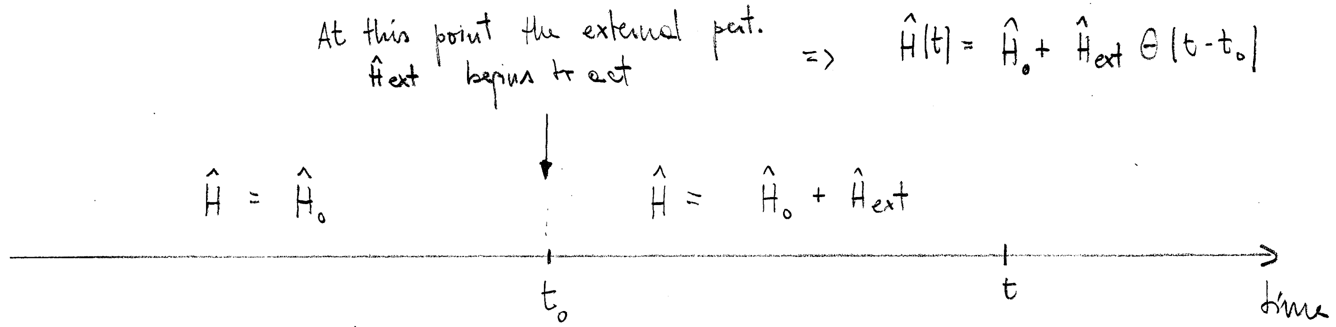
CHAPTER 8: LINEAR RESPONSE THEORY

The linear response theory is based on the idea that the response of a system to a weak perturbation is proportional to the perturbation itself. (e.g. $\rho_{ind,e} = \chi \phi_{ext}$). The general question one needs to answer is thus:

Given an external perturbation $\hat{H}_{ext}$ (e.g. an external electric or magnetic field) what is the expectation value $\langle \hat{A} \rangle$ of a given observable $\hat{A}$ to linear order in $\hat{H}_{ext}$?



Thermal equilibrium

$\langle \hat{A} \rangle_0 = \mathrm{Tr}\{\hat{A}\hat{\rho}_0\} = Z_0^{-1}\mathrm{Tr}\{\hat{A}e^{-\beta\hat{H}_0}\}$

Non-equilibrium state

$\langle \hat{A}(t) \rangle = \mathrm{Tr}\{\hat{A}\hat{\rho}(t)\} = ?$

8.1 The general Kubo formula

The solution to the problem is the general Kubo formula which we will derive here. Notice: we consider $\hat{H}_{ext}$ as a weak perturbation $\Rightarrow$ it is convenient to work with deviations from equilibrium. In other terms we solve the Liouville-von Neumann Eq. for $\hat{\rho}(t) = \hat{\rho}_0 + \delta\hat{\rho}(t)$. We start with:

$$\dot{\hat{\rho}}(t) = -\frac{i}{\hbar}[\hat{H}(t), \hat{\rho}(t)] = -\frac{i}{\hbar}[\hat{H}_0, \delta\hat{\rho}(t)] - \frac{i}{\hbar}[\hat{H}_{ext}(t), \hat{\rho}_0] + O(\hat{H}_{ext}^2) \quad (8.1)$$

where we have assumed that, we are only interested into the linear component of $\Delta\hat{\rho}$. Eq. (8.1) can be also written as:

$$i\Delta\dot{\hat{\rho}}(t) - \frac{1}{\hbar}[\hat{H}_0, \delta\hat{\rho}(t)] = \frac{1}{\hbar}[\hat{H}_{ext}(t), \hat{\rho}_0] \quad (8.2)$$

The differential equation (8.2) is solved by converting the LHS into:

$$e^{-\frac{i}{\hbar}\hat{H}_0 t}\left\{ i\frac{d}{dt}\left(e^{\frac{i}{\hbar}\hat{H}_0 t}\,\delta\hat{\rho}(t)\,e^{-\frac{i}{\hbar}\hat{H}_0 t}\right)\right\} e^{\frac{i}{\hbar}\hat{H}_0 t} = +\frac{1}{\hbar}\left[H_{ext}(t),\rho_0\right]$$

$\Downarrow$

$$i\frac{d}{dt}\left(e^{i/\hbar\,\hat{H}_0 t}\,\delta\hat{\rho}(t)\,e^{-i/\hbar\,\hat{H}_0 t}\right) = \frac{1}{\hbar}\,e^{i/\hbar\,\hat{H}_0 t}\left[H_{ext}(t),\rho_0\right]e^{-\frac{i}{\hbar}\hat{H}_0 t}$$

$\Downarrow$ By introducing the INTERACTION REPRESENTATION $\hat{O}_I(t) = e^{i\frac{\hat{H}_0 t}{\hbar}}\,\hat{O}_S(t)\,e^{-i\frac{\hat{H}_0 t}{\hbar}}$

$$\delta\dot{\rho}_I(t) = -\frac{i}{\hbar}\left[H_{ext,I}(t),\rho_0\right] \qquad (8.3)$$

Eq. (8.3) can be now easily solved by integration of both sides:

$$\delta\hat{\rho}_I(t) - \delta\hat{\rho}_I(t_0) = -\frac{i}{\hbar}\int_{t_0}^{t} dt'\left[\hat{H}_{ext,I}(t'),\hat{\rho}_0\right]$$

Having chosen t_0 as the initial time for integration $\delta\hat{\rho}_I(t_0) = 0$ and we can further proceed:

$$\delta\hat{\rho}(t) = -\frac{i}{\hbar}\int_{t_0}^{t} dt'\,e^{-i\hat{H}_0(t-t')/\hbar}\left[\hat{H}_{ext}(t'),\hat{\rho}_0\right]e^{+i\hat{H}_0(t-t')/\hbar}$$

Eventually, we calculate the response on the observable $\hat{A}(t)$

$$\delta\langle\hat{A}(t)\rangle \equiv \langle\hat{A}(t)\rangle - \langle\hat{A}(t)\rangle_0 \equiv \mathrm{Tr}\left\{\hat{A}(t)\,\delta\hat{\rho}(t)\right\} =$$

$$= -\frac{i}{\hbar}\int_{t_0}^{t} dt'\,\mathrm{Tr}\left\{\hat{A}(t)\,e^{-i\hat{H}_0(t-t')/\hbar}\left[\hat{H}_{ext}(t'),\hat{\rho}_0\right]e^{+i\hat{H}_0(t-t')/\hbar}\right\}$$

$$= -\frac{i}{\hbar}\int_{t_0}^{t} dt'\,\mathrm{Tr}\left\{\hat{A}_I(t)\left[\hat{H}_{ext,I}(t'),\rho_0\right]\right\} =$$

$$= -\frac{i}{\hbar}\int_{t_0}^{t} dt'\,\mathrm{Tr}\left\{\hat{A}_I(t)\,\hat{H}_{ext,I}(t')\,\hat{\rho}_0 - \underbrace{\hat{A}_I(t)\,\hat{\rho}_0\,\hat{H}_{ext,I}(t')}_{\text{cyclic property of the trace}}\right\}$$

Finally, one obtains the celebrated general Kubo formula (1957)

$$\begin{cases} \delta\langle \hat{A}(t)\rangle = \int_{t_0}^{\infty} dt' \, C^R_{AH_{ext}}(t,t') \\ \\ C^R_{AH_{ext}}(t,t') \equiv -\frac{i}{\hbar}\Theta(t-t')\left\langle \left[\hat{A}_I(t), \hat{H}_{ext,I}(t')\right]\right\rangle_0 \end{cases} \qquad (8.4)$$

← retarded correlator function

Notice:

- The inherent non-equilibrium quantity $\delta\langle \hat{A}(t)\rangle$ is expressed as a retarded correlation function of the system in equilibrium
- $\Theta(t-t')$ expresses the causality of the solution. i.e. the effects at time t can only be produced by causes at time $t' \leq t$.

Let us now consider the case in which $\hat{H}ext(t) = \hat{B} f(t)$, where $\hat{B}$ is a time independent operator and $f(t)$ is a c-number. Moreover we also assume that the observable $\hat{A}$ is NOT explicitly time dependent

$$\delta\langle A(t)\rangle = \int_{t_0}^{\infty} dt' \, -\frac{i}{\hbar}\Theta(t-t')\left\langle\left[\hat{A}_I(t), \hat{B}_I(t')\right]\right\rangle_0 f(t')$$

and

$$C^R_{AB}(t,t') = -\frac{i}{\hbar}\Theta(t-t')\left\langle\left[\hat{A}_I(t), \hat{B}_I(t')\right]\right\rangle_0 \underset{\uparrow}{=} C^R_{AB}(t-t')$$

cyclic inv of trace

It then follows, for $t_0 \to -\infty$

$$\widetilde{\delta\langle \hat{A}(\omega)\rangle} \equiv \int_{-\infty}^{+\infty} dt \, e^{i\omega t}\,\delta\langle \hat{A}(t)\rangle = \tilde{C}^R_{AB}(\omega)\,\tilde{f}(\omega) \qquad (8.5)$$

Notice:

- The usual definition of the Fourier transform would prescribe

$$\tilde{C}^R_{AB}(\omega) = \int_{-\infty}^{+\infty} dt \, e^{i\omega t}\, C^R_{AB}(t)$$

Since $C^R_{AB}(t)=0$ for $t<0$, convergence problems <u>could</u> arise only for $t\to\infty$. The problem is solved by inserting an infinitesimal convergence factor $\eta = 0^+$:

$$\tilde{C}^R_{AB}(\omega) = \int_{-\infty}^{+\infty} dt\; e^{i(\omega+i\eta)t}\, C^R_{AB}(t) \tag{8.6}$$

- When the external perturbation is position dependent

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

one readily finds $\quad \delta\widetilde{\langle \hat{A}(\omega)\rangle} = \int d\vec{r}\; \tilde{C}^R_{AB}(\omega,\vec{r})\, f(\vec{r},t)$

8.2 The Lehmann representation

Often correlation functions, like those entering the Kubo formula (8.4) cannot be calculated exactly because the eigenstates $\{|n\rangle\}$ and the eigenvalues $\{E_n\}$ of H_0 on which the trace has to be taken, are not known. Nevertheless, simply using the basis set $\{|n\rangle\}$ general properties of the correlation function can be demonstrated.

Let's consider the case of time independent (explicitly) operators:

$$C^R_{AB}(t,t') = -\frac{i}{\hbar}\theta(t-t')\, Z_0^{-1}\, \mathrm{Tr}\Big\{ e^{-\beta \hat{H}_0}\Big[e^{i/\hbar \hat{H}_0 t}\, \hat{A}\, e^{-i/\hbar \hat{H}_0(t-t')}\, \hat{B}\, e^{-i/\hbar \hat{H}_0 t'} - e^{i/\hbar \hat{H}_0 t'}\, \hat{B}\, e^{-i/\hbar \hat{H}_0(t'-t)}\, \hat{A}\, e^{-i/\hbar \hat{H}_0 t}\Big]\Big\} =$$

$$= -\frac{i}{\hbar}\theta(t-t')\, Z_0^{-1}\sum_{nn'} e^{-\beta E_n}\Big\{ \langle n|\hat{A}|n'\rangle\langle n'|\hat{B}|n\rangle\, e^{\frac{i}{\hbar}[(E_n-E_{n'})t + (E_{n'}-E_n)t']} + \\ - \langle n|\hat{B}|n'\rangle\langle n'|\hat{A}|n\rangle\, e^{\frac{i}{\hbar}[(E_n-E_{n'})t' + (E_{n'}-E_n)t]}\Big\}$$

$$= -\frac{i}{\hbar}\theta(t-t')\, Z_0^{-1}\sum_{nn'} e^{-\beta E_n}\Big\{ A_{nn'}B_{n'n}\, e^{+\frac{i}{\hbar}(E_n-E_{n'})(t-t')} - B_{nn'}A_{n'n}\, e^{\frac{i}{\hbar}(E_{n'}-E_n)(t-t')}$$

In other words, with $\tau = t - t'$

$$\tilde{C}^R_{AB}(\omega) = \int_{-\infty}^{+\infty} d\tau \, e^{i\omega\tau - \eta\tau} \, C^R_{AB}(\tau) =$$

$$= -\frac{i}{\hbar} \int_0^\infty d\tau \, e^{i\tau(\omega + i\eta)} \frac{1}{Z_0} \sum_{nn'} A_{nn'} B_{n'n} \left(e^{-\beta E_n + \frac{i}{\hbar}(E_n - E_{n'})\tau} + e^{-\beta E_{n'} + \frac{i}{\hbar}(E_n - E_{n'})\tau} \right)$$

$$= \frac{1}{Z_0} \sum_{nn'} \frac{\langle n | A | n' \rangle \langle n' | B | n \rangle}{\hbar\omega + E_n - E_{n'} + i\eta} \left(e^{-\beta E_n} - e^{-\beta E_{n'}} \right) \qquad (8.7)$$

Eq. (8.7) is the Lehmann representation of the retarded correlator C^R_{AB}.
Finally, by recalling the relation $\frac{1}{\omega + i\eta} = \mathcal{P}\left(\frac{1}{\omega}\right) - i\pi\delta(\omega)$ we obtain, for the autocorrelator $\tilde{C}^R_{AA}$

$$-\mathrm{Im}\, \tilde{C}^R_{AA}(\omega) = \frac{1}{Z_0} \sum_{nn'} |\langle n | A | n' \rangle|^2 \left(e^{-\beta E_n} - e^{-\beta E_{n'}} \right) \delta(\hbar\omega - (E_{n'} - E_n)) \qquad (8.8)$$

which, through the δ function, carries informations about the excitation energies of the system.

8.3 Application of the Kubo formula: the dielectric properties of solids

When dealing with charged particles, like for example the interacting electron gas, one is interested into its response to an external electro-magnetic perturbation $\varphi_{ext}(\vec{r}, t)$

i) The charge is redistributed and the system gets polarized

ii) The polarization induces a screening of the perturbation itself.

The $T\to 0$ limit of the (8.8) is important to understand it's role in the excitation processes:

$$\lim_{T\to 0} -\mathrm{Im}\,\tilde{C}^{R}_{AA}(\omega) = \lim_{T\to 0} \sum_{nn'} \frac{1}{Z_0} |\langle n|A|n'\rangle|^2 e^{-\beta E_n}\left(1 - e^{-\beta(E_{n'}-E_n)}\right)\delta(\hbar\omega-(E_{n'}-E_n))$$

$$= \lim_{T\to 0} \sum_{nn'} \frac{|\langle n|A|n'\rangle|^2}{\sum_m e^{-\beta E_m}} e^{-\beta E_n}\left(1 - \cancel{e^{-\beta\hbar\omega}}\right)\delta(\hbar\omega-(E_{n'}-E_n))$$

$$= \sum_n |\langle 0|A|n\rangle|^2\,\delta(\hbar\omega-(E_n-E_0)) .$$

Where $|0\rangle$ is the ground state associated to the ground state energy E_0 and we have factorized at numerator and denominator $e^{-\beta E_0}$ to exclude from the original sum the excited n states.

Definition: The (nonlocal) dielectric function or permittivity $\varepsilon(\vec{r},t;\vec{r}',t')$ expresses the proportionality between the external and the total potential:

$$\varphi_{ext}(\vec{r},t) = \int d\vec{r}' \int dt' \; \varepsilon(\vec{r},t;\vec{r}',t')\,\varphi_{tot}(\vec{r}',t') \tag{8.9}$$

Our purpose is to find ε within the linear response theory. To this end we introduce the external perturbation:

$$\begin{cases} \hat{H}_{ext} = \int d\vec{r}\; \varphi_{ext}(\vec{r},t)\,\hat{\rho}_e(\vec{r}) \\ \hat{\rho}_e(\vec{r}) = e\,\hat{\rho}(\vec{r}) \end{cases} \tag{8.10}$$

e: elementary charge; $\hat{\rho}$: particle density.

The variation of the charge density distribution due to the external perturbation is the induced charge:

$$\rho_{e,ind} = \delta\langle\hat{\rho}_e\rangle = \langle\hat{\rho}_e\rangle - \langle\hat{\rho}_e\rangle_0 \tag{8.11}$$

A direct application of the general Kubo formula (8.4) yields

$$\begin{cases} \rho_{e,ind} = \int d\vec{r}' \int_{t_0}^{\infty} dt' \; C^R_{\rho_e(\vec{r})\rho_e(\vec{r}')}(t,t')\,\varphi_{ext}(\vec{r}',t') \\ C^R_{\rho_e(\vec{r})\rho_e(\vec{r}')}(t,t') = -\frac{i}{\hbar}\,\theta(t-t')\,\langle[\hat{\rho}_{e,I}(\vec{r},t),\hat{\rho}_{e,I}(\vec{r}',t')]\rangle_0 \end{cases} \tag{8.12}$$

$\leftarrow$ density-density correlation function

Definition: The polarization function or polarizability $\chi^R(\vec{r},t;\vec{r}',t')$ expresses the proportionality between the induced charge density and the external potential:

$$\rho_{e,ind} = \int d\vec{r}' \int_{t_0}^{\infty} dt' \; \chi^R(\vec{r},t;\vec{r}',t')\,\varphi_{ext}(\vec{r}',t') \tag{8.13}$$

The comparison between (8.12) and (8.13) shows immediately:

$$\chi^R(\vec{r},t;\vec{r}',t') \equiv C^R_{\rho_e(\vec{r}),\rho_e(\vec{r}')}(t,t') = -\frac{i}{\hbar}\Theta(t-t')\langle[\hat{\rho}_{e,I}(\vec{r},t),\hat{\rho}_{e,I}(\vec{r},t')]\rangle;$$

(8.14)

Once the induced charge density is known, the induced potential follows:

$$\varphi_{ind}(\vec{r},t) = \int d\vec{r}'\, u_{ee}(\vec{r}-\vec{r}')\,\rho_{ind}(\vec{r}',t) \tag{8.15}$$

where $u_{ee}(\vec{r}) = \frac{1}{4\pi\varepsilon_0|\vec{r}|}$ is the Coulomb interaction. The total potential is the sum of the external and the induced one:

$$\varphi_{tot}(\vec{r},t) = \varphi_{ext}(\vec{r},t) + \int d\vec{r}'\int d\vec{r}''\int_{t_0}^{\infty} dt'\, u_{ee}(\vec{r}-\vec{r}')\,\chi^R(\vec{r}',t;\vec{r}'',t')\,\varphi_{ext}(\vec{r}'',t')$$

$$\Rightarrow \quad \varepsilon^{-1}(\vec{r},t;\vec{r}',t') = \delta(\vec{r}-\vec{r}')\,\delta(t-t') + \int d\vec{r}''\, u_{ee}(\vec{r}-\vec{r}'')\,\chi^R(\vec{r}'',t;\vec{r}',t')$$

(8.16)

In presence of time and space translationally invariant systems

$$\chi^R(\vec{r},t;\vec{r}',t') \equiv \chi^R(\vec{r}-\vec{r}';t-t')$$

It follows that

$$\tilde{\varphi}_{tot}(\vec{q},\omega) = \tilde{\varepsilon}^{-1}(\vec{q},\omega)\,\tilde{\varphi}_{ext}(\vec{q},\omega)$$

or

$$\tilde{\varphi}_{ext}(\vec{q},\omega) = \tilde{\varepsilon}(\vec{q},\omega)\,\tilde{\varphi}_{tot}(\vec{q},\omega)$$

with

$$\begin{cases} \tilde{\varepsilon}^{-1}(\vec{q},\omega) = 1 + \tilde{u}_{ee}(\vec{q})\,\tilde{\chi}^R(\vec{q},\omega) \\ \tilde{u}_{ee}(\vec{q}) = \frac{1}{\varepsilon_0 q^2} \end{cases} \tag{8.16b}$$

More specifically, how does the density-density correlator look like for translationally invariant systems?

We know that

$$\chi^R(\vec{r},t;\vec{r}',t') = \chi^R(\vec{r}-\vec{r}',t-t')$$

$$\vec{R} = (\vec{r}+\vec{r}')/2$$
$$\vec{\rho} = \vec{r}-\vec{r}'$$

$$\tilde{\chi}^R(\vec{q},t-t') = \frac{1}{V}\int d\vec{r}'\int d\vec{r}\;\chi^R(\vec{r}-\vec{r}',t-t')\,e^{-i\vec{q}(\vec{r}-\vec{r}')} =$$

$$= -\frac{i}{\hbar}\theta(t-t')\frac{1}{V}\int d\vec{R}\int d\vec{\rho}\;\langle[\hat{\rho}_{e,I}(\vec{R}+\tfrac{\vec{\rho}}{2},t),\hat{\rho}_{e,I}(\vec{R}-\tfrac{\vec{\rho}}{2},t')]\rangle_0\,e^{-i\vec{q}\cdot\vec{\rho}}$$

$$= -\frac{i}{\hbar}\theta(t-t')\frac{1}{V}\int d\vec{R}\int d\vec{\rho}\;\frac{1}{V^2}\sum_{\vec{q}_1\vec{q}_2}\langle[\hat{\rho}_{e,I}(\vec{q}_1,t),\hat{\rho}_{e,I}(\vec{q}_2,t')]\rangle_0\,.$$

$$e^{-i\vec{q}\vec{\rho}\;+i\vec{q}_1(\vec{R}+\frac{\vec{\rho}}{2})+i\vec{q}_2(\vec{R}-\frac{\vec{\rho}}{2})}$$

We analyze the integrals over $\vec{\rho}$ and $\vec{R}$

$$\frac{1}{V^3}\int d\vec{\rho}\int d\vec{R}\;\exp\left[i\vec{R}(\vec{q}_1+\vec{q}_2)+i\vec{\rho}\left(-\vec{q}+\frac{\vec{q}_1-\vec{q}_2}{2}\right)\right]$$

$$= \frac{1}{V^2}\int d\vec{\rho}\;\delta_{\vec{q}_1,-\vec{q}_2}\,e^{+i\vec{\rho}(\vec{q}_1-\vec{q})} = \frac{1}{V}\delta_{\vec{q}_1,\vec{q}}\,\delta_{\vec{q}_2,-\vec{q}}$$

All together

$$\tilde{\chi}^R(\vec{q},t-t') = -\frac{i}{\hbar}\theta(t-t')\frac{1}{V}\langle[\hat{\rho}_{e,I}(\vec{q},t),\hat{\rho}_{e,I}(-\vec{q},t')]\rangle_0 \qquad (8.17)$$

Notice that $\langle\;\rangle_0$ refers to the Hamiltonian in absence of the perturbation φ_{ext} but it <u>can include</u> e.g. the Coulomb interaction if the interacting e-gas is considered.

$\boxed{8.4}$ <u>Permittivity of a "free electron" gas</u>

As a first application of the Kubo formula let us calculate χ for a free el. gas.

$$\tilde{\chi}^R_0(\vec{q},t-t') = -\frac{i}{\hbar}\theta(t-t')\frac{1}{V}\langle[\hat{\rho}_{e,I}(\vec{q},t),\hat{\rho}_{e,I}(-\vec{q},t')]\rangle_0$$

$$\hat{H}_0 = \sum_{\vec{k}\sigma}\varepsilon_{\vec{k}}\,a^+_{\vec{k}\sigma}a_{\vec{k}\sigma} \Rightarrow \hat{\rho}_e(\vec{q},t) = -e\sum_{\vec{k}\sigma}a^+_{\vec{k}\sigma}a_{\vec{k}+\vec{q},\sigma}\,e^{\frac{i}{\hbar}(\varepsilon_{\vec{k}}-\varepsilon_{\vec{k}+\vec{q}})t}$$

(8.18)

It follows, for the polarizability:

$$\tilde{\chi}_0^R(\vec{q},t-t') = -\frac{i}{\hbar}\theta(t-t')\,\frac{e^2}{V}\sum_{\substack{\vec{k},\vec{k}'\\ \sigma,\sigma'}} \langle [a^+_{\vec{k}\sigma}a_{\vec{k}+\vec{q}\sigma},\, a^+_{\vec{k}'\sigma'}a_{\vec{k}'-\vec{q}\sigma'}]\rangle_0 \;\times$$

$$\times\; e^{i/\hbar(\varepsilon_{\vec{k}}-\varepsilon_{\vec{k}+\vec{q}})t + i/\hbar(\varepsilon_{\vec{k}'}-\varepsilon_{\vec{k}'-\vec{q}})t'}$$

$$= -\frac{i}{\hbar}\,\Theta(t-t')\,\frac{e^2}{V}\sum_{\vec{k}\sigma}\left[f(\varepsilon_{\vec{k}})-f(\varepsilon_{\vec{k}+\vec{q}})\right] e^{i/\hbar(\varepsilon_{\vec{k}}-\varepsilon_{\vec{k}+\vec{q}})(t-t')}$$

(8.19)

The second equality in eq. (8.19) is proven observing that

i) $$[a^+_\nu a_\mu,\, a^+_{\nu'}a_{\mu'}] = a^+_\nu [a_\mu,\, a^+_{\nu'}a_{\mu'}] + [a^+_\nu,\, a^+_{\nu'}a_{\mu'}]\,a_\mu$$

$$= -a^+_\nu\Big(a^+_{\nu'}\cancel{\{a_{\mu'},a_\mu\}} - \overbrace{\{a^+_{\nu'},a_\mu\}}^{\delta_{\nu'\mu}}a_{\mu'}\Big) +$$

$$-\,a^+_{\nu'}\underbrace{\{a_{\mu'},a^+_\nu\}}_{\delta_{\mu'\nu}}a_\mu + \cancel{\{a^+_{\nu'},a^+_\nu\}}a_{\mu'}a_\mu =$$

$$= a^+_\nu a_{\mu'}\delta_{\nu'\mu} - a^+_{\nu'}a_\mu\delta_{\mu'\nu}$$

Thus, for our case $[a^+_{\vec{k}\sigma}a_{\vec{k}+\vec{q}\sigma},\, a^+_{\vec{k}'\sigma'}a_{\vec{k}'-\vec{q}\sigma'}] =$

$$= a^+_{\vec{k}\sigma}a_{\vec{k}'-\vec{q}\sigma'}\,\delta_{\sigma\sigma'}\delta_{\vec{k}+\vec{q},\vec{k}'} - a^+_{\vec{k}'\sigma'}a_{\vec{k}+\vec{q}\sigma}\,\delta_{\sigma\sigma'}\delta_{\vec{k},\vec{k}'-\vec{q}}$$

$$= \left(a^+_{\vec{k}\sigma}a_{\vec{k}\sigma} - a^+_{\vec{k}+\vec{q}\sigma}a_{\vec{k}+\vec{q}\sigma}\right)\delta_{\sigma\sigma'}\delta_{\vec{k}+\vec{q},\vec{k}'} \qquad (8.19b)$$

ii) $\langle a^+_{\vec{k}\sigma}a_{\vec{k}\sigma}\rangle_0 = f(\varepsilon_{\vec{k}})$ where f is the Fermi distribution

From (8.19) we obtain the polarizability in the frequency momentum space:

$$\tilde{\chi}_0^R(\vec{q},\omega) = -\frac{i}{\hbar}\int_0^\infty d\tau\, e^{i\omega\tau}\,\frac{e^2}{V}\sum_{\vec{k}\sigma} f(\varepsilon_{\vec{k}})-f(\varepsilon_{\vec{k}+\vec{q}})\; e^{\frac{i}{\hbar}(\varepsilon_{\vec{k}}-\varepsilon_{\vec{k}+\vec{q}})\tau}\, e^{-\eta\tau}$$

$$= \frac{e^2}{\hbar V}\sum_{\vec{k}\sigma}\frac{[f(\varepsilon_{\vec{k}})-f(\varepsilon_{\vec{k}+\vec{q}})]}{\frac{\varepsilon_{\vec{k}}-\varepsilon_{\vec{k}+\vec{q}}}{\hbar}+\omega+i\eta} \quad \leftarrow \text{Lindhard function} \qquad (8.20)$$

It is useful to study the Lindhard function.

i) In the static, long wavelength limit: $\omega = 0$ $\vec{q} \to 0$

$$\chi_0^R(\vec{q},0) \xrightarrow[\vec{q}\to 0]{} 2e^2 \int \frac{d\vec{k}}{(2\pi)^3} \frac{\left(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}}\right)\frac{\partial f}{\partial \varepsilon_k}}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}}} = - \int d\varepsilon_{\vec{k}}\, d(\varepsilon_{\vec{k}}) \left[-\frac{\partial f}{\partial \varepsilon_k} \right]$$

$$\simeq - d(\varepsilon_F) \quad \text{since} \quad -\frac{\partial f}{\partial \varepsilon_k} \stackrel{\sim}{=} \delta(\varepsilon_k - \varepsilon_F)$$

ii) If we focus on the $\mathrm{Re}\, \chi_0^R(\vec{q},\omega)$ $k_B T \ll \varepsilon_F$

$$\mathrm{Re}\, \tilde{\chi}_0^R(\vec{q},\omega) = -\frac{e^2}{\hbar} \mathcal{P}\int_0^{k_F} \frac{dk}{2\pi^2} k^2 \int_{-1}^{1} d\lambda\, f(\varepsilon_{\vec{k}}) \left[\frac{1}{\hbar(q^2+2kq\lambda)/2m - \omega} + \frac{1}{\hbar(q^2-2kq\lambda)/2m + \omega} \right]$$

- Define dimensionless frequencies and momenta $x \equiv \frac{q}{2k_F}$ $x_0 \equiv \frac{\hbar\omega}{4\varepsilon_F}$
- Use standard logarithmic integrals

$$\int dx \frac{1}{ax+b} = \frac{1}{a}\ln(ax+b) \qquad \int dx \ln(ax+b) = \frac{1}{a}\left[(ax+b)\ln(ax+b) - ax\right]$$

$$\Rightarrow \quad \mathrm{Re}\, \tilde{\chi}_0^R(\vec{q},\omega) = -2e^2 d(\varepsilon_F) \left(\frac{1}{2} + \frac{f(x,x_0) + f(x,-x_0)}{8x} \right)$$

with $$f(x,x_0) \equiv \left[1 - \left(\frac{x_0}{x} - x\right)^2 \right] \ln \left| \frac{x + x^2 - x_0}{x - x^2 - x_0} \right|$$

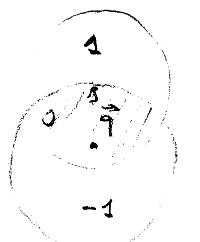
$$- \operatorname{Im} \tilde{\chi}_0^R(\vec{q},\omega) = \frac{\pi e^2}{8\pi^3} \cdot 2 \int d\vec{k} \left(f(\varepsilon_{\vec{k}}) - f(\varepsilon_{\vec{k}+\vec{q}}) \right) \delta\left(\hbar\omega - (\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}})\right) \tag{8.21}$$

If we compare the expression above with the general one obtained in the Lehmann representation we obtain which kind of excitation can be obtained due to the interaction of the non-interacting electron gas with an electro-magnetic field. They correspond to the combination of ω and $\vec{q}$ at which $\operatorname{Im}\tilde{\chi}_0^R(\vec{q},\omega) \neq 0$.

i) Consider $T = 0 \Rightarrow f(\varepsilon_{\vec{k}}) = \theta(k_F - |\vec{k}|)$

$$\theta(k_F - |\vec{k}|) - \theta(k_F - |\vec{k}+\vec{q}|) \neq 0$$

$$\begin{cases} k > k_F & |\vec{k}+\vec{q}| < k_F \Rightarrow \omega \\ k < k_F & |\vec{k}+\vec{q}| > k_F \Rightarrow \omega > \end{cases}$$



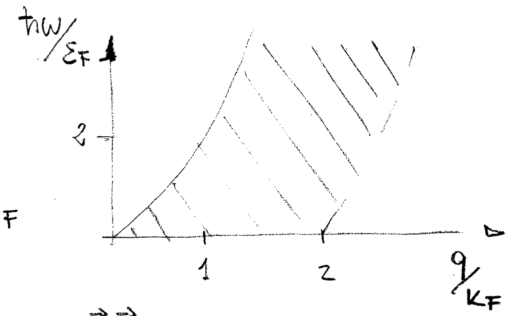
Once again we can give a geometrical interpretation

ii) Since $\operatorname{Im}\tilde{\chi}_0^R(\vec{q},\omega) = -\operatorname{Im}\tilde{\chi}_0^R(-\vec{q},-\omega) \Rightarrow$ we can concentrate on the case $\omega > 0$

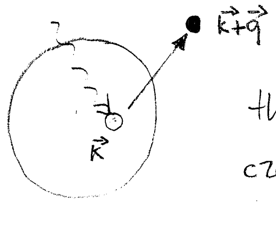
iii) $\hbar\omega > 0 \quad \hbar\omega = \varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} = \frac{\hbar^2}{2m}\left(|\vec{k}+\vec{q}|^2 - |\vec{k}|^2\right) = \frac{\hbar^2}{2m}\left(q^2 + 2\vec{k}\cdot\vec{q}\right)$

$$\begin{cases} \omega_{max} = \dfrac{\hbar q^2}{2m} + v_F q \\[2ex] \omega_{min} = \dfrac{\hbar q^2}{2m} - v_F q \end{cases}$$

and $q > 2k_F$ since $\omega > 0$!



$$\begin{cases} \dfrac{\hbar\omega_{max}}{\varepsilon_F} = \left(\dfrac{q}{k_F}\right)^2 + 2\left(\dfrac{q}{k_F}\right) \\[2ex] \dfrac{\hbar\omega_{min}}{\varepsilon_F} = \left(\dfrac{q}{k_F}\right)^2 - 2\left(\dfrac{q}{k_F}\right) \end{cases}$$



the incoming photon creates a particle-hole pair