The Memory Function Formalism: A Review

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November 30, 2017

Abstract

An introduction to the Zwanzig-Mori-Götze-Wölfle memory function formalism (or generalized Drude formalism) is presented. This formalism is used extensively in analyzing the experimentally obtained optical conductivity of strongly correlated systems like cuprates and Iron based superconductors etc. For a broader perspective both the generalised Langevin equation approach and the projection operator approach for the memory function formalism are given. The Götze-Wölfle perturbative expansion of memory function is presented and its application to the computation of the dynamical conductivity of metals is also reviewed. This review of the formalism contains all the mathematical details for pedagogical purposes.

“The first processes, therefore, in the effectual studies of the sciences, must be ones of simplification and reduction of the results of previous investigations to a form in which the mind can grasp them.”

– J.C. Maxwell

The pioneers of the memory function formalism

Figure 1: (a) Hazime Mori (1926–) (b) Ryogo Kubo (1920–1995) (c) Robert Zwanzig (1928-2014)

1 Introduction

A wider picture of the memory function formalism is presented. After sketching the standard derivation of the Drude formula of electrical conductivity from momentum relaxation equation, we introduce the Langevin equation for electrical conduction in metals. A derivation of the Drude formula from the Langevin equation is presented. By pointing out a fundamental problem with the Langevin equation, the problem of Drude formula is highlighted. Then generalised Langevin equation is introduced which rectifies the problem of the Langevin equation by incorporating the time dependent friction coefficient.

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Then generalised Drude formula is obtained from generalised Langevin equation in which constant Drude scattering rate is replaced by a frequency dependent scattering rate, which is popularly known as the memory function.

Then an alternative route to memory function formalism or generalised Drude formalism is sketched based on the Zwanzig-Mori projection operator method. A formal expression for the memory function in terms of the projection operator is given. We then introduce the Götze-Wölfle perturbation expansion of the memory function and review their formalism. Special cases of electron-impurity and electron-phonon interaction are revised in detail. We come back to the question of under what conditions frequency dependent Drude scattering rate can be taken as frequency independent parameter in standard Drude formula, and discuss the relevant conditions. Our overview provides a wider picture of this field of research, and nothing new is presented here. An attempt is made to put this beautiful field of research in a nutshell. We hope that this review will be useful for pedagogical purposes.

2 The Drude Model

The traditional way to introduce AC conductivity of a metal is to use the Drude formula. In the Drude model electrons in a metal are treated as classical particles (much like gas molecules) bumping with the stationary ion cores and constitute a random thermal motion. When an external electric field is applied, electrons are accelerated and gain momentum. The momentum gained from the field is dissipated due to the collisions with ion cores and they attain an average drift speed. Due to this finite drift speed an electric current is established in the sample. When external field is removed the drift speed vanishes and electrons go back to the thermally agitated motion. Thus under the action of applied field the equation of motion of electrons can be written as:

\[
m\frac{d^2\mathbf{r}}{dt^2} = -e\mathbf{E}(t) - m\frac{1}{\tau} \frac{d\mathbf{r}}{dt},
\]

which is nothing but Newton’s second law of motion including dissipation. The momentum of an electron is being degraded due to collision processes with the ion cores at the average rate \(\frac{1}{\tau}\). Considering the electric field \(\mathbf{E}(t)\) variation as \(\mathbf{E}_0 \cos(\omega t)\) and solving the equation of motion for momentum leads to

\[
\mathbf{p}(t) = -e \frac{\tau}{1 + \tau^2 \omega^2} \mathbf{E}_0 \cos(\omega t) - e \frac{\omega \tau^2}{1 + \tau^2 \omega^2} \mathbf{E}_0 \sin(\omega t)
\]

In phase response (dissipative) Out-of-phase response (reactive).

One can observe that the time dependent momentum constitutes two responses: (1) the in-phase response leading to dissipation that varies as \(\cos(\omega t)\), and (2) out-of-phase response which has \(\sin(\omega t)\) dependence. From the above equation of momentum, the current density is given by:

\[
\mathbf{j}(t) = -ne \frac{\mathbf{p}(t)}{m} = -ne^2 \frac{\tau}{m} \left( \frac{\tau}{1 + \tau^2 \omega^2} \mathbf{E}_0 \cos(\omega t) + \frac{\omega \tau^2}{1 + \tau^2 \omega^2} \mathbf{E}_0 \sin(\omega t) \right).
\]

The presence of current in the sample leads to dissipation of energy (Joule heating). The average heat dissipation is given as \(\frac{1}{2\pi} \int_0^{2\pi} dt \mathbf{j}(t) \cdot \mathbf{E}(t)\). Clearly, this Joule heating is only due to the dissipative component, and it vanishes due to the reactive components (average of \(\sin(\omega t) \cos(\omega t)\) over a period is zero). From equation (3) the dissipative part of the conductivity \((\bar{J} = \sigma \bar{E})\) reduces to

\[
\sigma_1(\omega) = \sigma_{DC} \frac{1}{1 + \tau^2 \omega^2}.
\]

On the other hand the reactive part of the conductivity becomes

\[
\sigma_2(\omega) = \sigma_{DC} \frac{\tau \omega}{1 + \tau^2 \omega^2}.
\]
In the following paragraph we will observe that Drude expression is valid when
1. Frequency $\omega$ is very small as compared to the characteristics energy scale in system (as discussed in section 6.2).
2. Scattering with ion cores is the dominant mechanism of momentum randomisation.

Below we will derive the Drude formula using a different approach and we will observe that the scattering rate $\frac{1}{\tau}$ ceases to be a constant, rather it depends on frequency and temperature.

3 The Langevin equation

In the present section we introduce an important subject of non-equilibrium statistical mechanics i.e., the Langevin equation, which provides the basis for the memory function (MF) formalism. Our purpose is to write ac conductivity (in a general case) in a form resembling the Drude formula derived from the Langevin equation. Such a representation can be obtained using the MF formalism which will be our subject in the next sections. To understand memory function formalism we have to first consider a phenomenological approach. Let us start with the simple Langevin equation. The Langevin equation describe the random motion of a Brownian particle. The Brownian particle can be a pollen grain in some fluid. The origin of the random motion of Brownian particles is due to the irregular bombardment of the particle by molecules of fluid. It can also be viewed from the density fluctuations of fluid at a spatial length scale of the Brownian particle size. The molecules of fluid also provide a drag force to Brownian particle along with the continuous random force. Thus, net force on the Brownian particles can be divided into two components (1) systematic drag force, and (2) random force. With this, equation of motion can be written as

$$\dot{u}(t) = -m\gamma u(t) + R(t) + E_0 \cos(\omega_0 t).$$

This is called the Langevin equation. This equation holds great significance not only to describe the motion of a Brownian particle, but its wide regime of applicability is beautifully expressed in [1] "Brownian motion is not merely random motion of a very fine particle; in general it is random motion of a physical quantity to be observed in a macrosystem".

Let us apply the Langevin equation to electrons in a metal which is biased by an external ac field. The presence of impurity potentials and phonons force electrons to move randomly in the metal. On applying external ac field ($E_0 \cos(\omega_0 t)$) the Langevin equation for an electron changes to

$$\dot{u}(t) = -m\gamma u(t) + R(t) + E_0 \cos(\omega_0 t).$$

Here $m$ is the mass of an electron and $\gamma$ is the friction coefficient. Write the above equation in the Laplace domain with $u(s) = \int_0^\infty dt u(t)e^{-st}$

$$-mu(0) + smu(s) = -m\gamma u(s) + R(s) + \frac{E_0}{2} \left( \frac{1}{s - i\omega_0} + \frac{1}{s + i\omega_0} \right).$$

On simplify it and performing the ensemble average we obtain

$$\langle u(s) \rangle = \frac{\langle u(0) \rangle}{s + \gamma} + \frac{E_0}{2m(s + \gamma)} \left( \frac{1}{s - i\omega_0} + \frac{1}{s + i\omega_0} \right).$$

The ensemble average of the random force $\langle R(t) \rangle = 0$. The above equation in the long time limit $t >> \frac{1}{\gamma}$ can be written in the form

$$\langle u(t) \rangle = \text{Re}\{\mu(\omega)E_0 e^{i\omega_0 t}\},$$

where $\mu$ is the ac conductivity of the system. $\mu(\omega)$ is defined as the real part of the static electric susceptibility $\chi(\omega)$ which represents the electric field response of the system to a time-dependent electric field.

$\mu(\omega) = \frac{\text{Re}\{\chi(\omega)\}}{\omega}$

The Johnson-Nyquist noise is a direct manifestation of this random motion.
where
\[ \mu(\omega) = \frac{1}{m} \frac{1}{i\omega + \gamma} \] (11)
is the expression for the electronic mobility. In the electrical conduction problem the terminal speed along the $x -$direction (say) gained by an electron due to the applied electric field is $u^e_t = -\mu(eE_x)$ (terminal speed = mobility $\times$ force i.e., Fick’s Law). The induced current density can be written in terms of mobility as $J_x = -neu^e_t = ne^2\mu E$. According to Ohm’s Law $J_x = \sigma_{xx}E_x$, thus $\sigma_{xx} = \sigma = ne^2\mu$.

From equation (11) of the mobility, the conductivity takes the form.
\[ \sigma(\omega) = \frac{ne^2}{m} \frac{1}{i\omega + \gamma}. \] (12)

The dc conductivity $\sigma(0) = ne^2/m\gamma$. Here $\gamma$ is to be identified with the Drude scattering rate $1/\tau$. This is the Drude formula that we derived in the previous section. From this derivation of the Drude formula an important insight can be gained. It will be shown in the following section that Langevin equation has a serious problem in a general setting. An understanding of the problem the Langevin equation will enable us to understand the problem of the Drude formula.

3.1 Problems of the Langevin equation

The Langevin equation (6) can be integrated and written as:
\[ u(t) = u(t_0)e^{-\gamma(t-t_0)} + \frac{1}{m} \int_{t_0}^{t} dt'e^{-\gamma(t-t')}R(t'). \] (13)

Multiply the above equation with $u(t_0)$ and shift $t$ to $t_0 + t$ in the above equation. Then ensemble average becomes
\[ \langle u(t_0)u(t_0 + t) \rangle = \langle u(t_0)^2 \rangle e^{-\gamma t} \] (14)
where we have used $\langle u(t_0) \rangle \langle R(t') \rangle = 0$. Further taking the time derivative of the above correlation function leads to
\[ \frac{d}{dt} \langle u(t_0)u(t_0 + t) \rangle = -\gamma \langle u(t_0)^2 \rangle e^{-\gamma t}. \] (15)

In the limit $t \to 0$ we have
\[ \langle u(t_0)u(t_0) \rangle = -\gamma \langle u(t_0)^2 \rangle \neq 0. \] (16)

Therefore, the time derivative with respect to the initial time($t_0$) of the velocity-velocity correlation function is not zero. It implies that according to the Langevin equation, the velocity correlation function depends on the initial time. But this is contrary to the requirement of stationarity in an equilibrium setting:
\[ \frac{d}{dt_0} \langle u(t_0)u(t_0 + t) \rangle = 0, \] (17)
i.e., the correlation function should not depend on the initial time $t_0$. It only dependent on the difference of time arguments. Simplifying the above equation by differentiating, and then taking the limit $t \to 0$ we get
\[ \langle u(t_0)u(t_0) \rangle = 0. \] (18)

Clearly, this is in contradiction to equation (16). Thus there is serious problem with the Langevin equation. From here it can be concluded that the Drude formula derived from the Langevin equation may give wrong results. It turns out that this conclusion is correct and the Drude scattering rate which is assumed to be constant is not constant in general setting and actually becomes a frequency dependent quantity. The following section points out this problem with the Drude formula.
4 The generalized Langevin equation and the memory function (time dependent friction coefficient)

From the previous section we notice that the standard Langevin equation is inconsistent with the stationarity condition. It turns out that this problem can be resolved if the friction coefficient in the Langevin equation is taken as time dependent. In other words constant friction rate \(-m\gamma\) in the standard Langevin equation is to be replaced by time dependent friction coefficient \(-m\gamma(t)\). This is equivalent to considering the collision history of the particle as will be made clear below. The modified Langevin equation which takes time dependent friction coefficient into account is called the generalised Langevin equation:

\[
m\ddot{\mu}(t) = -m \int_{-\infty}^{t} dt' M(t-t') u(t') + \underbrace{R(t)}_{\text{systematic part with memory}} + \underbrace{E(t)}_{\text{random part} \text{ external drive}}. \tag{19}
\]

Here a time dependent friction coefficient \(M(t)\) is introduced. We have phenomenologically introduced the generalized Langevin equation (GLE), however, it is well know fact in the non-equilibrium statistical mechanical literature that the GLE can be rigorously derived from equation of motion (EOM) of the brownian particle using projection operator method. We will not review this direction here, and interested readers can consult [2]. In the following steps we will derive a modified Drude formula from GLE.

Write GLE in Fourier transform \(u(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega u(\omega) e^{i\omega t} \) domain

\[
i\omega \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega u(\omega) e^{i\omega t} = - \int_{-\infty}^{t} dt' \left( \frac{1}{2\pi} \int_{-\infty}^{+\infty} M[\omega] e^{i\omega(t-t')} \right) \left( \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega' u(\omega') e^{i\omega' t'} \right) + \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega (E(\omega) + R(\omega)) e^{i\omega t}, \tag{20}
\]

where \(M[\omega]\) is defined as half-Fourier transform (or Fourier-Laplace transform)

\[
M[\omega] = \int_{0}^{\infty} dt M(t) e^{-i\omega t}. \tag{21}
\]

Here, \(M(t') = \text{finite} \quad \text{for} \quad t' \geq 0, \quad \text{and} \quad M(t') = 0 \quad \text{for} \quad t' < 0 \quad \text{(no memory of future)}. \) In equation [20], the upper limit of the integral over \(t'\) can be extended from \(t\) to \(+\infty\) as we set \(M(t < 0) = 0\) and then the integral over \(t'\) gives a delta function: \(\frac{1}{2\pi} \int_{-\infty}^{+\infty} dt' e^{i(\omega'-\omega)t'} = \delta(\omega' - \omega)\). This delta function removes the integral over \(\omega'\) and we get the frequency dependent velocity \(u(\omega)\) in the form :

\[
\langle u(\omega) \rangle = \frac{E(\omega)}{m(\omega^2 + M[\omega])}. \tag{22}
\]

In performing the ensemble average we set \(\langle R(t) \rangle = 0\), if \(E(t) = E_0 \cos(\omega_0 t)\), then by performing the inverse transformation\(^\text{ii}\) we get \(\langle u(t) \rangle = Re\mu(\omega_0) E_0 e^{i\omega_0 t}\). Here

\[
\mu(\omega) = \frac{1}{m} \frac{1}{\omega^2 + M[\omega]}, \tag{23}
\]

is called the dynamical mobility. The dynamical conductivity is related to dynamical mobility by \(\sigma(\omega) = ne^2 \mu(\omega)\). Thus

\[
\sigma(\omega) = \frac{ne^2}{m} \frac{1}{\omega^2 + M[\omega]} . \tag{24}
\]

\(^{\text{ii}}\)In the algebra one has to use \(M[-\omega] = M[\omega]^*\) which can be easily proved from the definition of \(M[\omega]\).
operators as shown in following section. The memory dependent friction gives Generalised Drude formula. On neglecting this memory we will get back the simple Drude formula. To demonstrate it let us consider the memory function to be a delta function in time i.e., \( M(t) = \gamma \delta(t + i0) \) (because \( M(t) \) is defined only for \( t > 0 \)). From equation (21) we can show that \( M[\omega] = \gamma \). On substitution it into equation (24) we get

\[
\sigma(\omega) = \frac{ne^2}{m} \frac{1}{i\omega + \gamma}.
\] (25)

This is the same conductivity, which we have obtained in the previous section (equation (12)). In a realistic situation \( M[\omega] \) can be a complicated frequency dependent function, and its computation can be an involved task. In the following section we derive GDF using projection operator technique and then in subsequent sections this technique will be used to derive \( M(\omega) \) for the important case of metals (using a pertubative procedure given by Wölfle-Götze[3]). Important point to remember from this section is that memoryless \( M(t) \) leads to simple Drude formula.

5 The Zwanzig-Mori projection operator formalism

In the present section we are going to derive generalised Drude formula using projection operator technique. This provides a powerful computational approach as the MF can be explicitly computed in many situations of interest. In the case of electron scattering in metals we will explicitly show that memory function becomes frequency independent in the low frequency limit and can be identified with the Drude scattering rate. To derive generalised Drude formula using memory function formalism, we need to introduce Mori-Zwanzig projection operators. We start with the Kubo formula [1, 4]

\[
\sigma_{\mu\nu}(\omega) = V \beta \int_0^\infty dt e^{i\omega t} \langle J_\nu(0) J_\mu(t) \rangle.
\] (26)

In the above equation we write \( J_\mu(t) = e^{iL_t} J_\mu(0) \) where \( L \) is the Liouville operator[4]. Thus

\[
\sigma_{\mu\nu}(\omega) = V \beta \int_0^\infty dt e^{i\omega t} \langle J_\nu(0) e^{iL_t} J_\mu(0) \rangle.
\] (27)

Time integration can be performed with the result:

\[
\sigma_{\mu\nu}(z) = V \beta \langle J_\nu \mid i \frac{z}{z + L} J_\mu \rangle.
\] (28)

Let us introduce the “Bra-Ket” notation of quantum mechanics for convenience, and define the scalar product of two “vector” \( A \) and \( B \) as

\[
\langle A | B \rangle = \langle A^* B \rangle,
\] (29)

where we define \( \langle ... \rangle = tr(\rho ... ) \) i.e. the thermodynamical ensemble average. On implementing this notation, equation (28) can be expressed as

\[
\sigma_{\mu\nu}(z) = V \beta \left\langle J_\nu \left| \frac{i}{z + L} J_\mu \right. \right\rangle.
\] (30)

Projection operator is defined as

\[
P \equiv \sum_{\mu'} \frac{1}{\langle J_{\mu'} | J_{\mu'} \rangle} | J_{\mu'} \rangle \langle J_{\mu'} |.
\] (31)

[3] The time evolution of a function of dynamical variables is expressed as \( \frac{d}{dt} f = -L f \), here \( L = i\{H, \} = i\frac{\partial H}{\partial \vec{q}} \frac{\partial}{\partial \vec{p}} - \frac{\partial H}{\partial \vec{p}} \frac{\partial}{\partial \vec{q}} \). \( H \) is the total Hamiltonian of the system. The solution of the above Liouville equation reads \( f(t) = e^{iLt} f(0) \).
This projection operator projects an arbitrary vector $J_\mu$ onto $J_\mu'$. It is easy to verify that $\mathcal{P}\mathcal{P} = \mathcal{P}$ (the essential property of projection). Introduce another projection operator $\mathcal{Q}$ such that $\mathcal{P} + \mathcal{Q} = \mathbb{1}$. Rewrite $\mathcal{L}$ in equation (30) as $\mathcal{L} = \mathcal{L}(\mathcal{P} + \mathcal{Q})$

$$\sigma_{\mu\nu}(z) = V\beta \left< \frac{i}{z + \mathcal{L} \mathcal{Q} + \mathcal{L} \mathcal{P}} \right| J_\nu \right| ^{-1} \left| J_\mu \right>.$$  

(32)

With the operator identity

$$\frac{1}{X + Y} = \frac{1}{X} - \frac{1}{X} \frac{1}{X + Y},$$  

(33)

$\sigma_{\mu\nu}(z)$ can be divided into two terms

$$\sigma_{\mu\nu}(z) = iV\beta \left< \frac{1}{z + \mathcal{L} \mathcal{Q}} \right| J_\mu \right| J_\nu \right> - iV\beta \left< \frac{1}{z + \mathcal{L} \mathcal{Q}} \mathcal{L} \mathcal{P} \frac{1}{z + \mathcal{L}} \right| J_\mu \right| J_\nu \right>.$$  

(34)

Write the first term as $\frac{1}{z(1 + \mathcal{L} \mathcal{Q})} = \frac{1}{z}(1 - \frac{1}{z} \mathcal{L} \mathcal{Q} + \frac{1}{z^2} \mathcal{L} \mathcal{Q} \mathcal{L} \mathcal{Q} - \ldots \ldots \ldots )$. Except the first term in the expansion, all higher terms vanishes. It is easy to observe this: $\mathcal{Q}|J_\mu\rangle = \mathbb{1}|J_\mu\rangle - \mathcal{P}|J_\mu\rangle = |J_\mu\rangle - |J_\mu\rangle = 0$. For the second term, insert for the "sandwiched" operator $\mathcal{P}$ from equation (31). Thus, the equation takes a new form

$$\sigma_{\mu\nu}(z) = i\chi \frac{1}{z} \mathcal{L} \mathcal{P} \mathcal{L} \mathcal{Q} \left< \frac{1}{z + \mathcal{L} \mathcal{Q}} \mathcal{L} \mathcal{P} \frac{1}{z + \mathcal{L}} \right| J_\mu \right| J_\nu \right>.$$  

(35)

Replacing the magnitude form of $\langle J_\nu|J_\mu \rangle$ by $\frac{\chi_0}{\beta V} \delta_{\nu\mu}$ \[1\] in both terms and manipulating the second term with projection operators, we obtain

$$\sigma_{\mu\nu}(z) = i\beta \left< \frac{1}{z} |J_\mu\rangle \right| J_\nu \right> - V\beta \chi_0^{-1} \sum_{\mu'} \langle J_\nu \left| \frac{i}{z + L} \right| J_\mu \right> \left< \frac{1}{z + \mathcal{L} \mathcal{Q}} \mathcal{L} \mathcal{P} \left| J_\mu \right> \right|.$$  

(36)

We notice that the second term of the above equation can be written as a product of conductivity and the memory function

$$\sigma(z) = i\chi_0 \frac{1}{z} - \frac{1}{z} \sigma(z) M(z),$$  

(37)

on simplifying

$$\sigma(z) = i\frac{\chi_0}{z + M(z)} = i\frac{\omega_p^2}{4\pi} \frac{1}{z + M(z)}.$$  

(38)

where $M(z)$ is the memory function

$$M(z) = V\beta \chi_0^{-1} \left< \frac{1}{z + \mathcal{L} \mathcal{Q}} \mathcal{L} \right| J \right>.$$  

(39)

On comparing the above equation (38) with GDF (equation (24)) we notice that the memory function can be expressed in terms of projection operator (equation (39)). In the following section we review the Götze-Wölfe perturbation method to evaluate the memory function.
6 The Götze-Wölfle (GW) Formalism

Expression given in the above section are formal and cannot be directly used for the computation of the memory function. In 1972, Götze and Wölfle[3] presented a perturbative method for the computation of the memory function. They applied their method to the computation of dynamical conductivity of metals. The purpose of this section is to present their method. Before giving the perturbative expansion for memory function we first derive a fundamental equation used by them, i.e.,

\[
\chi(z) = \chi_0 \frac{M(z)}{z + M(z)}. \tag{40}
\]

Here \(\chi(z)\) is the Fourier-Laplace transform of the current-current correlation function

\[
\chi(z) = iV \int_0^\infty dt e^{izt} \langle [J(t), J(0)] \rangle. \tag{41}
\]

Dynamical conductivity \(\sigma(z)\) can be written in terms of \(\chi(z)\) [4]

\[
\sigma(z) = i \omega \frac{z^2}{4 \pi z} - i \frac{z}{\chi(z)}. \tag{42}
\]

We have observed in the previous section that conductivity can be expressed in terms of memory function (equation(38)). An expression for \(\chi(z)\) in terms of \(M(z)\) can be obtained from equation (38) and (42):

\[
\chi(z) = \omega \frac{z^2}{4 \pi z} \frac{M(z)}{z + M(z)} = \chi_0 \frac{M(z)}{z + M(z)} \quad \text{or,} \quad M(z) = \frac{z \chi(z)}{\chi(0) - \chi(z)}. \tag{43}
\]

A more proof of equation (40) is given in the Appendix. Memory function can be computed if we compute \(\chi(z)\). The above expression is a non-perturbative (exact) expression of the memory function. In the next section we introduce the Götze-Wölfle (GW) perturbative method.

6.1 The Götze-Wölfle (GW) approximation for the memory function

For GW method for the computation of the memory function we need the following EOM [3]:

\[
z \langle\langle J; J \rangle \rangle_z = -\langle\langle [J, J] \rangle \rangle_z - \langle\langle [J, H]; J \rangle \rangle_z
= -\langle\langle [J, J] \rangle \rangle_z + \langle\langle [J, [J, H]] \rangle \rangle_z. \tag{44}
\]

Proof is as follows: We have

\[
z \langle\langle J; J \rangle \rangle_z = iV \int_0^\infty dt e^{izt} \langle [J(t), J] \rangle = V \int_0^\infty dt \langle [J(t), J] \rangle \frac{d}{dt} (e^{izt}). \tag{45}
\]

On integrating by parts and using \(J(t) = i[H, J]\), we obtain the first EOM. The second equation can be obtained by using the cyclic property of operators under trace operation. The equal time commutators \([J, J]\) in the above equation are zero. Thus, the first equation can be written as:

\[
z \chi(z) = -\langle\langle C; J \rangle \rangle_z, \tag{46}
\]

where we define \(C = [J, H]\). In the second equation of motion set \(J = C\) :

\[
z \langle\langle C; J \rangle \rangle_z = -\langle\langle C; J \rangle \rangle_z + \langle\langle C; C \rangle \rangle_z, \tag{47}
\]

or

\[
\langle\langle C; J \rangle \rangle_z = \frac{\langle\langle [C, J] \rangle \rangle_z - \langle\langle C; C \rangle \rangle_z}{z}. \tag{48}
\]
Put $z = 0$ in equation (47) and it leads to $\langle [C, J] \rangle = \langle (C; C) \rangle_0$. Using this and using equation (46), the equation (48) gives:

\[
z\chi(z) = \frac{1}{z}((\langle (C; C) \rangle_0 - \langle (C; C) \rangle_z).
\]  

(49)

This is an exact expression for the current-current correlation function. Now comes the issue of perturbative expansion. The correlation $\langle \langle (C; C) \rangle_z \rangle$ has terms proportional to the square of interaction as $C$ is proportional to $H_{\text{interaction}}$ ($C = [J, H] = [J, H_0 + H_{\text{int}}]$). If $H_{\text{int}}$ is a small perturbation, then one can linearize the above expression. In equation (43) one can expand $M(z)$ as $M(z) = \frac{z\chi(z)}{\chi(0)(1 - \frac{x(z)}{\chi(0)})} = \frac{z\chi(z)}{\chi(0)}(1 + \frac{x(z)}{\chi(0)} - ....)$. Under the condition of small perturbation $||H_{\text{int}}|| < ||H_0||$ one can keep the leading order term, and memory function can be approximately expressed as:

\[
M(z) \simeq \frac{1}{z\chi(0)}((\langle (C; C) \rangle_0 - \langle (C; C) \rangle_z).
\]  

(50)

This is the central equation used by GW for the computation of dynamical conductivity of a metal in which electron-impurity and electron-phonon scattering is treated as perturbation. In the next two subsections we review their calculation, and then return back to the issue of Drude scattering rate.

### 6.2 Impurity scattering

In this subsection we review the GW formalism as applied to the impurity scattering case [3]. The case of a simple metal (free electron gas) with impurity scattering is considered. The total Hamiltonian is written as

\[
H_{\text{total}} = H_{\text{electrons}} + H_{\text{electron-impurity}}
\]

\[
H_{\text{electrons}} = \sum_k \epsilon(k)c_k^\dagger c_k
\]

\[
H_{\text{electron-impurity}} = \frac{1}{N} \sum_{j,k,k'} \langle k|U^j|k' \rangle c_k^\dagger c_{k'}.
\]  

(51)

$N$ is the number of unit cells (we put cell volume to unity). The sum over $j$ is for all the randomly distributed impurities. $U^j$ is the electron scattering potential from $j$th impurity [3].

Our aim is to calculate memory function (which is generalised Drude scattering rate). We need to compute $C$, and the correlator $\langle \langle (C; C) \rangle_z \rangle$. The operator $C$ is defined as $[J, H_{\text{total}}]$. Current density is given by: $J = \sum_k v_x(k)c_k^\dagger c_k$, where $v_x(k)$ is the $x-$component of the electron velocity. We consider a case in which the external field is applied along the x-direction and the induced current is also measured in the same direction. As the current operator commutes with the free electron part of Hamiltonian, we get

\[
C = [J, H_{\text{electron-impurity}}] = \frac{1}{N} \sum_{j,k,k'} \langle k|U^j|k' \rangle (v_x(k) - v_x(k'))c_k^\dagger c_{k'}.
\]  

(52)

Define: $\phi(z) = \langle \langle (C; C) \rangle_z \rangle$ then equation (50) can be written as

\[
M(z) = \frac{1}{z\chi(0)}(\phi(0) - \phi(z)).
\]  

(53)

$\phi(z)$ will have correlators of the form: written as $\langle \langle c_k^\dagger c_{k'}^\dagger c_p c_p \rangle \rangle$.

\[
\langle \langle c_k^\dagger c_{k'}^\dagger c_p c_p \rangle \rangle = i \int_0^\infty dt e^{i z t} \langle \langle c_k^\dagger(t)c_k(t), c_p^\dagger c_p \rangle \rangle.
\]  

(54)
Using \( a_k(t) = c_k e^{-i \omega t} \), the time integration can be performed with the result

\[
- \frac{1}{z + \epsilon_k - \epsilon_{k'}} \langle [c_k^\dagger c_{k'}, c_k^\dagger p_{k'}^\dagger p] \rangle. \tag{55}
\]

By using anticommutation relations for \( c \) and \( c^\dagger \), thermal ensemble average can be found \cite{1}

\[
- \frac{1}{z + \epsilon_k - \epsilon_{k'}} (f(k) - f(k')). \tag{56}
\]

\( f(k) = \langle c_k^\dagger c_k \rangle \) is the Fermi-Dirac distribution function. With this simplified expression of correlator, \( \phi(z) \) can be written as

\[
\phi(z) = - \frac{2}{N} \sum_{i,j,k,k'} \langle k|U^i_1|k'\rangle \langle k'|U^j_1|k\rangle (v_x(k) - v_x(k'))^2 \frac{f(k) - f(k')}{z + \epsilon_k - \epsilon_{k'}}. \tag{57}
\]

The summations over \((i,j)\) run over the total number of impurities \((N_{imp})\). For \( i \neq j \), \( \phi(z) \) is proportional to \((N_{imp})^2\). If the impurity concentration \( c = \frac{N_{imp}}{N} \) is very small, then this term can be neglected as compared to the term proportional to \( c \) (the diagonal elements contribution). Thus, in the leading order:

\[
\phi(z) = - \frac{2}{N} \sum_{k,k'} \langle k|U^1_1|k'\rangle^2 (v_x(k) - v_x(k'))^2 \frac{f(k) - f(k')}{z + \epsilon_k - \epsilon_{k'}}. \tag{58}
\]

Here the summation over the impurity sites \( i \) is also performed because there are no correlation effects considered \cite{3, 4}. And the problem reduces to one impurity problem. Further simplification can be done using isotropy in the free electron case \( v^2 = 3v_x^2 \) and writing \( v = k/m \). Substituting equation (58) into equation (53) we get

\[
M(z) = \frac{2}{3z \chi_0 m^2 N} \sum_{k,k'} \langle k|U^1_1|k'\rangle^2 (k - k')^2 \frac{f(k) - f(k')}{\omega} \left( \frac{1}{z + \epsilon_k - \epsilon_{k'}} - \frac{1}{\epsilon_k - \epsilon_{k'}} \right). \tag{59}
\]

Substitute \( z = \omega + i \varepsilon \) and perform the limit \( \varepsilon \to 0 \), the above expression reduces to \cite{3, 4}

\[
ImM(\omega) = \frac{2}{3} \pi (\frac{N_{imp}}{N_e}) \frac{1}{m^2 N^2} \sum_{k,k'} |U(k,k')|^2 (k - k')^2 \frac{f(k) - f(k')}{\omega} \delta(\omega + \epsilon_k - \epsilon_{k'}). \tag{60}
\]

Using \( \frac{1}{N} \sum_k \to \int \frac{d^3k}{(2\pi)^3} \), equation (60) becomes

\[
ImM(\omega) = \frac{2}{3} \pi (\frac{N_{imp}}{N_e}) \frac{1}{m} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} |U(k,k',\theta)|^2 (k^2 + k'^2 - 2kk' \cos(\theta)) \times \left( \frac{f(k) - f(k')}{\omega} \right) \delta(\omega + \epsilon_k - \epsilon_{k'}). \tag{61}
\]

By changing variables \( \varepsilon = \frac{k^2}{2m} \) \((\hbar = 1)\) and performing the integration over \( \varepsilon' = \frac{k'^2}{2m} \) and using the properties of the delta function we obtain:

\[
ImM(\omega) = \frac{2}{3} \pi (\frac{N_{imp}}{N_e}) (\frac{2m}{2\pi})^3 \int_0^\infty d\varepsilon \sqrt{\varepsilon + \omega} \int_0^\pi d\theta \sin \theta |U(\varepsilon, \varepsilon + \omega, \theta)|^2 \times \left( 2\varepsilon + \omega - 2\sqrt{\varepsilon + \omega} \cos \theta \right) \left( \frac{f(\varepsilon) - f(\varepsilon + \omega)}{\omega} \right). \tag{62}
\]

\(^{iv}\)Use the identity \( \lim_{x \to 0} \frac{1}{x \pm i\varepsilon} = \frac{1}{\varepsilon} \mp i\pi \delta(\varepsilon) \).
This is a finite frequency result. In the limit \( \omega \to 0 \), the last factor gives a delta function and the integral over energy can be performed with the result

\[
ImM(0) = \frac{4}{3} \pi \left( \frac{N_{\text{imp}}}{N_e} \right) \left( \frac{2m}{2\pi} \right)^{3/2} \int_0^\pi d\theta \sin \theta |U(\epsilon_F, \theta)|^2 (1 - \cos \theta).
\]

With the angle dependence of the scattering potential taken into account it is clear that the scattering rate \((\frac{1}{\tau} = ImM(0))\) has very small contribution from small angle scattering \( (\text{when } \theta \text{ is small}) \). Thus, small angle scattering is not efficient in the momentum degradation. The very same conclusion is obtained when one deal with the solution of the Boltzmann equation beyond Relaxation Time Approximation (RTA) in an isotropic medium \([\text{RTA}]\). Thus the above expression from memory function formalism goes beyond the RTA \([\text{RTA}]\).

Next, consider that the scattering potential is independent of the angle between \(k\) and \(k'\). The above equation \(63\) can be further simplified:

\[
ImM(0) = \frac{2}{3} \pi \frac{N_{\text{imp}}}{N_e} (U \rho_F)^2 \epsilon_F.
\]

Thus the real part of conductivity from equation \(63\) is given by

\[
Re\sigma(\omega) = \frac{\omega_p^2}{4\pi} \frac{ImM(0)}{\omega^2 + (ImM(0))^2}.
\]

This is nothing but the Drude formula. We identify that

\[
\frac{1}{\tau} = ImM(0) = \frac{1}{\tau_{\text{Drude}}} = \frac{2}{3} \pi \frac{N_{\text{imp}}}{N_e} (U \rho_F)^2 \epsilon_F.
\]

Thus, the Drude scattering rate increases linearly (in the leading order) with impurity concentration and with the square power of the electron-impurity scattering potential. The most important point is that we recover the Drude formula in the low frequency limit. The low frequency here means \( \omega \ll \epsilon_F \) (the Fermi energy). If Fermi energy is in eV’s then the valid frequency regime of simple Drude formula is below say infrared frequencies. Thus

\[
\frac{1}{\tau} \text{ is frequency independent, when } \hbar \omega \ll \epsilon_F.
\]

This defines the regime of applicability of the Drude formula in metals \([\text{Drude}]\).

### 6.3 Phonon scattering

Next application of the WG formalism is the computation of the Memory Function (MF) in the case of electron-phonon scattering in metals. The leading cause of electrical resistance at ambient temperatures is due to the electron-phonon scattering. At ambient temperature electrical resistivity is linearly proportional to temperature i.e., \( \rho \propto T \). In a pure metallic sample at lower temperature \( (T \ll \Theta_D, \text{Debye Temperature}) \), resistivity is proportional to fifth power of temperature \( (\rho \propto T^5) \). These temperature dependencies have been experimentally verified. Theoretically these can be obtained from the solution of the Bloch-Boltzmann equation \([\text{Bloch-Boltzmann}]\). The Bloch-Boltzmann equation formulates the electron-phonon scattering in a semiclassical way. We will notice in this section that these temperature dependencies can also be obtained from memory function formalism. Before we start the calculation of the MF in the present case of electron-phonon scattering, let us note down its basic assumptions.

For conduction electrons, a free electron gas is assumed. The phonon considered are long wavelength longitudinal acoustic phonons. For electron-phonon interaction the Fröhlich Hamiltonian is used:

\[
H_0 = H_{el} + H_{ph},
\]

\[
H_{el-ph} = \sum_{k,k'} (D(k-k')c_{k}^\dagger c_{k'}b_{k-k'} + h.c.).
\]

\[
68
\]
Here $H_0$ is the free electron and free phonon part of the Hamiltonian with $H_{el} = \sum_k c_k^\dagger c_k$ and $H_{ph} = \sum_q \omega_q(b_q^\dagger b_q + 1/2)$. The second equation represents the electron phonon interaction. The coefficient $D(k - k')$ for acoustic phonon interaction is given by

$$D(q) = \frac{1}{\sqrt{2m_{ion} N\omega q}} q C_q,$$  \hspace{1cm} (69)

$N$ is the total number of unit cells, $m_{ion}$ is the ionic mass, and $\omega q$ is the phonon frequency. $C_q$ is the electron-phonon coupling constant and it is a slowly varying function of $q$ [7]. As before we work with units $\hbar = k_B = 1$. To compute the memory function we need to compute $C$:

$$C = [J_x, H_{el-ph}] = \sum_{k,k',p,p'} v_x(k)D(p - p')c_{k'}^\dagger c_pc_pb_{p'} - h.c.$$  \hspace{1cm} (70)

Using the anticommutation properties of $c_k$, and $c_k^\dagger$, and using the identity $[AB, C] = A[B, C] + [A, C]B$ we get

$$C = \sum_{p,p'} (v_x(p) - v_x(p'))D(p - p')c_{p'}^\dagger c_pc_pb_{p'} - h.c.$$  \hspace{1cm} (71)

Our next step is to calculate $\phi(z) = \langle \langle C; C \rangle \rangle_z$. Out of four terms in it only non-diagonal terms survive:

$$\phi(z) = -\sum_{k,k',p,p'} (v_x(k) - v_x(k'))(v_x(p) - v_x(p'))D(k - k')D^*(p - p')\langle \langle c_{k'}^\dagger c_{k'} b_{k-k'}; b_{p}^\dagger b_{p} c_{p}^\dagger c_{p} \rangle \rangle$$

$$-\sum_{k,k',p,p'} (v_x(k) - v_x(k'))(v_x(p) - v_x(p'))D^*(k - k')D(p - p')\langle \langle c_k^\dagger c_k b_{k-k'}^\dagger; b_{p} - b_{p}^\dagger c_{p}^\dagger c_{p} \rangle \rangle.$$  \hspace{1cm} (72)

The correlation function in its expanded notation is given by:

$$\langle \langle c_{k'}^\dagger c_{k'} b_{k-k'}; b_{p}^\dagger b_{p} c_{p}^\dagger c_{p} \rangle \rangle = i \int_0^\infty dt e^{i\omega t} \langle \langle [c_{k}(t)c_{k}^\dagger(t')]b_{k-k'}(t), b_{p}^\dagger b_{p} c_{p}^\dagger c_{p} \rangle \rangle.$$  \hspace{1cm} (73)

Using $c_k(t) = c_k e^{-i\omega t}$, the time integration and the ensemble average can be performed. The result is

$$\phi(z) = \frac{2}{3 m^2} \sum_{k,k'} |D(k - k')|^2 |k - k'|^2 \{f(1 - f')(1 + n_-) - (1 - f)f'n_-\}$$

$$\times \left( \frac{1}{\epsilon - \epsilon' - \omega + z} + \frac{1}{\epsilon - \epsilon' - \omega - z} \right).$$  \hspace{1cm} (74)

Here a factor of 2 in the coefficient comes from the spin summations. We have used short hand notation: $f$ means $f(k)$; $f'$ means $f(k')$; $n_-$ is for $n_{\omega_{k-k'}}$, and $\omega_-$ is for $\omega_{k-k'}$. On inserting the above equation into [63] and on simplifying we get:

$$ImM(\omega) = \frac{2}{3\pi} \frac{1}{m^2 \chi_0} \sum_{k,k'} |D(k - k')|^2 |k - k'|^2 (1 - f)f'n_-$$

$$\times \left( \frac{e^{\beta \omega} - 1}{\omega} \delta(\epsilon - \epsilon' - \omega + \omega) - \ldots \text{(terms with } \omega \to -\omega) \right).$$  \hspace{1cm} (75)
Convert momentum sums into integrals. To simplify the momentum integrals, change \(|k - k'|\) into \(q\) integral, by introducing \(\int dq \delta(q - |k - k'|)\) and writing integration variables \(k\) and \(k'\) as \(\sqrt{2me}\) and \(\sqrt{2me'}\), we obtain

\[
Im M(\omega) = \frac{2}{3\pi} N m^2 \frac{q}{\omega q} \int_0^\infty dq q^4 \int_0^\infty de \sqrt{e} \int_0^\infty de' \sqrt{e'} \int_0^\infty d\theta \sin \delta \left( q - \sqrt{2m} \sqrt{e + e' - 2\sqrt{ee'} \cos \theta} \right) \\
\times (1 - f) f' \left( \frac{e^{\beta \omega} - 1}{\omega} \delta(\epsilon - \epsilon' - \omega + \omega) - \dots \right).
\]

(76)

The integral over \(\theta\) can be simplified in the following way. The presence of the Fermi factors \((1 - f) f'\) cause the integrand to have a finite value only in a zone around the Fermi surface of a strip of width \(2k_B T\). And outside of this zone integrand is vanishingly small. Thus \(\epsilon\) and \(\epsilon'\) can be approximately replaced by \(\epsilon_F\). On implementing all these steps, the \(\theta\) integral reduces to:

\[
\int_0^\pi d\theta \sin \delta (q - \sqrt{2k_F} \sqrt{1 - \cos \theta}).
\]

(77)

This elementary integration can be performed with the result \(\frac{\pi}{q} f'\) (notice that \(0 < q < k_F\) ). Insert the value \(\frac{\pi}{q} f'\) of the \(\theta\)-integral into equation (76). Perform the \(\epsilon'\) integral using the property of the delta functions. Then, perform the integrations over \(\epsilon\) using elementary method\(\square\). Finally, we obtain

\[
Im M(\omega) = \frac{1}{8\pi^3 N(m m_{ion} k_F^5)^{-1}} \rho_F \int_0^{q_d} dq q^6 C_q^2 \left( \frac{1}{e^{\beta \omega} - 1} \right) \\
\times \left\{ (1 - \omega_q/\omega)(e^{\beta \omega} - 1)/e^{\beta (\omega - \omega_q)} - 1 + \dots \right\}.
\]

(78)

The above equation (78) is GW’s equation (54) in [3]. For further simplifications, we assume the linear approximation to phonon spectrum \(\omega_q = c_q \omega\) (i.e., the Debye approximation) and \(C_q\) is assumed constant \(C_q = \frac{1}{2}\) [3]. In the following subsections we analyse the above expression in various special cases of interest. We will notice that Bloch-Boltzmann equation results can also be obtained by this method. Let us first consider the D.C. case.

### 6.3.1 D.C. case

In the \(\omega \to 0\) limit, the expression in the curly brackets in the above equation (78) reduces to \(2\beta \omega_q/1 - e^{-\beta \omega_q}\). Thus

\[
Im M(0) = \frac{1}{4} \pi^3 N(m m_{ion} k_F^5)^{-1} \int_0^{q_d} dq q^6 e^{\beta \omega_q} / (e^{\beta \omega_q} - 1)^2.
\]

(79)

To simplify, write \(x = \beta \omega_q\), and \(\beta \omega_D = \Theta_D = \frac{\Theta_F}{T}\):

\[
Im M(0) = \frac{1}{4} \pi^3 N q_D^6 (m m_{ion} k_F^5 \Theta_D)^{-1} (T/\Theta_D)^5 J_5(\Theta_D/T), \quad \text{where} \ J_5(y) = \int_0^y dx x^5 e^x / (e^x - 1)^2.
\]

(80)

The above expression is the DC scattering rate (equivalent to the Drude scattering rate). It can be further analyzed into two special cases. In the high temperature limit, \(T >> \Theta_D\), we have \(J_5(y) \simeq \frac{1}{4} y^4\), thus

\[
Im M(0) = \frac{1}{16} \pi^3 N q_D^6 (m m_{ion} k_F^5 \Theta_D)^{-1} (T/\Theta_D) \propto T.
\]

(81)

\(\nu \int_0^\infty dx x^2 e^{-x} e^x = \pi^2/12\).
So, we observe that in high temperature approximation (when the temperature \( T \) is much greater than the Debye temperature \( \Theta_D \)), the scattering rate or, the imaginary part of the memory function has \( T^- \) linear temperature dependence. This agrees with the result as obtained from the Bloch-Boltzmann equation in the high temperature limit \([4, 5]\). In the low temperature limit, i.e, \( T << \Theta_D \), we have 
\[
J_5(y) \simeq 124.4, \quad \text{and the MF is}
\]
\[
ImM(0) = \frac{1}{\tau} = 31.1\pi^3 Nq_D^6(mm_{ion}k_F^5\Theta_D)^{-1}(T/\Theta_D)^5 \propto T^5.
\] (82)

This again agrees with the famous Bloch-Boltzmann’s \( T^5 \) law of phonon scattering. Thus all the known results in the DC limit are reproduced (Table 1:).

| Temperature limit | D.C. case |
|------------------|-----------|
| \( T >> \Theta_D \) | \( J_5(y) \simeq \frac{24}{5} \propto T \) |
| \( T << \Theta_D \) | \( \simeq 124.4 \propto T^5 \) |

### 6.3.2 A.C. case

The integral in equation (78) in \( \omega \neq 0 \) limit is difficult to perform (although it can be expressed in terms of PloyLog functions). We consider a simpler and relevant case of high frequencies \( \omega >> \Theta_D \), and \( \omega >> T \). Then the expression in curly brackets in equation (78) can be simplified to give \( e^{\beta_\omega q} + 1 \). On simplifying the integral over \( q \) we obtain

\[
ImM(\omega) \simeq \frac{1}{4}\pi^3 Nq_D^6(mm_{ion}k_F^5)^{-1}(T/\Theta_D)^5 J(\Theta_D/T), \quad J(y) = \frac{1}{2} \int_0^y dx x^4 \coth(x/2).
\] (83)

In the low temperature limit, i.e. \( T << \Theta_D \), we have \( J(y) \simeq \frac{1}{4} y^5 \), thus

\[
ImM(\omega) \simeq \frac{1}{40}\pi^3 Nq_D^6(mm_{ion}k_F^5)^{-1}.
\] (84)

We observe that at high frequency \( \omega >> \Theta_D \), but at lower temperature \( T << \Theta_D \), the scattering rate reduces to a constant value independent of frequency and temperature (Table 2:). And in the high temperature limit i.e., \( T >> \Theta_D \), we have \( J(y) \simeq \frac{1}{4} y^4 \). The temperature dependence of MF is given by

\[
ImM(\omega) \simeq \frac{1}{16}\pi^3 Nq_D^6(mm_{ion}k_F^5)^{-1}(T/\Theta_D) \propto T.
\] (85)

This behaviour is depicted in figure 2. An important point to be noticed is that even at zero temperature scattering rate is not zero. This non-zero scattering rate is due to an important mechanism called the Holstein mechanism.

In the limit \( T \to 0 \), equation (78) can be simplified for all values of \( \omega \). In this limit, the expression in the curly bracket in (78) gives \((1 - \omega_\xi/\omega)e^{3\omega_\xi} \) if \( \omega > \omega_\xi \), and \((\omega_\xi/\omega - 1)e^{3\omega_\xi} \) if \( \omega < \omega_\xi \). After performing the \( q \) integral we get:

\[
ImM(\omega) \simeq \frac{1}{240}\pi^3 Nq_D^6(mm_{ion}k_F^5\Theta_D)^{-1} \times \left\{ \begin{array}{ll} (\omega/\Theta_D)^5 & |\omega| < \Theta_D \\ 6 - 5(\omega_D/\omega) & |\omega| > \Theta_D. \end{array} \right.
\] (86)

In the limit \( T \to 0 \), the non-vanishing value of the generalised Drude scattering rate (or memory function) has a very important physical meaning as mentioned before. In a pure sample at zero temperature there are no thermally excited lattice vibrations or phonons, thus one would naively expect that electron scattering would be prohibited and the scattering rate would vanish. But it is shown for the first time by Ted Holstein that there is an important mechanism of momentum randomization...
even at zero temperature \([9]\). The mechanism involves the simultaneous absorption of a photon and
creation of an electron-hole pair along with an acoustic phonon. Thus the mechanism—now called
the Holstein mechanism—involves the creation of a phonon and it occurs at finite frequencies. From
equation (86) we observe that Götze-Wölfle formalism is capable of capturing this physical effect. At
low frequencies \(|\omega| < \Theta_D\), the scattering rate grows as \(\omega^5\) and then it saturates when \(\omega \gg \Theta_D\). The
transition happens around \(\Theta_D\) (Table 2). The generalised Drude scattering rate can be obtained from
the experimental data of reflectance using the memory function formalism. If experimentally obtained
scattering rate shows transition behaviour around \(\Theta_D\), then it can be derived that the dominating
scattering mechanism is due to phonons. This particular issue is very important in the field of strange
metals such as observed in normal states of cuprate high temperature superconductors. Absence of \(\Theta_D\)
points to other scattering mechanisms.

![Figure 2: A depiction of the Holstein mechanism](image)

Table 2: Temperature dependence of the memory function in the AC limit

| \((\omega \gg \Theta_D)\) Temperature limit | A.C. case |
|------------------------------------------|-----------|
| \(T \gg \Theta_D\)                     | \(J_5(y)\) | \(\text{Im} M(0)\) |
| \(T \ll \Theta_D\)                     | \(\cong y^4\) | \(\propto T\) |
|                                          | \(\cong \frac{y^2}{\omega^4}\) | independent of \(T\) |

We also notice that the generalised Drude scattering rate (equation (86)) strongly deviates from the
simple Drude scattering rate (which is just a constant parameter). From equation (87) the real part of
conductivity is given by:

\[
\text{Re}\sigma(\omega) = \frac{\omega_p^2}{4\pi} \frac{\text{Im} M(\omega)}{\omega^2 + (\text{Im} M(\omega))^2}. \tag{87}
\]

Where \(\text{Im} M(\omega)\) is given by the expression (86). If the sample also has dilute impurities, then in the
linear order \(\text{Im} M_{\text{total}}(\omega) = \text{Im} M_{\text{imp}}(\omega) + \text{Im} M(\omega)\), which in the \(\omega \rightarrow 0\) limit goes back to Drude
formula (equation (4)).

7 Summary of MF formalism

In this brief overview of the memory function formalism we sketched the derivations of the generalised
Drude formula by two methods. In the first method it is derived from the generalised Langevin equation.
An advantage of this route is that we are able to appreciate the problems of the standard Drude formula and the corresponding standard Langevin equation. Then in the second route we reviewed the Zwanzig-Mori projection operator method, and showed that dynamical conductivity from the Kubo formula can be written in a form resembling the generalised Drude formula. In doing that the memory function is expressed through projection operators. We then reviewed a very useful method for the computation of the memory function put forward by Götze-Wölfle (GW). Two applications of this method in the computation of dynamical conductivity of metals are reviewed. In the first application of the electron-impurity scattering we notice that the Drude scattering rate is frequency dependent. It can be taken as frequency independent only when the system is probed with frequencies much less than \( \frac{\epsilon}{\hbar} \). We also noticed that the DC scattering rate includes \( 1 - \cos \theta \) factor which stresses the importance of large angle scattering in momentum degradation. This factor appears in the solution of the Bloch-Boltzmann equation when vortex corrections are taken into account. In the electron-phonon scattering case we notice that in the DC limit the memory function formalism reproduces all the known results of the Bloch-Boltzmann equation (\( \rho \propto T \) when \( T >> \Theta_D \), and \( \rho \propto T^5 \) when \( T << \Theta_D \)). In the AC limit it also reproduces the Holstein mechanism of electromagnetic energy absorption at zero temperature.

8 Appendix: The Götze-Wölfle (GW) Formalism

We need to show that

\[
\chi(z) = \chi_0 \frac{M(z)}{z + M(z)},
\]

where \( \chi(z) \) is

\[
\chi(z) = iV \int_0^\infty dt e^{izt} \langle [J(t), J(0)] \rangle.
\]

Let us define

\[
\zeta(t) = i\langle [J(t), J(0)] \rangle.
\]

Using the cyclic property of trace \( \zeta(t) \) can be written as

\[
itr(\rho J(t) J) - itr(\rho J(t) J) = itr(J(t) [J, \rho]).
\]

Use Kubo’s Identity \( e^{\beta H} [J, e^{-\beta H}] = \int_0^\beta e^{\lambda H} [H, J] e^{-\lambda H} \), and write \( [J, \rho] \) it in the following way

\[
[J, \rho] = \int_0^\beta d\lambda \rho [H, J(-i\lambda)].
\]

Using \( \dot{A} = i[H, A] \), the above commutator takes the form

\[
[J, \rho] = -i \int_0^\beta d\lambda \rho \dot{J}(-i\lambda).
\]

Inserting this expression in equation (91), \( \zeta(t) \) takes the form

\[
\zeta(t) = \beta \langle \dot{J}(-i\lambda) J(t) \rangle^\circ.
\]

Here we have introduced a notation: \( \langle ... \rangle^\circ = \frac{1}{\beta} \int_0^\beta d\lambda tr(\rho...) \). With this, the equation (89) can be written as

\[
\chi(z) = V \int_0^\infty dt e^{izt} \zeta(t) = V \beta \int_0^\infty dt e^{izt} \langle \dot{J}(-i\lambda) J(t) \rangle^\circ.
\]
For the next part of the proof, we will use an alternative representation of conductivity from Kubo’s formula \[10\]:

\[
\sigma(z) = -\frac{\omega_p^2}{4\pi iz} - \frac{\beta V}{iz} \int_0^\infty dt e^{izt} \langle J(-i\lambda) \dot{J}(t) \rangle^\circ.
\]

(96)

We want to find a connection between the last two equations (95 and 96). Only problem is that the integrands differ w.r.t. time differentiation. To sort this out, we use the stationarity property of the current-current correlation function, i.e., \( \langle J(t_0) J(t_0 + t) \rangle \) must be independent from the initial time \( t_0 \) or

\[
\frac{d}{dt_0} \langle J(t_0) J(t_0 + t + i\lambda) \rangle^\circ = 0 = \langle \dot{J}(t_0) J(t_0 + t + i\lambda) \rangle^\circ + \langle J(t_0) \dot{J}(t_0 + t + i\lambda) \rangle^\circ.
\]

(97)

Thus at \( t_0 = 0 \)

\[
\langle \dot{J}(0) J(t + i\lambda) \rangle^\circ = -\langle J(0) \dot{J}(t + i\lambda) \rangle^\circ.
\]

(98)

Using this, from equation (95) and (96) we obtain the required result.

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