Linear Response Theory: Two Regimes, Two Equivalent Descriptions, and Two Parts of Electrical Conductivities

Xiaodong Hu*
Department of Physics, Boston College
(Dated: August 24, 2021)

In this letter, we will review the general theory of isothermal linear response adiabatic linear response. Taking adiabatic charge current response as one example, we will show that the standard form of the response function, consisting of paramagnetic (Drude) and diamagnetic parts, can also be obtained in the formulation of Luttinger [1]. Some other useful forms of Kubo formula are also derived for future reference.

当时共客长安，似二陆初来俱少年。有笔头千字，胸中万卷；致君尧舜，此事何难？

—— 苏轼「沁园春」

Contents

I. Linear Response Theory 1
A. Isothermal Response 2
B. Adiabatic Response 2
C. Example: Adiabatic Response of Charge Current 4
D. Drude Formula: Cancellation of Static Diamagnetic Response in Metals 6

II. Other Equivalent Forms of Kubo Formula 8
A. Kubo's Identities and Canonical Kubo Pair 8
B. Equivalent Forms of Kubo Formula 9
C. Equivalence bewteen Conductivity Obtained by Coupling with Vector Potentials and Electrical Potentials 9
D. Matsubara Green Function of Imaginary-frequencies 10

III. Appendix 10
A. f-sum Rule 10

References 11

I. LINEAR RESPONSE THEORY

The problem of linear-reponse is formulated as following:

Consider an system in equilibrium coupling with external driven forces through a perturbative fields $F(t)$ (switching on from t_0, for example)

$$\hat{H} = \hat{H}_0 + \hat{H}'(t) \equiv \hat{H}_0 + F(t)\hat{B}(t), \tag{1}$$

then for small fields $F(t)$, the meseasurable quantum average of the operator (in Schrödinger picture, for example)

$$\langle A\rangle(t) \equiv \frac{1}{\mathcal{Z}}\mathrm{Tr}\{\hat{\rho}_S(t)\hat{A}\} \equiv \frac{1}{\mathcal{Z}}\sum_\psi \langle\psi_S(t)|\hat{\rho}_S(t)\hat{A}|\psi_S(t)\rangle \tag{2}$$

can be expand to the first order of $F(t)$, which is believed to reflect the intrinsic properties of the material. However, depending on the treatment of the perturbation in (2), or more precisely whether we are in the *fast* or *slow* limit[1], we will fall into two regimes — the (usual) *adiabatic responses* and *isothermal responses*.

---

*Electronic address: `xiaodong.hu@bc.edu`

[1] Following [1], the perturbation is fast if the density matrix can be taken as the one in old equilibrium, while is slow if the system is always in (new) quasi-equilibrium.

A. Isothermal Response

For isothermal reponses, the perturbation is *slow* enough so that the system is always in quasi-equilibirum. So we can directly write down

$$\hat{\rho}(t) = \frac{1}{\mathcal{Z}} e^{-\beta \hat{H}} = \frac{1}{\mathcal{Z}} e^{-\beta(\hat{H}_0 + \hat{H}'(t))}. \tag{3}$$

But even the density matrix is known, it is still hard to expand to the first order of $F(t)$ and evaluate the quantum average for (2). Following [2], we can make use of the analogy of imaginary-time and inverse-temperature to define a function of β as

$$V(\beta) \equiv e^{-\beta \hat{H}} e^{\beta \hat{H}_0} = e^{-\beta(\hat{H}_0 + \hat{H}'(t))} e^{\beta \hat{H}_0}.$$

Clearly we have

$$\begin{aligned} \frac{\mathrm{d}V(\beta)}{\mathrm{d}\beta} &= e^{-\beta \hat{H}(t)} \hat{H}_0 e^{\beta \hat{H}_0} - e^{-\beta \hat{H}(t)} \hat{H}(t) e^{\beta \hat{H}_0} \equiv e^{-\beta \hat{H}(t)} \hat{H}'(t) e^{\beta \hat{H}_0} \\ &\equiv e^{-\beta \hat{H}(t)} e^{\beta \hat{H}_0} \cdot e^{-\beta \hat{H}_0} \hat{H}'(t) e^{\beta \hat{H}_0} \equiv V(\beta) \hat{H}'_I(t + i\hbar\beta), \end{aligned}$$

where $\hat{H}'_I(t + i\hbar\lambda) \equiv F(t)\hat{B}(i\hbar\lambda)$. This differential equation is equivalent to the integral equation (check by differentiation)

$$V(\beta) = 1 + \int_0^\beta \mathrm{d}\lambda\, V(\lambda) \hat{H}'_I(t + i\hbar\lambda), \tag{4}$$

which can be solved iteratively. To the first-order approximation, we can take $\hat{H}'(t) = 0$ in the definition of $V(\beta)$ (so to the zeroth order $V(\beta) = 1$), getting

$$V(\beta) \simeq 1 + \int_0^\beta \mathrm{d}\lambda\, \hat{H}'_I(t + i\hbar\lambda) \tag{5}$$

So

$$e^{-\beta \hat{H}(t)} \equiv V(\beta) e^{-\beta \hat{H}_0} \simeq \left(1 + \int_0^\beta \mathrm{d}\lambda\, \hat{H}'_I(t + i\hbar\lambda)\right) e^{-\beta \hat{H}_0} \tag{6}$$

and the variation of the quantum average of the operator $\hat{A}$ takes the form of

$$\delta\langle \hat{A} \rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}\{e^{-\beta \hat{H}(t)} \hat{A}\} - \frac{1}{\mathcal{Z}} \mathrm{Tr}\{e^{-\beta \hat{H}_0} \hat{A}\} = \int_0^\beta \mathrm{d}\lambda\, \langle \hat{A} \hat{H}'_I(t + i\hbar\lambda) \rangle_0 = \int_0^\beta \mathrm{d}\lambda \langle \hat{A} e^{-\beta \hat{H}_0} \hat{B} e^{\beta \hat{H}_0} \rangle F(t). \tag{7}$$

The *isothermal response*

$$\chi^T_{AB} \equiv \int_0^\beta \mathrm{d}\lambda\, \langle \hat{A} e^{-\lambda \hat{H}_0} \hat{B} e^{\lambda \hat{H}_0} \rangle \tag{8}$$

can be easily expressed in the energy basis: splitting into the cases when $m \neq n$ and $m = n$ and perform the integral over inverse-temperature, we have

$$\chi^T_{AB} = \sum_{m,n} \int_0^\beta \mathrm{d}\lambda\, e^{-\beta\varepsilon_n} A_{nm} e^{-\lambda\varepsilon_m} B_{mn} e^{-\lambda\varepsilon_n} = \sum_{\substack{m,n \\ m \neq n}} A_{nm} B_{mn} \frac{e^{-\beta\varepsilon_m} - e^{-\beta\varepsilon_n}}{\varepsilon_n - \varepsilon_m} - \beta \sum_n e^{-\beta\varepsilon_n} A_{nn} B_{nn}. \tag{9}$$

B. Adiabatic Response

For the more widely-used adiabatic responses, however, **we have no assumption on the form of the time-dependent density matrix, but can only determine it from the definition**

$$\dot{\hat{\rho}}_S(t) = \frac{1}{i\hbar} [\hat{H}_0 + \hat{H}'(t), \hat{\rho}_S(t)]. \tag{10}$$

Note 1. There are some literatures[2] going that the characteristic of the adiabatic response is that the density matrix can be assumed to stay as the same one in the old equilibrium $\hat{\rho}(t) = e^{-\beta \hat{H}_0}/\mathcal{Z}$ so that all-time dependence of adiabatic responses original from the time-evolved states. Such claim is true at least for linear response (giving the same result), but I am not sure if this is true for non-linear response as well. So I would not address in this way.

To solve the Liuville equation (10), it is helpful to switch into the interaction picture $\hat{\rho}_I(t) \equiv U_0^{-1}(t)\hat{\rho}_S(t)U_0(t) \equiv e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{\rho}_S(t)e^{-\frac{i}{\hbar}\hat{H}_0 t}$, leaving

$$\dot{\hat{\rho}}_I(t) = \frac{1}{i\hbar}U_0^{-1}(t)[\hat{H}'(t), U_0(t)\hat{\rho}_I(t)U_0^{-1}(t)]U_0(t) = \frac{1}{i\hbar}[\hat{H}'_I(t), \hat{\rho}_I(t)] \equiv \hat{L}'_I\hat{\rho}_I(t), \tag{11}$$

where the interaction picture operator $\hat{H}'_I(t) \equiv U_0^{-1}(t)\hat{H}'(t)U_0(t) \equiv e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{H}'(t)e^{-\frac{i}{\hbar}\hat{H}_0 t}$ and we introduce a Liouville operator $\hat{L}'_I\hat{\mathcal{O}} := \frac{1}{i\hbar}[\hat{H}'_I, \hat{\mathcal{O}}]$.

Differential equation (11) can be solved iteratetively: the zeroth-order solution is just the old equilibrium density matirix $\hat{\rho}_I(t_0) \equiv \hat{\rho}_S(t_0) \equiv \rho_0$, the first-order solution is obtained by inserting $\hat{\rho}_0$ into (11), the second order is obtained by inserting the first-order, and so on. Namely, $\hat{\rho}_I(t)$ can be expressed in terms of *Dyson series*

$$\begin{aligned}\hat{\rho}_I(t) &= \hat{\rho}_0 + \frac{1}{i\hbar}\int_{t_0}^{t} \mathrm{d}\tau\, \hat{L}'_I(\tau)\hat{\rho}_0 + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t}\mathrm{d}\tau_2 \int_{t_0}^{\tau_2}\mathrm{d}\tau_1\, \hat{L}'_I(\tau_2)\hat{L}'_I(\tau_1)\hat{\rho}_0 + \cdots . \\ &= \hat{\rho}_0 + \frac{1}{i\hbar}\int_{t_0}^{t} \mathrm{d}\tau\, [\hat{H}'_I(\tau), \hat{\rho}_0] + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t}\mathrm{d}\tau_2 \int_{t_0}^{\tau_2}\mathrm{d}\tau_1\, [\hat{H}'_I(\tau_2), [\hat{H}'_I(\tau_1), \hat{\rho}_0]] + \cdots .\end{aligned} \tag{12}$$

Therefore, the evaluation of (2) can be done in the interaction picture by cycling the trace

$$\begin{aligned}\langle\hat{A}\rangle(t) &\equiv \mathrm{Tr}\{\hat{\rho}_S(t)\hat{A}_S\} = \mathrm{Tr}\{\hat{\rho}_I(t)e^{\frac{i}{\hbar}H_0 t}\hat{A}_S e^{-\frac{i}{\hbar}H_0 t}\} \equiv \mathrm{Tr}\{\rho_I(t)\hat{A}_I(t)\} \\ &= \mathrm{Tr}\{\hat{\rho}_0\hat{A}_I(t)\} + \frac{1}{i\hbar}\int_{t_0}^{t}\mathrm{d}\tau\, \mathrm{Tr}\{[\hat{H}'_I(\tau), \hat{\rho}_0]\hat{A}_I(t)\} + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t}\mathrm{d}\tau_2 \int_{t_0}^{\tau_2}\mathrm{d}\tau_1\, \mathrm{Tr}\Big\{[\hat{H}'_I(\tau_2), [\hat{H}'_I(\tau_1), \hat{\rho}_0]]\hat{A}_I(t)\Big\} + \cdots \\ &= \langle\hat{A}\rangle_0 + \frac{1}{i\hbar}\int_{t_0}^{t}\mathrm{d}\tau\, \langle[\hat{A}_I(t), \hat{H}'_I(\tau)]\rangle_0 + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t}\mathrm{d}\tau_2 \int_{t_0}^{t_2}\mathrm{d}\tau_1\, \langle[[\hat{A}_I(t), \hat{H}'(\tau_2)], \hat{H}'_I(\tau_1)]\rangle_0 + \cdots ,\end{aligned} \tag{13}$$

where the first term (equilibrium average) is vanishing due to Bloch's theorem, and for the other terms identity

$$\mathrm{Tr}\{[A, B]C\} \equiv \mathrm{Tr}\{B[C, A]\}.$$

is used to take out $\hat{\rho}_0$ and recover the quantum average. Without loss of generality, from now on we take $t_0 \to -\infty$.

If $\hat{H}'(t)$ is introduced in the way of (1), the linear response is

$$\delta\langle\hat{A}\rangle^{(1)}(t) = \frac{1}{i\hbar}\int_{-\infty}^{t}\mathrm{d}t'\, \langle[\hat{A}_I(t), \hat{B}_I(t')]\rangle_0 \cdot F(t'), \tag{14}$$

or in terms of *retarded* Green function

$$\delta\langle\hat{A}\rangle^{(1)}(t) = \frac{1}{\hbar}\int_{-\infty}^{\infty}\mathrm{d}t' G^R_{AB}(t, t')F(t'), \quad G^R_{AB}(t, t') = (-i)\theta(t - t')\langle[\hat{A}_I(t), \hat{B}_I(t')]\rangle_0 \tag{15}$$

if the integral (14) is extended to the entire domain of time.

Note 2. Comparing (14) with (7), the most intuitive difference of isothermal response function and adiabatic response function is that the former one does not depend on time! This is resonable since the time-evolution of isothermal processes cannot be perceived by the system (it is always in quasi-equilibrium).

[2] Like Sec. 3.2.1 of [3] and Sec. 8.3 of [2].

Note that by cycling the time arguments of operator $\hat{A}$ and $\hat{B}$ in the retarded Green function, $G^R_{AB}(t,t') \equiv G^R_{AB}(t-t',0)$ so the R.H.S. of (15) has exactly the form of a *convolution*. According to convolution theorem[3], we have, in frequency domain,

$$\delta\langle\hat{A}\rangle(\omega) = \chi_{AB}(\omega)F(\omega), \tag{16}$$

where

$$\chi_{AB}(\omega) \equiv \mathbb{F}\left[\frac{1}{\hbar}G^R_{AB}(t,0)\right] \equiv \lim_{s\to 0^+}\frac{1}{\hbar}G^R_{AB}(\varpi) = \lim_{s\to 0^+}\frac{1}{i\hbar}\int_0^\infty \mathrm{d}t\,\langle[\hat{A}_I(t),B_I]\rangle_0 e^{i\varpi t}, \tag{17}$$

where an infinitesimal positive number is inserted $\varpi \equiv \omega + is$ because the retarded function $G^R_{AB}(\varpi)$ is analytical only on the upper-half plane of the frequency domain [4]. Another thing that needs to keep in mind is that unlike the integration domain in time space in (15), for response function in frequency space the integration is taken within $[0,+\infty)$.

Morever, if the system remains translation-invariant (this happens at least when we concern about only long wavelength physics) $\chi_{AB}(\boldsymbol{r},\boldsymbol{r'};\omega) \equiv \chi_{AB}(\boldsymbol{r}-\boldsymbol{r'};\omega)$, the response function in momentum space

$$\langle\hat{A}\rangle(\boldsymbol{q},\omega) = \chi_{AB}(\boldsymbol{q},\omega)F(\omega)$$

reads

$$\chi_{AB}(\boldsymbol{q},\omega) = \lim_{s\to 0^+}\frac{1}{i\hbar V}\int_0^\infty \mathrm{d}t\,\langle[\hat{A}_I(\boldsymbol{q},t),\hat{B}_I(-\boldsymbol{q},0)]\rangle_0 e^{i\varpi t}. \tag{18}$$

This is because (taking Fourier transformation to second-quantized operators)

$$\begin{aligned}\chi_{AB}(\boldsymbol{r},\boldsymbol{r'};\omega) &\equiv \lim_{s\to 0^+}\frac{1}{i\hbar V}\int_0^\infty \mathrm{d}t \sum_{\boldsymbol{k},\boldsymbol{k'}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}e^{i\boldsymbol{k'}\cdot\boldsymbol{r'}}\langle[\hat{A}_I(\boldsymbol{k},t),\hat{B}_I(\boldsymbol{k'},0)]\rangle_0 e^{i\varpi t} \\ &\equiv \lim_{s\to 0^+}\frac{1}{i\hbar V}\int_0^\infty \mathrm{d}t \sum_{\boldsymbol{k},\boldsymbol{k'}} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r'})}e^{i(\boldsymbol{k}+\boldsymbol{k'})\cdot\boldsymbol{r'}}\langle[\hat{A}_I(\boldsymbol{k},t),\hat{B}_I(\boldsymbol{k'},0)]\rangle_0 e^{i\varpi t}.\end{aligned}$$

is a function of $\boldsymbol{r}-\boldsymbol{r'}$ if and only if $\boldsymbol{k}+\boldsymbol{k'} \equiv 0$.

In the energy eigenstate, the response function takes the form of

$$\begin{aligned}\chi_{AB}(\omega) &= \lim_{s\to 0^+}\frac{1}{i\hbar}\int_0^\infty \mathrm{d}\tau \sum_{m,n}(e^{-\beta\varepsilon_n}-e^{-\beta\varepsilon_m})A_{nm}B_{mn}e^{\frac{i}{\hbar}(\varepsilon_n-\varepsilon_m)\tau}e^{i(\omega+is)\tau} \\ &= \lim_{s\to 0^+}\sum_{m,n}\frac{e^{-\beta\varepsilon_n}-e^{-\beta\varepsilon_m}}{\hbar\omega+\varepsilon_n-\varepsilon_m+is}A_{nm}B_{mn}.\end{aligned} \tag{19}$$

Comparing with (9), this time the denomenator is always well-defined so we do not have to split into the diagonal and off-diagonal parts before performing the integral.

Note 3. The off-diagonal part of isothermal response (9) is clear to coincides with the static limit of adiabatic response $\lim_{\omega\to 0}\chi_{AB}(\omega)$, while the diagonal part of (9) is exclusive. Anyway **in general isothermal responses do not have to be the same as the static limit of adiabatic responses — they are two quite different things.**

C. Example: Adiabatic Response of Charge Current

In this section, we will consider the electric current driven by an external electric field. In general such electric field depends on both scalar and vector potentials

$$\boldsymbol{E}(\boldsymbol{r},t) \equiv -\nabla\phi - \frac{\partial\boldsymbol{A}}{\partial t}.$$

[3] The Fourier transformation of a convolution of two functions is the multiplication of each's Fourier transformation.

Under the minimal coupling with external vector potential, the general continuum Hamiltonian with impurity potentials V_{imp} and interacting terms U (like four-fermion Coulomb interaction)

$$H = \int \mathrm{d}\boldsymbol{r}\, \psi^\dagger(\boldsymbol{r},t)\Big(-\frac{\hbar^2}{2m}\nabla^2 - \mu + V_{\text{imp}}(\boldsymbol{r})\Big)\psi(\boldsymbol{r},t) + U \tag{20}$$

becomes (we work in SI units so $A^\mu = (\frac{\phi}{c}, \boldsymbol{A})$)

$$\begin{aligned} H[A_\mu] &= \int \mathrm{d}\boldsymbol{r}\, \psi^\dagger(\boldsymbol{r},t)\left(\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\boldsymbol{A}(\boldsymbol{r},t)\right)^2 + \frac{q}{c}\phi(\boldsymbol{r},t) - \mu + V_{\text{imp}}\right)\psi(\boldsymbol{r},t) + U \\ &= H[0] - \frac{q\hbar}{2im}\int \mathrm{d}\boldsymbol{r}\left(\psi^\dagger(\boldsymbol{r},t)\boldsymbol{A}(\boldsymbol{r},t)\cdot\nabla\psi(\boldsymbol{r},t) - \nabla\psi^\dagger(\boldsymbol{r},t)\cdot\boldsymbol{A}(\boldsymbol{r},t)\psi(\boldsymbol{r},t)\right) \\ &\quad + \frac{q}{c}\int \mathrm{d}\boldsymbol{r}\,\psi^\dagger(\boldsymbol{r},t)\phi(\boldsymbol{r},t)\psi(\boldsymbol{r},t) + \frac{q^2}{2m}\int \mathrm{d}\boldsymbol{r}\,\psi^\dagger(\boldsymbol{r})\boldsymbol{A}(\boldsymbol{r},t)^2\psi(\boldsymbol{r}). \end{aligned} \tag{21}$$

By definition of charge current $J_\mu \equiv \dfrac{\delta S[A_\mu]}{\delta A_\mu}$, we get, in the metric $\mathrm{d}s^2 = -c^2\,\mathrm{d}t^2 + \mathrm{d}\boldsymbol{x}^2$

$$H[A_\mu] = H[0] - \boldsymbol{J}\cdot\boldsymbol{A} + A_0 J^0, \tag{22}$$

where

$$J^0(\boldsymbol{r},t) \equiv \frac{\delta H[A_\mu]}{\delta A_0} = \frac{\delta H}{\delta(\phi/c)} = q\psi^\dagger(\boldsymbol{r},t)\psi(\boldsymbol{r},t), \tag{23}$$

$$J^i(\boldsymbol{r},t) \equiv -\frac{\delta H[A_\mu]}{\delta A_i} = \frac{q\hbar}{2im}\Big(\psi^\dagger(\boldsymbol{r},t)(\partial^i\psi(\boldsymbol{r},t)) - (\partial^i\psi^\dagger(\boldsymbol{r},t))\psi(\boldsymbol{r},t)\Big) - \frac{q^2}{m}\psi^\dagger(\boldsymbol{r},t)A^i(\boldsymbol{r},t)\psi(\boldsymbol{r},t) =: J^{P,i}(\boldsymbol{r},t) + J^{D,i}(\boldsymbol{r},t), \tag{24}$$

where we introduce the *paramagnetic* part $\boldsymbol{J}^P$ (of order $\mathcal{O}((A_\mu)^0)$) and *diamagnetic* part $\boldsymbol{J}^D$ (of order $\mathcal{O}(A_\mu)$) of the charge current.

Keeping track of merely *linear* coupling of the Hamiltonian, i.e., separating the contribution of paramagnetic and diamagnetic parts in consideration of adabatic linear response, we can make use of the general result of adabatic linear response to write down the quantum average of total current at time t as

$$\begin{aligned} \langle J_\alpha(\boldsymbol{r},t)\rangle^{(1)} &= \langle J^P_\alpha(\boldsymbol{r},t)\rangle^{(1)} - \frac{q^2}{m}\langle\psi^\dagger(\boldsymbol{r},t)\psi(\boldsymbol{r},t)\rangle^{(0)}A_\alpha(\boldsymbol{r},t)(1-\delta_{\alpha 0}) \\ &= \frac{-1}{i\hbar}\int_{-\infty}^{0}\mathrm{d}t'\int\mathrm{d}\boldsymbol{r'}\,\langle[J^P_{\alpha,I}(\boldsymbol{r},t), J^P_{\beta,I}(\boldsymbol{r'},t')]\rangle_0 A_\beta(\boldsymbol{r'},t) - \frac{q^2}{m}n_0(1-\delta_{\alpha 0})A_\alpha(\boldsymbol{r},t) \\ &= \int\mathrm{d}\boldsymbol{r'}\int\mathrm{d}t'\left\{\frac{-1}{i\hbar}\theta(t-t')\langle[J^P_{\alpha,I}(\boldsymbol{r},t), J^P_{\beta,I}(\boldsymbol{r'},t')]\rangle_0 - \frac{q^2}{m}n_0\delta_{\alpha\beta}(1-\delta_{\alpha 0})\delta(\boldsymbol{r}-\boldsymbol{r'})\delta(t-t') + \right\}A^\beta(\boldsymbol{r'},t'), \end{aligned} \tag{25}$$

where in the first line we take the zeroth-order approximation for the diamagnetic part so that the particle density remains to be spacetime-independent $n(\boldsymbol{r},t) \equiv \langle\psi^\dagger(\boldsymbol{r},t)\psi(\boldsymbol{r},t)\rangle = n_0$ as the one in the old equilibrium (note that spacetime-fluctuation is all brought by the external stimulus). The extra minus sign for the adiabatic response of paramagnetic currents in the second line comes from the negative coupling with external vector potential (see (22)).

Since the expression in the curly brace in (25) is still a function of $t-t'$, then convolution theorem tells

$$\langle J_\alpha(\boldsymbol{r},\omega)\rangle^{(1)} = \int\mathrm{d}\boldsymbol{r'}\sigma_{\alpha\beta}(\boldsymbol{r},\boldsymbol{r'};\omega)E_\beta(\boldsymbol{r'},\omega), \tag{26}$$

with the conductivity matrix

$$\sigma_{\alpha\beta}(\boldsymbol{r},\boldsymbol{r'};\omega) = \frac{-1}{i\omega}\left[\chi^P_{\alpha\beta} + \frac{q^2}{m}n_0\delta_{\alpha\beta}(1-\delta_{\alpha 0})\delta(\boldsymbol{r}-\boldsymbol{r'})\right], \quad \chi^P_{\alpha\beta} \equiv \lim_{s\to 0^+}\frac{1}{i\hbar}\int_0^\infty\mathrm{d}t\,\langle[J^P_{\alpha,I}(\boldsymbol{r},t), J^P_{\beta,I}(\boldsymbol{r'},0)]\rangle_0 e^{i\varpi t}, \tag{27}$$

where we take the gauge $\phi = 0$ and express the electric field in terms of the vector potential $\boldsymbol{E}(\omega) = i\omega\boldsymbol{A}(\omega)$ in the frequency domain. Such step of gauge fixing can be done at the very beginning to simplify the form of the current operator (by setting $J^0 = 0$).

Anyway, if the material is furthermore homogeneous $\sigma_{\alpha\beta}(\boldsymbol{r},\boldsymbol{r'};\omega)\equiv\sigma_{\alpha\beta}(\boldsymbol{r}-\boldsymbol{r'};\omega)$, we have

$$\langle J_\alpha(\boldsymbol{q},\omega)\rangle^{(1)}=\frac{-1}{i\omega}\left\{\chi^P_{\alpha\beta}(\boldsymbol{q},\omega)+\frac{q^2}{m}n_0\delta_{\alpha\beta}(1-\delta_{\alpha 0})\right\}E^\beta(\boldsymbol{q},\omega), \tag{28}$$

with the paramagnetic response function

$$\chi^P_{\alpha\beta}(\boldsymbol{q},\omega)\equiv\lim_{s\to 0^+}\frac{1}{i\hbar V}\int_0^\infty \mathrm{d}t\,\langle[J^P_{\alpha,I}(\boldsymbol{q},t),J^P_{\beta,I}(-\boldsymbol{q},0)]\rangle_0 e^{i\varpi t}. \tag{29}$$

D. Drude Formula: Cancellation of Static Diamagnetic Response in Metals

DC limit (*slow limit*) of conductivity is taken in the order of

$$\sigma^{\mathrm{DC}}_{\alpha\beta}:=\lim_{\omega\to 0}\lim_{\boldsymbol{q}\to 0}\sigma_{\alpha\beta}(\boldsymbol{q},\omega). \tag{30}$$

A first glance of (28) tells that there is a divergence provided $\chi_{\alpha\beta}(\boldsymbol{q},\omega)$ was analytic, conflicting with the physical observations for large amounts of materials. However, we will show below that for band metals (where only intra-band processes dominate) such divergence is exactly cancelled by the term containing in the paramagnetic part. Denoting $I_{\alpha\beta}(t)\equiv\langle\hat{J}_\alpha(t)\hat{J}_\beta\rangle_0$ and expressiong the many-body current operator as a summation of single-particle current operator $\hat{J}_\alpha=\sum_{\mu\nu}J^{(1)}_\alpha\hat{a}^\dagger_\mu\hat{a}_\nu$, we have (only *connected* diagram contributes[4])

$$\begin{aligned}
I_{\alpha\beta}(t)-I_{\beta\alpha}(t)&=\sum_{1,2,3,4}\left\langle\langle 1|J^{(1)}_\alpha|2\rangle a^\dagger_1(t)a_2(t)\langle 3|J^{(1)}_\beta|4\rangle a^\dagger_3 a_4\right\rangle-(\alpha\leftrightarrow\beta)\\
&=\sum_{1,2,3,4}\langle 1|J^{(1)}_\alpha|2\rangle\langle 3|J^{(1)}_\beta|4\rangle\left\langle 4\left|\frac{e^{\frac{i}{\hbar}ht}}{1+e^{\beta h}}\right|1\right\rangle\left\langle 2\left|\frac{e^{-\frac{i}{\hbar}ht}}{1+e^{-\beta h}}\right|3\right\rangle-(\alpha\leftrightarrow\beta)\\
&=\sum_{m,n}e^{\frac{i}{\hbar}(\varepsilon_m-\varepsilon_n)t}\langle m|J^{(1)}_\alpha|n\rangle\langle n|J^{(1)}_\beta|m\rangle\left[\frac{1}{1+e^{\beta\varepsilon_m}}\frac{e^{\beta\varepsilon_n}}{1+e^{\beta\varepsilon_n}}-\frac{e^{\beta\varepsilon_m}}{1+e^{\beta\varepsilon_m}}\frac{1}{1+e^{\beta\varepsilon_n}}\right]\\
&=\sum_{m,n}e^{\frac{i}{\hbar}(\varepsilon_m-\varepsilon_n)t}\langle m|J^{(1)}_\alpha|n\rangle\langle n|J^{(1)}_\beta|m\rangle(f_m-f_n),
\end{aligned}$$

where in the second line we use, for free fermion $\hat{H}_0=\sum_{\alpha\beta}c^\dagger_\alpha h_{\alpha\beta}c_\beta$,

$$\begin{aligned}
\langle c^\dagger_\alpha(t)c_\beta\rangle&\equiv\left\langle e^{-\frac{i}{\hbar}\hat{H}_0 t}c^\dagger_\alpha e^{\frac{i}{\hbar}\hat{H}_0 t}c_\beta\right\rangle=\left\langle\left(c^\dagger_\alpha-i\frac{t}{\hbar}[\hat{H}_0,c^\dagger_\alpha]+\frac{t^2}{(2\hbar)!}[\hat{H}_0,[\hat{H}_0,c^\dagger_\alpha]]+\cdots\right)c_\beta\right\rangle\\
&=\sum_\gamma\left(e^{\frac{i}{\hbar}ht}\right)_{\gamma\alpha}\langle c^\dagger_\gamma c_\beta\rangle=\left\langle\beta\left|\frac{e^{\frac{i}{\hbar}ht}}{1+e^{\beta h}}\right|\alpha\right\rangle,
\end{aligned}$$

and similarly

$$\langle c_\alpha(t)c^\dagger_\beta\rangle=\sum_\gamma\left(e^{-\frac{i}{\hbar}ht}\right)_{\alpha\gamma}\langle c_\gamma c^\dagger_\beta\rangle=\left\langle\alpha\left|\frac{e^{-\frac{i}{\hbar}ht}}{1+e^{\beta h}}\right|\beta\right\rangle,$$

with h the first-quantized (single-particle) Hamiltonian. Thus by integrating out the time, the paramagnetic current-current response function reads

$$\chi^P_{\alpha\beta}(\boldsymbol{q},\omega)=\lim_{s\to 0^+}\frac{1}{i\hbar V}\int_0^\infty\mathrm{d}t\,(I_{\alpha\beta}(t)-I_{\beta\alpha(t)})e^{i\varpi t}=\lim_{s\to 0^+}\frac{1}{V}\sum_{m,n}(f_m-f_n)\frac{\langle m|J^{(1)}_\alpha(\boldsymbol{q})|n\rangle\langle n|J^{(1)}_\beta(-\boldsymbol{q})|m\rangle}{\hbar\varpi+\varepsilon_m-\varepsilon_n}. \tag{31}$$

---

[4] This fact is much clearer in path-integral formalism, see, for example, [5].

Re-expression the second-quantized paramagnetic current operator (24) as

$$J^P_\alpha = \sum_{\boldsymbol{r},\boldsymbol{r'}} \langle\psi|\boldsymbol{r}\rangle \frac{q}{2m}\Big(\langle\boldsymbol{r}|(-i\hbar\nabla')\boldsymbol{r'}\rangle + \langle(-i\hbar\nabla)\boldsymbol{r}|\boldsymbol{r'}\rangle\Big)\langle\boldsymbol{r'}|\psi\rangle,$$

we can immediately wirte down the single-particle current operator $\hat{J}_\alpha = \sum_{\mu\nu}\langle\mu|J^{(1)}_\alpha|\nu\rangle\psi^\dagger_\mu\psi_\nu$ for the i-th particle under the coordinate representation

$$J^{(1)}_\alpha(\boldsymbol{r}) = \frac{q}{2m}(\hat{p}_{i,\alpha}\delta(\boldsymbol{r}-\hat{\boldsymbol{r}}_i) + \delta(\boldsymbol{r}-\hat{\boldsymbol{r}}_i)\hat{p}_{i,\alpha}), \tag{32}$$

or in momentum representation

$$J^{(1)}_\alpha(\boldsymbol{q}) = \frac{q}{2m}(\hat{p}_{i,\alpha}e^{i\boldsymbol{q}\cdot\hat{\boldsymbol{r}}_i} + e^{i\boldsymbol{q}\cdot\hat{\boldsymbol{r}}_i}\hat{p}_{i,\alpha}). \tag{33}$$

Separating the denomenator (31) into two parts, we get

$$\chi^P_{\alpha\beta}(\boldsymbol{q},\omega) = \lim_{s\to0^+}\frac{q^2}{4m^2V}\sum_{m,n}(f_m-f_n)\frac{\langle m|p_\alpha e^{i\boldsymbol{q}\cdot\boldsymbol{r}} + e^{i\boldsymbol{q}\cdot\boldsymbol{r}}p_\alpha|n\rangle\langle n|p_\beta e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} + e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}p_\beta|m\rangle}{\hbar\varpi+\varepsilon_{mn}} \tag{34}$$

$$\equiv \lim_{s\to0^+}\frac{q^2}{m^2V}\sum_{m,n}(f_m-f_n)\langle m|p_\alpha e^{i\boldsymbol{q}\cdot\boldsymbol{r}} + e^{i\boldsymbol{q}\cdot\boldsymbol{r}}p_\alpha|n\rangle\langle n|p_\beta e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} + e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}p_\beta|m\rangle|\left[\frac{1}{\varepsilon_{mn}}\left(1-\frac{\hbar\varpi}{\hbar\varpi+\varepsilon_{mn}}\right)\right]. \tag{35}$$

It is clear that with the help of *f-sum rule* (the proof is given in the appendix)

$$\sum_{m,n}(f_m-f_n)\frac{\langle m|p_\alpha|n\rangle\langle n|p_\beta|m\rangle}{\varepsilon_{mn}} = -mN\delta_{\alpha\beta}, \tag{36}$$

the first part of response function

$$\chi^{P,\text{1st}}_{\alpha\beta}(\boldsymbol{q}\to\boldsymbol{0},\omega) \equiv \lim_{s\to0^+}\frac{q^2}{4m^2V}\sum_{m,n}(f_m-f_n)\frac{\langle m|p_\alpha e^{i\boldsymbol{q}\cdot\boldsymbol{r}} + e^{i\boldsymbol{q}\cdot\boldsymbol{r}}p_\alpha|n\rangle\langle n|p_\beta e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} + e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}p_\beta|m\rangle}{\varepsilon_m-\varepsilon_n}$$

$$= \lim_{s\to0^+}\frac{q^2}{m^2V}\sum_{m,n}(f_m-f_n)\frac{\langle m|p_\alpha|n\rangle\langle n|p_\beta|m\rangle}{\varepsilon_m-\varepsilon_n} = -\frac{q^2n}{m}\delta_{\alpha\beta} \tag{37}$$

cancel exactly with the the diamagnetic part in the conductivity tensor (27) in the uniform limit $\boldsymbol{q}\to\boldsymbol{0}$ (when we can safely omit the exponential $e^{i\boldsymbol{q}\cdot\boldsymbol{r}}$ for small $\boldsymbol{q}$), leaving only

$$\sigma_{\alpha\beta}(\boldsymbol{q}\to\boldsymbol{0},\omega) = \frac{-1}{i\omega}\chi^{P,\text{2nd}}_{\alpha\beta} = \lim_{s\to0^+}\frac{\hbar q^2}{i4m^2V}\sum_{m,n}(f_m-f_n)\frac{\langle m|p_\alpha e^{i\boldsymbol{q}\cdot\boldsymbol{r}} + e^{i\boldsymbol{q}\cdot\boldsymbol{r}}p_\alpha|n\rangle\langle n|p_\beta e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} + e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}p_\beta|m\rangle}{\varepsilon_{mn}(\hbar\varpi+\varepsilon_{mn})}. \tag{38}$$

The left task is to evaluate the quantum average in the Bloch states $|n\boldsymbol{k}\rangle$. For metals where intra-band processes dominate, we get (we will keep the exponential here since the zeroth-order is vanishing)

$$\sigma^{\text{intra}}_{\alpha\beta}(\boldsymbol{q},\omega) = \lim_{s\to0^+}\frac{\hbar q^2}{i4m^2V}\sum_n\sum_s\sum_{\boldsymbol{k},\boldsymbol{k'}}(f_{n\boldsymbol{k}}-f_{n\boldsymbol{k'}})\frac{\langle n\boldsymbol{k}|p_\alpha e^{i\boldsymbol{q}\cdot\boldsymbol{r}} + e^{i\boldsymbol{q}\cdot\boldsymbol{r}}p_\alpha|n\boldsymbol{k'}\rangle\langle n\boldsymbol{k'}|e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}p_\beta + e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}p_\beta|n\boldsymbol{k}\rangle}{(\varepsilon_{n\boldsymbol{k}}-\varepsilon_{n\boldsymbol{k'}})(\hbar\omega+is+\varepsilon_{n\boldsymbol{k}}-\varepsilon_{n\boldsymbol{k'}})}.$$

Using the definition of Block states $e^{i\boldsymbol{q}\cdot\boldsymbol{r}}|n\boldsymbol{k}\rangle \equiv e^{i\boldsymbol{q}\cdot\boldsymbol{r}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u_n(\boldsymbol{r}) = |n,\boldsymbol{k}+\boldsymbol{q}\rangle$, and for example $\langle n\boldsymbol{k}p_\alpha e^{i\boldsymbol{q}\cdot\boldsymbol{r}}|n\boldsymbol{k'}\rangle = \delta_{\boldsymbol{k},\boldsymbol{k'}+\boldsymbol{q}}m\langle n\boldsymbol{k}|v_\alpha|n\boldsymbol{k}\rangle$, we get

$$\sigma^{\text{intra}}_{\alpha\beta}(\boldsymbol{q},\omega) = \lim_{s\to0^+}\frac{2\hbar q^2}{iV}\sum_{n,\boldsymbol{k}}\frac{f_{n,\boldsymbol{k}}-f_{n,\boldsymbol{k}-\boldsymbol{q}}}{\varepsilon_{n,\boldsymbol{k}}-\varepsilon_{n,\boldsymbol{k'}-\boldsymbol{q}}}\frac{\langle n\boldsymbol{k}|v_\alpha|n\boldsymbol{k}\rangle\langle n\boldsymbol{k}|v_\beta|n\boldsymbol{k}\rangle}{\hbar\omega+is+\varepsilon_{n,\boldsymbol{k}}-\varepsilon_{n,\boldsymbol{k}-\boldsymbol{q}}}. \tag{39}$$

For $|\boldsymbol{q}\ll1|$, and quadratic dispersion, we get

$$\sigma^{\text{intra}}_{\alpha\beta}(\boldsymbol{q}\to\boldsymbol{0},\omega) \simeq \lim_{s\to0^+}\frac{2\hbar q^2}{iV}\sum_{n,\boldsymbol{k}}\left(\frac{\partial f_{n\boldsymbol{k}}}{\partial\varepsilon_{n\boldsymbol{k}}}\right)\frac{\langle n\boldsymbol{k}|v_\alpha|n\boldsymbol{k}\rangle\langle n\boldsymbol{k}|v_\beta|n\boldsymbol{k}\rangle}{\hbar\omega+is+\frac{\hbar^2}{m}\boldsymbol{k}\cdot\boldsymbol{q}}. \tag{40}$$

Equation (40) agrees with the result derived from the Boltzmann equation (if we identify the relaxation time $\tau \sim \hbar/s$).

If we further drop the linear-$\boldsymbol{q}$ term in (40), we get ($\eta \equiv s/\hbar \ll 1$)

$$\sigma_{\alpha\beta}^{\text{intra}}(\boldsymbol{q}\to\boldsymbol{0},\omega) \simeq \lim_{\eta\to 0^+}\frac{i}{\omega+i\eta}\times\frac{2q^2}{V}\sum_{n,\boldsymbol{k}}\left(-\frac{\partial f_{n\boldsymbol{k}}}{\partial\varepsilon_{n\boldsymbol{k}}}\right)\langle n\boldsymbol{k}|v_\alpha|n\boldsymbol{k}\rangle\langle n\boldsymbol{k}|v_\beta|n\boldsymbol{k}\rangle \equiv \lim_{\eta\to 0^+}\frac{i}{\omega+i\eta}\mathcal{D}_{\alpha\beta}, \tag{41}$$

where $\mathcal{D}_{\alpha\beta}$ is the *Drude weight*. Clearly the real part of the uniform limit of the conductivity tensor takes the form of Dirac delta function

$$\mathcal{R}e\,\sigma_{\alpha\beta}^{\text{intra}}(\boldsymbol{q}\to\boldsymbol{0},\omega) = \lim_{\eta\to 0^+}\frac{1}{\pi}\frac{\eta}{\omega^2+\eta^2}\times\pi\mathcal{D}_{\alpha\beta} = \delta(\omega)\pi\mathcal{D}. \tag{42}$$

In modern transport theory, we *define* the Drude weight as

Definition 1. (Drude-Weight)

$$\mathcal{D}_{\alpha\beta} := \lim_{\omega\to 0}\omega\,\mathcal{I}m\,\sigma_{\alpha\beta}(\omega). \tag{43}$$

Conversely, for (perfectly diamagnetic) superconductors, it is the paramagnetic part that vanishes in the DC limit, keeping the imaginary divergenent diamagnetic part. The detailed calculation of BCS superconductors can be found in Patrick Lee's lecture notes `https://ocw.mit.edu/courses/physics/8-512-theory-of-solids-ii-spring-2009/lecture-notes/MIT8_512s09_lec09.pdf`.

II. OTHER EQUIVALENT FORMS OF KUBO FORMULA

A. Kubo's Identities and Canonical Kubo Pair

In Kubo's original paper [6], he proved an identity:

Claim 1. (Kubo's First Identity) For any time-dependent operator (in interaction picture, for instance (for future use)) $\hat{X}_I(t) \equiv e^{\frac{i}{\hbar}\hat{H}_0(t-t_0)}\hat{X}_S(t_0)e^{-\frac{i}{\hbar}\hat{H}_0(t-t_0)}$ and density matrix $\hat{\rho}_0 = e^{-\beta\hat{H}_0}/\mathcal{Z}$, we have

$$\frac{1}{i\hbar}[\hat{X}_I(t),\hat{\rho}_0] \equiv -\hat{\rho}_0\int_0^\beta \mathrm{d}\lambda\,\dot{\hat{X}}_I(t-i\lambda\hbar), \quad \text{where} \quad \dot{\hat{X}}_I(t) \equiv \frac{1}{i\hbar}[\hat{X}_I(t),\hat{H}_0] \tag{44}$$

▷ Proving by direct check:

$$\begin{aligned}\text{RHS} &= -\hat{\rho}_0\int_0^\beta \mathrm{d}\lambda\,\frac{1}{i\hbar}[\hat{X}_I(t-i\lambda\hbar),\hat{H}_0] = -\frac{1}{i\hbar}\hat{\rho}_0\int_0^\beta\mathrm{d}\lambda\,\left[e^{\lambda\hat{H}_0}\hat{X}_I(t)e^{-\lambda\hat{H}_0},\hat{H}_0\right] = -\frac{1}{i\hbar}\hat{\rho}_0\int_0^\beta\mathrm{d}\lambda\,e^{\lambda\hat{H}_0}[\hat{X}_I(t),\hat{H}_0]e^{-\lambda\hat{H}_0}\\ &\equiv \frac{1}{i\hbar}\hat{\rho}_0\int_0^\beta\mathrm{d}\lambda\,\frac{\mathrm{d}}{\mathrm{d}\lambda}\left[e^{\lambda\hat{H}_0}\hat{X}_I(t)e^{-\lambda\hat{H}_0}\right] = \frac{1}{i\hbar}\left(\hat{\rho}_0e^{\beta\hat{H}_0}\hat{X}_I(t)e^{-\beta\hat{H}_0}-\hat{\rho}_0\hat{X}_I(t)\right) = \frac{1}{i\hbar}[\hat{X}_I(t),\hat{\rho}_0].\end{aligned}$$

□

If we introduce the *canonical Kubo pair* [7] (still for operators in interaction picture, for instance (for future use))

$$\langle\langle A;B\rangle\rangle := \frac{1}{\beta}\int_0^\beta\mathrm{d}\lambda\,\langle A_I(-i\hbar\lambda)B_I(0)\rangle_0. \tag{45}$$

then a neat form of *Kubo's second identity* can be immediately obtained

Corollary 1. (Kubo's Second Identity)

$$\beta\langle\langle[H_0,B];A(t)\rangle\rangle \equiv \langle[A_I(t),B_I(0)]\rangle_0. \tag{46}$$

▷ By Kubo's first identity (44), we have

$$\begin{aligned}\text{LHS} &= i\hbar\int_0^\beta\mathrm{d}\lambda\,\langle-\dot{\hat{B}}_I(-i\lambda\hbar)\hat{A}_I(t)\rangle = \mathrm{Tr}\left\{i\hbar\left(-\hat{\rho}\int_0^\beta\mathrm{d}\lambda\,\dot{\hat{B}}_I(-i\lambda\hbar)\right)\hat{A}_I\right\}\\ &= \mathrm{Tr}\{[\hat{B}(0),\hat{\rho}_0]\hat{A}_I(t)\} = \mathrm{Tr}\{\hat{\rho}_0[\hat{A}_I(t),\hat{B}_I(0)]\} = \text{RHS}.\end{aligned}$$

□

B. Equivalent Forms of Kubo Formula

There are many forms of Kubo formula used in literatures. In this section, we will try to derive all of them.

Applying Kubo's second identity to the general adiabatic response in frequency domain (17), the response function can be re-written as

$$\begin{aligned}\chi_{AB}(\omega) &= \lim_{s\to 0^+} \frac{1}{i\hbar}\int_0^{+\infty} \mathrm{d}t\,\langle[\hat{A}_I(t),\hat{B}_I(0)]\rangle e^{i\varpi t} = \lim_{s\to 0^+}\frac{\beta}{i\hbar}\int_0^{+\infty}\mathrm{d}t\,\langle\langle[H_0,B];A(t)\rangle\rangle e^{i\varpi t}\\ &\equiv \lim_{s\to 0^+}\frac{\beta}{i\hbar}\int_0^{+\infty}\mathrm{d}t\,e^{i\varpi t}\int_0^{\beta}\mathrm{d}\lambda\,\langle[H_0,B_I(-i\hbar\lambda)]A_I(t)\rangle.\end{aligned} \tag{47}$$

Particularly, for charge current response, if external sources is introduced in the way of Luttinger [1], i.e., $H_0 \mapsto H = H_0 + Q(\varphi,t)e^{i\omega t}$, or $\hat{B}(t)\equiv Q(\varphi,t)$, we have, the charge conductivity (in the language of Kapustin [8])

$$\begin{aligned}\sigma_{\gamma\varphi}(\omega) &= \lim_{s\to 0^+}\frac{\beta}{i\hbar}\int_0^{+\infty}\mathrm{d}t\,\langle\langle[H_0,Q(\varphi)];J(\delta\gamma,t)\rangle\rangle e^{i\varpi t}\\ &= \lim_{s\to 0^+}\beta\int_0^{+\infty}\mathrm{d}t\,\langle\langle J(\delta\varphi);J(\delta\gamma,t)\rangle\rangle e^{i\varpi t} \equiv \lim_{s\to 0^+}\beta\int_0^{+\infty}\mathrm{d}t\,\langle\langle J(\delta\gamma,t);J(\delta\varphi)\rangle\rangle e^{i\varpi t},\end{aligned} \tag{48}$$

where charge conservation law

$$\frac{\mathrm{d}Q(\varphi)}{\mathrm{d}t} = -(\partial J)(\varphi) \equiv J(\delta\varphi) \tag{49}$$

and symmetric properties of Kubo canonical pairs $\langle\langle A;B\rangle\rangle \equiv \langle B;A\rangle\rangle$ are used. For example, for static response $\omega = 0$, (48) coincides with Eq. (37) in [8].

C. Equivalence bewteen Conductivity Obtained by Coupling with Vector Potentials and Electrical Potentials

Electrical conductivities are separated by paramagnetic part and diamagnetic part as we have shown before. They are derived by coupling the system to external vector potentials (with the gauge choice $\varphi = 0$). Is such prescription the same as that proposed by Luttinger? In this section, we will anwser this question.

Using the fact that the retarded Green function (and its descendents by Kubo's identities) is analytic on the upper half plane, we can re-written (48) in another form that

$$\begin{aligned}\sigma_{\gamma\varphi}(\omega) &= \lim_{s\to 0^+}\int_0^{\infty}\mathrm{d}t\,e^{i\varpi t}\int_0^{\beta}\mathrm{d}\lambda\,\langle J(\delta\gamma,t-i\hbar\lambda)J(\delta\varphi)\rangle = \frac{-1}{i\hbar}\lim_{s\to 0^+}\int_0^{\infty}\mathrm{d}t\,e^{i\varpi t}\int_t^{t-i\hbar\beta}\mathrm{d}\tau\,\langle J(\delta\gamma,\tau)J(\delta\varphi)\rangle\\ &= \frac{-1}{i\hbar}\lim_{s\to 0^+}\int_0^{\infty}\mathrm{d}t\,e^{i\varpi t}\int_t^{\infty}\mathrm{d}t'\Big(\langle J(\delta\gamma,t')J(\delta\varphi)\rangle - \langle J(\delta\gamma,t-i\hbar\beta)J(\delta\varphi)\rangle\Big)\\ &= \frac{-1}{i\hbar}\lim_{s\to 0^+}\int_0^{\infty}\mathrm{d}t\,e^{i\varpi t}\int_t^{\infty}\mathrm{d}t'\ \mathrm{Tr}\Big\{\rho_0\Big(J(\delta\gamma,t')J(\delta\varphi) - e^{\beta H_0}J(\delta\gamma,t)e^{-\beta H_0}J(\delta\varphi)\Big)\Big\}\\ &= \frac{-1}{i\hbar}\lim_{s\to 0^+}\int_0^{\infty}\mathrm{d}t\,e^{i\varpi t}\int_t^{\infty}\mathrm{d}t'\ \mathrm{Tr}\Big\{\rho_0\Big(J(\delta\gamma,t')J(\delta\varphi) - J(\delta\varphi)J(\delta\gamma,t)\Big)\Big\}\\ &= \frac{-1}{i\hbar}\lim_{s\to 0^+}\int_0^{\infty}\mathrm{d}t\,e^{i\varpi t}\int_t^{\infty}\mathrm{d}t'\,\langle[J(\delta\gamma,t'),J(\delta\varphi)]\rangle.\end{aligned} \tag{50}$$

Integration by parts, we get

$$\begin{aligned}\sigma_{\gamma\varphi}(\omega) &= \lim_{s\to 0^+}\frac{1}{\hbar\varpi}\left\{e^{i\varpi t}\int_t^{\infty}\mathrm{d}t'\,\langle[J(\delta\gamma,t'),J(\delta\varphi)]\rangle\Big|_0^{\infty} - \int_0^{\infty}\mathrm{d}t\,e^{i\varpi t}\frac{\mathrm{d}}{\mathrm{d}t}\int_t^{\infty}\mathrm{d}t'\,\langle[J(\delta\gamma,t'),J(\delta\varphi)]\rangle\right\}\\ &= \lim_{s\to 0^+}\frac{-1}{i\varpi}\left\{\frac{-1}{i\hbar}\int_0^{\infty}\mathrm{d}t\,\langle[J(\delta\gamma,t),J(\delta\varphi)]\rangle + \frac{1}{i\hbar}\int_0^{\infty}\mathrm{d}t\,e^{i\varpi t}\langle[J(\delta\gamma,t),J(\delta\varphi)]\rangle\right\}\\ &\equiv \lim_{s\to 0^+}\frac{-1}{i\varpi}(\chi_{\gamma\varphi}(\omega) - \chi_{\gamma\varphi}(0))\end{aligned} \tag{51}$$

with the familiar response function

$$\chi_{\gamma\varphi}(\omega) \equiv \lim_{s\to 0^+} \frac{1}{i\hbar} \int_0^\infty \mathrm{d}t\, e^{i\varpi t} \langle [J(\delta\gamma, t), J(\delta\varphi)] \rangle \tag{52}$$

To show that (51) matches perfectly with the conductivity tensor (27) we have derived before, we have to show that $-\chi_{\gamma\varphi}(0)$ is nothing but the diamagnetic part of contribution. In fact, by taking similar steps as (31), we get

$$-\chi_{\gamma\varphi}(0) = \cdots = -\sum_{m,n} (f_m - f_n) \frac{\langle J_\gamma^{(1)}(\boldsymbol{q})|n\rangle\langle n|J_\varphi^{(1)}(-\boldsymbol{q})|m\rangle}{\varepsilon_m - \varepsilon_n}. \tag{53}$$

Again by inserting the single-particle current operator (33) and using f-sum rule, we confirm that $-\chi_{\gamma\varphi}(0)$ is indeed the diamagnetic part

$$-\chi_{\gamma\varphi}(0) = \frac{nq^2}{m}\delta_{\gamma\varphi}. \tag{54}$$

D. Matsubara Green Function of Imaginary-frequencies

Since (52) (or (29)) takes the form of retarded Green function $G^R_{J_\gamma J_\varphi}(\omega)$, we can also evaluate it with the help of Matsubara Green function (of current operators) on imaginary frequence domain

$$\mathcal{G}_{J_\gamma J_\varphi}(i\omega_n) \equiv \int_0^\beta \mathrm{d}\tau\, e^{i\omega_n\tau} \mathcal{G}_{J_\gamma J_\varphi}(\tau) \equiv \int_0^\beta \mathrm{d}\tau\, e^{i\omega_n\tau}(-1)\langle \mathcal{T}_\tau J(\delta\gamma,\tau) J(\delta\varphi)\rangle = -\int_0^\beta \mathrm{d}\tau\, e^{i\omega_n\tau}\langle J(\delta\gamma,\tau)J(\delta\varphi)\rangle.$$

and analytical continuation $\omega_n \to i\omega + 0^+$. The imaginary-time order is removed just because the integration is performed on $[0, \beta)$ (essentially this comes from the periodicity of the Matsubara Green function $\mathcal{G}(\tau) \equiv \mp\mathcal{G}(\tau + i\hbar\beta)$). This approach is gauranteed by the Lehmann spectral representation from there definition [9]. For instance, Scalapino *et al.* [10] employ such method to study the fast and slow limits for metals, insulators, and superconductors.

III. APPENDIX

A. f-sum Rule

In this section, we will give a proof of the identity (36) used in the main text. Let me quote it here again
Theorem 1. (f-sum Rule)

$$\sum_{m,n} (f_m - f_n) \frac{\langle m|p_\alpha|n\rangle\langle n|p_\beta|m\rangle}{\varepsilon_{mn}} = -mN\delta_{\alpha\beta}. \tag{55}$$

▷ Relabling the states, we have, equivalently

$$\begin{aligned}
\text{LHS} &= \sum_{m,n} f_m \frac{\langle m|p_\alpha|n\rangle\langle n|p_\beta|m\rangle + \langle m|p_\beta|n\rangle\langle n|p_\alpha|m\rangle}{\varepsilon_m - \varepsilon_n} \\
&= \sum_{m,n} f_m \frac{\frac{m}{-i\hbar}(\varepsilon_m - \varepsilon_n)}{\varepsilon_m - \varepsilon_n}\Big(\langle m|r_\alpha|n\rangle\langle n|p_\beta|m\rangle + \langle m|p_\beta|n\rangle\langle n|r_\alpha|m\rangle\Big) \\
&= \frac{m}{-i\hbar}\sum_m f_m \langle m|[r_\alpha, p_\beta]|m\rangle = -mN,
\end{aligned}$$

where in the second line we take the quantum average of the identity

$$[h, r_\alpha] = \frac{-i\hbar}{m} p_\alpha,$$

under the single-particle states $\langle m|$ and $|n\rangle$. This is always true if the single-particle Hamiltonian of the system takes the form $h = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r})$. □

Note 1. The term "f-sum rule" is abused in literature. In fact, the most fundamental form is for the commutator with charge densities [11]

$$[[h, n(\boldsymbol{q})], n(-\boldsymbol{q})] = \frac{Nq^2\hbar^2}{m}, \tag{56}$$

or

$$\sum_{m,n} (\varepsilon_m - \varepsilon_n)\langle m|n(\boldsymbol{q})|n\rangle\langle n|n(-\boldsymbol{q})|m\rangle = \frac{Nq^2\hbar^2}{2m}. \tag{57}$$

The proof share the same spirits here. Based on (56) we can then prove the widely-seen form

$$\int_{-\infty}^{\infty} \mathrm{d}\omega\, \sigma_{\alpha\beta}(\omega) = \delta_{\alpha\beta}\frac{n}{2m}. \tag{58}$$

[1] J. Luttinger, Physical Review **135**, A1505 (1964).
[2] L.-P. Lévy, *Magnetism and superconductivity* (Springer Science & Business Media, 2000).
[3] G. Giuliani and G. Vignale, *Quantum theory of the electron liquid* (Cambridge university press, 2005).
[4] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of quantum field theory in statistical physics* (Courier Corporation, 2012).
[5] E. Fradkin, *Field theories of condensed matter physics* (Cambridge University Press, 2013).
[6] R. Kubo, Journal of the Physical Society of Japan **12**, 570 (1957).
[7] R. Kubo, M. Toda, and N. Hashitsume, *Statistical physics II: nonequilibrium statistical mechanics*, vol. 31 (Springer Science & Business Media, 2012).
[8] A. Kapustin and L. Spodyneiko, Physical Review B **101**, 045137 (2020).
[9] G. Mahan, *Many-Particle Physics* (Plenum Press, 1990).
[10] D. J. Scalapino, S. R. White, and S. Zhang, Physical Review B **47**, 7995 (1993).
[11] P. W. Anderson, Physical review **110**, 827 (1958).