KUBO FORMULAE FOR THE CONDUCTIVITY

§ 1. Coupling between electromagnetic fields and matter – gauge invariance

$$\bar{E} = -\frac{\partial \bar{A}}{\partial t} - \bar{\nabla}\varphi \quad , \quad \bar{B} = \bar{\nabla}\times\bar{A} \qquad (*)$$

gauge transformation $\quad \bar{A} \to \bar{A} + \bar{\nabla}\Lambda$

many equivalent ways of representing the same physics $\quad \varphi \to \varphi - \frac{\partial \Lambda}{\partial t}$

This representation guarantees automatically

$$(*) \Rightarrow \begin{cases} \bar{\nabla}\cdot\bar{B} = 0 & \text{magnetic Gauss law} \\ \bar{\nabla}\times\bar{E} = -\frac{\partial \bar{B}}{\partial t} & \text{Faraday law} \end{cases}$$

A minimal-coupling of a matter and the EM fields

$$\boxed{\begin{aligned} p_\alpha = \frac{\hbar}{i}\bar{\nabla}_\alpha &\to \frac{\hbar}{i}\bar{\nabla}_\alpha - e\bar{A}(\bar{r}_\alpha, t) \\ i\hbar\frac{\partial}{\partial t} &\to i\hbar\frac{\partial}{\partial t} - e\varphi(\bar{r}_\alpha, t) \end{aligned}}$$

The Schrödinger equation

$$\left(i\hbar\frac{\partial}{\partial t} - e\varphi(\bar{r}_\alpha, t)\right)\Psi = \frac{1}{2m}\left(\frac{\hbar}{i}\bar{\nabla}_\alpha - e\bar{A}(\bar{r}_\alpha, t)\right)^2\Psi + V\Psi$$

in a different gauge

$$\left(i\hbar\frac{\partial}{\partial t} - e\varphi(\bar{r}_\alpha, t) + e\frac{\partial\Lambda(\bar{r}_\alpha, t)}{\partial t}\right)\Psi' =$$

$$= \frac{1}{2m}\left(\frac{\hbar}{i}\bar{\nabla}_\alpha - e\bar{A}(\bar{r}_\alpha t) - e\bar{\nabla}\Lambda(\bar{r}_\alpha, t)\right)^2\Psi' + V\Psi'$$

obviously $\quad \Psi' \neq \Psi$. But the physics must be the same in all gauges. Hence

$$\boxed{\Psi'(\bar{r}_\alpha t) = e^{\frac{i e\Lambda(\bar{r}_\alpha, t)}{\hbar}}\,\Psi(\bar{r}_\alpha, t)}$$

$$\left(\frac{\hbar}{i}\nabla - e\vec{A} - e\nabla\Lambda\right)\psi' = \left(\frac{\hbar}{i}\nabla - e\vec{A} - e\nabla\Lambda\right) e^{ie\Lambda/\hbar}\psi =$$

$$= \Big(\cancel{\frac{\hbar}{i}\frac{ie}{\hbar}\nabla\Lambda\, e^{ie\Lambda/\hbar}\psi} + \frac{\hbar}{i}(\nabla\psi)\, e^{ie\Lambda/\hbar}$$

$$- e^{ie\Lambda/\hbar}\psi\, e\vec{A} - \cancel{e^{ie\Lambda/\hbar}\psi\, e\nabla\Lambda} \Big) =$$

$$= e^{ie\Lambda/\hbar}\left(\frac{\hbar}{i}\nabla - e\vec{A}\right)\psi$$

$$\left(i\hbar\frac{\partial}{\partial t} - e\phi + e\frac{\partial\Lambda}{\partial t}\right)\psi' = \left(i\hbar\frac{\partial}{\partial t} - e\phi + e\frac{\partial\Lambda}{\partial t}\right) e^{ie\Lambda/\hbar}\psi =$$

$$= \Big(\cancel{i\hbar\frac{ie}{\hbar}\frac{\partial\Lambda}{\partial t} e^{ie\Lambda/\hbar}\psi} + e^{ie\Lambda/\hbar}\, i\hbar\frac{\partial\psi}{\partial t} - e\phi\, e^{ie\Lambda/\hbar}\psi +$$

$$+ \cancel{e\frac{\partial\Lambda}{\partial t} e^{ie\Lambda/\hbar}\psi} \Big) =$$

$$= e^{ie\Lambda/\hbar}\left(i\hbar\frac{\partial}{\partial t} - e\phi\right)\psi$$

Observables should be gauge invariant

$$\int d^3r\, \psi^* V \psi = \int d^3r\, \psi'^* V \psi'$$

but

$$\int d^3r\, \psi^* \frac{\hbar}{i}\vec{\nabla}\psi \neq \int d^3r\, \psi'^* \frac{\hbar}{i}\vec{\nabla}\psi'$$

not observable

On the other hand

$$\int d^3r\, \psi^* \left(\frac{\hbar}{i}\vec{\nabla} - e\vec{A}(\vec{r}_\alpha,t)\right)\psi = \int d^3r\, \psi'^* \left(\frac{\hbar}{i}\vec{\nabla} - e\vec{A}(\vec{r}_\alpha,t) - \vec{\nabla}\Lambda\right)\psi'$$

is gauge invariant → it is observable $\langle m\vec{v}\rangle$

§2. Response of the current to external vector and scalar potential

We need terms $\delta H(t) = \delta H(t)_\phi + \delta H(t)_{\vec{A}}$ added to the matter Hamiltonian in the presence of EM field.

Applying the minimal-coupling procedure

$$\frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla}_\alpha\right)^2 \rightarrow \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla}_\alpha - e\vec{A}(\vec{r}_\alpha,t)\right)^2 = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla}_\alpha - e\vec{A}\right)\left(\frac{\hbar}{i}\vec{\nabla}_\alpha - e\vec{A}\right) =$$

$$= \frac{1}{2m}\left(-\hbar^2\vec{\nabla}_\alpha^2 - \frac{\hbar e}{i}\vec{\nabla}_\alpha\vec{A} - e\frac{\hbar}{i}\vec{A}\cdot\vec{\nabla}_\alpha + e^2\vec{A}^2\right) =$$

$$= -\frac{\hbar^2}{2m}\vec{\nabla}_\alpha^2 - e\frac{\hbar}{2mi}\left(\vec{A}(\vec{r}_\alpha)\cdot\vec{\nabla}_\alpha + \vec{\nabla}_\alpha\vec{A}(\vec{r}_\alpha)\right) + \frac{e^2}{2m}\vec{A}^2(\vec{r}_\alpha)$$

Therefore,

1st quantization.

$$\delta \mathcal{H}(t)_{\vec{A}} = -\sum_{\alpha=1}^{N} \frac{e\hbar}{2mi}\left(\vec{A}(\vec{r}_\alpha,t)\cdot\vec{\nabla}_\alpha + \vec{\nabla}_\alpha \vec{A}(\vec{r}_\alpha,t)\right)$$

The paramagnetic current for particles with charge e

$\vec{p}_\alpha = \frac{\hbar}{i}\vec{\nabla}_\alpha$

$$\boxed{\vec{j}(\vec{r}) = \frac{e}{2m}\sum_{\alpha=1}^{N}\left[\delta(\vec{r}-\vec{r}_\alpha)\vec{p}_\alpha + \vec{p}_\alpha\,\delta(\vec{r}-\vec{r}_\alpha)\right]}$$

$\vec{j} = e\,\frac{\vec{p}}{m} = e\vec{v}$

hence

$$\delta \mathcal{H}(t)_{\vec{A}} = -\int d_3r\ \vec{A}(\vec{r},t)\cdot\vec{j}(\vec{r})$$

This current is the same as found in Schrödinger equation in the absence of EM field by demanding conservation of the probability density $\Psi^*\Psi$.

Unless the system is neutral $\vec{j}(\vec{r})$ is not observable since it is not gauge invariant.

The observable current operator $\vec{j}^{A}(\vec{r})$ is obtained from applying a minimal-coupling prescription to the paramagnetic current $\vec{j}$

$$\vec{j}(\vec{r}) \to \vec{j}^{A}(\vec{r}) = \frac{q}{2m}\sum_{\alpha=1}^{N}\left[\delta(\vec{r}-\vec{r}_\alpha)(\vec{p}_\alpha - e\vec{A}) + (\vec{p}_\alpha - q\vec{A})\delta(\vec{r}-\vec{r}_\alpha)\right] =$$

$$= \frac{q}{2m}\sum_{\alpha=1}^{N}\left[\delta(\vec{r}-\vec{r}_\alpha)\vec{p}_\alpha + \vec{p}_\alpha\,\delta(\vec{r}-\vec{r}_\alpha)\right] - \frac{q^2}{2m}\sum_{\alpha=1}^{N} 2\cdot\vec{A}(\vec{r}_\alpha)\delta(\vec{r}-\vec{r}_\alpha)$$

using a (charge) density operator

$$\boxed{\rho(\vec{r}) = e\,n(\vec{r}) = e\sum_{\alpha=1}^{N}\delta(\vec{r}-\vec{r}_\alpha)}$$

$$\vec{j}^{A}(\vec{r}) = \underbrace{\vec{j}(\vec{r})}_{\text{paramagnetic current}} - \underbrace{\frac{e}{m}\vec{A}(\vec{r})\,\rho(\vec{r})}_{\text{diamagnetic current}}$$

This is a gauge invariant operator → observable

(It can also be derived as $\vec{j}^{A} = q\vec{v} = \left(\frac{\partial L}{\partial \vec{A}}\right)_{\vec{r},\vec{v}} = -\left(\frac{\partial H}{\partial \vec{A}}\right)_{\vec{r},\vec{p}}$)

Finally,

$$\delta \mathcal{H}(t)_{\vec{A}} = -\int d^3r\, \vec{A}(\vec{r},t)\, \vec{j}^{A}(\vec{r},t)$$

Coupling to the scalar potential:

from $\left(i\hbar\frac{\partial}{\partial t} - e\,\phi(\vec{r}_i,t)\right)\psi = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla}_i - e\vec{A}(\vec{r}_i,t)\right)^2\psi + V\psi$

we have

$$\delta \mathcal{H}(t)_{\phi} = \int d^3r\, \phi(\vec{r},t)\,\rho(\vec{r})$$

Kubo formula for the current

$$\mathcal{H}(t) = \mathcal{H}_0 + \delta\mathcal{H}(t)$$

We need to determine $\langle \vec{j}^{\,\alpha} \rangle$ up to the first order in $\vec{A}$ and ϕ.

$$\rho_0 = \frac{1}{Z} e^{-\beta \mathcal{H}_0}, \quad \mathcal{H} = \mathcal{H}_0 - \mu N \text{ - grand canonical}$$

$$Z = \operatorname{Tr} e^{-\beta \mathcal{H}_0}$$

$$i\hbar \frac{\partial \rho(t)}{\partial t} = [\mathcal{H}(t), \rho(t)], \quad \mathcal{H}(t) = \mathcal{H}(t) - \mu N$$

Schrödinger picture

let $\rho(t) = \rho_0 + \rho'(t)$

↑ perturbed contribution due to $\delta\mathcal{H}$

using $[\mathcal{H}_0, \rho_0] = 0$ and up to the first order in $\delta\mathcal{H}$

$$i\hbar \frac{\partial \rho'(t)}{\partial t} = [\mathcal{H}_0, \rho'(t)] + [\delta\mathcal{H}(t), \rho_0]$$

In Dirac (interaction) picture

$$\rho_D(t) = \rho_0 + \rho_D'(t)$$

$$\rho_D'(t) = e^{i\mathcal{H}_0 t/\hbar} \rho'(t) e^{-i\mathcal{H}_0 t/\hbar}$$

$$i\hbar \frac{\partial \rho_D'(t)}{\partial t} = [\rho_D'(t), \mathcal{H}_0] + \underbrace{e^{i\mathcal{H}_0 t/\hbar} i\hbar \frac{\partial \rho'(t)}{\partial t} e^{-i\mathcal{H}_0 t/\hbar}}_{[\mathcal{H}_0, \rho_D'(t)] + [\delta\mathcal{H}_D(t), \rho_0]} =$$

$$= [\delta\mathcal{H}_D(t), \rho_0]$$

Solution, with b.c. $\rho_D'(t) \underset{t \to -\infty}{\longrightarrow} 0$

$$\rho_D'(t) = -\frac{i}{\hbar} \int_{-\infty}^{t} dt' \, [\delta\mathcal{H}_D(t'), \rho_0]$$

back to the Schrödinger picture

$$\rho(t) \simeq \rho_0 - \frac{i}{\hbar}\int_{-\infty}^{t} dt' e^{-i\frac{\mathcal{H}_0 t'}{\hbar}} [\delta\mathcal{H}_D(t'), \rho_0] e^{\frac{i}{\hbar}\mathcal{H}_0 t}$$

$$\langle \vec{j}^A \rangle = \mathrm{Tr}[\rho_0 \vec{j}^A] - \frac{i}{\hbar}\int_{-\infty}^{t} \mathrm{Tr}[e^{-i\mathcal{H}_0 t/\hbar} [\delta\mathcal{H}_D(t'), \rho_0] e^{i\mathcal{H}_0 t/\hbar} \vec{j}^A] =$$

$$= \mathrm{Tr}[\rho_0 \vec{j}^A] - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \, \mathrm{Tr}\left([\delta\mathcal{H}_D(t'), \rho_0] \, \vec{j}^A_D(t) \right)$$

$$\vec{j}^A_D(t) = e^{i\mathcal{H}_0 t/\hbar} \, \vec{j}^A \, e^{-i\mathcal{H}_0 t/\hbar}$$

using

$$\mathrm{Tr}([A,B]C) = \mathrm{Tr}(ABC - BAC) = \mathrm{Tr}(BCA - BAC) = \mathrm{Tr}(B[C,A])$$

$$\langle \vec{j}^A(\vec{r},t)\rangle = \mathrm{Tr}[\rho_0 \vec{j}^A(\vec{r}t)] - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \, \mathrm{Tr}\left(\rho_0 [\vec{j}^A_D(\vec{r}t), \delta\mathcal{H}_D(t')]\right)$$

$$\delta\hat{\mathcal{H}}(t) = -\int d^3r \, \vec{A}(\vec{r},t)\, \hat{\vec{j}}^A(\vec{r},t) + \int d^3r \, \phi(\vec{r},t)\, \hat{\rho}(\vec{r})$$

$$\langle \vec{j}^A(\vec{r},t)\rangle = \mathrm{Tr}[\rho_0 \vec{j}_D(\vec{r})] - \frac{q}{m}\vec{A}(\vec{r},t)\,\mathrm{Tr}[\rho_0 \hat{\rho}_D(\vec{r})] -$$

$$- \frac{i}{\hbar}\int_{-\infty}^{t} dt' \int d^3r' \, \mathrm{Tr}\Big(\rho_0 \Big[\vec{j}_D(\vec{r}t) - \frac{q}{m}\vec{A}(\vec{r},t)\rho_D(\vec{r}),$$

$$- \vec{A}(\vec{r}',t')\Big(\vec{j}_D(\vec{r}'t') - \frac{q}{m}\vec{A}(\vec{r}'t')\rho_D(\vec{r}')\Big) +$$

$$+ \phi(\vec{r}'t')\,\rho_D(\vec{r}')\Big]\Big)$$

- $\mathrm{Tr}[\rho_0 \vec{j}(\vec{r})] = 0$ in equilibrium
- $\mathrm{Tr}[\rho_0, \hat{\rho}(\vec{r})] = q\, n$ uniform charge density
  n - particle density
- keep only first order terms

$$\langle \vec{j}^{A}(\vec{r},t)\rangle = -\frac{e^2 n}{m}\vec{A}(\vec{r},t) -$$

$$-\frac{i}{\hbar}\int_{-\infty}^{t} dt' \int d\vec{r}'\, \mathrm{Tr}\Big(-\rho_0[\vec{j}_D(\vec{r},t), \vec{j}_D(\vec{r}',t')\cdot\vec{A}(\vec{r}',t')] +$$

$$\rho_0[\vec{j}_D(\vec{r},t), \rho_D(\vec{r}')\ \phi(\vec{r}'t')]\Big)$$

Introducing response functions

$$\chi^{R}_{j_a j_b}(\vec{r}t, \vec{r}'t') = i\,\theta(t-t')\,\mathrm{Tr}\big(\rho_0[j_{aD}(\vec{r}t), j_{bD}(\vec{r}'t')]\big)$$

$$\chi^{R}_{j_a \rho}(\vec{r}t, \vec{r}'t') = i\,\theta(t-t')\,\mathrm{Tr}\big(\rho_0[j_{aD}(\vec{r}t), \rho_D(\vec{r}'t')]\big)$$

$$\langle j^{A}_{a}(\vec{r}t)\rangle = -\frac{e^2 n}{m}A_a(\vec{r}t) + \frac{1}{\hbar}\int_{-\infty}^{\infty} dt' \int d^3r' \sum_{b=1}^{3}\chi^{R}_{j_a j_b}(\vec{r}t, \vec{r}'t')\,A_b(\vec{r}'t') -$$

$$-\frac{1}{\hbar}\int_{-\infty}^{\infty} dt' \int d^3r'\,\chi^{R}_{j_a\rho}(\vec{r}t, \vec{r}'t')\,\phi(\vec{r}'t')$$

a th component of the current

For translationally invariant systems $\vec{r}-\vec{r}'$

in equilibrium $t-t'$

We perform a Fourier transform

$$\langle j^{A}_{a}(\vec{k},\omega)\rangle = \sum_{b=1}^{3}\Big[\chi^{R}_{j_a j_b}(\vec{k},\omega) - \frac{e^2 n}{m}\delta_{ab}\Big]A_b(\vec{k},\omega) -$$

$$-\chi^{R}_{j_a\rho}(\vec{k}\,\omega)\,\phi(\vec{k},\omega)$$

where $\chi^{R}_{AB}(\omega) = \frac{i}{\hbar}\int_{0}^{\infty} dt\, e^{i(\omega+i0^+)t}\,\mathrm{Tr}\big(\rho_0[A(t), B(0)]\big)$

It does not look like a gauge invariant, depends on $\vec{A}$ and ϕ. But using current conservation it is gauge invariant equation.

§ 3. Kubo formula for the transverse conductivity

conductivity $\overline{\overline{\sigma}}$ tensor $\vec{j} = \overline{\overline{\sigma}}\,\vec{E}$

We need to go back to $\vec{E}$ and $\vec{B}$ fields.

$\vec{k}$ – wave vector, direction of propagation

In case of the transverse response $\vec{k}\cdot\vec{E}(\vec{k},\omega) = 0$

$\vec{B}$ is always transverse $\nabla\cdot\vec{B} = \nabla\cdot(\nabla\times\vec{A}) = 0$

$\hat{k} = \frac{\vec{k}}{|\vec{k}|}$ – unit vector $\qquad (\hat{k}\hat{k})_{ab} = \frac{k_a k_b}{k^2}$

↑ dyadic product

$$\vec{A}^L = \hat{k}\,(\hat{k}\cdot\vec{A}) = (\hat{k}\hat{k})\cdot\vec{A}$$

$$\vec{A}^T = (\mathbb{1} - \hat{k}\hat{k})\cdot\vec{A}$$

Similarly

$$\overline{\overline{\sigma}}^T(\vec{k},\omega) = (\mathbb{1} - \hat{k}\hat{k})\,\overline{\overline{\sigma}}(\vec{k},\omega)\,(\mathbb{1} - \hat{k}\hat{k})$$

$$\overline{\overline{\sigma}}^L(\vec{k},\omega) = \hat{k}\hat{k}\,\overline{\overline{\sigma}}(\vec{k},\omega)\,\hat{k}\hat{k}$$

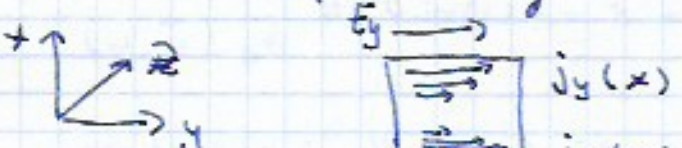
In normal systems $\overline{\overline{\sigma}} = \overline{\overline{\sigma}}^L + \overline{\overline{\sigma}}^T$ since

$$\hat{k}\hat{k}\,\overline{\overline{\sigma}}\,(\mathbb{1} - \hat{k}\hat{k}) = 0$$

In topological materials $\hat{k}\hat{k}\,\overline{\overline{\sigma}}\,(\mathbb{1} - \hat{k}\hat{k}) \neq 0$

(anomalous Hall effect).

Take a geometry



e.g. skin effect

gauge invariant

Then $\boxed{\langle j_y^A(k_x,\omega)\rangle = \sigma_{yy}(k_x,\omega)\,E_y(k_x,\omega)}$

Using that $\boxed{\vec{E} = -\frac{\partial\vec{A}}{\partial t} \leftrightarrow E_y(k_x,\omega) = i(\omega + i0^+)A_y(k_x,\omega)}$

$$\boxed{\sigma_{yy}(k_x,\omega) = \frac{1}{i(\omega+i0^+)}\left[\mathcal{K}^R_{j_y j_y}(k_x,\omega) - \frac{ne^2}{m}\right]}$$

PTO →

→ for a single Fourier component

$$A_y(\vec{r}, t) = e^{i\vec{k}\cdot\vec{r} - i(\omega + i0^+)t} A_y(\vec{k}, \omega)$$

→ $\omega + i0^+$ – the field is adiabatically switched on – causality

→ when $\vec{B} \neq 0$ then σ_{xy} – Hall or transverse conductivity is finite

It is a different definition, in fixed cartesian frame.

Our definition is with respect to propagation: relative direction of the current and its spatial dependence.

Decomposition into longitudinal and transverse part can be done by using unit vector $\hat{k} = \frac{\vec{k}}{k}$ in the direction of propagation

$\hat{k}_a \hat{k}_a = 1$

$$\hat{k}_a = \frac{k_a}{k} \quad , \quad k = \sqrt{\sum_a k_a k_a} = (k_a k_a)^{1/2}$$ summation convention

and two tensors of rank two

$$1_L = \hat{k}\hat{k} \qquad (1_L)_{ab} = \frac{k_a k_b}{k^2}$$

$$1_T = 1 - \hat{k}\hat{k} \qquad (1_T)_{ab} = \delta_{ab} - \frac{k_a k_b}{k^2}$$

note

.) $1_L + 1_T = 1 \qquad (1_L)_{ab} + (1_T)_{ab} = \delta_{ab}$

..) $(1_L \cdot 1_L)_{ab} = \hat{k}_a \hat{k}_c \hat{k}_c \hat{k}_b = \hat{k}_a \hat{k}_b = (1_L)_{ab}$

$$1_L \cdot 1_L = 1_L$$

...) $(1_T \cdot 1_T)_{ab} = (\delta_{ac} - \hat{k}_a \hat{k}_c)(\delta_{cb} - \hat{k}_c \hat{k}_b) =$

$= \delta_{ab} - \hat{k}_a \hat{k}_b - \hat{k}_a \hat{k}_b + \hat{k}_a \hat{k}_b = \delta_{ab} - \hat{k}_a \hat{k}_b = (1_T)_{ab}$

$$1_T \cdot 1_T = 1_T$$

1_L and 1_T are projection operators

$(1_L \cdot 1_T)_{ab} = (1_L)_{ac} (1_T)_{cb} = \hat{k}_a \hat{k}_c (\delta_{cb} - \hat{k}_c \hat{k}_b) =$

$= \hat{k}_a \hat{k}_b - \hat{k}_a \hat{k}_b = 0$

$(1_T \cdot 1_L)_{ab} = (1_T)_{ac} (1_L)_{cb} = (\delta_{ac} - \hat{k}_a \hat{k}_c) \hat{k}_c \hat{k}_b =$

$= \hat{k}_a \hat{k}_b - \hat{k}_a \hat{k}_b = 0$

projecting a vector

$$(A^L)_a = (1_L \cdot \bar{A})_a = (\hat{k}\hat{k}\,\bar{A})_a = \hat{k}_a \hat{k}_b A_b$$

$$(A^T)_a = (1_T \bar{A})_a = (\delta_{ab} - \hat{k}_a \hat{k}_b) A_b = A_a - \hat{k}_a \hat{k}_b A_b =$$

$$= (\hat{k} \times (\bar{A} \times \hat{k}))_a$$

projecting a tensor

$$\sigma_{ab}^T = (1_T \,\sigma\, 1_T)_{ab} = (1_T)_{ac}\, \sigma_{cd}\, (1_T)_{db} =$$

$$= (\delta_{ac} - \hat{k}_a \hat{k}_c)\, \sigma_{cd}\, (\delta_{db} - \hat{k}_d \hat{k}_b) =$$

$$= \sigma_{ab} - \hat{k}_a \hat{k}_c \sigma_{cb} - \sigma_{ad} \hat{k}_a \hat{k}_d +$$

$$+ \hat{k}_a \hat{k}_c\, \sigma_{cd}\, \hat{k}_d \hat{k}_b$$

$$\sigma_{ab}^L = (1_L \,\sigma\, 1_L)_{ab} = \hat{k}_a \hat{k}_c\, \sigma_{cd}\, \hat{k}_d \hat{k}_b$$

§4. Kubo formula for the longitudinal conductivity

gauge invariance leads to current conservation

$$\frac{\partial \rho(\vec{r},t)}{\partial t} = -\vec{\nabla}\cdot\vec{j}(\vec{r},t)$$

$$\frac{\partial \rho(\vec{k},t)}{\partial t} = -i\vec{k}\cdot\vec{j}(\vec{k},t)$$

because the same longitudinal electric field can be represented either by ϕ or by $\vec{A}$ so there must be a relation between ρ and $\vec{j}$

We use the current conservation to eliminate ρ

$$\frac{\partial}{\partial t}\chi^R_{j_x\rho}(k_x,t) = \delta(t)\frac{i}{\hbar V}\langle[j_x(k_x,0),\rho(-k_x,0)]\rangle +$$

$$+\,\theta(t)\frac{i}{\hbar V}(-ik_x)\langle[j_x(k_x,0),j_x(-k_x,-t)]\rangle$$

where we used $\frac{\partial\rho(-k_x,-t)}{\partial t} = -ik_x\, j_x(-k_x,-t)$

Using the definition of χ'' and f-sum rule

$$\frac{i}{\hbar V}\langle[j_x(k_x,0),\rho(-k_x,0)]\rangle = i\int\frac{d\omega}{\pi}\chi''_{j_x\rho}(k_x\omega) =$$

$$= i\int\frac{d\omega}{\pi}\frac{\omega}{k_x}\chi''_{\rho\rho}(k_x,\omega) =$$

$$= ik_x\frac{ne^2}{m}$$

Hence,
$$\boxed{-i(\omega+i0^+)\chi^R_{j_x\rho}(k_x,\omega) = ik_x\frac{ne^2}{m} - ik_x\chi^R_{j_xj_x}(k_x,\omega)}$$

Now,

$$\langle j_a^A(\vec{k},\omega)\rangle = \left[\chi^R_{j_a j_b}(\vec{k},\omega) - \frac{ne^2}{m}\delta_{ab}\right] A_b(\vec{k},\omega) - \chi^R_{j_a \rho}(\vec{k},\omega)\,\phi(\vec{k},\omega)$$

the longitudinal part is

$$\langle j_x^A(k_x,\omega)\rangle = \frac{1}{i(\omega+i0^+)}\left[\chi^R_{j_x j_x}(k_x\,\omega) - \frac{ne^2}{m}\right]\Big(i(\omega+i0^+)A_x(k_x,\omega) - i k_x \phi(k_x,\omega)\Big) =$$

or

$$= \left[\frac{1}{ik_x}\chi^R_{j_x\rho}(k_x,\omega)\right]\left(i(\omega+i0^+)A_x(k_x,\omega) - ik_x\phi(k_x\,\omega)\right)$$

Replacing gauge fields by field intensity

$$E_x(k_x\,\omega) = i(\omega+i0^+)A_x(k_x,\omega) - i k_x \phi(k_x,\omega)$$

$$\langle j_x^A(k_x,\omega)\rangle = \sigma_{xx}(k_x,\omega)\,E_x(k_x,\omega)$$

$$\boxed{\sigma_{xx}(k_x\,\omega) = \frac{1}{i(\omega+i0^+)}\left[\chi^R_{j_x j_x}(k_x,\omega) - \frac{ne^2}{m}\right] = \frac{1}{ie_x}\chi^R_{j_x\rho}(k_x,\omega)}$$