), \rho_{\mathrm{I}}(t')\right] F(t') \tag{3.7}$$

Jet it is clear why the interection picture is used. The integrand depends on the Hamiltonian of the pertubation only in linear order which is a perfect starting point for a iterativ solution procedure. Starting with the zeroth order the density operator is trivially the density operator at thermical equilibrium. Inserting the zeroth order on the right hand side of equation (3.7) yield the first order of the density operator, a. s.ø. In linear response theory the iteration is cutted off after the first order. Inserting this in equation (3.5) and defining the dynamical susceptibility

$$\chi_{\mathrm{AB}}(t - t') = \frac{i}{\hbar}\Theta(t - t') \left\langle \left[A_{\mathrm{I}}(t - t'), B_{\mathrm{I}}(0)\right] \right\rangle_{H_0} \tag{3.8}$$

yield the Kubo formula

$$\delta \langle \mathrm{A}(t) \rangle := \langle \mathrm{A} \rangle (t) - \langle \mathrm{A}(t) \rangle_{H_0} \approx \int_{-\infty}^{\infty} \mathrm{d}t' \, \chi_{\mathrm{AB}}(t - t') F(t'), \tag{3.9}$$

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

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3.2.2 Kubo relaxation function

After a general equation for the deviation of an observable A from the equilibrium value was established, we want to investigate a certain kind of pertubation. Let us assume $F(t) = \Theta(-t) \cdot F \cdot e^{-s\tau}$ the time evolution function of a pertubation, which is switched on adiabatically at $t = -\infty$ and switched off at $t = 0$. Inserting this in equation (3.9) and substituting $\tau = t - t'$ yield $\delta \langle \mathrm{A}(t) \rangle = \Phi_{AB}(t) \cdot F e^{st}$ with the Kubo relaxation function

$$\Phi_{\mathrm{AB}}(t) = \frac{i}{\hbar} \lim_{s \to 0} \int_{t}^{\infty} \mathrm{d}\tau \, \langle [\mathrm{A}_{\mathrm{I}}(\tau), \mathrm{B}_{\mathrm{I}}(0)] \rangle_0 \, e^{-s\tau}. \tag{3.10}$$

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

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

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

$$\big\langle\big[\mathrm{A}(t),\mathrm{B}(t')\big]\big\rangle = \frac{1}{Z}\,\mathrm{Tr}\big\{[\rho,\mathrm{A}(t)]\mathrm{B}(t')\big\}, \tag{3.11}$$

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

$$\begin{aligned}
& i[\rho,\mathrm{A}(t)] = i\Big[\rho\mathrm{A}(t) - \mathrm{A}(t)\rho\Big] \\
\Leftrightarrow\ & i[\rho,\mathrm{A}(t)] = i\Big[\rho\mathrm{A}(t) - e^{-\beta H}e^{\beta\mathrm{H}}\mathrm{A}(t)e^{-\beta\mathrm{H}}\Big] \\
\Leftrightarrow\ & i[\rho,\mathrm{A}(t)] = -i\rho\int_0^\beta \mathrm{d}\lambda\,\frac{\mathrm{d}}{\mathrm{d}\lambda}e^{\lambda\mathrm{H}}\mathrm{A}(t)e^{-\lambda\mathrm{H}} \\
\Leftrightarrow\ & i[\rho,\mathrm{A}(t)] = -i\rho\int_0^\beta \mathrm{d}\lambda\,\Big[\mathrm{H}e^{i\tilde{\lambda}\mathrm{H}/\hbar}\mathrm{A}(t)e^{-i\tilde{\lambda}\mathrm{H}/\hbar} - e^{i\tilde{\lambda}\mathrm{H}/\hbar}\mathrm{A}(t)e^{-i\tilde{\lambda}\mathrm{H}/\hbar}\mathrm{H}\Big] \\
\Leftrightarrow\ & i[\rho,\mathrm{A}(t)] = -i\rho\int_0^\beta \mathrm{d}\lambda\,\Big[\mathrm{H},\mathrm{A}(t+\tilde{\lambda})\Big] \\
\Leftrightarrow\ & \frac{i}{\hbar}[\rho,\mathrm{A}(t)] = -\rho\int_0^\beta \mathrm{d}\lambda\,\dot{\mathrm{A}}(t+\tilde{\lambda}) = -\rho\int_0^\beta \mathrm{d}\lambda\,\dot{\mathrm{A}}(t-i\lambda\hbar),
\end{aligned} \tag{3.12}$$

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

Now inserting equation (3.11) and (3.12) in the Kubo relaxation function (3.10) yield the searching form of the Kubo relaxation function, where the right hand side of the following compuation has to be integrated by parts, dedicated with PI.

$$
\begin{aligned}
&\Phi_{\mathrm{AB}}(t) = \frac{i}{\hbar} \lim_{s\to 0} \int_t^\infty \mathrm{d}\tau \, \langle [\mathrm{A_I}(\tau), \mathrm{B_I}(0)] \rangle_0 \, e^{-s\tau} \\
\overset{(3.11)}{\Leftrightarrow} \quad &\Phi_{\mathrm{AB}}(t) = \frac{i}{\hbar} \lim_{s\to 0} \int_t^\infty \mathrm{d}\tau \, \frac{1}{Z_0} \, \mathrm{Tr}\{[\rho_0, \mathrm{A_I}(\tau)]\mathrm{B_I}(0)\} e^{-s\tau} \\
\overset{(3.12)}{\Leftrightarrow} \quad &\Phi_{\mathrm{AB}}(t) = -\lim_{s\to 0} \int_0^\beta \mathrm{d}\lambda \int_t^\infty \mathrm{d}\tau \left\langle \dot{\mathrm{A}}_{\mathrm{I}}(\tau - i\lambda\hbar)\mathrm{B_I}(0) \right\rangle_0 e^{-s\tau} \\
\overset{\mathrm{PI}}{\Leftrightarrow} \quad &\Phi_{\mathrm{AB}}(t) = -\lim_{s\to 0} \int_0^\beta \mathrm{d}\lambda \left\langle \left[\mathrm{A_I}(\tau - i\lambda\hbar) e^{-s\tau} \Big|_t^\infty + s \int_t^\infty \mathrm{d}\tau \, \dot{\mathrm{A}}_{\mathrm{I}}(\tau - i\lambda\hbar) e^{-s\tau} \right] \mathrm{B_I}(0) \right\rangle_0 \\
\Leftrightarrow \quad &\Phi_{\mathrm{AB}}(t) = \int_0^\beta \mathrm{d}\lambda \, \langle \mathrm{A_I}(t - i\lambda\hbar)\mathrm{B_I}(0) \rangle_0 = \int_0^\beta \mathrm{d}\lambda \, \langle \mathrm{A_I}(t)\mathrm{B_I}(i\lambda\hbar) \rangle_0 \qquad (3.13)
\end{aligned}
$$

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

3.2.3 Kramer-Kronig-relation

3.2.4 spectral representation

4 Calculation

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

make link to chapter spin-fermion-model

4.1 Infinite conductivity in systems with unbroken translation symmetry

After Drude published his theory about the electrical transport in metals [Dru00] in the beginning of the last century it is well known that a broken translation symmetry is needed to get a finite static conductivity. Because of Neother's theorem it is also well known that a unbroken symmetry always implies a conserved quantity. In the case of translation symmetry this quantity is the momentum. Phenomenas breaking the translation symmetry are for example impurity scattering, electron-electron scattering and umklapp scattering. Let us firstly assume the standard spin-fermion-model without a translation symmetry breaking pertubation. In chapter () it is showed that in the used model the momentum is conserved but the currunt isn't conserved. This property is needed to calculate the static conductivity.

link to chapter spin-fermion-model

In general the static conductivity is given by taking the small frequencie limit of the conductivity and the conductivity itself is given by the current-current correlation function (J-J correlation function), which reslut directly from the linear response theory.

$$\sigma_{\mathrm{dc}} = \lim_{z\to 0} \sigma(z) = \lim_{z\to 0} \beta\, \mathcal{C}_{\mathrm{JJ}}(z) \tag{4.1}$$

The memory matrix formalism is used to calculate the J-J correlation function. Before we attend us to the calculation of the correlation function we have to think about the set of operators introduced by defining the projection operator. This set of operators has to be choosen for each calculation seperatly depending of the model and the quantity of interest. In our case we choose only a set of two operators namly the momentum and the current, because we want to figure out the influnece of the momentum on the current. That means the projector $\mathcal{P}$ projects into the two dimensional sub-Hilbertspace, spanned P and J. Lets go back to the correlation function, defined by equation (), where the sum over k und l is implied. Because our interest is focused on the J-J correlation function each index j and l is set to J.

reference to correlation function

$$\mathcal{C}_{\mathrm{JJ}}(z) = \frac{i}{\beta}\left[z\delta_{i\mathrm{J}} + i\beta\big(\dot{\mathrm{A}}_i\big|\hat{Q}\frac{i}{z-\hat{Q}\hat{L}\hat{Q}}\hat{Q}\big|\dot{\mathrm{A}}_k\big)\chi^{-1}_{k\mathrm{J}}\right]^{-1}\chi_{i\mathrm{J}}, \tag{4.2}$$

Now the sum over k is performed explicitly where both contriubtions for J and P vanish. Let us look seperatly on J and P starting with the latter case. In our observed model the momentum is conserved and so the time deriviative of P is zero. No more words are needed to see that the expactation value doesn't contribute. In the case of J the time derivative doesn't vanish so the two dimensional sub-Hilbertspace and the action of J in this Hilbertspace has to be consider. In the investigated system the whole current lives in the J-P Hilbertspace to any time, so no single part of J is transported out of the Hilbertspace. The appering operator $\mathcal{Q}$ is the inverse of $\mathcal{P}$ and therefore projected out of the J-P Hilbertspace. Combining both statements it is clear that $\mathcal{Q}|\dot{\mathrm{J}}) = 0$. The only resulting term choosing $i = J$ is

$$\mathcal{C}_{\mathrm{JJ}}(z) = \frac{i}{\beta} z^{-1} \chi_{\mathrm{JJ}}(\omega = 0) = \frac{i}{z} \mathcal{C}_{\mathrm{JJ}}(t = 0), \tag{4.3}$$

reference to scalar product

where the correlation function at $t = 0$ is given by the scalar product $(\mathrm{J}(0)|\mathrm{J}(0))$ defined in equation (). During the motivation of the previous chapter we explained that each observalbe can be split in one secular and one non-secular part. This is equatable with splitting a vector in a parallel and a perpendicular component, respectivily.

$$|\mathrm{J}) = |\mathrm{J}_{||}) + |\mathrm{J}_{\perp}) \tag{4.4}$$

What does this mean in physical language? In the investigated system the current isn't conserved, but nevertheless a part of him is it. This part is represented by the secular part and has to be parallel with the momentum. Therfore the projection from J at P yield the parallel component of J.

$$|\mathrm{J}_{||}) = \mathcal{P}|\mathrm{J}) = \frac{|\mathrm{P})(\mathrm{P}|}{(\mathrm{P}|\mathrm{P})}|\mathrm{J}) = \frac{\chi_{\mathrm{PJ}}}{\chi_{\mathrm{PP}}}|\mathrm{P}) \tag{4.5}$$

Firstly this give us the oppertunity to write the J-J correlation function into two parts one parrallel and one perpendicular correlation function using equation (4.4). The mixed correlation functions are zero by construction because $|\mathrm{J}_{||})$ and $|\mathrm{J}_{\perp})$ are orthogonal and therfore the scalar product of both is zero.

$$\mathcal{C}_{\mathrm{JJ}}(t = 0) = \big(\mathrm{J}(0)\big|\mathrm{J}(0)\big) = \big(\mathrm{J}_{||}\big|\mathrm{J}_{||}\big) + \big(\mathrm{J}_{\perp}\big|\mathrm{J}_{\perp}\big) \tag{4.6}$$

In a next step equation (4.5) is used to write the parallel J-J correlation function in a expression depending on the P-P correlation function which is nothing else $(\mathrm{P}|\mathrm{P})$.

$$\mathcal{C}_{\mathrm{JJ}}(t = 0) = \frac{|\chi_{\mathrm{PJ}}|^2}{|\chi_{\mathrm{PP}}|^2} \mathcal{C}_{\mathrm{PP}}(t = 0) + \big(\mathrm{J}_{\perp}\big|\mathrm{J}_{\perp}\big) \tag{4.7}$$

Now let us insert back this expression into equation (4.3) which give us multipling by β the conductivity

$$\sigma(z) = \frac{|\chi_{\mathrm{PJ}}|^2}{|\chi_{\mathrm{PP}}|} \frac{i}{z} + \sigma_{\mathrm{reg}}(z) \tag{4.8}$$

where the regular conductivity $\sigma_{\text{reg}}(z) = \frac{i\beta}{z}\big(\mathrm{J}_\perp\big|\mathrm{J}_\perp\big)$ is introduced. The physical meaning of $\sigma_{\text{reg}}(z)$ is discussed in a view steps, if we have the final expression for the conductivity. In the whole calculation there wasn't made a condition on z, so the equation for the conductivity is valid for each z in the complex plane. In reality the conductivity isn't depending on an complex frequency. Physical quantities are always real. Therefore we have to set $z = \omega + i\eta$, where $\omega \in \mathbb{R}$ and the limit $\eta \to 0$ is implied. Using $\frac{1}{\omega+i\eta} = \mathcal{P}\frac{1}{\omega} - i\pi\delta(\omega)$ the conductivity is given by

$$\sigma(\omega) = \frac{|\chi_{\text{PJ}}|^2}{|\chi_{\text{PP}}|}\left(\mathcal{P}\frac{i}{\omega} + \pi\delta(\omega)\right) + \sigma_{\text{reg}}(\omega) \tag{4.9}$$

where in this special case $\mathcal{P}$ sympolizied that the prinzipal value is taken. Equation (4.9) yield us exactly the expected result. For small frequencies the main contribution is generated by the δ-distribution, so the conductivity becomes infinity. This isn't really surprising because the translation symmetry isn't broken in the investigated system. If voltage is applied on a system like ours the electrons accelerate infinite long. There is nothing they can scatter on and loss some momentum. The electrons accelerate more and more and this results in an infinite conductivity. Only in a system with broken translation symmetry it's possible for the electrons to loss some momentum by scattering with the lattice for example. This results in a finite conductivity, so the δ-peak becomes smaller. The factor in front of the δ-distribution is the so called Drude-wight.
Let us now talk about the regular part of the conductivity. We don't want here to calculate some explicite expression, a small physical discussion about this part should be enough at this point. In every physical system there are some kind of effects which are always there and it's nearly impossible to suppress them. These effects are noise, fluctuations and other effects influenced by random forces. All of them are summarized in the regular conductivity.

4.2 Finite conductivity because of breaking the translation symmetry by umklapp scattering

After we saw that the conductivity is infinite in a system with conserved momentum, we consider now a system with broken translation symmetrie resulting in unconserved momentum. The regarded translation symmetry breaking pertubation considers umklapp scattering introduced by the Hamiltonian

$$H_{\text{U}} = \sum_{\mathbf{G}} \mathrm{J}_{\mathbf{G}} \int_{\text{BZ}} \frac{\mathrm{d}\mathbf{k}}{(2\pi)^2}\, \Phi_\mu(\mathbf{k},\tau)\Phi_\mu(-\mathbf{k}+\mathbf{G},\tau) \tag{4.10}$$

in chapter (). The electrical conductivity is like in the above section directly given by the current-current correlation function multiplied with β. In the previous chapter a general valid and exact expression for correlation functions was established.

link to umklapp scattering

$$\mathcal{C}_{lj}(z) = i\Big[z\delta_{il} - \Omega_{il} + i\Sigma_{il}(z)\Big]^{-1}\mathcal{C}_{ij}(t=0) \tag{4.11}$$

link to equation

with Ω_{il} and $\Sigma_{il}(z)$ given by equation (). Setting $l = j = J$ yield us the needed J-J correlation function. Now we have to look the squared brackets. In the definition of the functions Ω_{il} and $\Sigma_{il}(z)$ a sum over the set of operators defined by the
The equilibrium-Hamiltonian and the umklapp-Hamiltonian are both symmetrical under time reversal and the operators

5 Conclusion

A Properties of the Kubo relaxation function

In section 3.2.2 the Kubo relaxation function

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

and the three relations

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

connecting the dynamical susceptibility χ_{AB} with Φ_{AB} are introduced. In the following we want to proof these three relations.
The first one is easly gotten by derivating the Kubo relaxation function with respect to t and comparing the result with the definition of the dynamical susceptibility (3.8).

$$-\Theta(t) \frac{\mathrm{d}}{\mathrm{d}t} \Phi_{\mathrm{AB}}(t) = \frac{i}{\hbar} \Theta(t) \, \langle [\mathrm{A_I}(t), \mathrm{B_I}(0)] \rangle_0 = \chi_{\mathrm{AB}}(t) \tag{A.2}$$

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

$$\Phi_{\mathrm{AB}}(\omega) = \int \mathrm{d}t \, \Phi_{\mathrm{AB}}(t) e^{i\omega t} \tag{A.3}$$

In this definition of the Laplace transformation compared to (3.3) we set $s = -i\omega$ which correspond to a rotation of $\frac{\pi}{2}$ of the definition space . Using (A.3) after setting $t = 0$ in (A.1) yield

reference to a book of laplace transformation

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

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

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

$$\Leftrightarrow \ \Phi_{\mathrm{AB}}(t=0) = \chi_{\mathrm{AB}}(\omega=0), \tag{A.4}$$

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

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

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

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

$$\Leftrightarrow \ \Phi_{\mathrm{AB}}(\omega) = \frac{1}{i\omega} \big[\chi_{\mathrm{AB}}(\omega) - \chi_{\mathrm{AB}}(\omega=0)\big] \tag{A.5}$$

In the first step the right hand side is integrated by parts and in last step the first relation and (A.3) is used. So the third relation gives us the dependence between the Kubo relaxation function and the dynamical susceptibility in frequency space.

B Analysis of Matsubara-sums

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

B.1 Simple poles

Let us assume a Matsubara-sum like

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

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

Todo list

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