Lecture notes: Linear Response Theory

Habib Rostami

Nordita, Stocholm University: October 2020

Contents

1 Correlation functions are the experimental observable

The probe will couple to the system through an interaction potential which in the leading order can be written as a linear coupling to an operator $\hat{A}$ with an classical field strength F

$$\hat{V} = F\hat{A} + c.c. \tag{1}$$

What is usually measured in experiment is proportional to the transition probability which at zero temperature follows the Fermi's golden role

$$\sum_n |\langle\psi_n|F\hat{A}|\psi_0\rangle|^2\delta(\omega-\omega_{n0}) = |F|^2 S(\omega) \tag{2}$$

where at $T=0$ we have

$$S(\omega) = \sum_n |\langle\psi_n|\hat{A}|\psi_0\rangle|^2\delta(\omega-\omega_{n0}) \tag{3}$$

At finite temperature the equilibrium distribution function P_m must be taken into account

$$S(\omega) = \sum_{nm} P_m|\langle\psi_n|\hat{A}|\psi_m\rangle|^2\delta(\omega-\omega_{nm}) \tag{4}$$

After Fourier transform we obtain

$$S(\tau) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega S(\omega) e^{-i\omega t} \tag{5}$$

$$S(\tau) = \frac{1}{2\pi}\sum_{nm} P_m |\langle\psi_n|\hat{A}|\psi_m\rangle|^2 e^{-i\omega_{nm}\tau} \tag{6}$$

$$S(\tau) = \frac{1}{2\pi}\sum_{nm} P_m \langle\psi_m|\hat{A}(\tau)|\psi_n\rangle\langle\psi_n|\hat{A}^\dagger|\psi_m\rangle \tag{7}$$

$$S(\tau) = \frac{1}{2\pi}\sum_{m} P_m \langle\psi_m|\hat{A}(\tau)\hat{A}^\dagger(0)|\psi_m\rangle = \langle\hat{A}(\tau)\hat{A}^\dagger(0)\rangle \tag{8}$$

$$\boxed{S(\tau) = \frac{1}{2\pi}\langle\hat{A}(\tau)\hat{A}^\dagger(0)\rangle} \tag{9}$$

2 Linear response function in terms of correlation function

We consider an interacting system in the thermal equilibrium described by Hamiltonian $\hat{h}$ and temperature T.

$$\hat{h}|\varphi_n\rangle = \varepsilon_n|\varphi_n\rangle \tag{10}$$

Energy levels are populated by canonical distribution

$$P_n = \frac{e^{-\beta\varepsilon_n}}{\sum_n e^{-\beta\varepsilon_n}} \tag{11}$$

with $\beta = 1/T$ after adapting the notation $k_\mathrm{B} = 1$ for the Boltzmann's constant. Macroscopic value of an arbitrary operator $\hat{A}$ follows

$$\langle\hat{A}\rangle_h = \sum_n P_n \langle\varphi_n|\hat{A}|\varphi_n\rangle \tag{12}$$

Now we expose the system with an external probe which can interact with our system through a perturbation potential $\hat{V}(t)$. Therefore, the total Hamiltonian is given by

$$\hat{H}(t) = \hat{h} + \hat{V}(t)e^{\eta t} \tag{13}$$

The term $e^{\eta t}$ with $\eta \to 0^+$ is added to turn on the perturbation in an adiabatic manner (i.e. very slowly). In fact it implies the total Hamiltonian approach to the equilibrium hamiltonian in the remote past: $\lim_{t\to-\infty}\hat{H} \to \hat{h}$. The adiabatic switch-on ensure that the P_n function will not change in the presence of probe. Note that this is an approximation and mostly valid when the probe energy (or frequency) is much larger than the thermalization rate. However, with some care it can be used also for the static perturbation potential. However, ground state eigenfunction will be evolved in time based on the following Schrödinger's equation (after setting $\hbar = 1$ for the reduced Planck's constant):

$$i\frac{\partial}{\partial t}|\psi_n(t)\rangle = \hat{H}(t)|\psi_n(t)\rangle \tag{14}$$

with the boundary condition at t_0: $|\psi_n(t_0)\rangle = |\varphi_n\rangle$. Therefore, using the time-evolution operator $\hat{U}(t, t_0)$ we have

$$|\psi_n(t)\rangle = \hat{U}(t, t_0)|\varphi_n\rangle \tag{15}$$

where

$$i\frac{\partial}{\partial t}\hat{U}(t, t_0) = \hat{H}(t)\hat{U}(t, t_0) \tag{16}$$

The macroscopic fluctuation an arbitrary operator with respect to its equilibrium value is given by

$$\delta A(t) = \langle \hat{A} \rangle_H - \langle \hat{A} \rangle_h \tag{17}$$

Note that

$$\langle \hat{A} \rangle_H = \sum_n P_n \langle \psi_n(t) | \hat{A} | \psi_n(t) \rangle \tag{18}$$

Now we just need to estimate time-evolution operator. In the absence of interaction $\hat{V}$, we have

$$i \frac{\partial}{\partial t} \hat{U}_h(t, t_0) = \hat{h} \hat{U}_h(t, t_0) \to \hat{U}_h(t, t_0) = e^{-i\hat{h}(t-t_0)} \ . \tag{19}$$

We define

$$\hat{U}(t, t_0) = \hat{U}_h(t, t_0) \hat{U}_V(t, t_0) \tag{20}$$

where

$$i \frac{\partial}{\partial t} \hat{U}_V(t, t_0) = \hat{V}(t; t - t_0) e^{\eta t} \hat{U}_V(t, t_0). \tag{21}$$

Within the interaction-picture we have

$$\hat{V}(t; t - t_0) = \hat{U}_h^\dagger(t, t_0) \hat{V}(t) \hat{U}_h(t, t_0) \tag{22}$$

Using the boundary condition $|\psi_n(t_0)\rangle = |\varphi_n\rangle$ we have $\hat{U}_V(t_0, t_0) = 1$. The equation of motion for $\hat{U}_V$ can be solved in a perturbative manner (i.e. Dyson series). For the case of linear response theory we just need to solve it up to the linear order in $\hat{V}$:

$$\hat{U}_V(t, t_0) = 1 - i \int_{t_0}^{t} \hat{V}(t'; t' - t_0) e^{\eta t'} dt' + \mathcal{O}(\hat{V}^2) \tag{23}$$

Therefore,

$$\hat{U}(t, t_0) \approx e^{-i\hat{h}(t-t_0)} \left\{ 1 - i \int_{t_0}^{t} \hat{V}(t'; t' - t_0) e^{\eta t'} dt' \right\} \tag{24}$$

$$\begin{aligned}
\langle \hat{A} \rangle_H &\approx \left\langle \left(1 + i \int_{t_0}^{t} \hat{V}(t'; t' - t_0) e^{\eta t'} dt' \right) e^{i\hat{h}(t-t_0)} \hat{A} e^{-i\hat{h}(t-t_0)} \left(1 - i \int_{t_0}^{t} \hat{V}(t'; t' - t_0) e^{\eta t'} dt' \right) \right\rangle_h \\
&= \langle \hat{A}(t - t_0) \rangle_h - i \int_{t_0}^{t} dt' \langle [\hat{A}(t - t_0), \hat{V}(t', t' - t_0)] \rangle_h e^{\eta t'} \\
&= \langle \hat{A} \rangle_h - i \int_{t_0}^{t} dt' \langle [\hat{A}(t - t'), \hat{V}(t', 0)] \rangle_h e^{\eta t'}
\end{aligned} \tag{25}$$

Therefore, we have

$$\delta A(t) = -i \int_0^{t-t_0} dt' \langle [\hat{A}(\tau), \hat{V}(t - \tau, 0)] \rangle_h e^{\eta(t-\tau)} \tag{26}$$

We set $t_0 \to -\infty$ and we use $\tau = t - t' > 0$:

$$\delta A(t) = -i \int_0^{\infty} d\tau \langle [\hat{A}(\tau), \hat{V}(t - \tau, 0)] \rangle_h e^{\eta(t-\tau)} \tag{27}$$

$$\hat{V}(t - \tau, 0) = F(t - \tau) \hat{B}(0) \tag{28}$$

$$\delta A(t) = \int_0^{\infty} d\tau \langle [\hat{A}(\tau), \hat{B}(0)] \rangle_h F(t - \tau) e^{\eta(t-\tau)} \tag{29}$$

$$\boxed{\delta A(t) = \int_{-\infty}^{+\infty} d\tau \chi_{AB}(\tau) F(t - \tau) e^{\eta(t-\tau)}} \tag{30}$$

$$\boxed{\chi_{AB}(\tau) = -i\Theta(\tau)\langle[\hat{A}(\tau), \hat{B}(0)]\rangle_h} \tag{31}$$

$$\boxed{F(t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega F(\omega)e^{-i\omega t}} \tag{32}$$

$$\delta A(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \int_{-\infty}^{+\infty} d\tau \chi_{AB}(\tau)F(\omega)e^{-i\omega(t-\tau)}e^{\eta(t-\tau)} \tag{33}$$

$$\delta A(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega e^{-i(\omega+i\eta)t}F(\omega)\int_{-\infty}^{+\infty} d\tau \chi_{AB}(\tau)e^{i(\omega+i\eta)\tau} \tag{34}$$

$$\boxed{\chi_{AB}(\omega) = \int_{-\infty}^{+\infty} d\tau \chi_{AB}(\tau)e^{i(\omega+i\eta)\tau}} \tag{35}$$

$$\begin{aligned}
\chi_{AB}(\omega) &= -i\int_0^{\infty} d\tau e^{i(\omega+i\eta)\tau}\langle[\hat{A}(\tau), \hat{B}(0)]\rangle_h \\
&= -i\int_0^{\infty} d\tau e^{i(\omega+i\eta)\tau}\sum_{nm} P_n(A_{nm}(\tau)B_{mn} - B_{nm}A_{mn}(\tau)) \\
&= -i\int_0^{\infty} d\tau e^{i(\omega+i\eta)\tau}\sum_{nm} P_n(A_{nm}B_{mn}e^{i\varepsilon_{nm}\tau} - B_{nm}A_{mn}e^{-i\varepsilon_{nm}\tau}) \\
&= -i\sum_{nm}(P_n - P_m)A_{nm}B_{mn}\int_0^{\infty} d\tau e^{i(\varepsilon_{nm}+\omega+i\eta)\tau} \\
&= \sum_{nm}(P_n - P_m)\frac{A_{nm}B_{mn}}{\varepsilon_{nm}+\omega+i\eta}
\end{aligned} \tag{36}$$

$$\boxed{\chi_{AB}(\omega) = \sum_{mn}\frac{P_m - P_n}{\omega - \varepsilon_{nm} + i\eta}A_{mn}B_{nm}} \tag{37}$$

3 Symmetry properties

Any static response function is real valued and since for $P_{nm} = P_n - P_m < 0$ for $\varepsilon_{nm} = \varepsilon_n - \varepsilon_m > 0$ we have the following inequality

$$\chi_{AA^\dagger}(\omega = 0) = \sum_{nm}\frac{P_{nm}}{\varepsilon_{nm}}|A_{mn}|^2 \leq 0 \tag{38}$$

Moreover, we have

$$\chi_{AB}(\omega = 0) = \sum_{nm}\frac{P_{nm}}{\varepsilon_{nm}}A_{mn}B_{nm} = \sum_{nm}\frac{P_{mn}}{\varepsilon_{mn}}B_{mn}A_{nm} = \chi_{BA}(\omega = 0) \tag{39}$$

Another general property of the linear response function reads

$$\chi_{AB}(-\omega) = [\chi_{A^\dagger B^\dagger}(\omega)]^* \tag{40}$$

Proof:

$$\begin{aligned}
[\chi_{A^\dagger B^\dagger}(\omega)]^* &= \sum_{mn}\frac{P_m - P_n}{\omega - \varepsilon_{nm} - i\eta}(A^\dagger)^*_{mn}(B^\dagger)^*_{nm} = \sum_{mn}\frac{P_m - P_n}{\omega - \varepsilon_{nm} - i\eta}A_{nm}B_{mn} \\
&= \sum_{mn}\frac{P_n - P_m}{\omega + \varepsilon_{nm} - i\eta}A_{mn}B_{nm} \\
&= \sum_{mn}\frac{P_m - P_n}{-\omega - \varepsilon_{nm} + i\eta}A_{mn}B_{nm} = \chi_{AB}(-\omega)
\end{aligned} \tag{41}$$

Finally, one of the most important symmetry property is Onsager relation:

$$\chi_{AB}(\omega, \mathbf{B}) = \chi_{B^t A^t}(\omega, -\mathbf{B}) \tag{42}$$

where $\hat{A}^t = (\hat{A}^\dagger)^*$ stand for the transpose of operator $\hat{A}$. First we check the transpose of observable operators:

$$i^t = (i^\dagger)^* = (-i)^* = i \tag{43}$$
$$\mathbf{r}^t \to (\mathbf{r}^\dagger)^* = \mathbf{r} \tag{44}$$
$$\hat{\mathbf{p}}^t \to (\hat{\mathbf{p}}^\dagger)^* = (-i\nabla)^* = -\mathbf{p} \tag{45}$$

and

$$[\hat{n}(\mathbf{r})]^t = \hat{n}(\mathbf{r}) \tag{46}$$
$$[\hat{\mathbf{j}}(\mathbf{r})]^t = -\hat{\mathbf{j}}(\mathbf{r}) \tag{47}$$

$$\hat{n}^t_{\mathbf{q}} = \int d\mathbf{r}\ \hat{n}^t(\mathbf{r})[e^{i\mathbf{q}\cdot\mathbf{r}}]^t = \int d\mathbf{r}\ \hat{n}(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}} = \hat{n}_{\mathbf{q}} \tag{48}$$
$$\hat{\mathbf{j}}^t_{\mathbf{q}} = \int d\mathbf{r}\ \hat{\mathbf{j}}^t(\mathbf{r})[e^{i\mathbf{q}\cdot\mathbf{r}}]^t = -\int d\mathbf{r}\ \hat{\mathbf{j}}(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}} = -\hat{\mathbf{j}}_{\mathbf{q}} \tag{49}$$

Proof: In the presence of time reversal symmetry (e.g. zero magnetic field $\mathbf{B} = 0$) for an spin-less system we have

$$\psi_n(\mathbf{r}) = \langle \mathbf{r}|\psi_n\rangle = \psi_n^*(\mathbf{r}) = \langle \psi_n|\mathbf{r}\rangle \tag{50}$$

which implies

$$(A^t)_{nm} = \langle\psi_n|A^t|\psi_m\rangle = \langle\psi_m|A^*|\psi_n\rangle^* = \langle\psi_m|A|\psi_n\rangle = A_{mn} \tag{51}$$

Therefore, we have

$$\begin{aligned}\chi_{B^t A^t}(\omega) &= \sum_{mn} \frac{P_m - P_n}{\omega - \varepsilon_{nm} + i\eta}(B^t)_{mn}(A^t)_{nm} = \sum_{mn} \frac{P_m - P_n}{\omega - \varepsilon_{nm} + i\eta} B_{nm}A_{mn} \\ &= \chi_{AB}(\omega)\end{aligned} \tag{52}$$

In the presence of the magnetic field we have

$$\psi_n(\mathbf{r}, \mathbf{B}) = \psi_n^*(\mathbf{r}, -\mathbf{B}) \tag{53}$$

4 Dissipation

Let us consider a coupling of an external field to operator $\hat{A}$:

$$\hat{H}(t) = \hat{h} + F(t)\hat{A}^\dagger + F^*(t)\hat{A} \tag{54}$$

The time-averaged power transfer from the external field to the system (absorbance power) is a period of time Δt is given by

$$W = \frac{1}{\Delta t}\int_{-\Delta t/2}^{\Delta t/2} dt \frac{\partial\langle\hat{H}(t)\rangle_H}{\partial t} \tag{55}$$

Noting that

$$\frac{\partial\langle\hat{H}(t)\rangle_H}{\partial t} = \left\langle \frac{\partial\hat{H}(t)}{\partial t}\right\rangle_H \tag{56}$$

Therefore, we find

$$W = \frac{1}{\Delta t}\int_{-\Delta t/2}^{\Delta t/2} dt \left\{\frac{\partial F(t)}{\partial t}\langle\hat{A}^\dagger\rangle_H + c.c.\right\} \tag{57}$$

Let us consider a periodic driving field

$$F(t) = F(\omega)e^{-i\omega t} \quad , \quad \Delta t = \frac{2\pi}{\omega} \tag{58}$$

Using the linear response response function, we have

$$\langle \hat{A}^\dagger \rangle_H = \langle \hat{A}^\dagger \rangle_h + \chi_{A^\dagger A}(\omega)F^*(\omega)e^{i\omega t} + \chi_{A^\dagger A^\dagger}(\omega)F(\omega)e^{-i\omega t} \tag{59}$$

Therefore, we obtain

$$W = i|F(\omega)|^2\omega \left\{\chi_{A^\dagger A}(\omega) - [\chi_{A^\dagger A}(\omega)]^*\right\} \tag{60}$$

$$\boxed{W = -2\omega \text{Im}[\chi_{A^\dagger A}(\omega)]|F(\omega)|^2} \tag{61}$$

Note that

$$\text{Im}[\chi_{A^\dagger A}(\omega)] = \pi \sum_{mn} |A_{nm}|^2 (P_n - P_m)\delta(\omega - \varepsilon_{nm}) \tag{62}$$

Note that $\varepsilon_n > \varepsilon_m$ we have $P_n < P_m$ and accordingly we obtain

$$\boxed{\omega \text{Im}[\chi_{A^\dagger A}(\omega)] < 0} \tag{63}$$

Therefore, we find $W > 0$.

5 Causality: Kramers–Krönig relationship

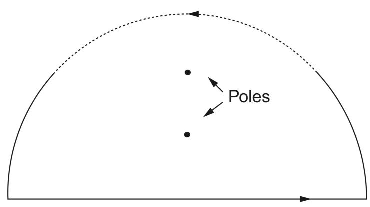

Figure 1: Contour C enclosing the upper half complex plane and the real axis.

We remind the following integration using contour techniques:

$$\int_{-\infty}^{\infty} f(x)e^{iax}dx = \oint_C f(z)e^{iaz}dz = 2\pi i \sum \text{residues of } e^{iaz}f(z) \text{ in contour } C. \tag{64}$$

- $a > 0$
- $\lim_{|z|\to\infty} f(z) \to 0$

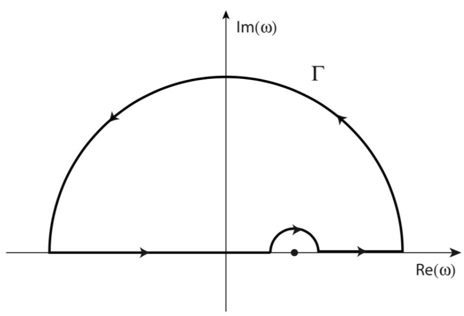

Figure 2: Contour C enclosing the upper half complex plane and excluding a pole at $z = \omega$ on the real axsis.

For retarded (casual) response function we have

$$\chi_{AB}(\tau<0) = \int_{-\infty}^{+\infty} d\omega \chi_{AB}(\omega) e^{-i\omega\tau} = \oint_C d\omega \chi_{AB}(\omega) e^{-i\omega\tau}$$
$$= \oint_C d\omega \chi_{AB}(\omega) e^{i\omega|\tau|} = 0 \quad (65)$$

Therefore, for the upper half complex frequency plane including the real axis (i.e. $\text{Im}[\omega] \geq 0$), the response function $\chi_{AB}(\omega)$ must be analytic implying that all poles and branch cuts of $\chi_{AB}(\omega)$ must in the lower-half plane. Based on the Lehmann representation of the response function given in Eq. (37) we have a branch cut (quasiparticle continuum) just below the real axis in the lower-half plane. In extended there is also possible to observe simple pole in the lower-half plane representing collective excitations (e.g. sound and plasmon modes). In order to observe collective excitations we need to take the thermodynamical limit and perform the momentum integration. Collective modes pole occur at $\omega = \omega_q - i\Gamma_q$ with $\Gamma_q > 0$ being the Landau damping (inverse life-time) of the collective mode with dispersion $\omega \sim \omega_q$. Since the casual response function is analytic in the upper-half plane, we have

$$\oint_C dz \frac{\chi_{AB}(z)}{z-\omega} = 0 \quad (66)$$

Using the fact that $\chi_{AB}(|z| \to \infty) \to 0$, we obtain

$$\mathcal{P} \int_{-\infty}^{+\infty} d\nu \frac{\chi_{AB}(\nu)}{\nu - \omega} - i\pi\chi_{AB}(\omega) = 0 \quad (67)$$

Using the fact that the real and imaginary parts of the response function are even and odd function of frequency, respectively, one can prove

$$\text{Re}[\chi_{AB}(\omega)] = \frac{2}{\pi}\mathcal{P}\int_0^{\infty} \frac{\nu \text{Im}[\chi_{AB}(\nu)]}{\nu^2-\omega^2} d\nu \quad (68)$$

6 2-level system

We consider $\hat{H}(t) = \hat{h} + \hat{V}(t)$ where

$$\hat{h} = \frac{\varepsilon_g}{2}\hat{\sigma}_z \quad (69)$$
$$\hat{V}(t) = E(t) d_{cv} \hat{\sigma}_x \quad (70)$$

where $\hat{d} = -e\hat{x}$ and $d_{cv} = \langle c|(-e\hat{x})|v\rangle$. Lets assume density of two-level atoms is equal to n_0 and $P(t) = n_0\langle(-e\hat{x})\rangle_H$ is the total polarization. Therefore, the polarization (total dipole per volume) is given by $\mathcal{P}(\omega) = \chi(\omega)E(\omega)$ where

$$\chi(\omega) = n_0|d_{cv}|^2(P_c - P_v)\left\{\frac{1}{\omega+\varepsilon_g+i\eta} - \frac{1}{\omega-\varepsilon_g+i\eta}\right\} \quad (71)$$

We assume $P_c = 0$ and $P_v = 1$ which implies

$$\chi(\omega) = n_0|d_{cv}|^2\left\{\frac{1}{\omega-\varepsilon_g+i\eta} - \frac{1}{\omega+\varepsilon_g+i\eta}\right\} \quad (72)$$

Displacement vector is defined:

$$D(\omega) = E(\omega) + 4\pi\mathcal{P}(\omega) = (1+4\pi\chi(\omega))E(\omega) = \epsilon(\omega)E(\omega) \quad (73)$$

where the dynamical dielectric constant is given by

$$\epsilon(\omega) = 1 + 4\pi\chi(\omega) = 1 + 4\pi n_0|d_{cv}|^2\left\{\frac{1}{\omega-\varepsilon_g+i\eta} - \frac{1}{\omega+\varepsilon_g+i\eta}\right\} = \epsilon'(\omega) + i\epsilon''(\omega) \quad (74)$$

The absorption coefficient is related to the imaginary part of the dielectric function:

$$\alpha(\omega) \propto \omega\epsilon''(\omega) = (4\pi^2 n_0|d_{cv}|^2)\omega\left\{\delta(\omega-\varepsilon_g) - \delta(\omega+\varepsilon_g)\right\} \quad (75)$$

7 Dynamical structure factor: fluctuation-dissipation theorem

We define a quantity called dynamical structure factor:

$$S_{AA^\dagger}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \langle \hat{A}(t)\hat{A}^\dagger(0)\rangle_h e^{i\omega t} dt \tag{76}$$

If we decompose $\hat{A} = A_0 + \delta\hat{A}$ where $\langle \delta A\rangle_h = 0$ is the fluctuation part. Therefore, we have

$$S_{AA^\dagger}(\omega) = |\hat{A}_0|^2\delta(\omega) + \frac{1}{2\pi}\int_{-\infty}^{+\infty} \langle \delta\hat{A}(t)\delta\hat{A}^\dagger(0)\rangle_h e^{i\omega t} dt \tag{77}$$

which implies for $\omega \neq 0$, $S_{AA^\dagger}(\omega)$ conveys the information about dynamics of the fluctuation part of $\hat{A}$ operator. It is easy to show that

$$S_{AA^\dagger}(\omega) = \sum_{nm} P_m |A_{mn}|^2 \delta(\omega - \varepsilon_{nm}) \quad , \quad P_m = \frac{e^{-\beta\varepsilon_m}}{\sum_m e^{-\beta\varepsilon_m}} \tag{78}$$

$$S_{AA^\dagger}(-\omega) = \sum_{nm} P_m |A_{mn}|^2 \delta(-\omega - \varepsilon_{nm}) = \sum_{nm} P_n |A_{nm}|^2 \delta(-\omega + \varepsilon_{nm}) \tag{79}$$

Note that for $\omega = \omega_{nm}$ we have $P_n = P_m e^{-\beta\omega}$ and therefore we find

$$\boxed{\text{Detailed balance:} \quad \frac{S_{AA^\dagger}(-\omega)}{S_{AA^\dagger}(\omega)} = e^{-\beta\omega}} \tag{80}$$

Moreover, it is easy to show the following relation known as the fluctuation-dissipation theorem:

$$\boxed{\mathrm{Im}[\chi_{AA^\dagger}(\omega)] = -\pi(1 - e^{-\beta\omega}) S_{AA^\dagger}(\omega)} \tag{81}$$

For $\omega > 0$:

$$S_{AA^\dagger}(\omega) \text{ stands for the absorption spectrum} \tag{82}$$

$$S_{AA^\dagger}(-\omega) \text{ stands for the stimulated emission spectrum} \tag{83}$$

Two conclusions from the fluctuation-dissipation theorem: (i) At finite temperature a power absorption (i.e. dissipation) from an external field is always accompanied by a stimulated emission (i.e. fluctuation) in order to keep the system in the thermal equilibrium. (ii) At zero temperature there is no stimulated emission.

The static (instaneous) structure factor is defined as the frequency integral of the dynamical structure factor

$$S_{AA^\dagger} = \langle \hat{A}(0)\hat{A}^\dagger(0)\rangle_h = \int_{-\infty}^{+\infty} S_{AA^\dagger}(\omega) d\omega \tag{84}$$

Particularly, the static density structure factor is very important quantity in quantifying crystalline

$$S(\mathbf{q}) = \frac{1}{N}\int_{-\infty}^{\infty} S_{n_\mathbf{q} n_\mathbf{q}^\dagger}(\omega) = \frac{\langle \hat{n}_\mathbf{q}^\dagger \hat{n}_\mathbf{q}\rangle_h}{N} \tag{85}$$

Having density operator as $\hat{n}(\mathbf{r}) = \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i)$ with N being the total number of particles, we note

$$\hat{n}_\mathbf{q} = \int d\mathbf{r} \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i) e^{-i\mathbf{q}\cdot\mathbf{r}} = \sum_{i=1}^N e^{-i\mathbf{q}\cdot\mathbf{r}_i} \tag{86}$$

Therefore, we obtain

$$\boxed{S(\mathbf{q}) = \frac{1}{N}\sum_{i=1}^N \sum_{j=1}^N e^{-i\mathbf{q}\cdot(\mathbf{r}_j - \mathbf{r}_i)} = \frac{1}{N}\left|\sum_{j=1}^N e^{-i\mathbf{q}\cdot\mathbf{r}_j}\right|^2} \tag{87}$$

The static density structure factor can be utilized to evaluate pair-correlation function that contain in classical and quantum liquids. For example in isotropic liquid we have

$$g(r) = g(\mathbf{r}, 0) = 1 + \frac{1}{N}\sum_\mathbf{q} \int [S(q) - 1] e^{i\mathbf{q}\cdot\mathbf{r}} \tag{88}$$

where the pair-correlation function is defined in terms of the density-density correlation function:

$$g(\mathbf{r}_1, \mathbf{r}_2) = \frac{\langle \hat{n}(\mathbf{r}_2)\hat{n}(\mathbf{r}_1)\rangle_h}{n(\mathbf{r}_2)n(\mathbf{r}_1)} - \frac{\delta(\mathbf{r}_2 - \mathbf{r}_1)}{n(\mathbf{r}_1)} \tag{89}$$

8 Density response

Let us consider an external scalar potential which couples to particle density as

$$\hat{V}(t) = \int d\mathbf{r}\; V_{\text{ext}}(\mathbf{r},t)\hat{n}(\mathbf{r}) \tag{90}$$

where the density operator is given by

$$\hat{n}(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r} - \hat{\mathbf{r}}_i) \tag{91}$$

and in the Fourier space it reads

$$\hat{n}_{\mathbf{q}} = \int d\mathbf{r}\; \hat{n}(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} = \sum_i e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}_i} \tag{92}$$

The induced time-dependent density thus follows

$$n_1(\mathbf{r},t) = \langle \hat{n}(\mathbf{r})\rangle_H - \langle \hat{n}(\mathbf{r})\rangle_h = \int d\tau \int d\mathbf{r}' \chi_{nn}(\mathbf{r},\mathbf{r}',\tau) V_{\text{ext}}(\mathbf{r}', t-\tau) \tag{93}$$

where the density-density response function reads

$$\chi_{nn}(\mathbf{r},\mathbf{r}',\tau) = \chi_{n(\mathbf{r})n(\mathbf{r}')}(\tau) = -i\Theta(\tau)\langle[\hat{n}(\mathbf{r},\tau), \hat{n}(\mathbf{r}',0)]\rangle_h \tag{94}$$

Note that

$$\hat{n}(\mathbf{r},\tau) = e^{i\tau\hat{h}} \hat{n}(\mathbf{r}) e^{-i\tau\hat{h}} \tag{95}$$

$$\chi_{nn}(\mathbf{q},\mathbf{q}',\omega) = \int d\mathbf{r} \int d\mathbf{r}' \int d\tau e^{i\mathbf{q}\cdot\mathbf{r}} e^{i\mathbf{q}'\cdot\mathbf{r}'} e^{i\omega t} \chi_{nn}(\mathbf{r},\mathbf{r}',\tau) \tag{96}$$

For translationally invariant system we have $\chi_{nn}(\mathbf{r},\mathbf{r}',\tau)$ just depends on $\mathbf{r}-\mathbf{r}'$. We use change of variables as follows

$$\mathbf{r} = \mathbf{R} - \frac{\boldsymbol{\rho}}{2} \tag{97}$$

$$\mathbf{r}' = \mathbf{R} + \frac{\boldsymbol{\rho}}{2} \tag{98}$$

and note that

$$\int d\mathbf{R} e^{i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{R}} = L^d \delta_{\mathbf{q},-\mathbf{q}'} \tag{99}$$

and therefore we have

$$\chi_{nn}(\mathbf{q},\mathbf{q}',\omega) = \chi_{n_{\mathbf{q}}n_{\mathbf{q}'}}(\omega) = L^d \delta_{\mathbf{q},-\mathbf{q}'} \chi_{nn}(\mathbf{q},\omega) \tag{100}$$

where

$$\chi_{nn}(\mathbf{q},\omega) = \frac{1}{L^d}\chi_{n_{\mathbf{q}}n_{-\mathbf{q}}}(\omega) = \frac{1}{L^d}\sum_{nm} \frac{P_m - P_n}{\omega - \varepsilon_{nm} + i\eta} |(\hat{n}_{\mathbf{q}})_{nm}|^2 \tag{101}$$

In the non-interacting model $\psi_{n\mathbf{k}}(\mathbf{r})$ are plain (or Bloch) wave

$$|n\rangle \to |n,\mathbf{k}\rangle = |u_{n\mathbf{k}}\rangle \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{L^{d/2}} \tag{102}$$

$$P_n \to f_n(\mathbf{k}) \qquad \text{Fermi-Dirac distribution function} \tag{103}$$

where n stands for any discrete, such as band, indices and $\mathbf{k}$ is the wave vector. Note that

$$(\hat{n}_{\mathbf{q}})_{nm} \to \langle n,\mathbf{k}|\hat{n}_{\mathbf{q}}|m,\mathbf{k}'\rangle = \langle n,\mathbf{k}|e^{-i\mathbf{q}\cdot\mathbf{r}}|m,\mathbf{k}'\rangle = \langle u_{n\mathbf{k}}|u_{m\mathbf{k}'}\rangle \delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}} \tag{104}$$

Therefore, we find

$$\chi^{(0)}_{nn}(\mathbf{q},\omega) = \frac{1}{L^d}\sum_{\mathbf{k}}\sum_{nm} \frac{f_m(\mathbf{k}+\mathbf{q}) - f_n(\mathbf{k})}{\omega + \varepsilon_m(\mathbf{k}+\mathbf{q}) - \varepsilon_n(\mathbf{k}) + i\eta} |\langle u_{n\mathbf{k}}|u_{m\mathbf{k}+\mathbf{q}}\rangle|^2 \tag{105}$$

in which the Fermi distribution function follows

$$f_n(\mathbf{k}) = \frac{1}{1 + e^{\beta\varepsilon_n(\mathbf{k})}} \tag{106}$$

Note that the chemical potential μ is already taken into account in the definition of the Hamiltonian (e.g. $\hat{h}(\mathbf{k}) = k^2/2m - \mu$). Note that

$$\frac{1}{L^d}\sum_{\mathbf{k}} \to \int \frac{d^d\mathbf{k}}{(2\pi)^d} \tag{107}$$

8.1 Lindhard function in 1D

We consider as 1D parabolic model $\varepsilon(k) = k^2/2m - \mu = (k^2 - k_F^2)/2m$ and we set $\omega = 0$. Therefore we find

$$\begin{aligned}\chi_{nn}(q) &= \int \frac{dk}{2\pi}\frac{f(k+q)-f(k)}{\varepsilon(k+q)-\varepsilon(k)} = \int \frac{dk}{2\pi} f(k)\left\{\frac{1}{\varepsilon(k)-\varepsilon(k-q)} + \frac{1}{\varepsilon(k)-\varepsilon(k+q)}\right\} \\ &= 2m\int_{-k_F}^{k_F}\frac{dk}{2\pi}\left\{\frac{1}{k^2-(k-q)^2} + \frac{1}{k^2-(k+q)^2}\right\} \\ &= \frac{m}{\pi q}\ln\left|\frac{q-2k_F}{q+2k_F}\right| \end{aligned} \quad (108)$$

Peierls instability :

$$\ddot{Q}_q + \Omega^2(q)Q_q \propto \sqrt{\Omega(q)}n_q \quad (109)$$

$$\Phi_q \propto \sqrt{\Omega(q)}Q_q \quad (110)$$

$$n_q = \chi(q)\Phi_q \propto \chi(q)\sqrt{\Omega(q)}Q_q \quad (111)$$

Therefore, the phonon energy will be renormalized as follows

$$\Omega^2_{\text{ren}}(q) - \Omega^2(q) \propto \Omega(q)\chi(q) \quad (112)$$

Transition temperature T_{CDW} is the temperature at which $\Omega^2_{\text{ren}}(q = 2k_F) = 0$. The Phonon mode become soften, highly populated, and the system become unstable and a structure phase transition occurs to harden the phonon mode again.

8.2 Symmetry properties

Onsager relation:

$$\chi_{n_{\mathbf{q}}n_{-\mathbf{q}}}(\omega) = \chi_{n_{-\mathbf{q}}n_{\mathbf{q}}}(\omega) \rightarrow \chi_{nn}(\mathbf{q},\omega) = \chi_{nn}(-\mathbf{q},\omega) \quad (113)$$

Moreover we have

$$\chi_{nn}(\mathbf{q},\omega) = [\chi_{nn}(\mathbf{q},-\omega)]^* \quad (114)$$

8.3 Proper response function and RPA dielectric constant

Redistribution of density due to long range interaction can cause the screening of the external potential. The screened potential then reads

$$V_{sc}(\mathbf{r},t) = V_{ext}(\mathbf{r},t) + V_{ind}(\mathbf{r},t) \quad (115)$$

In the Hartree approximation we can estimate the induced potential due to the induced density

$$V_{ind}(\mathbf{r},t) = \int d\mathbf{r}' v_{ee}(|\mathbf{r}-\mathbf{r}'|)n_1(\mathbf{r}',t) \quad , \quad v_{ee}(r) = \frac{e^2}{r} \quad (116)$$

which implies

$$V_{ind}(\mathbf{q},\omega) = v_q n_1(\mathbf{q},\omega) \quad (117)$$

with v_q being the Fourier transform of the electron-electron interaction potential $v_{ee}(r)$. Using the linear response theory we have

$$n_1(\mathbf{q},\omega) = \chi_{nn}(\mathbf{q},\omega)V_{ext}(\mathbf{q},\omega) \quad (118)$$

Therefore, we find

$$V_{sc}(\mathbf{q},\omega) = [1 + v_q\chi_{nn}(\mathbf{q},\omega)]V_{ext}(\mathbf{q},\omega) \quad (119)$$

Now we define the *proper* response function as follows

$$n_1(\mathbf{q},\omega) = \tilde{\chi}_{nn}(\mathbf{q},\omega)V_{sc}(\mathbf{q},\omega) = \tilde{\chi}_{nn}(\mathbf{q},\omega)[1 + v_q\chi_{nn}(\mathbf{q},\omega)]V_{ext}(\mathbf{q},\omega) \quad (120)$$

Therefore, we find

$$\chi_{nn}(\mathbf{q},\omega) = \tilde{\chi}_{nn}(\mathbf{q},\omega)[1 + v_q\chi_{nn}(\mathbf{q},\omega)] \tag{121}$$

which implies

$$\chi_{nn}(\mathbf{q},\omega) = \frac{\tilde{\chi}_{nn}(\mathbf{q},\omega)}{1 - v_q\tilde{\chi}_{nn}(\mathbf{q},\omega)} \tag{122}$$

Moreover, the screened potential follows

$$V_{sc}(\mathbf{q},\omega) = \frac{V_{ext}(\mathbf{q},\omega)}{\epsilon(\mathbf{q},\omega)} \tag{123}$$

where the dielectric function is given in terms of the proper response function

$$\epsilon(\mathbf{q},\omega) = 1 - v_q\tilde{\chi}_{nn}(\mathbf{q},\omega) \tag{124}$$

The Random Phase Approximation (RPA) is to approximate the proper density-density response function with the non-interacting one:

$$\epsilon_{\mathrm{RPA}}(\mathbf{q},\omega) = 1 - v_q\chi^{(0)}_{nn}(\mathbf{q},\omega) \tag{125}$$

and

$$\chi^{\mathrm{RPA}}_{nn}(\mathbf{q},\omega) = \frac{\chi^{(0)}_{nn}(\mathbf{q},\omega)}{\epsilon_{\mathrm{RPA}}(\mathbf{q},\omega)} \tag{126}$$

8.4 Static screening

$$\epsilon^{\mathrm{static}}_{\mathrm{RPA}}(\mathbf{q}) = 1 - v_q\chi^{(0)}_{nn}(\mathbf{q}) \tag{127}$$

For small exchange momentum q:

$$\begin{aligned}
\lim_{q\to 0}\chi^{(0)}_{nn}(\mathbf{q}) &= \lim_{q\to 0}\frac{1}{L^d}\sum_{\mathbf{k}}\sum_{nm}\frac{f_m(\mathbf{k}+\mathbf{q}) - f_n(\mathbf{k})}{\varepsilon_m(\mathbf{k}+\mathbf{q}) - \varepsilon_n(\mathbf{k})}|\langle u_{n\mathbf{k}}|u_{m\mathbf{k}+\mathbf{q}}\rangle|^2 \\
&= \lim_{q\to 0}\frac{1}{L^d}\sum_{\mathbf{k}}\sum_{m}\frac{f_m(\mathbf{k}+\mathbf{q}) - f_m(\mathbf{k})}{\varepsilon_m(\mathbf{k}+\mathbf{q}) - \varepsilon_m(\mathbf{k})} \\
&= \frac{1}{L^d}\sum_{\mathbf{k}}\sum_{m}\frac{\partial f_m(\mathbf{k})}{\partial\varepsilon_m(\mathbf{k})} = -\frac{1}{L^d}\sum_{\mathbf{k}}\sum_{m}\delta(0 - \varepsilon_m(\mathbf{k})) \\
&= -N(0)
\end{aligned} \tag{128}$$

Note that the last manipulation is done at zero temperature and $N(0)$ is the density of states at the Fermi surface. Moreover, we remind that

$$\text{In 2D} : v_q = \frac{2\pi e^2}{q} \tag{129}$$

$$\text{In 3D} : v_q = \frac{4\pi e^2}{q^2} \tag{130}$$

$$\text{In D=2,3} : v_q = (2\pi e^2)\frac{D-1}{q^{D-1}} \tag{131}$$

Therefore, for small q we have

$$\text{In 2D} : \epsilon^{\mathrm{static}}_{\mathrm{RPA}}(\mathbf{q}) \approx 1 + \frac{2\pi e^2 N(0)}{q} \tag{132}$$

$$\text{In 3D} : \epsilon^{\mathrm{static}}_{\mathrm{RPA}}(\mathbf{q}) \approx 1 + \frac{4\pi e^2 N(0)}{q^2} \tag{133}$$

Static screened inter-particle interaction (i.e. Thomas-Fermi screening) is given by $v^{sc}_q = v_q/\epsilon^{\mathrm{static}}_{\mathrm{RPA}}(\mathbf{q})$:

$$\text{In 2D} : v^{sc}_q = \frac{2\pi e^2}{q + 2\pi e^2 N(0)} \tag{134}$$

$$\text{In 3D} : v^{sc}_q = \frac{4\pi e^2}{q^2 + 4\pi e^2 N(0)} \tag{135}$$

Screening of charged impurity and Friedel oscillation:

8.5 Collective mode: plasmon

Collective mode is exist when the response function diverges for a particular dispersion of $\omega = \Omega_q$. This because in the absence of external field we can have a density fluctuation only if a collective mode is excited . Therefore, the collective mode dispersion and life-time can be obtained in RPA level as follows

$$1 - v_q \chi^{(0)}_{nn}(\mathbf{q}, \Omega_q) = 0 \quad , \quad n_1 \sim e^{i(\mathbf{q}\cdot\mathbf{r} - \Omega_q t)} \tag{136}$$

It can be shown that the dynamical density structure factor at zero temperature contains a simple delta function pole:

$$S^{\rm RPA}_{nn}(q,\omega) = -\frac{1}{\pi}{\rm Im}[\chi^{\rm RPA}_{nn}(\mathbf{q}, \Omega_q)] \approx \frac{\Omega_q}{2v_q}\delta(\omega - \Omega_q)\ . \tag{137}$$

9 Current response

In response to an external scalar or vector potential field we can in principal generate an electric current in our system. The current can be calculated by utilizing the linear response theory. The permutation potential energy can be written in two possible gauges:

$$\hat{V}(t) = \int d\mathbf{r}'\varphi(\mathbf{r}', t)\hat{n}(\mathbf{r}') \quad \text{or} \quad \hat{V}(t) = e\int d\mathbf{r}'\mathbf{A}_\alpha(\mathbf{r}', t)\hat{j}_\alpha(\mathbf{r}') \tag{138}$$

where the electric and magnetic field follow (we set speed of light $c = 1$):

$$\mathbf{E}(\mathbf{r}, t) = -\boldsymbol{\nabla}\varphi(\mathbf{r}, t) - \partial_t\mathbf{A}(\mathbf{r}, t) \tag{139}$$

$$\mathbf{B}(\mathbf{r}, t) = \boldsymbol{\nabla}\times\mathbf{A}(\mathbf{r}, t) \tag{140}$$

However, it is always possible to eliminate the scalar potential using a gauge transformation

$$\varphi(\mathbf{r}, t) \to \varphi(\mathbf{r}, t) - \partial_t\Lambda(\mathbf{r}, t) \tag{141}$$

$$\mathbf{A}(\mathbf{r}, t) \to \mathbf{A}(\mathbf{r}, t) + \boldsymbol{\nabla}\Lambda(\mathbf{r}, t) \tag{142}$$

We choose vector potential gauge since it is more complete in describing inhomogeneous external probe. For a simple free electron model the vector potential is added as the minimal coupling (Peierls substitution) as $\mathbf{p} \to \mathbf{p} - q\mathbf{A}$ with $q = -e$ as the electron charge:

$$\frac{p^2}{2m} \to \frac{(\mathbf{p} + e\mathbf{A})^2}{2m} = \frac{p^2}{2m} + e\frac{\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}}{2m} + \frac{e^2A^2}{2m} \tag{143}$$

$$\begin{aligned} H(t) = \sum_i \frac{(\hat{\mathbf{p}}_i + e\mathbf{A}(\hat{\mathbf{r}}_i, t))^2}{2m} &= \sum_i \frac{p_i^2}{2m} + \frac{e^2}{2m}\int d\mathbf{r}\sum_i \delta(\mathbf{r} - \hat{\mathbf{r}}_i)A^2(\mathbf{r}, t) \\ &+ e\int d\mathbf{r}\left\{\sum_i \frac{\hat{\mathbf{p}}_i\delta(\mathbf{r} - \hat{\mathbf{r}}_i) + \delta(\mathbf{r} - \hat{\mathbf{r}}_i)\hat{\mathbf{p}}_i}{2m}\right\}\cdot\mathbf{A}(\mathbf{r}, t) \end{aligned} \tag{144}$$

For many-particle system we define then the charge-current operator as follows

$$\hat{\mathbf{j}}(\mathbf{r}) = \frac{1}{2}\sum_i \{\hat{\mathbf{v}}_i\delta(\mathbf{r} - \hat{\mathbf{r}}_i) + \delta(\mathbf{r} - \hat{\mathbf{r}}_i)\hat{\mathbf{v}}_i\} \tag{145}$$

in whcih

$$\mathbf{v}_i = \mathbf{v}(\hat{\mathbf{p}}_i + e\mathbf{A}(\mathbf{r}_i, t)) \tag{146}$$

where the velocity operator follows

$$\hat{\mathbf{v}}(\mathbf{p}) = \frac{\partial\hat{h}(\mathbf{p})}{\partial\mathbf{p}} = \frac{\hat{\mathbf{p}}}{m} \tag{147}$$

We can decompose

$$\hat{\mathbf{j}}(\mathbf{r}) = \hat{\mathbf{j}}^p(\mathbf{r}) + \hat{\mathbf{j}}^d(\mathbf{r}) \tag{148}$$

where the paramagnetic current component reads

$$\hat{\mathbf{j}}^p(\mathbf{r}) = \frac{1}{2}\sum_i \{\hat{\mathbf{v}}(\mathbf{p}_i)\delta(\mathbf{r}-\hat{\mathbf{r}}_i) + \delta(\mathbf{r}-\hat{\mathbf{r}}_i)\hat{\mathbf{v}}(\mathbf{p}_i)\} \tag{149}$$

and the second contibution follows

$$\hat{\mathbf{j}}^d(\mathbf{r}) = \frac{1}{2}\sum_i \left\{\hat{\mathbf{v}}_i^d\delta(\mathbf{r}-\hat{\mathbf{r}}_i) + \delta(\mathbf{r}-\hat{\mathbf{r}}_i)\hat{\mathbf{v}}_i^d\right\} \tag{150}$$

Note that

$$\hat{\mathbf{v}}_i^d = \hat{\mathbf{v}}(\mathbf{p}_i + e\mathbf{A}(\mathbf{r}_i,t)) - \hat{\mathbf{v}}(\mathbf{p}_i) \tag{151}$$

Therefore, in simple parabolic dispersion model, the diamagnetic current component reads

$$\hat{\mathbf{j}}^d(\mathbf{r}) = \frac{e}{m}\sum_i \mathbf{A}(\hat{\mathbf{r}}_i,t)\delta(\mathbf{r}-\hat{\mathbf{r}}_i) = \frac{e}{m}\mathbf{A}(\mathbf{r},t)\hat{n}(\mathbf{r}) \tag{152}$$

The macroscopic current generated by external vector potential reads

$$j_\alpha(\mathbf{r},t) = \langle \hat{j}^p_\alpha(\mathbf{r})\rangle_H + \langle \hat{j}^d_\alpha(\mathbf{r})\rangle_H \tag{153}$$

In the linear response approximation we obtain

$$j^p_\alpha(\mathbf{r},t) = \langle \hat{j}^p_\alpha(\mathbf{r})\rangle_H = e\int d\tau \int d\mathbf{r}'\; \chi_{j^p_\alpha j^p_\beta}(\mathbf{r},\mathbf{r}',\tau)A_\beta(\mathbf{r}',t-\tau) \tag{154}$$

where

$$\chi_{j^p_\alpha j^p_\beta}(\mathbf{r},\mathbf{r}',\tau) = -i\Theta(\tau)\langle[\hat{j}^p_\alpha(\mathbf{r},\tau),\hat{j}^p_\beta(\mathbf{r}',0)]\rangle_H \tag{155}$$

The diamagnetic contribution reads (for parabolic model)

$$-ej^d_\alpha(\mathbf{r},t) = -e\langle \hat{j}^p_\alpha(\mathbf{r})\rangle_h = (-e^2)\chi^{dia}_{\alpha\beta}A_\beta(\mathbf{r},t) \tag{156}$$

in which we have

$$\chi^{dia}_{\alpha\beta} = \frac{n}{m}\delta_{\alpha\beta} \tag{157}$$

where $n = \langle n(\mathbf{r})\rangle_h$ is the equilibrium particle density. In the translationally invariant system we have

$$-ej^p_\alpha(\mathbf{q},\omega) = (-e^2)\chi^{para}_{\alpha\beta}(\mathbf{q},\omega)A_\beta(\mathbf{q},\omega) \tag{158}$$

where

$$\chi^{para}_{\alpha\beta}(\mathbf{q},\omega) = \frac{1}{L^d}\chi_{j^p_\alpha(\mathbf{q})j^p_\beta(-\mathbf{q})}(\omega) \tag{159}$$

In the non-interacting approximation we obtain

$$\begin{aligned}\chi^{para;(0)}_{\alpha\beta}(\mathbf{q},\omega) = {} & \frac{1}{L^d}\sum_{\mathbf{k}}\sum_{mn}\frac{f_m(\mathbf{k}+\mathbf{q}) - f_n(\mathbf{k})}{\omega + \varepsilon_m(\mathbf{k}+\mathbf{q}) - \varepsilon_n(\mathbf{k}) + i\eta} \\ & \times \langle m,\mathbf{k}+\mathbf{q}|\hat{j}^p_\alpha(\mathbf{q})|n,\mathbf{k}\rangle\langle n,\mathbf{k}|\hat{j}^p_\beta(-\mathbf{q})|m,\mathbf{k}+\mathbf{q}\rangle\end{aligned} \tag{160}$$

Eventually, the linear charge current can be written in response to the external electric field

$$J_\alpha(\mathbf{q},\omega) = -ej_\alpha(\mathbf{q},\omega) = \sigma_{\alpha\beta}(\mathbf{q},\omega)E_\beta(\mathbf{q},\omega) \tag{161}$$

where $A_\beta = -iE_\beta/\omega$ and therefore the linear conductivity reads

$$\boxed{\sigma_{\alpha\beta}(\mathbf{q},\omega) = ie^2\frac{\chi^{para}_{\alpha\beta}(\mathbf{q},\omega) + \chi^{dia}_{\alpha\beta}}{\omega}} \tag{162}$$

9.1 Gauge invariance

1) For homogenous external electric field ($\mathbf{q} = 0$) both scalar and vector potential gauge must give the same result which one can postulate it and arrive at the following relationship:

$$\chi^{dia}_{\alpha\beta} = -\chi^{para}_{\alpha\beta}(\mathbf{q}=0,\omega=0) \tag{163}$$

9.2 Linear optical conductivity

The optical conductivity is obtained by taking the limit $q \to 0$ and using the gauge invariance relation:

$$\sigma_{\alpha\beta}(\omega) = ie^2 \frac{\chi^{para}_{\alpha\beta}(\omega) - \chi^{para}_{\alpha\beta}(0)}{\omega} \tag{164}$$

In the non-interacting approximation we obtain

$$\boxed{\sigma^{(0)}_{\alpha\beta}(\omega) = -ie^2 \frac{1}{L^d} \sum_{\mathbf{k}} \sum_{mn} \frac{f_m(\mathbf{k}) - f_n(\mathbf{k})}{\varepsilon_m(\mathbf{k}) - \varepsilon_n(\mathbf{k})} \frac{\langle m, \mathbf{k} | \hat{j}^p_\alpha | n, \mathbf{k} \rangle \langle n, \mathbf{k} | \hat{j}^p_\beta | m, \mathbf{k} \rangle}{\omega + \varepsilon_m(\mathbf{k}) - \varepsilon_n(\mathbf{k}) + i\eta}} \tag{165}$$

10 Optical conductivity of SSH model

$$\hat{H} = \begin{bmatrix} 0 & v + we^{-ik} \\ v + we^{ik} & 0 \end{bmatrix} \tag{166}$$

$$\varepsilon_\pm = \pm\sqrt{v^2 + w^2 + 2vw\cos(k)} \quad , \quad |\pm\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \pm e^{-i\phi_k} \end{bmatrix} \tag{167}$$

where

$$\tan(\phi_k) = \frac{w\sin(k)}{v + w\cos(k)} \tag{168}$$

$$\hat{j}(q = 0) = \partial_k \hat{H} = iw \begin{pmatrix} 0 & -e^{-ik} \\ e^{ik} & 0 \end{pmatrix} \tag{169}$$

$$\sigma(\omega) = -ie^2 \frac{1}{L} \sum_{\mathbf{k}} \frac{f_+ - f_-}{\varepsilon_+ - \varepsilon_-} |\langle + | \hat{j} | - \rangle|^2 \left\{ \frac{1}{\omega + \varepsilon_+ - \varepsilon_- + i\eta} + \frac{1}{\omega + \varepsilon_- - \varepsilon_+ + i\eta} \right\} \tag{170}$$

$$\varepsilon_+ - \varepsilon_- = 2\sqrt{v^2 + w^2 + 2vw\cos(k)} \tag{171}$$

$$|\langle +, k | \hat{j} | -, k \rangle|^2 = \frac{w^2[w + v\cos(k)]^2}{v^2 + w^2 + 2vw\cos(k)} \tag{172}$$

lets set $f_+ = 0, f_- = 1$.

$$\sigma(\omega) = i\frac{e^2}{2\pi} \int_{-\pi}^{\pi} dk \frac{w^2[w + v\cos(k)]^2}{[v^2 + w^2 + 2vw\cos(k)]^{3/2}} \frac{\omega_+}{\omega_+^2 - 4[v^2 + w^2 + 2vw\cos(k)]} \tag{173}$$

For the case of $w = v = 1$ we have:

$$\sigma(\omega) = \frac{e^2}{4\pi} \frac{i\omega_+ \tan^{-1}\left(\frac{4}{\sqrt{\omega_+^2 - 16}}\right)}{\sqrt{\omega_+^2 - 16}} \tag{174}$$

Note that $\omega_+ = \omega + i0^+$.
Winding number:

$$N_{\text{wind}} = \frac{1}{2\pi i} \int_{-\pi}^{\pi} \frac{\partial \ln[v + we^{ik}]}{\partial k} \tag{175}$$

$$|v| > |w| \quad \to \quad N_{\text{wind}} = 0 \tag{176}$$

$$|v| < |w| \quad \to \quad N_{\text{wind}} = 1 \tag{177}$$

11 Final essay subjects related to the "Linear Response Theory" lecture

- **Review projects initiate by reference textbooks and papers. You may find more references to expand your discussion on the subject.**
- **Calculation/Review projects contain a short calculation doable in a few days together with result discussion and the review of the relevant concepts. You can receive guidance at the calculation step.**
- **You should deliver a presentation on your project by the end of the course.**
- **Deadline for submitting the report is the end of November.**
- **The report/essay should be summited as a PDF file.**

List of projects

1. (Calculation/Review) Static density-density susceptibility (Lindhard function) of the Su-Schrieffer Heeger (SSH) model: Peierls instability, charge density waves
2. (Calculation/Review) Optical conductivity of 2D massless Dirac systems: metal, semimetal, and insulator
3. (Review) Optical sum rules, the f-sum rule, the compressibility sum rule
4. (Review) Onsager reciprocal relations: the case of thermal currents
5. (Review) Mean-field theory of linear response
6. (Review) Random Phase Approximation (RPA) density-density response function: screening, Friedel oscillation
7. (Review) RPA density-density response function: collective modes such as plasmon and zero sound
8. (Review) Linear response function and band topology: adiabatic geometric phases, Berry curvature
9. (Review) Thermoelectric effects: Seebeck effect, Peltier effect, Thomson effect, and Nernst effect
10. (Review) Landauer-Buttiker formalism for ballistic transport
11. (Review) Hydrodynamics transport of electron liquids: the case of graphene
12. (Review) Linear response theory for tunneling current, Scanning Tunneling Microscopy (STM)
13. (Review) Semiconductor Bloch equation: time- and Angle-Resolved Photoemission Spectroscopy (ARPES), Optical stark effect

12 References

- G. Giuliani and G. Vignale, *Quantum theory of the electron liquid*, (Cambridge university press, 2005).
- Philippe Nozieres, *Theory Of Interacting Fermi Systems*, (CRC Press,1998).