Kubo / Linear response

Density matrix $\hat{\rho} = \sum_i |i\rangle \rho_i \langle i|$

Since $|i\rangle_t = e^{-i\mathcal{H}t}|i\rangle$

we have dynamics $\hat{\rho}(t) = e^{-i\mathcal{H}t}\hat{\rho}(t=0)\, e^{i\mathcal{H}t}$

or Liouville's eq-n:

$$\boxed{i\hbar\, \partial_t \hat{\rho} = [\hat{\mathcal{H}}, \hat{\rho}]}$$

Linear response: $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{V}$ and calculate "response" in the first in perturbation order ($\hat{\rho} = \hat{\rho}_0 + \delta\hat{\rho} + \dots$, $\delta\hat{\rho} \sim \hat{V}$)

$$i\hbar\, \partial_t \delta\hat{\rho} = [\hat{V}, \hat{\rho}_0] + [\hat{\mathcal{H}}_0, \delta\hat{\rho}]$$

$$\delta\hat{\rho}(t) = -\frac{i}{\hbar}\int_{-\infty}^{t} dt'\, e^{-i\hat{\mathcal{H}}_0 t}[\hat{V}(t'), \hat{\rho}_0]\, e^{i\hat{\mathcal{H}}_0 t}, \quad \hat{V}(t') = e^{i\hat{\mathcal{H}}_0 t'}\hat{V} e^{-i\hat{\mathcal{H}}_0 t'}$$

Any observable $O(t) = \mathrm{tr}\, \hat{\rho}(t)\hat{O} \approx \mathrm{tr}\, \hat{\rho}_0 \hat{O} + \mathrm{tr}\, \delta\hat{\rho}(t)\hat{O}$

If $\langle \hat{O} \rangle_0 \equiv \mathrm{tr}\, \hat{\rho}_0 \hat{O} = 0$ then

$$\boxed{O(t) = -\frac{i}{\hbar}\int_{-\infty}^{t} dt' \langle [\hat{O}(t), \hat{V}(t')] \rangle}$$

Kubo formula

K-2

Electric current: observable

$$\vec{j}(\vec{r},t) = \frac{e}{2m}\langle \hat{\psi}^+ \vec{P}\hat{\psi} + h.c.\rangle = \cancel{t}r\, \hat{\vec{j}}'(\vec{r},t)\cdot\hat{\rho}$$

In the presence of vector potential

$$\hat{\vec{P}} = \hat{\vec{p}} - \frac{e}{c}\vec{A}, \quad \vec{p} = -i\hbar\nabla \;;\; \hat{\vec{j}}' = \hat{\vec{j}} - \frac{e^2}{mc}\vec{A}\cdot\hat{\psi}^+\hat{\psi}$$

In the linear response

$$\vec{j}(\vec{r},t) \approx tr\,\delta\hat{\rho}(t)\cdot\hat{\vec{j}}(\vec{r},t) - \frac{e^2}{mc}\vec{A}\; tr\,\hat{\rho}_0\,\hat{\psi}^+(\vec{r},t)\hat{\psi}(\vec{r},t)$$

The Kubo formula for the electric current:

$$\vec{j}(\vec{r},t) = -\frac{ne^2}{mc}\vec{A} - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \langle[\hat{\vec{j}}(\vec{r},t), \hat{V}(t')]\rangle$$

The perturbation

$$\mathcal{H} = \int d^3r\, \hat{\psi}^+\left[\frac{1}{2m}\left(\hat{\vec{p}} - \frac{e}{c}\vec{A}\right)^2 + V\right]\hat{\psi} + int$$

$$\Rightarrow \hat{V}(t) = -\frac{1}{c}\int d^3r\, \hat{\vec{j}}(\vec{r},t)\vec{A}(\vec{r},t)$$

$$\boxed{j_\mu(\vec{r},t) = -\frac{ne^2}{mc}A_\mu(\vec{r},t) + \frac{i}{\hbar c}\int_{-\infty}^{t} dt' \int d^3r' \langle[\hat{j}_\mu(\vec{r},t), \hat{j}_\nu(\vec{r}',t')]\rangle A_\nu(\vec{r}',t')}$$

K-3

It was assumed that the choice of the gauge $\varphi = 0$!

$$\vec{E} = -\frac{1}{c}\partial_t \vec{A} \Rightarrow \vec{E}(\vec{r},\omega) = \frac{i\omega}{c}\vec{A}(\vec{r},\omega)$$

For a monochromatic perturbation $\vec{E} \sim \vec{E}(\omega) e^{-i\omega t}$

$$j_\mu(\vec{r},\omega) = -\frac{ne^2}{mi\omega} E_\mu(\vec{r},\omega) + \frac{1}{\hbar\omega}\int_0^\infty dt' \int d^3r' e^{i\omega t}\langle [\hat{j}_\mu(\vec{r},t), \hat{j}_\nu(\vec{r}',0)]\rangle E_\nu(\vec{r}',\omega)$$

$$j_\mu(\vec{r}) = \int d^3r' \, \Pi_{\mu\nu}(\vec{r},\vec{r}') \underbrace{E_\nu(\vec{r}')}_{\text{sum over}}$$

Dissipative part $\oint dt (j_\omega e^{-i\omega t} + c.c.)(E_\omega e^{-i\omega t} + c.c.) \sim \mathrm{Re}\,\Pi$

Dissipative current (or subtracting displacement current)

$$j_\mu^{dis}(\vec{r}) = \int d^3r' \, \sigma_{\mu\nu}(\vec{r},\vec{r}') E_\nu(\vec{r}')$$

$$\sigma_{\mu\nu}(\vec{r},\vec{r}') = \frac{1}{\hbar\omega}\mathrm{Re}\int_0^\infty dt \, e^{i\omega t}\langle [\hat{j}_\mu(\vec{r},t), \hat{j}_\nu(\vec{r}',0)]\rangle$$

K-4

1D-current: reduction to Landauer formula (non-interacting electrons!)

$$\sigma_\omega(x,x') = \frac{1}{\hbar\omega} \mathrm{Re} \int_0^\infty dt\, e^{i\omega t} \langle [\hat{j}(x t), \hat{j}(x')] \rangle$$

The field operator

$$\hat{\psi}(x,t) = \sum_\mu \psi_\mu(x)\, \hat{a}_\mu e^{-i\varepsilon_\mu t}$$

eigenstates

$$\langle [\hat{j}(xt), \hat{j}(x')] \rangle = \sum j_{\mu\nu}(x)\, j_{\mu'\nu'}(x')\, e^{i(\varepsilon_\mu - \varepsilon_\nu)t} \langle [\hat{a}_\mu^+ \hat{a}_\nu, \hat{a}_{\mu'}^+ \hat{a}_{\nu'}] \rangle$$

$$\parallel$$

Using that $\Longrightarrow \langle \delta_{\mu'\nu} \hat{a}_\mu^+ \hat{a}_{\nu'} - \delta_{\mu\nu'} \hat{a}_{\mu'}^+ \hat{a}_\nu \rangle$

we get

$$\boxed{\sigma_\omega(x,x') = \frac{1}{\hbar\omega} \mathrm{Re}\, i \sum j_{\mu\nu}(x)\, j_{\nu\mu}(x') \frac{f_\mu - f_\nu}{\varepsilon_\mu - \varepsilon_\nu + \hbar\omega + i0}}$$

Notice that $j_{\mu\nu} = \frac{e\hbar}{2mi}\left(\bar{\psi}_\mu \partial_x \psi_\nu - \partial_x \bar{\psi}_\mu \cdot \psi_\nu\right)$

so $\overline{j_{\mu\nu}(x)} = j_{\nu\mu}(x)$

K-5

$$\sigma_\omega(x,x') = -\frac{1}{\cancel{\hbar}\omega}\,\mathrm{Im}\,\underbrace{\sum j_{\mu\nu}(x)\, j_{\nu\mu}(x')\,(f_\mu - f_\nu)\left[\mathcal{P}\frac{1}{\varepsilon_\mu - \varepsilon_\nu + \hbar\omega} - i\pi\delta(\varepsilon_\mu - \varepsilon_\nu + \omega)\right]}_{A(\omega)}$$

$$A(\omega) - \bar{A}(\omega) = \sum j_{\mu\nu}(x)\, j_{\nu\mu}(x')\,(f_\mu - f_\nu)\,\frac{-2\omega}{(\varepsilon_\mu - \varepsilon_\nu)^2 + \omega^2}$$

In the $\omega \to 0$ limit (dc-conductivity) contribution from principal value ($A(\omega)$) vanishes!

$$\sigma(x,x') = \lim_{\omega\to 0} \sigma_\omega(x,x') = \lim_{\omega\to 0}\frac{\pi}{\cancel{\hbar}\omega}\sum_{\mu\nu} j_{\mu\nu}(x)\, j_{\nu\mu}(x')\,(f_\mu - f_\nu)\,\delta(\varepsilon_\mu - \varepsilon_\nu + \omega)$$

$$f_\mu - f_\nu = f(\varepsilon_\mu) - f(\varepsilon_\nu = \varepsilon_\mu + \hbar\omega) \approx -f'(\varepsilon_\mu)\,\hbar\omega$$

Finally, taking dc-limit

$$\boxed{\sigma = \pi\hbar \sum_{\mu\nu} j_{\mu\nu}(x)\, j_{\nu\mu}(x')\,(-f'(\varepsilon_\mu))\,\delta(\varepsilon_\mu - \varepsilon_\nu)}$$

$$\left\{\begin{aligned} \sum_\mu &= \sum_\alpha \int d\varepsilon\, \nu_\alpha(\varepsilon) \\ &= \frac{1}{2}\sum_\alpha \int d\varepsilon\, \nu(\varepsilon) \end{aligned}\right.$$

$$= \frac{\pi\hbar}{4}\int d\varepsilon\, \nu^2(\varepsilon)\left(-\frac{\partial f}{\partial \varepsilon}\right) j_{\alpha\beta}(x;\varepsilon)\, j_{\beta\alpha}(x';\varepsilon)$$

K-6

Since both α- and p-states are eigenstates with the same eigenenergy

$$\partial_x \hat{j}_{\alpha p}(x;\varepsilon) = 0$$

and
$$\sigma = \frac{\pi\hbar}{4}\int d\varepsilon\, \nu^2(\varepsilon)\left(-\frac{\partial f}{\partial \varepsilon}\right) \mathrm{tr}\, \hat{j}^2$$

The j-matrix in scattering states basis

$$\hat{j} = ev\begin{pmatrix} T & \bar{r}t \\ r\bar{t} & T \end{pmatrix}$$

and
$$\sigma = \frac{\pi\hbar}{4}\int \frac{d\varepsilon}{(\pi\hbar v)^2}(-f')\, e^2 v^2 \cdot 2(T^2 + RT)$$

$$\boxed{\sigma = \frac{e^2}{2\pi\hbar}\int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon}\right) T(\varepsilon)} \leftarrow$$

the same as Landauer!