CHAPTER 3, LINEAR RESPONSE THEORY

Ch. 6 Bruus e Flensberg

(or Kubo formalism)

Ch. 2.3 di Ventra

The situation we have in mind is a system initially in global equilibrium and subject to a <u>weak</u> external perturbation (e.g. electromagnetic field) after a time $t \geq t_0$.

3.1. KUBO FORMULA

Questions:

- What is the expectation value $\langle \hat{A} \rangle$ of an operator $\hat{A}$ to linear order in the external perturbation $\hat{H}_{ext}$?
- How to evaluate non-equilibrium averages?

Global equilibrium — Non-equilibrium

$\hat{H}(t) = \hat{H}_0$ — $\hat{H}(t) = \hat{H}_0 + \hat{H}_{ext}\,\theta(t-t_0)$

t_0 — t

$$\langle \hat{A} \rangle_0 = \mathrm{Tr}\{\hat{A}\hat{\rho}_0\} \qquad \langle \hat{A} \rangle_t = \mathrm{Tr}\{\hat{A}\hat{\rho}(t)\} = ?$$

with

$$\hat{\rho}_0 = \frac{e^{-\beta \hat{H}_0}}{Z_c} \quad \text{canonical ensemble}$$

or

$$\hat{\rho}_0 = \frac{e^{-\beta(\hat{H}_0 - \mu \hat{N}_0)}}{Z_{gc}} \quad \text{grand canonical ensemble}$$

e.g. if $\hat{H}_{ext} \propto$ electromagnetic field it is sufficient to work in canonical ensemble

if $\hat{H}_{ext} \propto$ tunneling coupling to reservoirs $\Rightarrow$ grand canonical

Strategy: $\hat{H}_{ext}$ is weak $\rightarrow$ deviation of $\hat{\varrho}(t)$ from equilibrium form $\hat{\varrho}_0$ included up to linear order in $\hat{H}_{ext}$

$\Rightarrow$ i) $\hat{\varrho}(t) = \hat{\varrho}_0 + \Delta\hat{\varrho}(t) + O(\hat{H}_{ext}^2)$ (3.1)

Consider the Liouville von-Neumann equation for $\hat{H}(t)$:

$$\dot{\hat{\varrho}}(t) = -\frac{i}{\hbar}[\hat{H}(t), \hat{\varrho}(t)] = -\frac{i}{\hbar}[\hat{H}_0, \Delta\hat{\varrho}(t)] - \frac{i}{\hbar}[\hat{H}_{ext}, \hat{\varrho}_0] + O(\hat{H}_{ext}^2)$$

ii) Because we know all properties of the system in the absence of $\hat{H}_{ext}$, it is convenient to first evaluate the statistical operator in the <u>interaction</u> <u>picture</u>:

$$\hat{\varrho}_I(t) \equiv e^{+i\hat{H}_0\frac{t}{\hbar}}\,\hat{\varrho}(t)\,e^{-i\hat{H}_0\frac{t}{\hbar}} \qquad (3.2)$$

as well as the interaction

$$\hat{H}_{ext,I}(t) = e^{i\hat{H}_0 t/\hbar}\,\hat{H}_{ext}(t)\,e^{-i\hat{H}_0 t/\hbar} \qquad (3.3)$$

$\hookrightarrow$ <u>Liouville von-Neumann eq.</u> <u>in interaction picture</u>

$$\boxed{\frac{\partial}{\partial t}\hat{\varrho}_I(t) = \Delta\dot{\hat{\varrho}}_I(t) = -\frac{i}{\hbar}[\hat{H}_{ext,I}(t), \hat{\varrho}_I(t)]} \qquad (3.4)$$

A formal solution is

$$\Delta\hat{\varrho}_I(t) = \underset{\overset{\parallel}{0}}{\Delta\hat{\varrho}_I(t_0)} - \frac{i}{\hbar}\int_{t_0}^{t} dt' \, [\hat{H}_{ext,I}(t'), \hat{\varrho}_I(t')]$$

and hence to first order in $\hat{H}_{ext,I}$

$$\begin{cases} \Delta\hat{\varrho}_I(t) = -\frac{i}{\hbar}\int_{t_0}^{t} dt' \, [\hat{H}_{ext,I}(t'), \hat{\varrho}_0] + O(\hat{H}_{ext}^2) \\ \Delta\hat{\varrho}(t) = e^{-i\hat{H}_0 t/\hbar} \, \Delta\hat{\varrho}_I(t) \, e^{+i\hat{H}_0 t/\hbar} \end{cases}$$

iii) It follows the Kubo formula

$$\boxed{\langle\hat{A}\rangle_t - \langle\hat{A}\rangle_0 = -\frac{i}{\hbar}\int_{t_0}^{\infty} dt' \, \theta(t-t') \, \langle[\hat{A}_I(t), \hat{H}_{ext,I}(t')]\rangle_0} \quad (3.5)$$

⇒ The inherent non-equilibrium quantity $\langle\hat{A}\rangle_t$ is expressed as a retarded correlation of the system in equilibrium

In fact $\theta(t-t')$ expresses causality of the solution

(3.5) is the

KUBO FORMULA IN FREQUENCY DOMAIN

Consider the case in which

$$\hat{H}_{ext}(t) = \hat{B}\, f(t)$$

c-number

time-independent operator

From (3.5) it follows

$$\delta\langle \hat{A}(t)\rangle \equiv \langle \hat{A}\rangle_t - \langle \hat{A}_0\rangle = -\frac{i}{\hbar}\int_{t_0}^{\infty} dt'\, \theta(t-t')\langle [\hat{A}_I(t), \hat{B}_I(t')]\rangle_0\, f(t') \quad (3.6)$$

with

$$\chi^R_{AB}(t,t') \equiv -\frac{i}{\hbar}\theta(t-t')\langle [\hat{A}_I(t), \hat{B}_I(t')]\rangle_0$$

response function or susceptibility (retarderd correlation function)

$$\hookrightarrow \boxed{\chi^R_{AB}(t,t') = C^R_{AB}(t-t')} \quad (3.7)$$ due to cyclic invariance of the trace (see next page)

Setting $t_0 = -\infty$ and taking the Fourier transform of (3.6) we get

$$\boxed{\delta\langle \tilde{\hat{A}}(\omega)\rangle = \int_{-\infty}^{+\infty} dt\, e^{i\omega t}\, \delta\langle \hat{A}(t)\rangle = \tilde{\chi}^R_{AB}(\omega)\, \tilde{f}(\omega)} \quad (3.8)$$

Note: because $\chi^R_{AB}(t)$ is a retarded correlation function, it decays at $-\infty$. We insure a proper behavior also for $+\infty$ by introducing an infinitesimal convergence factor:

$$\tilde{\chi}^R_{AB}(\omega) \equiv \int_{-\infty}^{+\infty} dt\, e^{i\omega t - \eta t}\, \chi^R_{AB}(t), \quad \eta = 0^+$$

POSITION DEPENDENT PERTURBATION

$$\hat{H}_{ext}(t) = \int d\vec{r}\ \hat{B}(\vec{r})\ f(\vec{r},t)$$

yields

$$\delta\langle \tilde{\hat{A}}(\omega)\rangle = \int d\vec{r}\ \tilde{\chi}^R_{A\,B(\vec{r})}(\omega)\ \tilde{f}(\vec{r},\omega)$$

CYCLIC INVARIANCE

$$\chi^R_{AB}(t,t') = \frac{i}{\hbar}\theta(t-t')\ \langle [\hat{A}_I(t), \hat{B}_I(t')]\rangle_0$$

$$= -\frac{i}{\hbar}\theta(t-t')\ \mathrm{Tr}\left\{ \frac{e^{-\beta\hat{H}_0}}{Z}\left(e^{i\hat{H}_0 t/\hbar}\hat{A}\underbrace{e^{-i\hat{H}_0\frac{t}{\hbar}}\ e^{i\hat{H}_0\frac{t'}{\hbar}}}_{e^{-i\hat{H}_0\frac{(t-t')}{\hbar}}}\hat{B}\, e^{-i\hat{H}_0\frac{t'}{\hbar}} - \hat{B}_I(t')\hat{A}_I(t)\right)\right\}$$

$$= -\frac{i}{\hbar}\theta(t-t')\ \mathrm{Tr}\left\{ \frac{e^{-\beta\hat{H}_0}}{Z}\left(e^{i\hat{H}_0\frac{(t-t')}{\hbar}}\hat{A}\, e^{-i\hat{H}_0\frac{(t-t')}{\hbar}}\hat{B} - \hat{B}_I(t')\hat{A}_I(t)\right)\right\}$$

$$= -\frac{i}{\hbar}\theta(t-t')\ \langle [\hat{A}_I(t-t'), \hat{B}_I(0)]\rangle_0$$

3.2 Lehmann representation

The Lehmann representation is the representation of the eigenstates of $\hat{H}_0$.

We set $\hat{H}_0 |m\rangle = E_m |m\rangle$,

$$E_n - E_m = E_{nm} = \hbar \omega_{nm} \quad , \quad \hat{\rho}(t_0) = \sum_m \frac{e^{-\beta E_m}}{Z} |m\rangle\langle m| \quad (*)$$

It is useful to proof exact properties of correlation functions like e.g. $\chi_{AB}(t)$

$$\chi_{AB}(t) = -\frac{i}{\hbar}\,\theta(t)\,\langle [\hat{A}_I(t), B_I(0)]\rangle_0 =$$

$$= -\frac{i}{\hbar}\,\theta(t)\,\mathrm{Tr}\{\hat{\rho}(t_0)\hat{A}_I(t)\hat{B}_I(0) - \hat{\rho}(t_0)\hat{B}_I(0)\hat{A}_I(t)\}$$

$$= -\frac{i}{\hbar}\,\theta(t)\sum_m \langle m|\,\hat{\rho}(t_0)\hat{A}_I(t)\,B_I(0) - \hat{\rho}(t_0)\hat{B}_I(0)\hat{A}_I(t)|m\rangle$$

$$\mathbb{1} = \sum_n |n\rangle\langle n| \qquad \qquad \mathbb{1} = \sum_n |n\rangle\langle n|$$

use:
$$\hat{A}_I(t) = e^{+i\hat{H}_0 t/\hbar}\,\hat{A}_I\,e^{-i\hat{H}_0 t/\hbar}$$

(*) grand canonical case, for a particle conserving $\hat{H}_0$

$$\begin{cases} |m\rangle \to |m, N\rangle \quad , \quad \text{many body state with } N \text{ particles} \\ \hat{\rho}(t_0) \to \sum_m \frac{e^{-\beta(E_m - \mu N)}}{Z} |m N\rangle\langle m N| \end{cases}$$

Lehmann representation and symmetry properties of $\tilde{\chi}_{AB}(\omega)$

(cf. Giuliani and Vignale "Quantum theory of the electron liquid" Ch. 3.2) 3.3, 3.4

We gain insight into the structure of the response function χ_{AB} by expanding the commutator in a complete set of eigenstates of H_0

$$\langle [\hat{A}(\tau), \hat{B}] \rangle_0 = \sum_{m,n} \rho_{mm} \left(e^{i\omega_{mn}\tau} A_{mn} B_{nm} - e^{i\omega_{nm}\tau} B_{mn} A_{nm} \right)$$

$$= \sum_{mn} (\rho_{mm} - \rho_{nn}) \, e^{i\omega_{mn}\tau} A_{mn} B_{nm}$$

$$\uparrow \rho_{mm} = \frac{e^{-\beta E_m}}{Z}$$

$$\Rightarrow \boxed{\tilde{\chi}_{AB}(\omega) = \frac{1}{\hbar} \sum_{mn} \frac{\rho_{mm} - \rho_{nn}}{\omega - \omega_{nm} + i\eta} A_{mn} B_{nm}} \quad (3.9)$$

Hence for a finite system $\Rightarrow$ Singularities of a response function are simple poles, located infinitesimally below the real axis at the transition frequencies of the system (••); (•••)

χ_{AA^+} Take $B = A^+$ and use $\lim_{\eta \to 0} \frac{1}{\omega - y + i\eta} = P \frac{1}{\omega - y} - i\pi \delta(\omega - y)$ (*)

$$\Rightarrow \mathrm{Re}\, \tilde{\chi}_{AA^+}(\omega) = \frac{1}{\hbar} P \sum_{mn} \frac{|A_{mn}|^2}{\omega - \omega_{nm}} (\rho_{mm} - \rho_{nn}) \equiv \tilde{\chi}'_{AA^+}(\omega)$$

$$\mathrm{Im}\, \tilde{\chi}_{AA^+}(\omega) = -\frac{\pi}{\hbar} \sum_{mn} (\rho_{mm} - \rho_{nn}) |A_{mn}|^2 \delta(\omega - \omega_{nm}) \equiv \tilde{\chi}''_{AA^+}(\omega)$$

and, in particular

$$\boxed{\tilde{\chi}'_{AA^+}(\omega) = \tilde{\chi}'_{A^+A}(-\omega), \quad \tilde{\chi}''_{AA^+}(\omega) = -\tilde{\chi}''_{A^+A}(-\omega)} \quad (3.10)$$

$\omega = 0$: Static case

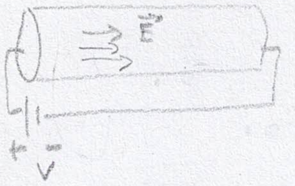
$$\begin{cases} \mathrm{Im}\, \tilde{\chi}_{AA^+}(\omega = 0) = 0 & \text{Because } (\rho_{mm} - \rho_{nn}) \delta(\omega_{nm}) = 0 \\ \mathrm{Re}\, \tilde{\chi}_{AA^+}(\omega = 0) \leq 0 & \end{cases}$$

(*) $$P \int_{-\infty}^{+\infty} d\omega \frac{f(\omega)}{\omega - y} = \lim_{\eta \to 0^+} \left(\int_{-\infty}^{y-\eta} d\omega \frac{f(\omega)}{\omega - y} + \int_{y+\eta}^{\infty} d\omega \frac{f(\omega)}{\omega - y} \right)$$

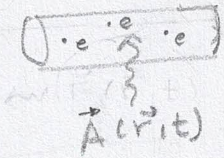
(••) For a continuum system additional poles, signaling collective excitations can arise

3.3. APPLICATION 1. CONDUCTIVITY

Viewpoint 1



or



$\vec{J}(\vec{r},t) = ?$

i) Perturbation $\hat{H}_{ext}$ associated to $\vec{E}$?

Consider the action of an electromagnetic field with associated vector potential $\vec{A}(\vec{r},t)$ and potential $\phi(\vec{r},t)$:

$$\begin{cases} \vec{E}(\vec{r},t) = -\vec{\nabla}\phi(\vec{r},t) - \frac{1}{c}\partial_t \vec{A}(\vec{r},t) & (3.11) \\ \vec{B}(\vec{r},t) = \vec{\nabla}\times\vec{A} \end{cases}$$

Hamiltonian of a system of N electrons + electromgn. field

$$\hat{H} = \sum_{i=1}^{N} \frac{\left(\hat{\vec{P}}_i - \frac{e}{c}A(\hat{\vec{r}}_i,t)\right)^2}{2m} + e\sum_{i=1}^{N}\phi(\hat{\vec{r}}_i,t) + \underbrace{V(\hat{\vec{r}}_1,\hat{\vec{r}}_2,\hat{\vec{r}}_3,\dots,\hat{\vec{r}}_N)}_{\text{can include e.g. e-e interactions}} \qquad (3.12)$$

Notice that

$$\left(\hat{\vec{P}}_i - \frac{e}{c}A(\hat{\vec{r}}_i,t)\right)\left(\hat{\vec{P}}_i - \frac{e}{c}A(\hat{\vec{r}}_i,t)\right) = \hat{P}_i^2 + \frac{e^2}{c^2}A^2(\hat{\vec{r}}_i) - \hat{\vec{P}}_i\cdot\frac{e}{c}\vec{A} - \frac{e}{c}\vec{A}\cdot\hat{\vec{P}}_i$$

and recall the definition (2.8), (2.9) of the current density operator

$$\begin{cases} \hat{\vec{J}}(\vec{r},t) = \hat{\vec{J}}_p(\vec{r},t) \underbrace{- \frac{e^2}{mc}\hat{n}(\vec{r})A(\vec{r},t)}_{\vec{J}_d} & (2.8) \\ \hat{\vec{J}}_p(\vec{r},t) = \frac{e}{2m}\sum_i \left\{\delta(\vec{r}-\hat{\vec{r}}_i), \hat{\vec{P}}_i\right\} & (2.9) \end{cases}$$

where $\hat{n}(\vec{r}) = \sum_{i=1}^{N}\delta(\vec{r}-\hat{\vec{r}}_i)$ (2.7)

Then

$$\hat{H} = \hat{H}_0 \underbrace{- \frac{1}{c}\int d\vec{r}\,' \,\hat{\vec{J}}_p(r') \cdot \vec{A}(\vec{r}\,',t) + e\int d\vec{r}\,' \,\hat{m}(\vec{r}\,')\,\phi(\vec{r}\,',t)}_{\hat{H}_{ext}} + O(A^2) \tag{3.13}$$

linear response

↳ electromag. field couples to a system of charged particles through $\hat{\vec{J}}_p$ & $\hat{m}$.

- Let us work in a gauge where $\phi = 0$ at any time.

- Recall that our formulae are invariant under the gauge transformation

$$\phi \to \phi - \frac{1}{c}\frac{\partial \Lambda}{\partial t}, \qquad \vec{A} \to \vec{A} + \vec{\nabla}\Lambda \qquad (*)$$

not voltage ☺

- Due to gauge invariance, any scalar potential $V(\vec{r},t) = -e\Phi$ can be represented by a longitudinal potential $\vec{A}(\vec{r},t)$ using

$$\vec{A}(\vec{r},t) = -\frac{c}{e}\int_{t_0}^{t} dt'\, \vec{\nabla} V(\vec{r},t') \Rightarrow \vec{A}(\vec{q}\,t) = -\frac{c}{e}\, i\vec{q}\int_{t_0}^{t} V(\vec{q},t')\,dt' \quad (**)$$

$$= -c\int dt'\,\vec{E}(\vec{q},t')$$

Longitudinal means $\vec{\nabla}\cdot\vec{A} \neq 0$, $\vec{\nabla}\times\vec{A} = 0$

i.e., according to $(*)$, being the gradient of a scalar function, $\vec{A}(\vec{q}) \parallel \vec{q}$

Transverse potentials satisfy $\vec{A}(\vec{q}) \perp \vec{q}$ and are used to describe static $\vec{B}$ —

It follows:

$$\boxed{\hat{H}^{(t)}_{ext} = -\frac{1}{c}\int d\vec{r}\,'\,\hat{\vec{J}}_p(\vec{r}\,')\cdot\vec{A}(\vec{r}\,',t)} \tag{3.14}$$

$\Rightarrow$ we are in the position of evaluating $\langle \hat{\vec{J}} \rangle(t)$ using Kubo formula

$(**)$ $V(\vec{r}) = \int d\vec{q}\; e^{i\vec{q}\cdot\vec{r}}\, V(\vec{q}) \Rightarrow \nabla V(\vec{r}) = i\int d\vec{q}\; \vec{q}\, V(\vec{q})\, e^{i\vec{q}\cdot\vec{r}}$

Further, $\vec{E} = -\vec{\nabla}\phi = \frac{1}{e}\vec{\nabla}V \Rightarrow \vec{E}(q) = \frac{i}{e}\vec{q}\,V(\vec{q})$

Gauge invariance : response to a scalar potential

Often we are interested to a dc-response to a scalar potential ϕ.

From $\vec{E} = -\vec{\nabla}\Phi - \frac{1}{c}\partial_t \vec{A}$, it means we look at the case in which $\vec{E} = -\vec{\nabla}\Phi$ or, if Φ was gauged away, to the case of a pure longitudinal vector potential $\vec{A}$:

$$\vec{A}(\vec{r},t) = -\frac{c}{e}\int_{t_0}^{t} dt' \, \vec{\nabla} V(\vec{r},t') = +c\int_{t_0}^{t} dt' \, \vec{\nabla}\phi$$

$$\text{or } \quad \tilde{\vec{A}}(\vec{q},\omega) = -\frac{c}{e}\,\frac{i\vec{q}}{i\omega}\,\tilde{V}(\vec{q},\omega) = \left(-\frac{ic}{\omega}\tilde{\vec{E}}(\vec{q},\omega)\right) \equiv \vec{A}_L(\vec{q},\omega)$$

$$\tilde{\vec{E}}(\vec{q},\omega) = +e\, i\vec{q}\, \tilde{V}(\vec{q},\omega)$$

$$\tilde{E}_\beta(\vec{q},\omega) = e\, iq_\beta \, \tilde{V}(\vec{q},\omega)$$

The perturbation (3.14) then reads

$$\boxed{\hat{H}^{(t)}_{ext} = -\frac{1}{c}\int d\vec{r}\,'\, \hat{\vec{J}}_p(\vec{r}\,')\cdot \vec{A}_L(\vec{r}\,';t)} \quad (3.14b)$$

Note: This expression is equivalent to (cf. Eq. (3.13))

$$\boxed{\hat{H}'_{ext} = e\int d\vec{r}\,'\, \hat{n}(\vec{r}\,')\,\phi(\vec{r}\,',t)}$$

↳ for a uniform and static electric field

$$\vec{E}(\vec{r},t) = \vec{E} = -\vec{\nabla}\phi \quad \hookrightarrow \quad \phi(\vec{r},t) = -\vec{r}\cdot\vec{E} \qquad (-\vec{\nabla}\phi = (E_x, E_y \ldots$$

Hence $\boxed{\hat{H}'_{ext} = -e\int d\vec{r}\, \hat{n}(\vec{r})\, \vec{r}\cdot\vec{E}}$ (3.14c) ($\hat{n}\vec{r}$ dipole operator)

CURRENT RESPONSE FUNCTION

We wish to evaluate the change $\delta\langle \hat{\vec{J}} \rangle$ due to $\hat{H}_{ext}$ in (3.14);

$$\delta\langle \hat{\vec{J}} \rangle = \langle \hat{\vec{J}} \rangle - \langle \hat{\vec{J}} \rangle_0 = \langle \hat{\vec{J}}_p + \hat{\vec{J}}_d \rangle - \underbrace{\langle \hat{\vec{J}} \rangle_0}_{= 0 \text{ at equilibrium}}$$

moreover

$$\langle \hat{\vec{J}}_d \rangle = -\frac{e^2}{mc} \langle \hat{n}(\vec{r}) \rangle \vec{A}(\vec{r},t) = -\frac{e^2}{mc} \underbrace{\langle \hat{n}(\vec{r}) \rangle_0}_{= n_0(\vec{r})} \vec{A}(\vec{r},t) + o(A^2)$$

$\Rightarrow$ We only need $\langle \vec{J}_p \rangle$. Using Kubo formula

$$\vec{J}_p = \langle \hat{\vec{J}}_p \rangle = -\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt' \, \theta(t-t') \langle [\hat{\vec{J}}_{p,I}(t), \hat{H}_{ext,I}(t')] \rangle_0 \qquad (3.15)$$

and in components

$$\begin{cases} J_{p\alpha}(\vec{r},t) = \langle \hat{J}_{p\alpha}(\vec{r},t) \rangle = -\frac{1}{c} \sum_\beta \int d\vec{r}' \int dt' \, \chi^{R\alpha\beta}_{J_pJ_p}(\vec{r},\vec{r}',t-t') A_\beta(\vec{r}',t') & (3.16) \\ \chi^{R\alpha\beta}_{J_pJ_p}(\vec{r},\vec{r}',t-t') = -\frac{i}{\hbar} \theta(t-t') \langle [\hat{J}_{p\alpha}(\vec{r},t), \hat{J}_{p\beta}(\vec{r}',t')] \rangle_0 & (3.17) \end{cases}$$

paramagnetic current-current response function

By adding the diamagnetic contribution

$$\boxed{\begin{cases} J_\alpha(\vec{r},t) = J_{p\alpha} + J_{d\alpha} = -\frac{1}{c} \sum_\beta \int d\vec{r}' \int_{-\infty}^{+\infty} dt' \, \chi^{\alpha\beta}_J(\vec{r},\vec{r}',t-t') A_\beta(\vec{r}',t') \\ \chi^{\alpha\beta}_J(\vec{r},\vec{r}',t-t') = \chi^{R\alpha\beta}_{J_pJ_p} + \frac{e^2 n_0(\vec{r})}{m} \delta(\vec{r}-\vec{r}')\delta(t-t')\delta_{\alpha\beta} \end{cases}} \quad (3.18)$$

iii) CONDUCTIVITY

From $\vec{E}(\vec{r},t) = -\frac{1}{c}\frac{\partial \vec{A}(\vec{r},t)}{\partial t} \Rightarrow \vec{A}(\vec{r},t) = -c\int_{t_0}^{t} dt' \, \vec{E}(\vec{r},t')$

and hence taking the Fourier transform

$$\tilde{\vec{A}}(\vec{r},\omega) = -\frac{ic}{\omega}\tilde{\vec{E}}(\vec{r},\omega)$$

with $\begin{cases} \mathcal{F}\{a(t)\} = \tilde{a}(\omega) = \int_{-\infty}^{+\infty} dt \, e^{i\omega t} a(t) \\ a(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \tilde{a}(\omega) \end{cases}$

⇒ frequency domain

$$\tilde{J}_\alpha(\vec{r},\omega) = \int_{-\infty}^{+\infty} dt \, e^{i\omega t} J_\alpha(\vec{r},t)$$

and hence

$$\tilde{J}_\alpha(\vec{r},\omega) = -\frac{1}{c}\sum_\beta \int d\vec{r}\,' \tilde{\chi}_J^{\alpha\beta}(\vec{r},\vec{r}\,';\omega)\tilde{A}_\beta(\vec{r}\,',\omega)$$

$$= \frac{i}{\omega}\sum_\beta \int d\vec{r}\,' \tilde{\chi}_J^{\alpha\beta}(\vec{r},\vec{r}\,';\omega) E_\beta(\vec{r}\,',\omega)$$

$$\equiv \sum_\beta \int d\vec{r}\,' \tilde{\sigma}_{\alpha\beta}(\vec{r},\vec{r}\,',\omega)\tilde{E}_\beta(\vec{r}\,',\omega)$$

conductivity tensor, cf. (2.4) !!!

with

$$\boxed{\tilde{\sigma}_{\alpha\beta}(\vec{r},\vec{r}\,',\omega) = \frac{i}{\omega}\tilde{\chi}_J^{\alpha\beta}(\vec{r},\vec{r}\,';\omega) = \frac{i}{\omega}\left[\tilde{\chi}^{\alpha\beta}_{J_pJ_p} + \frac{n_0(\vec{r})e^2}{m}\delta(\vec{r}-\vec{r}\,')\delta_{\alpha\beta}\right]} \quad (3.19)$$

Translational invariant systems: $\sigma_{\alpha\beta}(\vec{r},\vec{r}\,';\omega) = \sigma_{\alpha\beta}(\vec{r}-\vec{r}\,';\omega)$ and $n_0(\vec{r}) = n$

$$\Rightarrow \boxed{\tilde{\sigma}_{\alpha\beta}(\vec{q},\omega) = \frac{i}{\omega}\left(\tilde{\chi}^{\alpha\beta}_{J_pJ_p}(\vec{q},\omega) + \frac{n_0e^2}{m}\delta_{\alpha\beta}\right)} \quad (3.20) \Rightarrow \boxed{\tilde{J}_\alpha(\vec{q},\omega) = \sum_\beta \tilde{\sigma}_{\alpha\beta}(q,\omega)\tilde{E}_\beta(\vec{q}} \quad (3.21)$$

Note: Properties of response functions in $\vec{q}$ space

Define

$$\chi_{AB}(\vec{q},\vec{q}\,';t) \equiv \frac{1}{V}\int d\vec{r}\, e^{-i\vec{q}\cdot\vec{r}} \int d\vec{r}\,'\, e^{i\vec{q}\,'\cdot\vec{r}\,'}\, \chi_{AB}(\vec{r},\vec{r}\,';t)$$

It depends generally on $\vec{q}$ and $\vec{q}\,'$:

$$\chi_{AB}(\vec{q},\vec{q}\,';t) = -\frac{i}{\hbar}\,\theta(t)\,\langle[\hat{A}(+\vec{q}),\hat{B}(-\vec{q}\,')]\rangle$$

i) The case of translational invariant (homogeneous) systems

$$\chi_{AB}(\vec{q},\vec{q}\,';t) = \frac{1}{V}\int d\vec{r}\, e^{-i\vec{q}\cdot\vec{r}} \int d\vec{r}\,'\, e^{i\vec{q}\,'\cdot\vec{r}\,'}\, \chi_{AB}(\vec{r},\vec{r}\,';t)$$

$$= \frac{1}{V}\int d\vec{r}\,'\, e^{-i(\vec{q}-\vec{q}\,')\cdot\vec{r}} \int d\vec{r}\,'\, e^{i\vec{q}\,'\cdot(\vec{r}\,'-\vec{r})}\, \chi_{AB}(\vec{r},\vec{r}\,';t)$$

$$= \frac{1}{V}\int d\vec{r}\; e^{-i\,\vec{q}-\vec{q}\,'\cdot\vec{r}} \underbrace{\int d\vec{r}\,''\, e^{-i\vec{q}\,'\cdot\vec{r}\,''}}_{\vec{r}\,''=\vec{r}-\vec{r}\,'}\; \underbrace{\chi_{AB}(\vec{r}\,'+\vec{r}\,'',\vec{r}\,';t)}_{\text{translational invariant}\to\text{depends on difference}}$$

$$= \delta_{\vec{q},\vec{q}\,'}\int d\vec{r}\,''\, e^{-i\vec{q}\,'\cdot\vec{r}\,''}\,\chi_{AB}(\vec{r}\,'+\vec{r}\,'',\vec{r}\,';t) = \chi_{AB}(\vec{q},t)\,\delta_{\vec{q}\vec{q}\,'}$$

ii) The property $\chi_{AB}(\vec{q},\vec{q}\,';t) = \chi_{AB}(\vec{q},t)\,\delta_{\vec{q}\vec{q}\,'}$

holds true also for disordered "self-averaging" systems. As seen later, for such systems some properties only depend on the impurity density, and not on their location.

DC-limit : $\omega \to 0$

Consider $\tilde{\sigma}_{\alpha\beta}(\vec{q},\omega) = \frac{i}{\omega}\left(\tilde{\chi}^{R\alpha\beta}_{J_pJ_p}(\vec{q},\omega) + \frac{n_0 e^2}{m}\delta_{\alpha\beta}\right)$

Clearly, the diamagnetic term diverges when $\omega \to 0$.

Thus, depending on the low frequency behavior of $\tilde{\chi}^{R}_{J_pJ_p}$,

various cases can occur

i) homogeneous & isotropic systems (Vignale Ch. 3.4)

$$\boxed{\lim_{q\to 0}\lim_{\omega\to 0}\tilde{\chi}^{\alpha\beta}_{J}(\vec{q},\omega=0) = \lim_{q\to 0}\tilde{\chi}^{R\alpha\beta}_{J_pJ_p}(\vec{q},\omega\to 0) + \frac{n_0 e^2}{m}\delta_{\alpha\beta} = 0}$$

known as diamagnetic sum rule :

the real, long wave ($q\to 0$) part of $\tilde{\chi}^{R\alpha\beta}_{J_pJ_p}(\vec{q},\omega=0)$

exactly compensates the diamagnetic part

$$\Rightarrow \lim_{q\to 0}\lim_{\omega\to 0}\tilde{\sigma}_{\alpha\beta}(\vec{q},\omega) = -\lim_{q\to 0}\frac{\mathrm{Im}\,\tilde{\chi}^{R\alpha\beta}_{J_pJ_p}(\vec{q},\omega\to 0)}{\omega}$$

ii) superconductors

due to the presence of long range order, the diamagnetic sum rule does not hold for a superconductor

Electrical conductivity in response to a uniform electric field : $q \to 0$

$$\tilde{\sigma}_{\alpha\beta}(\vec{q}=0,\omega) = \frac{i}{\omega}\left[\tilde{\chi}^{R\,\alpha\beta}_{J_p J_p}(q=0,\omega) + \frac{e^2 n_0}{m}\delta_{\alpha\beta}\right]$$

homogeneous systems

$$\boxed{\tilde{\sigma}_{\alpha\beta}(q=0,\omega) = \frac{ie^2}{\omega}\frac{n_0}{m}\delta_{\alpha\beta}}$$ due to $\tilde{\chi}^{R\,\alpha\beta}_{J_p J_p}(q=0,\omega) = 0$ (*)

$\Rightarrow \lim\limits_{\omega \to 0} \tilde{\sigma}_{\alpha\beta}(0,\omega) = \infty$ i.e. the conductivity is infinite (no dissipation)

$\Rightarrow$ i) impurities are needed to get a finite conductivity

ii) the limits $q \to 0, \omega \to 0$ and $\omega \to 0, q \to 0$ do not commute

superconductors

Similar to the case of a homogeneous electron liquid, also for sc $\tilde{\sigma}_{\alpha\beta}(q=0,\omega)$ is purely imaginary

(this is due to a particular rigidity of the ground state)

(*) consequence of translational invariance $[\hat{H}, \hat{\vec{P}}] = 0$, with $\hat{\vec{P}}$ total momentum operator

For applications : see e.g. conductivity of homogeneous electron gas in the next pages 11f, 11g

↳ behavior of the Lindhard function $\tilde{\chi}_0(\vec{q},\omega)$ (*)

note: diamagnetic sum rule is easy to show in this case cf. page 11g

note: the property

$$\tilde{\chi}^R_{J_p J_p}(\vec{q}=0,\omega) = 0 \qquad \forall\, \omega \neq 0$$

also follows easily for the free electron gas, since the Lindhard function $\tilde{\chi}_0$ is proportional to

$$\frac{f(\varepsilon_{\vec{k}}) - f(\varepsilon_{\vec{k}+\vec{q}})}{(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{q}})/\hbar + \omega + i\eta}$$

note: if $\omega \neq 0$ this quantity is only non zero if

$$k > k_F \quad \& \quad |\vec{k}+\vec{q}| < k_F \quad \Rightarrow \omega < 0$$

$$(\text{or} \quad k < k_F \quad \text{and} \quad |\vec{k}+\vec{q}| > k_F \Rightarrow \omega > 0)$$

This corresponds to the creation of an electron-hole pair in the Fermi gas through emission/absorption of a photon from the electromagn. field

(*) 2nd quantization needed → intermezzo Ch. 3.5

Conductivity of a homogeneous, non interacting, fermionic system

- $\hat{H}_0 = \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}}\, c^+_{\vec{k}\sigma} c_{\vec{k}\sigma}$

$$\hat{n}(\vec{r}) = \frac{1}{V}\sum_{\vec{q}}\sum_{\vec{k}\sigma} \hat{c}^+_{\vec{k}\sigma}\hat{c}_{\vec{k}+\vec{q}\,\sigma}\, e^{i\vec{q}\cdot\vec{r}} \quad \left(= \frac{1}{V}\sum_{\vec{q}}\sum_{\vec{k}\sigma} \hat{c}^+_{\vec{k}-\vec{q}\,\sigma}\hat{c}_{\vec{k}\sigma}\, e^{i\vec{q}\cdot\vec{r}} \right)$$

$$\hat{\vec{J}}_{p\sigma}(\vec{r}) = e\frac{(-i\hbar)}{2m}\left[\hat{\psi}^+_\sigma(\vec{r})\vec{\nabla}\hat{\psi}_\sigma(\vec{r}) - \vec{\nabla}\hat{\psi}^+_\sigma(\vec{r})\hat{\psi}_\sigma(\vec{r})\right]$$

$$\underset{(*)}{=} \frac{\hbar e}{2mV}\sum_{q\vec{k}\sigma}(2\vec{k}+\vec{q})\hat{c}^+_{\vec{k}\sigma}\hat{c}_{\vec{k}+\vec{q}\,\sigma}\, e^{i\vec{q}\cdot\vec{r}} \quad \left(= \frac{\hbar}{2mV}\sum_{\vec{k}\sigma}(2\vec{k}-\vec{q})\hat{c}^+_{\vec{k}-\vec{q}\,\sigma}\hat{c}_{\vec{k}\sigma}\, e^{-i\vec{q}\cdot\vec{r}} \right)$$

(*) cf. Proof page (a)

$\equiv \frac{1}{V}\sum_{\vec{q}} \hat{\vec{J}}_p(q)\, e^{i\vec{q}\cdot\vec{r}}$ operatorial parts of $\hat{n}(\vec{r})$ and $\hat{\vec{J}}_p(\vec{r})$ are the same

- homogeneous gas is translationally invariant $\Rightarrow \chi^{\alpha\beta}(\vec{r},\vec{r}') = f^{\alpha\beta}(\vec{r}-\vec{r}')$

cf page 11.b

$$\chi^{R\alpha\beta}_{J_pJ_p}(\vec{q}, t-t') = \int d\vec{r}\, e^{-i\vec{q}\cdot(\vec{r}-\vec{r}')}\chi^{R\alpha\beta}_{J_pJ_p}(\vec{r}-\vec{r}', t-t')$$

$$= -\frac{i}{\hbar}\theta(t-t')\frac{1}{V}\langle[\hat{J}_{p\alpha}(\vec{q},t), \hat{J}_{p\beta}(-\vec{q},t')]\rangle_0$$

reads proof notes

$$\chi^{R\alpha\beta}_{J_pJ_p} = -\frac{i}{\hbar}\theta(t-t')\frac{\hbar^2 e^2}{4m^2}\frac{1}{V}\sum_{\vec{k}\sigma}\sum_{\vec{k}'\sigma'}(2\vec{k}+\vec{q})_\alpha(2\vec{k}'-\vec{q})_\beta \cdot$$

$$\cdot\langle[\hat{c}^+_{\vec{k}\sigma}(t)\hat{c}_{\vec{k}+\vec{q}\,\sigma}(t), \hat{c}^+_{\vec{k}'\sigma}(t')\hat{c}_{\vec{k}'-\vec{q},\sigma}]\rangle_0$$

$$= -\frac{i}{\hbar}\theta(t-t')\frac{\hbar^2}{4m^2}\frac{e^2}{V}\sum_{\vec{k}'\sigma'}(2\vec{k}'+\vec{q})_\alpha(2\vec{k}'+\vec{q})_\beta\, e^{\frac{i}{\hbar}(\varepsilon_{k'}-\varepsilon_{k'+q})(t-t')}[f(\varepsilon_{\vec{k}'}) - f(\varepsilon_{\vec{k}'+\vec{q}})]$$

$$\boxed{\Rightarrow \tilde{\chi}^{R\alpha\beta}_{J_pJ_p}(\vec{q},\omega) = \frac{1}{\hbar}\frac{\hbar^2 e^2}{4m^2V}\sum_{\vec{k}\sigma}(2\vec{k}+\vec{q})_\alpha(2\vec{k}+\vec{q})_\beta\frac{f(\varepsilon_{\vec{k}}) - f(\varepsilon_{\vec{k}+\vec{q}})}{(\varepsilon_{\vec{k}}-\varepsilon_{\vec{k}+\vec{q}})/\hbar + \omega + i\eta} \equiv e^2\tilde{\chi}_0}$$

$\tilde{\chi}_0(\vec{q},\omega) \equiv$ Lindhard function

long wave length limit $q \to 0$ and static case $\omega \to 0$

$$\lim_{q\to 0} \lim_{\omega \to 0} \chi^{R\,\alpha\beta}_{J_pJ_p}(\vec q,\omega) = -\frac{e^2\hbar}{4m^2V}\sum_{\vec k\sigma} 2k_\alpha 2k_\beta \left(\frac{-\partial f}{\partial \varepsilon}\right)_{\varepsilon=\varepsilon_{\vec k}}$$

$\lim_{q\to 0} \lim_{\omega \to 0} \ne$ order of limits matter

$$= -\frac{e^2\hbar^2}{m^2V}\,\delta_{\alpha\beta}\sum_{\vec k\sigma} k_\alpha k_\beta \left(\frac{-\partial f}{\partial \varepsilon}\right)_{\varepsilon=\varepsilon_k}$$

off-diagonal contribution sums up to zero

$$= -\frac{\hbar^2 e^2}{m^2V}\,\delta_{\alpha\beta}\,\frac{1}{3}\sum_{\vec k\sigma} k^2 \left(\frac{-\partial f}{\partial \varepsilon}\right)_{\varepsilon=\varepsilon_k}$$

homogeneity

$$\Rightarrow \chi^{R\,\alpha\beta}_{J_pJ_p}(q=0,\omega=0) = -\frac{e^2}{m}\,\delta_{\alpha\beta}\,\frac{2}{3V}\sum_{\vec k\sigma}\varepsilon(k)\left(-\frac{\partial f}{\partial \varepsilon}\right)_{\varepsilon=\varepsilon_k}$$

$$= -\frac{e^2}{m}\,\delta_{\alpha\beta}\,\frac{2}{3V}\cdot 2\int d\varepsilon\, \mathcal{D}(\varepsilon)\,\varepsilon\left(-\frac{\partial f}{\partial \varepsilon}\right)$$

$$= -\frac{e^2}{m}\,\delta_{\alpha\beta}\,\frac{4}{3V}\,\mathcal{D}(\varepsilon_F)\,\varepsilon_F$$

low temperatures $-\frac{\partial f}{\partial \varepsilon} \simeq \delta(\varepsilon-\varepsilon_F)$

Remember: $\mathcal{D}(\varepsilon_F) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\varepsilon_F^{1/2}$, $k_F^2 = \frac{2m\varepsilon_F}{\hbar^2}$, $k_F^3 = 3\pi^2 n$

$$\Rightarrow \tilde\chi^{\alpha\beta}_{J_pJ_p}(0,0) = -\frac{e^2}{m}\,n\,\delta_{\alpha\beta}$$

which exactly compensates the diamagnetic contribution!

$$\Rightarrow \boxed{\tilde\chi^{\alpha\beta}_{J}(0,0) = \tilde\chi^{\alpha\beta}_{J_pP}(0,0) + \frac{ne^2}{m}\,\delta_{\alpha\beta} \equiv 0}$$

diamagnetic sum rule

3.4 APPLICATION 2. CONDUCTANCE

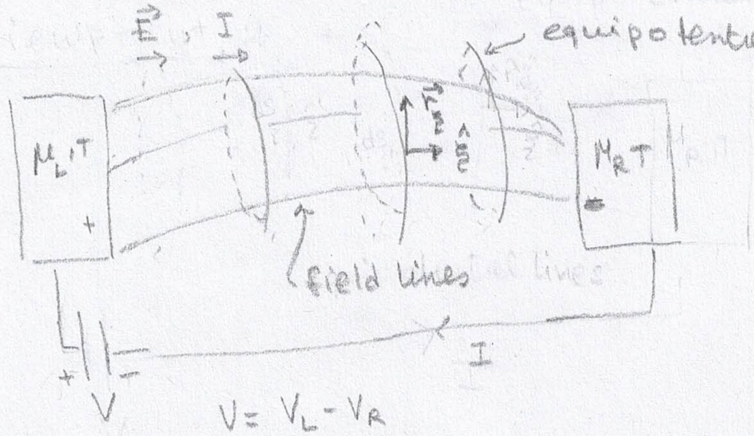
Bruus & Flensberg Ch. 6.3

We have just seen that Kubo formula yields Eq. (3.21),

$$\tilde{J}_\alpha(\vec q, \omega) = \sum_\beta \tilde{\sigma}_{\alpha\beta}(\vec q, \omega)\, E_\beta(\vec q, \omega)$$, with $\tilde{\sigma}_{\alpha\beta}$ the conductivity

being an intrinsic property of the material.

In viewpoint 2. Here we do not look at $\tilde\sigma$ but rather at the conductance, the proportionality between current and voltage. We have already seen that the simple relation $G = \sigma \frac{A}{L}$ might not apply for mesoscopic systems $\Rightarrow$ we must use a Kubo formula for G!



$$I = GV + O(V^2)$$

coordinate system $\vec r_\xi$, $\hat\xi$

$\vec r_\xi \in$ equipotential surface

$\hat\xi \perp$ equipot. surface (// field line)

$\Rightarrow$ G is the linear response coefficient relating I to V

According to (2.1)

$\vec r = (\xi, \vec r_\xi)$

$$I(t) = \int_S d\vec s \cdot \vec J(\vec r, t) = \int_{S_\xi} ds_\xi\, \hat\xi \cdot \vec J(\xi, \vec r_\xi, t) \quad (3.22)$$

where, since the surface is arbitrary, we choose a surface of constant electrostatic potential (equipotential surface) and the coordinate system $(\xi, \vec r_\xi)$

i) DC-response

Due to $\vec{E} = -\vec{\nabla}\phi - \partial_t A(\vec{r},t)$

↳ for a static perturbation, is $\vec{E} = -\vec{\nabla}\phi$;

it follows that $\vec{E}$ vanishes on an equipotential surface

and is perpendicular to it:

$$\vec{E} = \hat{\xi}\, E(\xi) \quad (3.23) \quad (\text{independent of } \vec{r}_\xi)$$

Hence, the stationary current (DC-current) reads

$$\underset{\substack{\uparrow\\ \text{current at position } \xi}}{I_{st}(\xi)} = \int_{S_\xi} dS_\xi\, \hat{\xi}\cdot \vec{J}_{st}(\xi, \vec{r}_\xi) = I_{st} \ \underline{\text{independent of } \xi}\,!^{(*)}$$

or

$$I_{st} = \int_{S_\xi} dS_\xi\, \hat{\xi}\cdot \int d\vec{r}'\, \tilde{\sigma}(\vec{r},\vec{r}';\omega=0)\, \vec{E}(\vec{r}')$$

$$= \int_{S_\xi} dS_\xi\, \hat{\xi}\cdot \int dS_{\xi'} \int d\xi' \lim_{\omega\to 0} \tilde{\sigma}(\xi', \vec{r}_{\xi'}, \xi, \vec{r}_{\xi}, \omega)\, E(\xi')\, \hat{\xi}'$$

Remember Kubo formula for $\tilde{\sigma}(\vec{r},\vec{r}',\omega)$ Eq. (3.19)

$$\left\{ \begin{aligned} &\tilde{\sigma}_{\alpha\beta}(\vec{r},\vec{r}';\omega) = \frac{i}{\omega}\left[\tilde{\chi}^{R\alpha\beta}_{J_pJ_p}(\vec{r},\vec{r}',\omega) + \frac{n_0(\vec{r})e^2\,\delta(\vec{r}-\vec{r}')}{m}\delta_{\alpha\beta}\right] \quad (3.19)\\ &\tilde{\chi}^{R\alpha\beta}_{J_pJ_p}(\vec{r},\vec{r}',t) = -\frac{i}{\hbar}\langle[\hat{J}^\alpha_{p_I}(\vec{r},t), \hat{J}^\beta_{p_I}(\vec{r}',0)]\rangle_0\,\theta(t) \end{aligned}\right.$$

$$\leadsto \tilde{\chi}^R_{J_pJ_p}(\vec{r},\vec{r}',t) = -\frac{i}{\hbar}\theta(t)\langle[\hat{\vec{J}}_{p_I}(\vec{r},t), \hat{\vec{J}}_{p_I}(\vec{r}',0)]\rangle_0$$

(*) can be seen from the continuity equation

Further, since the current is real, what determines it is the real part of the first term in (3.19) (*)

$$\Rightarrow I_{st}(\xi) = I_{st} = \lim_{\omega \to 0} \int d\xi' \, \mathrm{Re}\left[\frac{i}{\omega} \tilde{\chi}^R_{I(\xi) I(\xi')}(\omega) \right] E(\xi') \quad (3.24)$$

Because of current conservation, the DC-current may be calculated at any point and is independent of ξ ⇒ also $\chi^R_{I(\xi)I(\xi')}$ cannot depend on ξ. Similarly, because of the reciprocity relation (cf. Eq. (3.9) for $\omega = 0$)

$$\tilde{\chi}^R_{AB}(\omega=0) = \tilde{\chi}^R_{BA}(\omega=0),$$

the function $\tilde{\chi}^R_{I(\xi)I(\xi')}(\omega \to 0)$ cannot depend on ξ' either

$$\vec{E} = -\vec{\nabla}\Phi$$

$$\Rightarrow I_e = \lim_{\omega \to 0} \mathrm{Re}\left[\frac{i}{\omega} \tilde{\chi}^R_{II}(\omega) \right] \int d\xi' \, E(\xi') = -(\Phi_R - \Phi_L) = \Phi_L - \Phi_R =$$

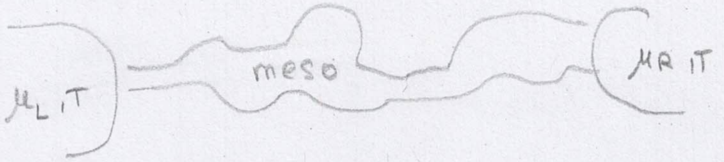
$$= \lim_{\omega \to 0} \mathrm{Re}\left[\frac{i}{\omega} \chi^R_{II}(\omega) \right] [V] \equiv G V$$

$$\Rightarrow \boxed{G = \lim_{\omega \to 0} \mathrm{Re}\left[\frac{i}{\omega} \tilde{\chi}^R_{II}(\omega) \right]} \; (3.26) \text{ with } \boxed{\chi^R_{II}(t) = -\frac{i}{\hbar}\theta(t)\langle[\hat{I}(t), \hat{I}(0)]\rangle_0} \; (3.25)$$

(*) What about the contribution coming from $\mathrm{Im}\,\tilde{\sigma}$?

Fazit: the expression (3.26) with (3,25) are very general and applicable to any mesoscopic system

We have mapped the nonequilibrium transport problem onto a global equilibrium one



$\mu_L = \mu_0 + \eta_L eV$

$\mu_R = \mu_0 + \eta_R eV$

linear response $eV \to 0$

$\mu_L - \mu_R = (\eta_L - \eta_R) eV \equiv eV$

e.g. $\eta_L = 1/2$, $\eta_R = -1/2$

global equilibrium properties of mesoscopic conductor with a fermionic bath of chemical potential μ_0 & temperature T

Summary:

$$G = \lim_{\omega \to 0} \mathrm{Re}\left[\frac{i}{\omega} \tilde{\chi}_{II}(\omega)\right] \qquad (3.26)$$

with

$$\chi^R_{II}(t) = -\frac{i}{\hbar} \theta(t) \langle [\hat{I}(t), \hat{I}(0)] \rangle_0 \qquad (3.25)$$

current-current response function

and

$$\langle \cdots \rangle_0 = \mathrm{Tr}\{\hat{\rho} \cdots\} \quad \text{and} \quad \hat{\rho} = \frac{e^{-\beta(\hat{H} - \mu_0 \hat{N})}}{Z}$$

grandcanonical density operator

Finally, $\hat{H}$ is the Hamiltonian of the mesoscopic conductor + reservoirs ; $\hat{N}$ is the total particle number

Outlook . The formula we have derived is very general and can be used to derive the conductance of any mesoscopic system.

In the following chapter 4 we shall use it to describe ballistic & noninteracting mesoscopic conductors.

One application will be e.g. again the Quantum point contact (QPC) but also more complicated geometries.

. Prerequisite for doing this is to express the Hamiltonian $\hat{H}$ and the particle operator $\hat{N}$ in second quantization

Likewise, for the operators

$$\hat{\vec{J}}(\vec{r},t) \quad , \quad \hat{n}(\vec{r},t) \quad , \quad \hat{I}(\vec{r},t)$$

current density   density   current

3.5 INTERMEZZO : SECOND QUANTIZATION

Consider a system of N particles described by one-body and two-body operators. A standard example are N interacting electrons

$$\hat{H} = \underbrace{\sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \sum_{i=1}^{N} u(\vec{r}_i)}_{1\text{-body } \hat{T}+\hat{U}=\hat{H}_0} + \underbrace{\frac{1}{2}\sum_{i\neq j} v(\hat{\vec{r}}_i - \hat{\vec{r}}_j)}_{2\text{-body } \hat{V}} \qquad (3.27)$$

To express $\hat{H}$ in second quantization we need to specify

i) the statistics of the particle ⇝ fermions / bosons

ii) to choose a complete set $\{|\lambda\rangle\}$ of single-particle states

It is convenient to group 1-body operators in a 1-body Hamiltonian $\hat{H}_0$:

$$\hat{T} = \sum_{i=1}^{N} \hat{t}_i = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} \quad , \quad \hat{H}_0 = \hat{T} + \hat{U} = \sum_{i=1}^{N} \hat{h}_i \qquad (3.28)$$

The full Hamiltonian $\hat{H} = \hat{H}_0 + V$ then reads in 2nd Q

$$\boxed{\hat{H} = \sum_{\mu\lambda} \varepsilon_{\mu\lambda}\, \hat{c}^+_\mu \hat{c}_\lambda + \frac{1}{2}\sum_{\mu\mu'\lambda\lambda'} v_{\mu\mu'\lambda\lambda'}\, \hat{c}^+_\mu \hat{c}^+_{\mu'} \hat{c}_{\lambda'} \hat{c}_\lambda} \qquad (3.29)$$

with

$$\varepsilon_{\mu\lambda} = \langle\mu|\hat{h}|\lambda\rangle = \langle\mu|\hat{t}+\hat{u}|\lambda\rangle \quad , \quad v_{\mu\mu'\lambda\lambda'} = \langle\mu|\langle\mu'|\hat{v}|\lambda\rangle|\lambda'\rangle$$

$\Rightarrow$ $\varepsilon_{\mu\lambda}$ and $v_{\mu\mu',\lambda\lambda'}$ are the matrix elements of the operators $\hat{h} = \hat{t} + \hat{u}$ and $\hat{v}$ in the chosen basis.

- The statistics enters through the requirements

$$[\hat{c}_\lambda, \hat{c}^+_\mu]_\xi = \hat{c}_\lambda \hat{c}^+_\mu + \xi\, \hat{c}^+_\mu \hat{c}_\lambda = \delta_{\lambda\mu} \qquad (3.30)$$

with $\xi = \pm$ for fermions / bosons

For further details $\Rightarrow$ lecture notes on 2nd Q.