Chapter 4.2. Screening in Interacting Electron gas.

4.2: Interacting electronic gas,
Random Phase Approximation
Thomas - Fermi Screening
Dielectric function
Plasmon.

Ref: Subir Sachdev Youtube Lectures on quantum theory of solid
G. Mahan book
P. Phillips book.
G. Vignale book.

4.3 Interacting Electron Gas

We will now study how the density-density fluctuation spectrum modifies due to long-range Coulomb interaction. In fact, we will discover that the long-range coulomb interaction will rather be screened into short range interaction. Another interesting property we will discover is that the particle-hole continuum will modify to sharp dispersions and they are called plasmons. This can absorb light for much longer period, but has a dispersion called plasmon dispersion.

→ We write the interacting Hamiltonian in the 2nd quantized form:

$$H_0 = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \frac{1}{2V} \sum_{\substack{k,k',q \\ \sigma\sigma'}} v(q)\, c^\dagger_{k+q,\sigma} c^\dagger_{k'-q,\sigma'} c_{k'\sigma'} c_{k\sigma} \quad \text{---(25a)}$$

where $\varepsilon_k = \frac{\hbar^2 k^2}{2m} - \mu$ for electron gas, or can be generalized to tight binding dispersion.

$$v(q) = \frac{4\pi}{q^2}$$ for long range Coulomb interaction. We set $e=-1$ for electron charge.

We rewrite the last term in terms of the density operator

$\rho(q) = n(q) = \sum_{k,\sigma} c^\dagger_{k+q,\sigma} c_{k\sigma}$ (we set the charge of electron $e=-1$).

$$H_{int} = \frac{1}{2V} \sum_q v(q)\, \rho(q)\, \rho(-q). \quad \text{---(25b)}$$

→ The external perturbation is $H' = \int d^3r\, \phi_{ext}(\vec{r},t)\, \rho(\vec{r})$ ---(25c)

(The electrons charge $q=-e$ is absorbed in ϕ_{ext}.)

- Its easier to see the effect of the external potential to the electron density by associating an external charge density $\rho_{ext}(\vec{r},t)$ corresponding to the external potential, energy $\phi_{ext}(\vec{r},t)$ using the Poisson's equation $\nabla^2\phi_{ext} = -e\rho_{ext}$:

$$\phi_{ext}(q,\omega) = \frac{4\pi e^2}{q^2}\rho_{ext}(q,\omega) \quad \text{--- (26a)}$$

Note that for the intrinsic electron density fluctuation, this external potential is related to the nucleous charge density, which we approximated to be uniform in space & time. Otherwise, for external gate voltage, we can also associate such a charge density $e n_{ext}(q,\omega)$, atleast mathematically, to facilitate the understanding of its impact on the electron density in the usual electromagnetic theory language.

- Substituting eq (26a) in (25c), we see that H' is like an Coulomb interaction as H_{int} in eq (25b), but between external and internal charge density. This gives a hint to define an effective / total charge density as follows.
- Now the induced charge density of electrons $\delta\langle\rho(q,\omega)\rangle$, which is the variation of the electron charge density with respect to its value before the $\phi_{ext}(r,t)$ was turned on, ie, at $t=0$. According to the Linear response theory we discussed in eq(17a), the induced charge density is proportional to the external potential as

$f(q,t)$ term,

$$\rho_{ind}(q,\omega) = \delta\langle\rho(q,\omega)\rangle = \chi(q,\omega)\,\phi_{ext}(q,\omega) \quad \text{--- (17a)}$$

$$= \frac{4\pi}{q^2}\chi(q,\omega)\,\rho_{ext}(q,\omega), \quad \text{from eq (26a)} \quad \text{--- (26b)}$$

$v(q)$ to make it general

Here, $\chi(q,\omega)$ is the exact density-density correlator of the interacting electron gas. ($\rho_{ind} = 0$ for $\phi_{ext} = 0$ as it should be).

- Then the total charge density:

$$\rho_{tot}(q,\omega) = \rho_{ext}(q,\omega) + \rho_{ind}(q,\omega)$$
$$= \left[1 + v(q)\,\chi(q,\omega)\right] \rho_{ext}(q,\omega)$$
$$= \frac{1}{\epsilon(q,\omega)}\, \rho_{ext}(q,\omega) \quad \text{--- (26c)}$$

where, in the last line, we used the definition of the dielectric function (eq(3)), that the displacement vector $D(q,\omega) = \epsilon(q,\omega)\, E(q,\omega)$, and $D(q,\omega) = -i\frac{4\pi}{q}\rho_{ext}(q,\omega)$ & $E(q,\omega) = -i\frac{4\pi}{q}\rho_{tot}(q,\omega)$.

- This gives a mechanism of the dielectric response of a material as the density-density fluctuation due to external potential within the Kubo formula as

$$\boxed{\frac{1}{\epsilon(q,\omega)} = 1 + v(q)\,\chi(q,\omega)} \quad \text{--- (27)}$$

We notice that although there are density fluctuation of non-interacting electron χ_0 due to external perturbation, but it does not contribute to the dielectric function of a material. Its only the interaction term that gives a dielectric response due to density-density fluctuation. Its important to emphasize that χ in eq (27) is the <u>interacting</u> electron density fluctuation, if we replace it with non-interaction electron's density fluctuation χ_0, that we just calculated above, will give wrong result in the sense it will be inconsistent with experiment. This is because without interaction electrons do not talk to each other and hence do not screen each other.

- Since χ is complex, in general, incorporating the absorption/dissipation of energy in the system, the dielectric function is also complex and its imaginary part is completely determined by $\text{Im}\,\chi$. This sounds a bit odd in eq(26c) for the charge density which is real. There one includes the real part of ε. Experimentally, one measures both real and imaginary ε. One can define a refractive index of a material with complex ε, where the imaginary part corresponds to the absorption of the light within the material. Nowadays people discovered metamaterials whose refractive index is negative, suggesting $\varepsilon < 0$. This is a different story.

- Now if we think of the coulomb interaction seen to the external charge due to the total charge of the material, we see that the interaction is screened as

$$v_{sc}(q,\omega) = \frac{v(q)}{\varepsilon(q,\omega)} = \frac{4\pi}{q^2\,\varepsilon(q,\omega)} \quad \text{---(28)}$$

The coulomb repulsion is now reduced as $\varepsilon > 1$, and is also frequency dependent. It's like we have applied an electrostatic potential at some frequency ω, which is analog to an external charge density wave at wavevector q which is oscillating at a frequency ω. This external charge attracts (or repels) other charges of the medium and the total charge density (induced + external) oscillates at the same wavevector q and frequency. The net Coulomb interaction comming out from this total charge density is smaller than the one exerted by a factor of the dielectric function $\varepsilon(q,\omega)$.

- So, the entire thing has to be calculated self-consistently that the interacting electron density depends on the screened coulomb interaction and screened coulomb interaction depends on interacting electron density. This is in general a much harder problem to compute the interacting electron density and a topic of present research. There are Feynmann diagram methods to write down all of these in a neat way and one defines self-energy correction to the electron density based on perturbation method. self-consistency is generally very challenging.

The simpler approximation one does is a time-dependent mean-field (time-dependent Hartree approximation) which is popularly known as the Random Phase Approximation (RPA).

4.2.A Random Phase Approximation (RPA)

(Also known as time-dependent Hartree-~~Fock~~ Approximation or Coherent Potential Approximation, time-dependent mean-field theory, ...)

Recall the interacting Hamiltonian with the perturbation in the Fourier space

$$H = \underbrace{\sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \frac{1}{2V}\sum_q v(q)\, \rho(q)\, \rho(-q)}_{H_0} + \underbrace{\frac{1}{V}\sum_q \phi_{ext}(q,t)\, \rho(-q)}_{H'(t)} \quad \text{--- (29)}$$

We are interested in the ground state of H_0. The ground state wavefunction is a single particle Hartree-Fock state $|\Psi_{H.F}(t)\rangle$. Then we can factorize the interaction part into product of expectation values of two operators. We will only keep the Hartree term as our first approximation. (Because exchange term captures quantum fluctuations so, we assume quantum fluctuations are suppressed in the density-density correlation function of present interest. Indeed in most materials that is the case.)

We will now employ the mean field theory - whose basic idea is to rescale an operator with respect to its mean value: $\rho(q) = \langle \rho(q)\rangle_0 + \delta\rho(q)$. In the present case we take $\rho_{ind}(q,t) = \langle \rho(q)\rangle_0$ as the mean induced density, which obtains its time-dependence from the state. Then the deviation/fluctuation of the density around this mean value obtained by the operator $\rho(q)$.

$$\underset{\uparrow \text{ operator}}{\rho(q)} \rightarrow \underset{\substack{\uparrow \text{ number} \\ \langle \Psi(q,t)|\hat\rho_{ind}(q)|\Psi(q,t)\rangle}}{\rho_{ind}(q,t)} + \underset{\uparrow \text{ operator}}{\rho(q)} \quad \text{-- (30)}$$

This is the key approximation of the time-dependent mean field theory. Then the interaction term factors out as

$$\rho(q)\,\rho(-q) \rightarrow \left(\rho_{ind}(q,t) + \rho(q)\right)\left(\rho_{ind}(-q,t) + \rho(q)\right)$$
$$= \rho_{ind}(q,t)\,\rho_{ind}(-q,t) + \rho_{ind}(q,t)\,\rho(q) + \rho_{ind}(-q,t)\,\rho(-q) + \mathcal{O}(\rho^2)$$

This term is just a number and shifts the overall energy. So, we will not include it explicitly.

Then plugging this equation in the Hamiltonian we get

$$H_{RPA} = \sum_k \varepsilon_k c^{+}_{k\sigma} c_{k\sigma} + \frac{1}{V}\sum_q v(q)\,\rho_{ind}(q,t)\,\rho(-q) + \frac{1}{V}\sum_q \underbrace{\phi_{ext}(q,t)}_{\frac{4\pi}{q^2}\rho_{ext}(q,t)}\,\rho(-q)$$

$$= \sum_k \varepsilon_k c^{+}_{k\sigma} c_{k\sigma} + \frac{1}{V}\sum_q \phi_{tot}(q,t)\,\rho(-q) \quad \text{--- (31)}$$

When we started out in eq(29), the electron density sees only the external potential ϕ_{ext}, but after applying the mean field theory on the Coulomb interaction, the same electron density sees a total potential which differs from the external one by including the induced charge of the electron density as

$$\phi_{tot}(q,t) = \phi_{ext}(q,t) + v(q)\,\rho_{ind}(q,t). \quad \text{--- (32)}$$

- Now, the RPA Hamiltonian in eq(31) is just a non-interacting electron gas under an electrostatic time-dependent potential $\phi_{tot}(q,t)$. This Hamiltonian is exactly same as the non-interacting theory we have solved in the previous section. Now we employ Kubo formula, in which the induced charge density is related to

$\phi_{ext}(q,t)$ through the non-interacting / Lindhard response function:

$$\rho_{ind}(q,\omega) = \chi_0(q,\omega)\,\phi_{tot}(q,\omega) \quad \text{--- (33)}$$

This is the key outcome of the RPA approximation. Substituting eq (32) in eq (33) and manipulating for ρ_{ind} we get

$$\rho_{ind}(q,\omega) = \frac{\chi_0(q,\omega)}{1-v(q)\,\chi_0(q,\omega)}\,\phi_{ext}(q,\omega)$$

$$= \chi_{RPA}(q,\omega)\,\phi_{ext}(q,\omega) \quad \text{--- (34a)}$$

where

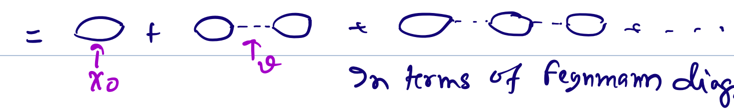
$$\chi_{RPA}(q,\omega) = \frac{\chi_0(q,\omega)}{1-v(q)\,\chi_0(q,\omega)} \quad \text{--- (34b)}$$

So, the induced charge density response to the total / screened potential as free electron, where to the external potential through χ_{RPA} susceptibility.

The binomial expansion of eq (34b) gives:

$$\chi_{RPA}(q,\omega) = \chi_0(q,\omega)\sum_{n=0}^{\infty}\left(v(q)\,\chi_0(q,\omega)\right)^{2}$$

$$= \chi_0 + v\,\chi_0^2 + v^2\chi_0^3 + \cdots \qquad [q,\omega \text{ dep implicit}]$$



In terms of Feynmann diagram.

The above expansion reveals that the many-body RPA response function is nothing but summation over infinite number of fluctuations of non-interacting density. RPA theory was not initially taken seriously untill it was reproduced by perturbation theory using Feynmann diagram. RPA theory ignores exchange term in the mean-field theory as well as is not self-consistent. Otherwise, its a pretty good approximation as long as the denominator is positive definite. At $1 - v(q)\chi_0(q, \omega) = 0$, one has divergence and hence is a good approximation if the interaction is <u>weak</u> $v(q) \leq \chi_0^{-1}(q, \omega)$. At $\omega \to 0$, the $1 - v(q)\chi_0(q, 0) = 0$ is called the Stoner instability, as we will discuss later.

- Now from the definition of the dielectric constant (eq 27). By substituting $\chi = \chi_{RPA}$, we get

$$\varepsilon_{RPA}(q, \omega) = \frac{1}{1 + v(q)\chi_{RPA}(q, \omega)} = 1 - v(q)\chi_0(q, \omega) \qquad \text{— (34c)}$$

We see something interesting that while the interacting susceptibility appears in the denominator in ε, the non-interaction one appears in the numerator and with a <u>negative</u> sign. Therefore, the RPA interacting response is very different from the non-interacting one for any finite strength of the coulomb interaction $v(q)$.

4.3 Screening:

As we saw in eq (28), dielectric constant $\varepsilon(q,\omega)$ appears in the denominator of the Coulomb interaction

$$v_{\text{screened}}(q,\omega) = \frac{v(q)}{\epsilon(q,\omega)} \quad \text{--- (28)}$$

Within the RPA approximation, we have $\varepsilon(q,\omega) = 1 - v(q)\,\chi_0(q,\omega)$.

Static screening

Static screening meaning $\omega \to 0$. We brought the test charge way back in time, and we are asking how does the electron density response to that charge: $\varepsilon(q,0)$

Thomas Fermi Approximation: In this case we also set $q \to 0$, i.e. the uniform electrostatic potential. We have computed before $\chi_0(0,0) = -d(\varepsilon_F)$, where $d(\varepsilon_F)$ is the density of states at ε_F.

Then

$$\epsilon_{RPA}(q,0) = 1 + v(q)\,d(\varepsilon_F)$$
$$= 1 + \frac{4\pi e^2}{q^2} d(\varepsilon_F) = 1 + \frac{q_{TF}^2}{q^2}. \quad \text{--- (35a)}$$

(The Thomas-Fermi screening is actually derived for the long range Coulomb repulsion $v(q) = 4\pi e^2/q^2$. The trouble with this theory is that we set $q \to 0$ in the response function, but not in the dielectric constant. Therefore, this is not such a good approximation and we can do better below. But the final result is incredibly simple and occasionally work.

q_{TF} is called the T.F wave vector $\boxed{q_{T.F.} = \sqrt{4\pi e^2 d(\varepsilon_F)} = \sqrt{\frac{2.434}{r_s}}\frac{1}{a_0}}$

So, q_{TF} is associated with some length scale whose physical role is interesting. To figure that out we perform an inverse Fourier transformation of the screened Coulomb interaction :

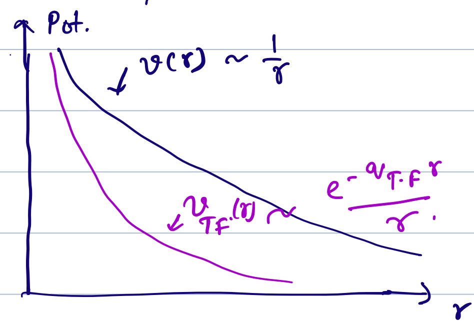
$$v_{RPA}(q) = \frac{4\pi e^2}{q^2 + q_{TF}^2} \quad \text{--- (35b)}$$

$$v_{RPA}(r) = \frac{1}{V}\int \frac{d^3q}{(2\pi)^3} \frac{4\pi e^2}{q^2 + q_{TF}^2} e^{i q \cdot r}$$ (This integration must be familiar to all of us).

$$= \frac{e^2}{4\pi} \cdot \frac{e^{-q_{TF} r}}{r} \quad \text{--- (35c)}$$

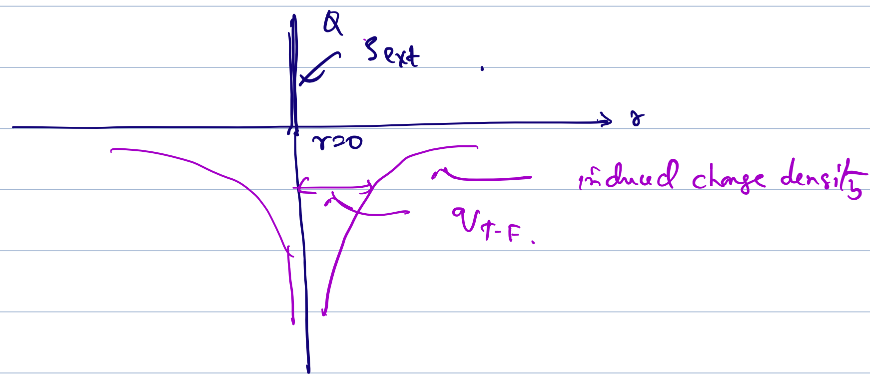
$$= \frac{e^2}{4\pi} \frac{e^{-\alpha \frac{r}{a_0}}}{r}, \quad \alpha = \sqrt{\frac{2.434}{r_s}} \sim 1 \text{ in metal.}$$

Now we see that the Coulomb interaction is exponentially decreasing with r, and $\hbar / q_{TF}$ gives the screening length of the coulomb interaction. (Recall a similar Yukawa potential was derived for the nuclear strong force).



Suppose we take a completely local external charge $\rho_{ext}(r) = Q\, \delta^{(3)}(r)$ then the induced charge density is

$$\rho_{ind}^{(TF)}(r) = -Q\, q_{TF}^2 \frac{e^{-q_{TF} r}}{r}.$$



At $r \to 0$ where the test charge is inserted, we see that $\rho_{ind} \to \infty$, with opposite sign of the charge. This means the test charge is completly screened by the electron in a metal. This is not surprising because electrons are free to move around in a metal (free fermion). So, all the negative charge rush to the test charge to conterbalance the test charge. We can easily verify that $\int \rho_{ind}(r)\, d^3r = \rho_{ind}(q=0) = -q$. So, we have a perfect screening with the T-F approximation.

As we mentioned, Thomas Fermi Approximation has the inconsistency of setting $q \to 0$ in the bare susceptibility, but not in the dielectric constant. The T.F approximation is also semiclassical approximation and does not consider a Fermi surface and exclusion principles. In other words, it does not consider the quantum fluctuations. They are however important as they tend to slow down the decay of the screened charge.

- For metal $r_s \sim 2-6$. Hence $q_{TF}^{-1} \sim 0.34\sqrt{r_s}\,\mathring{A} \approx 0.45 - 0.9\,\mathring{A}$. This is much smaller than the lattice constant $\sim 3\,\mathring{A}$ and also smaller than the interelectron distance $r_s a_0$ in an electron liquid/gas. On the otherhand, the Thomas-Fermi Theory - which is the $q \to 0$ limit theory does not correctly predict the behavior at large distance as we will see below.

⊛ Friedel Oscillation: We now relax the $q=0$ limit and consider all q in the susceptibility and $\varepsilon(q)$ for $\omega \to 0$.

We computed

$$\chi_0(q,0) = -d(\varepsilon_F)\, F\left(\frac{q}{2k_F}\right)$$

where $$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln \frac{1+x}{1-x}.$$

We discussed that $F(x)$ has a singularity at $x=1$, i.e., $q=2k_F$ in which its first derivative diverges logarithmically. For this case, the screening of a point charge Q at $r=0$ [i.e., $\rho_{ext} = Q\,\delta^3(0)$] looks like

$$\rho_{ind}(r) = -Q \int \frac{d^3q}{(2\pi)^3} \frac{q_{TF}^2\, F(q/2k_F)}{q^2 + q_{TF}^2\, F(q/2k_F)}\, e^{i\vec{q}\cdot\vec{r}} \quad \text{---(36)}$$

An important point to remember that any singularity, i.e., pole in a function is like a "localization" of that function, which yields a delocalized behavior in its Fourier space. Therefore, the singularity in F-function in q-space gives rise to a long distance property in real space. $F(q/2k_F)$ actually has a branch cut due to its log behavior. We want to see what does it corresponds to in the $\rho_{ind}(r)$:

$$\rho_{ind}(r) = \frac{-Q}{2\pi^2 r} \int_0^\infty dq\, q\, \sin(qr)\, \frac{q_{TF}^2\, F(q/2k_F)}{q^2 + q_{TF}^2\, F(q/2k_F)}.$$

↑ This term arises after doing the angular integration of $\int e^{iqr\cos\theta}\, d\theta$.

In the case of Thomas-Fermi approximation $q \to 0$, $F \to 1$, and then the exponential part $e^{i\vec{q}\cdot\vec{r}}$ oscillates rapidly at $r \to \infty$ and in the integration it cancels out. But now the singularity in F does not cancel out the integral. We have to look at the analytic structure of F to figure out its long distance behavior, so we need to go to the complex plane. To close the contour it better to go to $-\infty$ to ∞. Thankfully, $F(x)$ is an even function, and the entire integrand is also even in q. So, we extend the integrand from $-\infty$ to $+\infty$ with a factor of 2. So,

$$\delta_{Ind}(r) = -\frac{Q}{2\pi^2 r^2} \, \mathrm{Im}\int_{-\infty}^{\infty} dq \; q e^{iqr} \frac{q_{TF}^2 \, F(q/2k_F)}{q^2 + q_{TF}^2 \, F(q/2k_F)} .$$

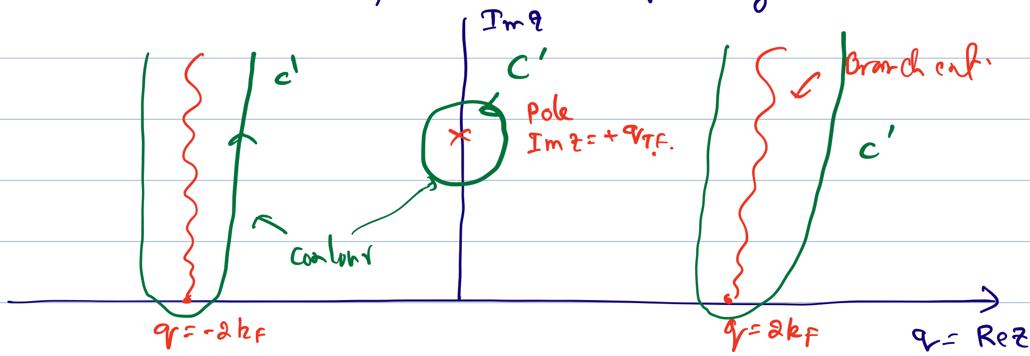
we want to do a contour integration of the following now:

$$I = \oint dz \; z e^{izr} \frac{q_{TF}^2 \, F(z/2k_F)}{z^2 + q_{TF}^2 \, F(z/2k_F)}$$

→ $e^{izr} \to 0$ if we close the contour on the upper half plane because $e^{-\mathrm{Im}z\, r} \to 0$ as $r \to \infty$.

→ $z^2 + q_{TF}^2 F(z/2k_F) \to 0$ at $z = +i q_{TF}$. This was the singularity which produces the $1/r$ behavior of the coulomb interaction.

→ But now we need to worry about the branch cut at $\mathrm{Re}\, z = q = \pm 2k_F$. So, we choose the following contour:



→ The pole part gives a $1/r$ as discussed above.

→ The new contribution is the branch cut part. The integration on the contour around the branch cut decays along the imaginary axis except at $q = \pm 2k_F$. This part in fact gives a strong contribution - which is oscillatory $e^{i2k_F r}$.

After performing the integration we get :

$$\rho_{ind}(r \to \infty) \sim Q \frac{\cos(2k_F r)}{r^3} \quad \text{--- (37)}$$

This is the main result of this calculation that the induced charge density oscillated due to particle-hole excitations exactly at $2k_F$. This is called the Friedel oscillation. This is actually observed easily in Scanning Tunneling Microscopy measurement.

- So, in fact we have two important behavior that we discovered that at $q \to q_{T-F}$, the induced charge density exponentially decays at $r \to \infty$ whereas at $q = 2F$, the charge density oscillates rapidly as $r \to \infty$. As we sum over all q, both contributions are present.
- The induced charge however perfectly screens the test charge Q as we sum over all q. This can be seen by integrating over $\int \rho_{ind}(r) d^3r = -Q$.
- The physics of this peculiar behavior for fermions is of course their quantum nature that as electrons try to screen the test charge, they have to follow the exclusion principle. The electrons inside the Fermi sea does not participate much in static screening. The electrons on the Fermi surface only scatter with all q-values upto $q = 2k_F$. All the other scattered electrons density decays exponentially except at $q = 2k_F$ which oscillates due to the singularity in the response function.

4.4. Dynamical Screening and Plasma Oscillations.

For the non-interacting susceptibility (χ_0) we observed that there are particle-hole continuum of excitation - which are short-lived and not bound states. At large $\omega \to \infty$, we saw a power law decay $\chi \sim nq^2/m\omega^2$.

Now we want to see the dynamical response of the RPA susceptibility. For the dynamical response, we will again be looking at the resonance condition in the imaginary part of χ_{RPA}. We have

$$\chi''_{RPA}(q,\omega) = \frac{\chi_0''(1-v\chi_0')}{(1-v\chi_0')^2 + v^2\chi_0''^2} \quad --- (38).$$

(q and ω dependence on χ_0 & v are implicit. χ_0', χ_0'' correspond to real and imaginary parts of χ_0.)

- First thing we notice is that χ''_{RPA} is directly proportional to χ_0'', i.e., to the particle-hole resonance spectrum. Therefore, the primary origin of having absorption/response in the interacting electron system is also the particle-hole excitation.

- We obtain a new resonance condition in the RPA case, given by
$$1 - v(q)\chi_0'(q,\omega) = 0.$$
This is completely different from the particle-hole continuum, and called the Plasmons. In fact, this is a sharp resonance with a dispersion (not a continuum), with long-lifetime. The resonance occurs at large frequency, $\omega \gg v_F q$ (why above $v_F q$? because, otherwise χ_0'' term causes decay of the resonance). We substitute

value of $\chi_0'(q, \omega \to \infty) = nq^2/m\omega^2$ in the above equation, which gives

$$1 - \frac{4\pi e^2}{q^2} \frac{nq^2}{m\omega^2} = 0$$

$$\Rightarrow \boxed{\omega_p = \sqrt{4\pi e^2 \frac{n}{m}} = \text{Plasma frequency.}} \quad \text{--- (39)}$$

Substituting $\chi_0' = nq^2/m\omega^2 = \frac{q^2}{4\pi e^2}\left(\frac{\omega_p}{\omega}\right)^2$ in χ_{RPA}, we get

$$\boxed{\chi_{RPA}(q,\omega) = \frac{4\pi e^2 q^2 (\omega_p/\omega)^2}{1 - \omega_p^2/\omega^2} = 4\pi e^2 \omega_p^2 \frac{q^2}{\omega^2 - \omega_p^2} = \frac{n}{m} \frac{q^2}{\omega^2 - \omega_p^2}} \quad \text{--- (40)}$$

Several comments are in order:

(i) The plasma frequency ω_p is completely dispersionless, i.e., local in real space. This is due to the cancellation of the q^2 term in eq (39) in 3D. (In 2D, the Coulomb interaction is not $1/q^2$, but $\sim \frac{1}{q}$. This gives a dispersive and gapless plasma mode).

(ii) The prefactor nq^2/m is sometimes called the oscillator strength which goes to zero $q \to 0$. The other term $1/(\omega^2 - \omega_p^2)$ is like a simple harmonic oscillator without any damping. So, its an energy conserving oscillation / resonance that the non-interacting electron density will experience if one shine an photon at the plasma frequency $\omega = \omega_p$. So, this is a complete absorption of photon energy at $\omega = \omega_p$ which will result in an undamped oscillation of electron density with long range Coulomb interactions. Note that the electron density oscillates at this frequency for all wavevectors (since ω_p does not depend on q), only the oscillator strength depends on q^2. So, ω_p is a fundamental frequency of any metal, depending on the charge density 'n' only.

(iii) $\omega < \omega_p$, $\chi_{RPA} < 0$, which is not allowed, ei, the interacting electrons in a metal does not respond to the photons at frequency less than its plasma frequency. So, the photons will be reflected completely at $\omega < \omega_p$ in a metal.

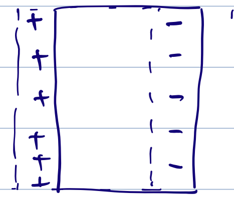
At $\omega = \omega_p$, all photons will be absorbed by the metal causing long-lived (undamped) density oscillation.

At $\omega > \omega_p$, there will be some absorption for $\omega < v_F q$ and at frequency $\omega > v_F q$, the density oscillation will decay into the particle-hole continuum (χ_0''), which gives the broadening of the resonance in eq (38).

For a density $n \sim 10^{23}$ electrons $/cm^3$, $\omega_p \sim 10^{16}\ sec^{-1}$ or

$\hbar\omega \sim 12$ eV This is very large and most metals are hence reflective.

We can get a semiclassical picture of the plasma resonance as follows. As the electrons move, on a positive background, they sort of create electric dipole moments. So, the electric field of thin capacitor plate of charge density ne is $4\pi n e x$, by Gauss law. Then the Newton's equation of motion is

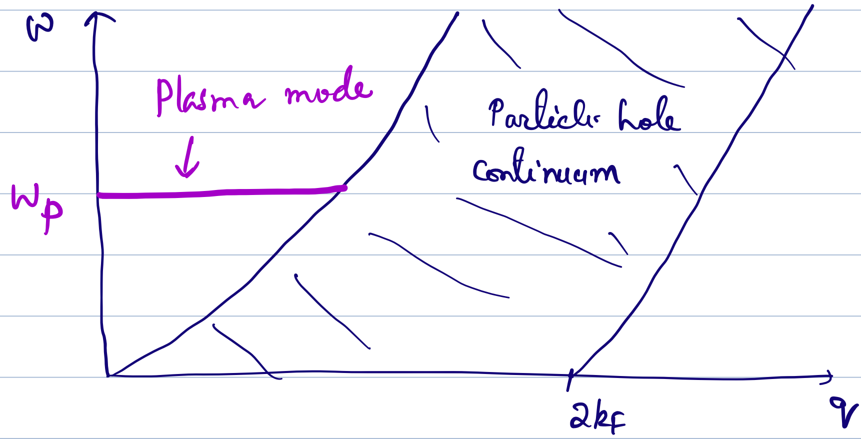


$$m\frac{d^2x}{dt^2} = -4\pi n e x = -eE$$

$$\Rightarrow \frac{d^2x}{dt^2} = -\omega_p^2 x.$$

So, one gets harmonic oscillator motion of collective oscillation of all electrons and positive charge centers (dipoles) at one natural frequency ω_p. There is no wave nature of the electron gas - they all osscillates around the positive charge centers at a coherent harmonic oscillator motion.

(iv) So the plasma mode is the collective mode of oscillations of all electrons at small wavevector (large distances) due to coulomb interactions. As we increase the wavevector, q, go to short wavelength fluctuations, $v_F q > \hbar\omega_p \sim v_F q_{TF}$, the electrons start to behave as non-interacting electrons. Then one has simple particle-hole continuum and the plasma oscillations are damped.



(ii) These plasma like collective oscillations of electron density is actually bosons - called Plasmons. (This is similar to collective oscillations of EM fields for photon or collective oscillations of nucleons called phonons or collective oscillations of spins - called magnons). This is interesting. We started with fermionic particles and obtained a many body ground state - fermi sea. The excitations around a Fermi sea is single Fermions, particle-hole continuum, and now we found something very novel bosonic excitations.

Another interpretation of plasma is that as the photons goes inside a metal, it becomes massive and plasma frequency is the Higgs mass of photon:

$$w^2 = c^2 k^2 + w_p^2$$

4.5 : Spectral Representation. (Kramers-Kronig Relation).

The spectral representation is a very powerful and general technique, which is applied to many other quantities/propagators such as Green's function, response function etc. We will learn it briefly and apply it to the Kubo formula. The spectral representation — roughly speaking — meaning representing these function in terms of the spectral lines — which are the energy eigenstates here. In many cases, we really cannot solve a many body eigenstate and hence do not really have a way to compute these function in spectral representation. But for mathematical derivation and interpretation, a spectral representation comes very handy. Moreover, in some cases, the results can be written in terms of "trace" which is independent of basis choice, and one can do the computation in any suitable basis. Knowing the energy eigenstates makes it easier to incorporate the temperature dependence via partition function quite easily.

- Let us now say $|n\rangle$ are the complete energy eigenstates of the Hamiltonian H that we can compute. Then $|n\rangle$ are orthonormalized as $\langle n|m\rangle = \delta_{nm}$, and present a complete Hilbert space $\sum_n |n\rangle\langle n| = \mathbb{1}$. Then the partition function is $Z = \sum_n e^{-\beta E_n}$, $\beta = \frac{1}{k_B T}$. And the trace of an operator $\hat{O}$ is defined as $Tr(\hat{O}) = \sum_n \langle n|\hat{O}|n\rangle$ and the expectation value of an operator at some thermal equilibrium is

$$\langle \hat{O} \rangle = \frac{1}{Z} \sum_n e^{-\beta E_n} \langle n | \hat{O} | n \rangle . \quad --- (41)$$

At $T \to 0$, only state that contributes is the ground state, because all particles must go to the ground state and its Boltzmann weight $e^{-\beta E_0}/Z \to 1$ for $E_0 \to 0$ as $\beta \to \infty$.

- Let us now apply this method to the Kubo formula:

$$\chi(q,\omega) = -\frac{i}{\hbar} \int_0^\infty dt \; e^{i\omega t} \langle [S(q,t), S(-q,0)] \rangle . \quad -- (42)$$

Recall that the integral goes from 0 to ∞, since χ is retarded.

We evaluate the expectation value of the commutator by using eq (41) and obtain:

$$\langle [S(q,t), S(-q,0)] \rangle = \frac{1}{Z} \sum_n \left[\langle n | S(q,t) \, S(-q,0) | n \rangle - (q \to -q) \right] e^{-\beta E_n}$$

insert $\sum_m |m\rangle\langle m| = \mathbb{I}$ and use the Heisenberg representation $S(q,t) = e^{iHt} S(q,0) e^{-iHt}$ $[\hbar = 1]$

$$= \frac{1}{Z} \sum_n e^{-\beta E_n} \left[\sum_m \langle n | e^{iHt} S(q,0) e^{-iHt} |m\rangle \; e^{-iE_m t} |m\rangle \langle m | S(-q,0) | n \rangle - (q \to -q) \right]$$

$$= \frac{1}{Z} \sum_{n,m} e^{-\beta E_n} \left[\langle n | S(q,0) | m \rangle \langle m | S(-q,0) | n \rangle \times e^{i(E_n - E_m)t} - (q \to -q) \right].$$

[Show that $\langle n | S(q,0) | m \rangle = \langle m | S(-q,0) | n \rangle^*$.].

$$= \frac{1}{Z} \sum_{n,m} e^{-\beta E_n} \left| \langle n | S(q,0) | m \rangle \right|^2 \left[e^{i(E_n - E_m)t} - e^{-i(E_n - E_m)t} \right].$$

so we get

$$\chi(q,\omega) = -\frac{i}{Z\hbar}\sum_{n,m}\int_0^\infty dt\, e^{i\omega t}\left|\langle n|\delta(q,0)|m\rangle\right| e^{-\beta E_n}\left[e^{i(E_n-E_m)t} - e^{-i(E_n-E_m)t}\right]$$

--- (43a)

(Since n & m are dummy indices, both being summed over, so we can exchange $n \leftrightarrow m$ in the 2nd term. Then we get

$$\chi(q,\omega) = -\frac{i}{Z\hbar}\sum_{n,m}\int_0^t dt\, e^{i\omega t}\left|\langle n|\delta(q,0)|m\rangle\right|^2\left(e^{-\beta E_n} - e^{-\beta E_m}\right) e^{i(E_n-E_m)t}$$

--- (43b)

- These two expressions are the same, but seem to convey very different physical processes.

(43a) The first term is like an energy absorption or a transition from $n \to m$ state, while the 2nd term is like an energy emission from $m \to n$ state. One can also view them as time-reversed terms of each other, as they do appear in some other derivations. In that way, the two terms will be regarded as retarded ($t > 0$ effect is after the cause) and advanced ($t < 0$, effect is before the cause), and we are subtracting them in the response function. If the two terms are the same (ie the time-reversal symmetry is present), then there is no dissipation.

(43b) In this equation, the time part remains the same, conveying only one transition process, while one is subtracting the thermal occupation probability between the initial and final states.

In equilibrium, the quantum tunneling (in time) between two states is equivalent to change in thermal occupation density of those states. This is something to do with the ergodicity hypothesis of the quantum statistical theory.

This ergodicity / equilibrium condition is embedded in a hidden analyticity of the complex response function. This can be exposed by defining an imaginary time (τ) for the temperature as $\beta \to -i\tau$. Then we can interpret the two terms as classical tunneling in imaginary time with one as retarded and the other one as advanced. We can do the entire calculation in imaginary time (or imaginary frequency - called the Matsubara frequency), and the final result can be obtained in real time via analytical continuation from imaginary frequency to real frequency $i\omega \to \omega \pm i\eta$ ($\eta \to 0$ is added for convergence as before and also shown below). This is because if the function is analytic (single valued), then it does not matter where the poles are as long as they lie within the contour of integration.

Such an imaginary time formalism often done in the Green's function formalism. In different books you will encounter either eq(43a) or (43b) depending on the different approaches invoked, but they are mathematically the same.

- We will show the results for both eqs (43 a) + (43 b).

The time integral can be done easily as

$$\int_0^t dt \; e^{i(\omega + E_n - E_m) - \eta t} = \frac{i}{\omega + E_n - E_m + i\eta}$$

↑ a decay term is introduced for convergence of the integral at long time.

Then we get from eqs (43 a) & (43 b) as

$$\chi(q, \omega) = \frac{1}{Z\hbar} \sum_{n,m} |\langle n|S(q,0)|m\rangle|^2 e^{-\beta E_n} \left[\frac{1}{\omega + E_n - E_m + i\eta} - \frac{1}{\omega - E_n + E_m - i\eta} \right] \quad \text{--- (44a)}$$

(opposite sign as this is retarded.)

$$= \frac{1}{Z\hbar} \sum_{n,m} |\langle n|S(q,0)|m\rangle|^2 \frac{e^{-\beta E_n} - e^{-\beta E_m}}{\omega + E_n - E_m + i\eta} \quad \text{--- (44b)}$$

- Now, we use the identity.

$$\lim_{\eta \to 0} \frac{1}{x + i\eta} = \mathcal{P}\left(\frac{1}{x}\right) - i\pi\delta(x).$$

This gives

$$\mathrm{Im}\,\chi(q, \omega) = -\frac{\pi}{Z\hbar} \sum_{n,m} |\langle n|S(q,0)|m\rangle|^2 e^{-\beta E_n} \left[\delta(\omega + E_n - E_m) - \delta(\omega - E_n + E_m) \right] \quad \text{--- (45a)}$$

$$= -\frac{\pi}{Z\hbar} \sum_{n,m} |\langle n|S(q,0)|m\rangle|^2 \left(e^{-\beta E_n} - e^{-\beta E_m} \right) \delta(\omega - E_n + E_m) \quad \text{--- (45b)}$$

$$= -\frac{\pi}{Z\hbar} \left(1 - e^{-\beta\omega} \right) \sum_{n,m} |\langle n|S(q,0)|m\rangle|^2 e^{-\beta E_n} \delta(\omega - E_n + E_m) \quad \text{--- (45b)}'$$

In the last equation we have substituted

$$e^{-\beta E_n} - e^{-\beta E_m} = e^{-\beta E_n}\left[1 - e^{-\beta(E_m - E_n)}\right] = e^{-\beta E_n}(1 - e^{-\beta\hbar\omega}).$$

- Now it is possible to write eq(44) in the so-called Spectral Representation (Spectral decomposition / Lehmann Representation in terms of the spectral weight / spectral function $A(q,\omega) = -\,\mathrm{Im}\,\chi(q,\omega)$ as

$$\chi(q,\omega) = \int_{-\infty}^{\infty} \frac{d\Omega}{\pi} \frac{\mathrm{Im}\,\chi(q,\Omega)}{\Omega - \omega - i\eta} \quad \text{---(46)}$$

(It's easy to substitute eq (46) in eq(45) to obtain eq(44).)

This equation (44a) is also called the Kramers-Kronig relation which is tied to the analyticity of the complex function and is another form of the Cauchy-Reimann equation (See Homework)

- The spectral function $A(q,\Omega)$ is odd in frequency:

$$A(q,-\Omega) = -A(q,\Omega).$$

This oddness of the function is sometimes known as the Onsager's reciprocal theorem.

- As $T \to 0$ and $\Omega > 0$;

$$A(q, \Omega) = -\pi \sum_n |\langle 0| S(q, 0) |n\rangle|^2 \, \delta(\Omega - E_n + E_0) \quad \text{---(44c)}$$

where E_0 is the ground state energy. This is clear because as $T \to 0$, the particles are in the ground state and hence the initial state is $|0\rangle$.

Eq (44c) is the same as the Fermi's Golden rule that one can derive from it as well. In QM-II course, we have learned to derive the Fermi's Golden rule that if we have a time-dependent perturbation $S(q, \Omega)$, what's the probability of making a transition from its ground state to all possible excited states.

- The purpose of deriving these spectral representation of the response function is to easily derive some more properties of the response function.

4.6 : Dissipation (or Absorption) = Im part of the Response Function χ. $\chi''(q,\omega)$

We claimed many times that $\text{Im}\,\chi(q,\omega)$ encode the energy dissipation or absorption by the material from the incident potential. Here we will start with the Fermi's Golden rule to compute the change in energy and present it in terms of $\text{Im}\,\chi(q,\omega)$.

In the presence of an external potential $\phi_{ext}(q,\omega)$, the change in average energy is $\sim \int \Delta E\, S(\Delta E)$, where $S(\Delta E)$ is the probability of making a specific transition of energy ΔE, which we write in terms of the Fermi's Golden rule. So, we have

$$\frac{d\langle H\rangle}{dt} = \int \frac{d^3q}{(2\pi)^3}\int \frac{d\omega}{2\pi}\cdot(2\pi)\,\frac{e^{-\beta E_m}}{Z}\,\left|\langle m|\,S(q,0)\,|n\rangle\right|^2$$

classical prob at T; quantum matrix-element.

$$\times\Big[(E_n-E_m)\,\delta(\omega+E_m-E_n) - (E_m-E_n)\,\delta(\omega-E_m+E_n)\Big]$$

energy absorption; stimulated emission

$$\times\ \left|\phi_{ext}(q,\omega)\right|^2.$$

These two terms are like the commutator of density operators.

$$= -\int\frac{d^3q}{2\pi}\int_0^{\omega}\frac{d\omega}{2\pi}\,\left|\phi_{ext}(q,\omega)\right|^2\,\omega\,\text{Im}\,\chi(q,\omega) \quad \text{--- (45)}$$

from eq(45a) after some manipulation.

4.7 Fluctuation / Correlation function / Structure Factor / [Scattering rate].

$S(q, \omega)$

Above we discussed the dissipation (of energy) defined by the imaginary part of the susceptibility - which is the commutator between density operators at different time (and position).

The fluctuation is determined by the first part of the commutator as

$$S(q, \omega) = \int_{-\infty}^{\infty} dt \, e^{i\omega t} \langle \delta(q, t) \, \delta(-q, 0) \rangle \quad \text{---(46)}.$$

← (the integral is from $-\infty$ to $+\infty$) — just a product, not the commutator.

$S(q, \omega)$ is often called the "S of q and ω" or the "structure factor".
$S(q, \omega)$ is actually a measure of the scattering cross-section for external electrons / x-rays to scatter by wavevector q and emitted energy ω.
Basically, we are computing the scattering probability for an electron to scatter by the external electron / photon / neutron etc that we impart on.
This is different from the susceptibility which measures the probability of energy absorption.

(Scattering cross-section is computed by the Born approximation which involves the scattering probability, scattering angle and some phase factor. Structure constant does not capture the phase factor. So, its like $S(q, \omega) \sim |\sigma(q, \omega)|^2$, where σ is the scattering crosssection).

- Now employing the spectral representation analysis as we did before, we obtain

$$S(q,\omega) = \frac{2\pi}{Z} \sum_{n,m} |\langle m| S(q,0) |n\rangle|^2 \, e^{-\beta E_n} \, \delta(\omega - E_n + E_m). \quad \text{--- (47)}$$

In another way of saying, the energy dissipation measures the residual energy loss after subtracting the probability of energy emission from the probability of energy absorption. But dissipation measures only the probability of energy emission for $\omega > 0$ (or the absorption for $\omega < 0$). This is like as the X-ray / neutron is incident on the matter, its energy is lost by $\omega > 0$ and momentum is lost by $q > 0$, compared to the reflected X-ray / neutron. Then this energy and momentum is absorbed by the electron which is now in its excited state. If the outgoing photon / neutron gain energy $\omega < 0$, then this additional energy has come from an electron being moved from its excited state to a lower energy state.

- In X-ray scattering, Raman scattering, neutron scattering etc we measure the structure factor $S(q,\omega)$.

(4.8) Fluctuation - Dissipation Theorem: [Ref. P. Colemann book chapter 8]

The fluctuation-dissipation theorem we may have encountered, knowingly or unknowingly, in other context such as in probability theory and/or statistical physics, solid state physics and so on. Dissipation is like friction, resistance, diffusion, and energy absorption/dissipation in the above concept. And fluctuation is like noise - the random/scattering of variation of some quantity in time. How some random variation affect the entire system in a system where all degrees of freedom are correlated and hence lead to absorption/dissipation (of energy mainly but can be general otherwise) in the system.

Since we have already computed the dissipation part in eq (45b) and fluctuation in eq (47), now by relating them we obtain the famous Fluctuation - Dissipation Theorem:

$$S(q,\omega) = -\frac{2\hbar \, \mathrm{Im}\, \chi(q,\omega)}{1-e^{-\beta\omega}} \quad \text{---} (48)$$

$$= 2\hbar \left[1+n_B(\omega)\right] \mathrm{Im}\, \chi(q,\omega).$$

The denominator in the Bose factor n_B (sometimes called the detailed balance of the Bose factor).

- The fluctuation-dissipation theorem is a general property of any Hamiltonian system in thermal equilibrium. This is as fundamental as, say, the continuity equation for non-dissipative system.

- At very small frequency, $\omega \ll k_B T$ i.e. $\beta\omega \ll 1$, we obtain

$$\boxed{S(q,\omega) = -\frac{2k_B T}{\omega} \, \mathrm{Im}\, \chi(q,\omega)} \quad \text{--- (49).}$$

This is actually the classical limit, as the bose factor is replaced by the "equipartition" like term here. In fact, in the classical statistical theorem one obtains the same relation.

- Einstein used such a relation for Brownian motion description (even though the Fluctuation-Dissipation theory was not formalized by then) in relating the diffusivity (fluctuation) of metal to its conductivity (dissipation). This is roughly relating how many particles will diffuse due to random Brownian motion to the number of particles that will drift to the other side giving conductivity. This is valid if the system is in thermal equilibrium.

- The "Johnson-Nyquist noise" in a wire is another example of the fluctuation-dissipation theorem. It replaces the noise in a wire to the resistance and temperature. The noise is the measure of fluctuation and the resistance is the measure of dissipation.

H.W. Consider a forced harmonic oscillator

$$m(\ddot{x} + w_0^2 x) + \eta \dot{x} = f(t)$$

← time-dependent force – noise → Fluctuation.

↑ friction/dissipation

Use linear response theory to define the response function $\chi(w)$ as $x(w) = \chi(w) f(w)$.
Then compute the fluctuation spectrum $S(w)$ as the standard deviation $\langle x(t) x(0) \rangle$, where the average is taken over thermal ensemble (Maxwell Boltzmann or use equipartition theorem).
Then show that the fluctuation-dissipation theorem in eq (49) is maintained here, which gives a relation between the force f and the friction η and temperature T: $\langle |f(w_0)|^2 \rangle = 2 k_B T \eta$

From P. Coleman's book:

Table. 10.1 Selected Spectroscopies .

	NAME	SPECTRUM	$\hat{A}$	Questions and Issues
ELECTRON	STM $\frac{dI}{dV}$	$\frac{dI}{dV}(\mathbf{x}) \propto A(\mathbf{x},\omega)\vert_{\omega=e\mathrm{V}}$	$\psi(x)$	Surface probe. $T \sim 0$ measurement. Is the surface different?
	ARPES	$I(\mathbf{k},\omega) \propto f(-\omega)A(\mathbf{k},-\omega)$	$c_{\mathbf{k}\sigma}(t)$	$p_\perp$ unresolved. Surface probe. No magnetic field
	Inverse PES	$I(\omega) \propto \sum_{\mathbf{k}}[1-f(\omega)]A(\mathbf{k},\omega)$	$c^\dagger{}_{\mathbf{k}\sigma}(t)$	p unresolved. Surface probe.
SPIN	χ_{DC} Uniform Susceptibility	$\chi_{DC} = \int \frac{d\omega}{\pi\omega}\chi''(\mathbf{q}=0,\omega)$	M	$\chi \sim \frac{1}{T}$ local moments. $\chi \sim$ cons paramagnet
	Inelastic Neutron Scattering $\frac{d^2\sigma}{d\Omega d\omega}$	$S(\mathbf{q},\omega) = \frac{1}{1-e^{-\beta\omega}}\chi''(\mathbf{q},\omega)$	$S(\mathbf{q},t)$	What is the background? Quality of crystal?
	NMR Knight Shift $\frac{1}{T_1}$	$K_{contact} \propto \chi_{\mathrm{local}}$ $T\int_q F(\mathbf{q})\frac{\chi''(\mathbf{q},\omega)}{\omega}\Big\vert_{\omega=\omega_N}$	$S(\mathbf{x},t)$	How is the orbital part subtracted? How does powdering affect sample?
CHARGE	Resistivity ρ	$\rho = \frac{1}{\sigma(0)}$	$\vec{j}(q=0)$	What is the resistance ratio? (R_{300}/R_0)
	Optical Conductivity	$\sigma(\omega) = \frac{1}{-i\omega}[\langle j(\omega')j(-\omega')\rangle]_0^\omega$	$\vec{j}(\omega)$	Reflectivity: How was the Kramer's Krönig done? Spectral weight transfer?

(4.9) The f-sum rule :

The f-sum rule comes from the sum rule in spectral line theorem, that is the sum over all possible transitions is fixed. Its also related to analyticity of the response function.

According to the f-sum rule, the integrated spectral weight of the response function must equate to the number of electrons in the system.

Mathematically, the f-sum rule looks like

$$\int_0^\infty d\Omega \; \Omega \, \mathrm{Im}\, \chi(q,\omega) = \frac{\pi}{Z} \sum_{n,m} |\langle n| \delta(q,0) |m\rangle|^2 \left[e^{-\beta E_m} - e^{-\beta E_n}\right] \times \int d\Omega \; \Omega \; \delta(\Omega - E_n + E_m).$$

[using eq (4.5 b)]

$$= \frac{1}{Z} \sum_{n,m} |\langle n| \delta(q,0) |m\rangle|^2 (E_n - E_m) \times \left[e^{-\beta E_m} - e^{-\beta E_n}\right]$$

Now, we want to go back from the spectral representation to the commutator algebra. To do that we have to collect the $|m\rangle\langle m|$ terms and replace it with $\mathbb{I}$.

$$|\langle n| \delta(q,0)|m\rangle|^2 (E_n - E_m) = \underbrace{(E_n - E_m)\langle n| \delta(q)|m\rangle}_{\langle n|[\delta(q,0),H]|m\rangle} \langle m| \delta(-q,0)|n\rangle$$

as $H|n\rangle = E_n|n\rangle$.

$$= \langle n| [\delta(q,0), H] |m\rangle \langle m| \delta(-q,0)|n\rangle.$$

We do the same for the other term and obtain

$$= \frac{1}{Z} \sum_{mn} \Big[e^{-\beta E_m} \langle n| [\delta(q,0), H] |m\rangle \langle m| \delta(-q,0)|n\rangle - e^{-\beta E_n} \langle n| [\delta(q,0), H] |m\rangle \langle m| \delta(-q,0)|n\rangle \Big].$$

$$= \frac{1}{Z} \sum_n e^{-\beta E_n} \Big[\langle n | [\rho(q,0), H] \rho(-q,0) | n \rangle - \langle n | \rho(-q,0) [\rho(q,0), H] | n \rangle \Big]$$

$$= \langle [[\rho(q,0), H], \rho(-q,0)] \rangle$$ according to the definition of the expectation value at thermal equilibrium. — ... (58)

- Now we notice that for any generic Hamiltonian in which any interaction which is governed by density, such as Coulomb interaction, will not contribute here because of the commutator. So, we will get a generic result that the value of this double commutator depends on the band structure only, i.e. on the kinetic energy of the Hamiltonian.

Lets consider the coulomb interaction Hamiltonian

$$H = \underbrace{\sum_{k,\sigma} \varepsilon_k c^{\dagger}_{k\sigma} c_{k\sigma}}_{H_K} + \underbrace{\frac{1}{2V} \sum_q v(q)\, \rho(q)\, \rho(-q)}_{H_{int.}}$$

where $\rho(q) = \sum_{k,\sigma} c^{\dagger}_{k+q\,\sigma} c_{k\sigma}$.

- $[\rho(q), H_{int}] = 0$,
- $[\rho(q), H_K] = \sum_{k,k',\sigma\sigma'} \varepsilon_{k'} [c^{\dagger}_{k+q\sigma} c_{k\sigma}, c^{\dagger}_{k'\sigma'} c_{k'\sigma'}]$

where $\varepsilon_{k'} [c^{\dagger}_{k+q\sigma} c_{k\sigma}, c^{\dagger}_{k'\sigma'} c_{k'\sigma'}]$

$$= \varepsilon_{k'} c^{\dagger}_{k+q\sigma} \underbrace{c_{k\sigma} c^{\dagger}_{k'\sigma'}}_{\delta_{kk'}\delta_{\sigma\sigma'} - c^{\dagger}_{k'\sigma'} c_{k\sigma}} c_{k'\sigma'} - \varepsilon_{k'} c^{\dagger}_{k'\sigma'} \underbrace{c_{k'\sigma'} c^{\dagger}_{k+q\sigma}}_{\delta_{k+q\,k'}\delta_{\sigma\sigma'} - c^{\dagger}_{k+q\sigma} c_{k'\sigma'}} c_{k\sigma}.$$

$$= \varepsilon_k \left[c^{\dagger}_{k+q\sigma} c_{k\sigma} - c^{\dagger}_{k+q\sigma} c^{\dagger}_{k'\sigma'} c_{k\sigma} c_{k'\sigma'} \right] - \varepsilon_{k+q} \left[c^{\dagger}_{k+q\sigma} c_{k\sigma} + c^{\dagger}_{k'\sigma'} c^{\dagger}_{k+q\sigma} c_{k'\sigma'} c_{k\sigma} \right]$$

$$= (\varepsilon_k - \varepsilon_{k+q})\, c^{\dagger}_{k+q\sigma} c_{k\sigma}$$

- $$[[S(q), H_K], S(-q)] = \sum_{\substack{kk' \\ \sigma\sigma'}} (\varepsilon_k - \varepsilon_{k+q}) \left[c^{\dagger}_{k+q\sigma} c_{k\sigma},\; c^{\dagger}_{k'-q\sigma'} c_{k'\sigma'} \right].$$

$$(\varepsilon_k - \varepsilon_{k+q}) \left(c^{\dagger}_{k+q\sigma} c_{k\sigma} c^{\dagger}_{k'-q\sigma'} c_{k'\sigma'} - c^{\dagger}_{k'-q\sigma'} c_{k'\sigma'} c^{\dagger}_{k+q\sigma} c_{k\sigma} \right)$$

$\delta_{kk'-q}\delta_{\sigma\sigma'} - c^{\dagger}_{k'-q\sigma'} c_{k\sigma}$ $\quad$ $\delta_{k+qk'}\delta_{\sigma\sigma'} - c^{\dagger}_{k+q\sigma} c_{k'\sigma'}$

$$= (\varepsilon_k - \varepsilon_{k+q})\, c^{\dagger}_{k+q\sigma} c_{k+q\sigma} - (\varepsilon_k - \varepsilon_{k+q})\, c^{\dagger}_{k\sigma} c_{k\sigma}.$$

$$= -2(\varepsilon_{k+q} - \varepsilon_k)\, c^{\dagger}_{k\sigma} c_{k\sigma}$$ with a change of variable in the 2nd term

- substituting this form in eq (50) we get

$$\langle [[S(q), H], S(-q)] \rangle = -2 \sum_{k,\sigma} (\varepsilon_{k+q} - \varepsilon_k) \langle n_{k\sigma} \rangle$$

$\langle n_{k\sigma} \rangle = f(\varepsilon_k)$ ← Fermi Dirac distribution funct.

$$= -\frac{2\hbar^2 q^2}{2m} \sum_{k,\sigma} f(\varepsilon_k)$$

$\sum_{k,\sigma} f(\varepsilon_k)$: n = number density

for $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$, $\varepsilon_k - \varepsilon_{k+q} = \frac{\hbar^2 q^2}{2m} - \frac{\hbar^2}{2m} 2\vec{k}\cdot\vec{q}$.

drops out as summation over $\vec{k}$ from $-\pi/a$ to π/a gives zero.

$$= -\frac{\hbar^2 q^2}{m} n.$$

Therefore, we obtain the universal relation that

$$\int_0^\infty d\Omega \; \Omega \; \mathrm{Im}\, \chi(q, \Omega) = -\frac{\hbar^2 q^2}{m} n \quad \text{--- (51).}$$

- This is the famous f-sum rule for the response function. The key feature of the f-sum rule is that it is universal, depending only on the non-interaction dispersion — or the sum over the bare energy difference at this q-value $\sum_k (\epsilon_k - \epsilon_{k+q})$, and the bare electron mass m and the number of electron in the system. The relation remains universal for any density-density interaction one puts.

- Physically what this relation implying is that as we perturb the density of the system with some energy ω and at some wavevector q, electrons get excited across the Fermi surface and if we sum over all such excitations, it must equate to the total number of electrons in the system, something like the total number of excitations that is possible. Its only the Fermi statistics that matters for the scattering process, not the Coulomb or any other interaction that commutes with the density operator at that q-vector.

- The f-sum rule is also a consequence of the Kramers-Kronig relation - which is to do with the analyticity of the response function. From eq (49a)

$$\chi(q, \omega) = \int_{-\infty}^{\infty} \frac{d\Omega}{\pi} \frac{\mathrm{Im}\, \chi(q, \Omega)}{\Omega - \omega - i\eta}.$$

Now take $\omega \to \infty$ limit: $\frac{1}{\Omega - \omega} = -\frac{1}{\omega} - \frac{\Omega}{\omega^2} - \cdots$ (binomial expansion)

Now $\text{Im}\chi$ is odd under $\Omega \to -\Omega$ as we saw before. So, the first term vanishes. The 2nd term contributes as

$$\chi(q,\omega) = -\frac{1}{\omega^2}\int_{-\infty}^{\infty} \frac{d\Omega}{\pi}\, \Omega\, \text{Im}\chi(q,\omega)$$

$$= -\frac{1}{\omega^2}\underbrace{\int_{-\infty}^{\infty} \frac{d\Omega}{\pi}\, \Omega\, \text{Im}\chi(q,\omega)}_{-\frac{\hbar^2 q^2}{m} n}$$

$$= \frac{\hbar^2 q^2}{m\omega^2} n = \frac{\hbar^2 q^2}{4\pi e^2 \omega^2} \omega_p^2, \qquad \omega_p^2 = \frac{4\pi e^2}{m} n.$$

This is exactly the result we obtained in the non-interacting susceptibility at $\omega \to 0$, and also for the RPA susceptibility for $\omega > v_F q$ limit. This is an exact result for a closed system which does not violate causality that the total absorption in the continuum is related to the plasma frequency.

- The same sum rule is obtained for any other response function such as neutron scattering spectrum, optical conductivity. Through optical conductivity — which is defined by the current-current commutator also relates to the Plasma frequency through the optical f-sum rule. — Home work.