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# MEMORY FUNCTION FORMALISM APPLIED TO ELECTRONIC TRANSPORT IN DISORDERED SYSTEMS

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Memory function formalism is briefly reviewed and applied to electronic transport using the projection operator technique. The resistivity of a disordered 2-D electron gas under strong magnetic field is obtained in terms of the force-force correlation function.

Memory functions have been extensively studied in the past in relation with hydrodynamical processes /1/. During the last decade their use has been extended to electronic transport properties in disordered materials /2/ and more recently to the interesting problem of conduction of disordered 2-D system /3,4/. The fact that they play the role of a self-energy of a many-particle propagator, and therefore the resonance structure is already built in, makes their expansion in a small parameter-like impurity concentration valid for all range of frequencies. In this paper we will review their definitions and apply the formalism to the case of 2-D electron gas under a strong magnetic field.

The linear response theory establishes that the dynamics of spontaneous fluctuations about the equilibrium can be described in terms of correlation functions. Let's consider a quantity  $m(\vec{r},t)$  obeying the conservation equation.

$$\frac{\partial}{\partial t} m(\vec{r}, t) + \vec{\nabla} \times \vec{j}(\vec{r}, t) = 0. \quad (1)$$

The above equation relating density and current is not enough to solve for  $m(\vec{r}, t)$ . We need a second equation that establishes that the current will flow from regions of higher to lower density. This is the so called constitutive equation

$$\langle \vec{j}(\vec{r}, t) \rangle = -D \vec{\nabla} \langle m(\vec{r}, t) \rangle. \quad (2)$$

Here  $D$  is the diffusion coefficient. The average  $\langle \rangle$  is a non-equilibrium average to be properly defined.

We know that at thermal equilibrium  $\langle m(\vec{r}, t) \rangle = \text{constant}$ ,  $\langle \vec{j}(\vec{r}, t) \rangle_{\text{eq}} = 0$ . The conservation equation and the constitutive equation together lead to the diffusion equation

$$\frac{\partial}{\partial t} \langle m(\vec{r}, t) \rangle - D \nabla^2 \langle m(\vec{r}, t) \rangle = 0 \quad (3)$$

valid only if the property  $m(\vec{r}, t)$  varies slowly in space and time. It can be solved by Laplace transforming in time and Fourier transforming in space to yield

$$\langle m(\vec{k}, z) \rangle = i(z + iDk^2)^{-1} \langle m(\vec{k}, t = 0) \rangle \quad (4)$$

or

$$\langle m(\vec{k}, z) \rangle = e^{-Dk^2 t} \langle m(\vec{k}, t = 0) \rangle. \quad (5)$$

The pole at  $-iDk^2$  characterise a hydrodynamic mode corresponding to a lifetime  $\tau(k) = (Dk^2)^{-1}$ .

At this point let's define the autocorrelation function

$$S(\vec{r}, t) = \langle m(\vec{r}, t) m(\vec{0}, 0) \rangle_{\text{eq}}. \quad (6)$$

It is well defined as a thermal equilibrium average. Its Laplace transform

$$\tilde{S}(\vec{k}, z) = \int_0^{\infty} dt \int d\vec{r} e^{izt} e^{-i\vec{k} \cdot \vec{r}} S(\vec{r}, t) \quad \text{Im}z > 0 \quad (7)$$

and its Fourier transform (spectral density)

$$S(\vec{k}, \omega) = \int_{-\infty}^{+\infty} dt \int d\vec{r} e^{i\omega t} e^{-i\vec{k} \cdot \vec{r}} S(\vec{r}, t) \quad (8)$$

are related by

$$\tilde{S}(\vec{k}, z) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\omega \frac{S(\vec{k}, \omega)}{\omega - z}. \quad (9)$$

If we assume that the constitutive equation is valid in an operational sense, i.e., even if we omit  $\langle \rangle_{\text{non-eq}}$ , we obtain

$$[\partial_t - D \nabla^2] S(\vec{r}, t) = 0 \quad (10)$$

as proposed by Onsager in 1931. Then

$$\tilde{S}(\vec{k}, z) = i(z + iDk^2)^{-1} S(\vec{k}, t = 0). \quad (11)$$

The constitutive equation can be further improved to include causality:

$$\langle \vec{J}(\vec{r}, t) \rangle = - \int_0^t dt' D(t-t') \vec{\nabla} \langle m(\vec{r}, t') \rangle \quad (12)$$

or

$$\langle \vec{J}(\vec{r}, t) \rangle = - \int_0^t dt' \int d\vec{r}' D(\vec{r}-\vec{r}', t-t') \vec{\nabla}' \langle m(\vec{r}', t') \rangle. \quad (13)$$

In these cases  $D$  is called a memory function.

In 1972 Götze and Wölfle /2/ applied their holomorphic memory function to obtain the homogeneous dynamical conductivity of metals,

$$\sigma(z) = - \frac{ie^2}{z} \chi(z) + \frac{i\omega_p^2}{4\pi z}, \quad (14)$$

where  $\omega_p$  is the plasma frequency ( $\omega_p^2 = 4\pi e^2 N/m$ ) and  $\chi(z)$  is the current-current correlation function:

$$\delta_{xy} \chi(z) \equiv - \langle \langle j_i; j_j \rangle \rangle_z = -i \int e^{izt} \langle [j_i(t), j_j(0)] \rangle dt, \quad (15)$$

Since the conductivity has to remain finite in the limit of  $\omega$  going to zero,

$$\chi_0 = \omega_p^2 / 4\pi e^2 = N/m \quad (16)$$

and

$$\sigma(z) = - \frac{ie^2}{z} (\chi(z) - \chi_0). \quad (17)$$

Defining a holomorphic relaxation function

$$M(z) = z\chi(z) / [\chi_0 - \chi(z)] \quad (18)$$

then,

$$\sigma(z) = \frac{i}{4\pi} \omega_p^2 \frac{1}{z + M(z)}. \quad (19)$$

$M(z)$  works like a self-energy of the two particle propagator that appears in  $\sigma(z)$ .

For vanishing impurity concentrations the total current  $\vec{j}$  is a constant of motion. In this case  $\chi(z)$  and  $M(z)$  vanish. Assuming a regular dependence of  $M$  on the concentration  $n_i$ , then

$$M(z) = \frac{n_i}{z\chi_0} [\phi(z) - \phi(z=0)], \quad (20)$$

where  $\phi(z)$  is the force-force correlation function. This result reproduces Drude's model ( $\omega \rightarrow 0$ )

$$\sigma(\omega) = \frac{iNe^2}{m} (\omega + e\tau^{-1})^{-1}. \quad (21)$$

Transport properties of 2-D electron gas has attracted much attention during the last years, both due to the interest on localization in 2-D and to the discover of the quantum Hall effect and the surprise of the anomalous quantized Hall effect. Among the extensive arsenal used, memory function formalism has not been put aside. So, Shiwa and Isihara /4/ and Ying and da Cunha Lima /3/ have studied the transport properties of a 2-D electron systems under strong magnetic field using a memory function-projection operator technique. The experimentally measured quantities are  $\rho_{xx}$  and  $\rho_{xy}$ . It is not clear if the inversion of the conductivity tensor  $\underline{\sigma}$ , which has been averaged over all impurity configurations, yields the appropriate quantity for comparison with experiments. So, we aim directly to the calculation of the resistivity first and then perform the impurity average.

Let us start with the Hamiltonian for an electron gas under an external field, given by the vector potential  $\vec{A}$  and in the presence of impurities with scattering potential given by the Fourier transform  $U(q)$ .

$$H = \sum_i \frac{1}{2m} [\vec{p}_i + \frac{e}{c} \vec{A}(\vec{r}_i)]^2 + \sum_{i>j} V(\vec{r}_i - \vec{r}_j) + \sum_{q,j,l} U(\vec{q}) e^{iq \cdot (\vec{r}_j - \vec{R}_l)}, \quad (22)$$

where  $\vec{R}_l$  denotes impurities positions.

Next we transform this Hamiltonian into center of mass (CM) and relative coordinates

$$H = \frac{1}{2M} [\vec{P} + \frac{Ne}{c} \vec{A}(\vec{R})]^2 + H_r + \sum_{qj} e^{i\vec{q}\cdot\vec{R}} (q) e^{i\vec{q}\cdot(\vec{r}_j - R_e)}. \quad (23)$$

We have used respectively N and M to denote the number (density) of electrons and the total mass,  $M = Nm$ .  $\vec{P}$  and  $\vec{R}$  are the momentum and the position of the CM.  $H_r$  contains only relative coordinates. Using Kubo's expression for the conductivity (conductance) tensor, we have ( $\alpha, \beta = x, y$ )

$$\sigma_{\alpha\beta}(\omega) = \frac{i}{\omega} \frac{Ne}{m} \delta_{\alpha\beta} + \frac{i}{\omega} \left(\frac{e}{m}\right)^2 \int_{-\infty}^{+\infty} dt e^{i\omega t} Q_{\alpha\beta}(t), \quad (24)$$

where

$$Q_{\alpha\beta}(t) = i\theta(t) \langle [\pi_{\alpha}(t), \pi_{\beta}(0)] \rangle, \quad (25)$$

with  $\pi_x = i\partial/\partial x$  and  $\pi_y = -i\partial/\partial y + M\omega_c X$ . We have used the gauge  $\vec{A}(\vec{R}) = (0, HX, 0)$ .  $\omega_c$  is the cyclotron frequency,  $\omega_c = eH/mc$ .

Defining the Laplace transform

$$\chi_{\alpha\beta}(z) = i \int_0^{\infty} e^{izt} \langle [\pi_{\alpha}(t), \pi_{\beta}(0)] \rangle dt, \quad \text{Im } z > 0, \quad (26)$$

the conductivity becomes

$$\sigma_{\alpha\beta}(z) = \frac{iNe^2}{mz} \delta_{\alpha\beta} - \frac{ie^2}{m^2z} \chi_{\alpha\beta}(z). \quad (27)$$

We define the momentum-momentum correlation function

$$C_{\alpha\beta}(t) = \langle \pi_{\alpha}(t) | \pi_{\beta}(0) \rangle \quad (28)$$

using the following definition of the scalar product

$$\langle A|B \rangle = \beta^{-1} \int_0^\beta d\lambda \langle A^+ B(i\lambda) \rangle. \quad (29)$$

Using the fluctuation-dissipation theorem the Laplace transform  $C_{\alpha\beta}(z)$  is related with  $\chi_{\alpha\beta}(z)$  according to

$$\chi_{\alpha\beta}(z) = i\beta Z C_{\alpha\beta}(z) + \chi_{\alpha\beta}(0), \quad (0 \equiv 0 + i0^+). \quad (30)$$

Using the fact that  $\sigma$  remains finite as  $\omega \rightarrow 0$ ,

$$\chi_{\alpha\beta} \equiv \chi_{\alpha\beta}(0) = Nm \delta_{\alpha\beta} \quad (31)$$

and

$$\sigma_{\alpha\beta}(z) = \frac{e^2\beta}{m^2} C_{\alpha\beta}(z). \quad (32)$$

At this point we invert  $\underline{\sigma}$  to obtain the resistivity tensor

$$\rho_{\alpha\beta}(z) = \frac{m^2}{e^2\beta} C_{\alpha\beta}^{-1}(z). \quad (33)$$

The correlation function is now solved by means of the memory function-projection operator technique. Let's define

$$\hat{P} = \sum_{\alpha\beta} |\pi_\alpha \rangle \beta \chi_{\alpha\beta}^{-1} \langle \pi_\beta | \quad (34)$$

and  $\hat{Q} = 1 - \hat{P}$ . Then  $C_{\alpha\beta}(z)$  obeys the equation /1/

$$[z \underline{1} - \underline{\Omega} + i \underline{\Sigma}(z)] \underline{C}(z) = i\beta^{-1} \underline{\chi}, \quad (35)$$

where

$$\underline{\Omega} = \underline{\omega} \underline{\chi}^{-1}, \quad \omega_{\alpha\beta} = i\beta \langle \pi_\alpha | \pi_\beta \rangle = \langle [\pi_\alpha, \pi_\beta] \rangle, \quad (36)$$

$$\underline{\Sigma}(z) = \underline{S}(z) \underline{\chi}^{-1}, \quad S_{\alpha\beta}(z) = \beta \langle \pi_\alpha | \hat{Q} \frac{1}{z - \hat{Q}L\hat{Q}} | \pi_\beta \rangle. \quad (37)$$



L is the Liouville  $L \Psi = [H, \Psi]$ . As a consequence,

$$\underline{\rho}(z) = - \frac{im}{Ne^2} [z\underline{1} - \underline{\Omega} + \underline{M}(z)], \quad (38)$$

with  $\underline{M}(z) = \underline{\sum}(f)$ . In the absence of magnetic field  $\underline{\Omega}$  is zero and  $\underline{M}(z)$  is diagonal. The above expression becomes the reciprocal of the Götze and Wolfle's conductivity.

With the Hamiltonian given by Eq. (23) we obtain

$$\underline{\Omega} = -iN\omega_c \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (39)$$

It does not contribute to the longitudinal resistivity. The off-diagonal elements immediately generate the term  $m\omega_c/ne^2$  in the transverse resistivity. Expanding the operator  $(z - \hat{Q}L\hat{Q})^{-1}$  we obtain for the memory-function

$$M_{\alpha\beta}(z) = i\beta M^{-1} \int_0^\infty \langle U_\alpha | e^{-it\hat{Q}L} | U_\beta \rangle e^{izt} dt, \quad (40)$$

where  $-U_\alpha$  is the component  $\alpha$  of the generalized force acting on the CM due to impurity scattering, i.e.,

$$U_\alpha \equiv \frac{\partial U}{\partial R_\alpha} = \sum_{\vec{q}, l} i q_\alpha e^{i\vec{q} \times \vec{R} l} U(q) \rho(q) \quad (41)$$

and  $\rho(\vec{q})$  is the electron density  $\rho(\vec{q}) = \sum_j e^{i\vec{q} \times \vec{r}_j}$ .

At this point we assume that the dynamics of the generalized force is governed by the full Liouville operator

$$e^{itQL} | U_\alpha \rangle = e^{itL} | U_\alpha \rangle = | U_\alpha(t) \rangle. \quad (42)$$

In this case

$$M(z) = \frac{i\beta}{Nm} \int_0^{\infty} \langle U_{\alpha}(t) U_{\beta} \rangle e^{izt} dt. \quad (43)$$

Defining the (retarded) force-force correlation function according to

$$\pi_{\alpha\beta}^R(\omega) = i \int_{-\infty}^{+\infty} \theta(t) \langle [U_{\alpha}(t), U_{\beta}(0)] \rangle e^{i\omega t} dt \quad (44)$$

we obtain

$$M_{\alpha\beta}(\omega + i0^+) = -\frac{1}{Nm\omega} [\pi_{\alpha\beta}^R(\omega) - \pi_{\alpha\beta}^R(0)], \quad (45)$$

that is nothing but GW's expression in a matrix form.

For low impurity concentration a standard approach to the configurational average leads to

$$\pi_{\alpha\beta}^R(\omega) = n_i \sum_{\vec{q}} q_{\alpha} q_{\beta} U^2(q) \bar{S}(q, \omega), \quad (46)$$

where  $S(q, \omega)$  is the retarded density-density correlation function

$$S(\vec{q}, \omega) = i \int_{-0}^{+\infty} \theta(t) \langle [\rho(\vec{q}, t), \rho(-\vec{q}, 0)] \rangle e^{i\omega t} dt. \quad (47)$$

Collecting those equations together, we have for the resistivity

$$\bar{\rho}_{xx}(\omega) = \frac{i m \omega}{Ne^2} + \frac{i}{n^2 e^2} \frac{1}{\omega} [\bar{\pi}_{xx}(\omega) - \bar{\pi}_{xx}(0)], \quad (48)$$

$$\rho_{xx}(\omega) = \frac{m \omega_c}{Ne^2} + \frac{i}{N^2 e^2} \frac{1}{\omega} [\bar{\pi}_{xy}(\omega) - \bar{\pi}_{xy}(0)]. \quad (49)$$

What is left at this point is to calculate the average density-density correlation function and perform the summation on the wave vector in Eq (46). Many processes can be used. One is to use the memory

function formalism repeatedly. Another possibility is to perform a diagrammatic perturbative expansion on  $S(\vec{q}, \omega)$ . In the present case of strong magnetic field, Landau quasi-particle Green's functions in the self-consistent Born approximation form a convenient basis to express the one-particle propagator. In fact, current-current diagrams have been worked out by Houghton et al. /5/ and a great effort can be saved in the present case by using many of their results.

An important test for the present theory consists in trying to recover Drude's result when we make the limit of  $H$  going to zero. In another work presented in this Symposium it is shown that the lowest order diagram is enough to reproduce Drude's formula.

#### REFERENCES

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FIGURE CAPTIONS

Fig. 1 - Diagram for  $\overline{\pi}_{\alpha\beta}^0(i\Omega)$ .

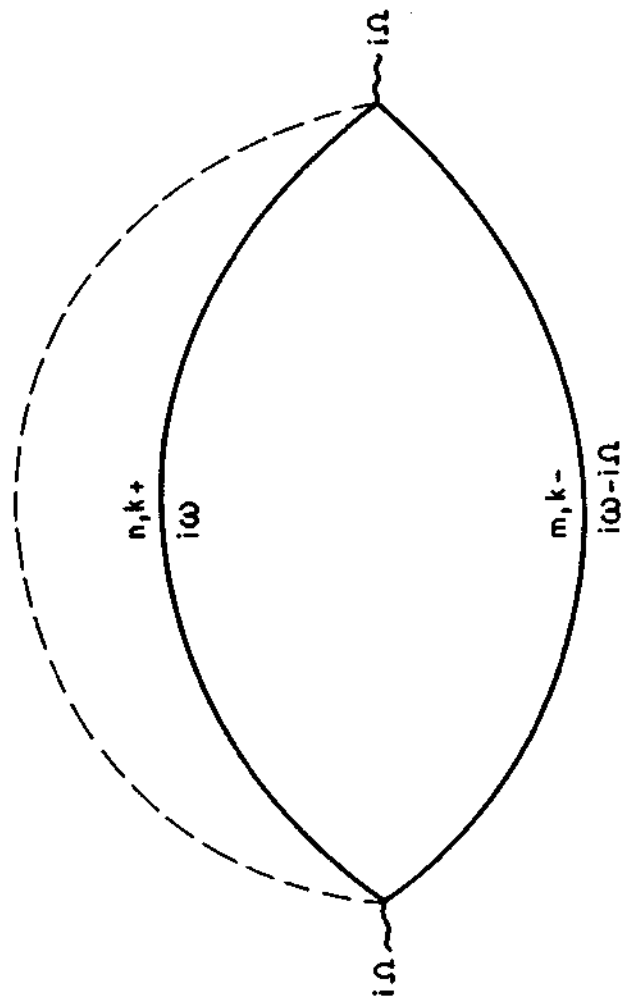


Fig. 1 - I.C. da Cunha Lima