Chapter 4: Linear Response Theory (Kubo Formula) and applications

4.1A: Linear Response Theory.

4.1B: Non-interacting electron gas, Lindhard function, Particle hole Continuum

Ref: Subir Sachdev Youtube Lectures on quantum theory of solid

G. Mahan book

P. Phillips book.

G. Vignalle book.

In the previous chapter, we had a fixed uniform positive charge background on which electrons are moving. This was an unphysical setting, because charges are mobile and thus when the mobile charges see a point (test) charge, they are attracted to/repelled from the test charge (depending on opposite/same sign of the test charge). Imagine we insert a positive test charge on an electron gas. Because electrons are mobile, so, they will be attracted towards this test charge and create a region of large electron density near the positive charge. Then if we add another positive test charge at a distance, the 2nd positive charge will see a much reduced effective positive charge at the other test charge, due to the electron cloud around it. This will reduce the effective Coulomb interaction substantially. Such an effect is captured by introducing the dielectric constant ε in the electricity and magnetism course. This is called screening.

Generally, electrons are mobile, with its velocity not being uniform in a lattice. Electrons slow down near a nucleus/ion, move faster away from it. Moreover, at finite temperature, the electron density fluctuates. The density fluctuates (analog to vibration) collectively, and one obtains modes - like the phonon modes for nucleus vibrations/fluctuations. These collective density fluctuations have wavevectors - called plasma waves and the quantized density fluctuations are called plasmons. These fluctuations also causes screening - called dynamical screening. The resulting dielectric constant depends on wavevector and frequency $\varepsilon(q, \omega)$ and one obtains frequency dependent Coulomb interaction $U(q, \omega) \sim e^2/q^2 \varepsilon(q, \omega)$.

These fluctuations also causes dissipation (like friction). Such effects are captured by fluctuation - dissipation theorems. In more modern language, we learn it via simpler Linear Response Theory - called Kubo formula. In Kubo formula we obtain, complex dielectric function, with its real part capturing the plasma dispersion and the imaginary part captures dissipation. Because, the complex ε - function is analytic, both the fluctuation & dissipation are related to each other - hence we recover the Fluctuation - Dissipation theory.

⊛ Introduction to Screening & Dielectric constant. – G. Mahan.

Lets assume we add an external test charge Q, given by some density $Q = \int d^3r\, \rho_{ext}(r)$ in a metal (e-gas). A test charge can be regarded as some local fluctuation of the (uniform/ mean) charge density or impurity. This test charge distribution causes an electric field, and the mobile electrons must distribute themselves to cancel this electric field, so that the system is stabilized. The amount of electron charge to be screened around the test charge is $-Q$ (with some length scale). Its important to note that the total charge must be cancelled, not their charge density at each position. So, lets say the screened/ induced electron density is $\rho_{ind}(r)$, such that the electrostatic potential due to the total charge density $\rho_{tot}(\vec{r}) = \rho_{ext}(\vec{r}) + \rho_{ind}(\vec{r})$, is

$$\phi(r) = \int d^3r' \frac{\rho_{tot}(\vec{r}')}{|\vec{r}-\vec{r}'|} \quad \text{---} (1)$$

The screened charge is not necessarily in bound state due to the electric field from the charge, they can be mobile and $\rho_{ind}(\vec{r})$ is then the equilibrium or instantaneous charge density (we will consider its dynamics later in this chapter). So, the mobile charge (in a metal) spends more time near the test charge (if its attractive), than in other places. When these motions are averaged in time, there is more electron density near a test charge (nucleus), than in other places. So, the density fluctuates in both space & time.

In a simple picture, one can think of it as follows. The electrostatic potential energy $e\phi(r)$ causes a spatial variation of the chemical potential $\mu(r)$ and in its response the charge density is modulated $n(r)$. Their ratio is called the compressibility $\chi \sim \partial n / \partial \mu$, which we are essentially going to evaluate here.

The classical picture is similar to the EM theory. The external charge is related to displacement vector $\vec{D}$, while the total charge is related to the electric field $\vec{E}$, via Gauss law:

$$\vec{\nabla} \cdot \vec{D}(\vec{r}) = 4\pi \rho_{ext}(\vec{r}) \quad \text{--(2a)}$$

$$\vec{\nabla} \cdot \vec{E}(\vec{r}) = 4\pi \rho_{tot}(\vec{r}) \quad \text{--(2b)}$$

Their Fourier transformation gives:

$$i\vec{q} \cdot \vec{D}(\vec{q}) = 4\pi \rho_{ext}(\vec{q})$$

$$i\vec{q} \cdot \vec{E}(\vec{q}) = 4\pi \rho_{tot}(\vec{q})$$

Consider the longitudinal components of E & $\vec{D}$ (along the propagation direction of $\vec{q}$). Then the dielectric constant is defined by the kernel:

$$\varepsilon(q) = \lim_{\rho_{ind}\to 0} \frac{D_\ell(q)}{E_\ell(q)} = \lim_{\rho_{ind}\to 0} \frac{\rho_{ext}(\vec{q})}{\rho_{tot}(\vec{q})} \quad \text{--(3)}$$

(ℓ = longitudinal)

$\varepsilon(q)$ is a property of the material, and is governed by the charge density fluctuation. In a linear screening model, one assumes, this definition holds for non-zero ρ_{ind}. Then using Gauss law $E_\ell(r) = -\nabla_\ell \phi(r)$ or $E_\ell(q) = -iq\,\phi(q)$, where $\phi(q)$ is the electrostatic potential, we obtain

$$\phi(\vec{q}) = \frac{4\pi}{q^2} S_{tot}(\vec{q}) \quad \text{--(4a)}$$

$$= \frac{4\pi}{q^2} \frac{S_{ext}(\vec{q})}{\varepsilon(\vec{q})}. \quad \text{--- (4b)}$$

Below, we perform a quick, static calculation of $\varepsilon(q)$ in the $q \to 0$, i.e., long-wavelength density variation case - which is valid when the electrostatic potential $\phi(r)$ varies very slowly in space. This is called the Thomas-Fermi approximation. Then we will formalize it better within the Linear response theory (Kubo formula) for all wavelength and frequency dependence of $\varepsilon(q, \omega)$ calculation. These density fluctuations are called plasmons.

- One may mistakenly think that the screening is only occurring in response to an external electric field or charge density. This is not true. Electrons in a metal are always screened due to charge density fluctuation and positive background, and hence to an another electron, the given electron's charge density is much reduced, which effectively screened the Coulomb interaction as written by

$$v_{screened} = \frac{v_0(q)}{\varepsilon(q)}, \quad \text{where } v_0(q) = \frac{4\pi e^2}{q^2}.$$

So, $\varepsilon(q)$ is an internal properties of the system.

- The response to an external perturbation (generally electric/magnetic field) in the density/current fluctuation is computed within the Linear Response Theory (Kubo formula).

Linear Response Theory (Kubo Formula)

S. Sachdev, Youtube (Lec 6).

The external perturbation can be time-dependent such as time-dependent electric field, and/or it can be thought of being turned on at some time t_0, and the system was in its ground state or in some thermal equilibrium before the perturbation. So, we will invoke a time-dependent perturbation theory. The time-dependent perturbation theory uses interaction picture for convenience.

- Schrödinger Picture (S.P.): $H|\Psi(t)\rangle = i\hbar \frac{\partial}{\partial t}\Psi(t)$.

$$\Rightarrow \quad |\Psi(t)\rangle = e^{-iHt/\hbar}\,|\Psi(0)\rangle .$$

States are time dependent, but operators are time-independent.

- Heisenberg Picture (H.P.) $\quad i\hbar \frac{\partial}{\partial t} A(t) = [H, A(t)]$.

$$\Rightarrow \quad A(t) = e^{iHt/\hbar}\, A(0)\, e^{-iHt/\hbar} .$$

States are time-independent, but operators are time-dependent.

The expectation values of physical operators are invariant:

$$\underbrace{\langle \Psi(t)|A(0)|\Psi(t)\rangle}_{\text{S.P.}} = \underbrace{\langle \Psi(0)|A(t)|\Psi(0)\rangle}_{\text{H.P.}}$$

- Interaction picture (I.P.) $\quad H(t) = H_0 + V(t) \quad$ ---(1)

Any perturbation $V(t)$ will be treated as "interaction" although H_0 also has its many-body interaction in it.

Here both state and operators evolve in time, but differently.

$$\underbrace{|\Psi_I(t)\rangle}_{\text{state in I.P.}} = e^{iH_0t/\hbar}\underbrace{|\psi_s(t)\rangle}_{\text{state in S.P.}} = \underbrace{e^{iH_0t/\hbar}e^{-iHt/\hbar}}_{\sim e^{-iVt/\hbar} \text{ if } [V, H_0]=0}|\psi(0)\rangle \quad ---(2)$$

$$A_I(t) = e^{iH_0t/\hbar}\underbrace{A(t)}_{\text{S.P. where } A(t) \text{ is time dependent to begin with in S.P.}} e^{-iH_0t/\hbar} \quad ---(3)$$

(Note that the time evolution to states & operators of the S.P is done with the non-perturbed Hamiltonian H_0, not the full Hamiltonian).

This gives the time-evolution equation of motion of $V_I(t) = e^{iH_0t/\hbar}V(t)e^{-iH_0t/\hbar}$,

$$i\hbar\frac{\partial}{\partial t}|\Psi_I(t)\rangle = V_I(t)|\Psi_I(t)\rangle. \quad ---(4)$$

Then the solution of eq (4) is

$$|\Psi_I(t)\rangle = \underbrace{U(t,t_0)}|\Psi_I(t_0)\rangle$$

where the unitary time evolution operator of the state in the interaction picture:

$$U(t,t_0) = T_t \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t}V_I(t')dt'\right] \quad ---(5)$$

where the time-ordering operator is introduced since $V_I(t)$ does not necessarily commute with itself at a different time.

⊛ The equation (5) is exact for any "interaction" term V_I. The linear response theory basically stems from the approximation in $U(t,t_0)$ by keeping only the first two terms:

$$U(t,t_0) \approx I - \frac{i}{\hbar}\int_{t_0}^{t}V_I(t')dt' + \mathcal{O}((V_I\Delta t)^2) \quad --(6)$$

Basically this is an acceptable solution if the perturbation V_I is small, and/or, if the time interval $\delta t = t - t_0$ is infinitesimally small.

4.1 A Linear Response Theory (formal definition):

- The theory is applicable to calculations of the modifications of ground state properties due to intrinsic fluctuations of quantities such as charge density / current density etc. But for the calculational trick, we first assume there is an external perturbation to cause that fluctuation and at the end we remove that external field. So, we take H_0 to be our many-body full Hamiltonian (time-independent), and $H(t)$ is an external perturbation which starts at t_0. So, the full time dependent Hamiltonian is

$$H(t) = H_0 + V(t)\,\theta(t-t'), \quad \text{where } \theta(t-t_0) \text{ is the usual step function.} \quad \text{---}(7)$$

- Let say we know the full eigenspectrum of H_0 as

$$H_0|\Psi_n\rangle = E_n|\Psi_n\rangle, \quad \text{---}(8).$$

and we are interested in the time evolution of the $|\Psi_n\rangle$ states of H_0 at $t>t_0$. In the interaction picture, using eq (6) we have

$$|\Psi_n^{(I)}(t)\rangle = \left(\mathbb{I} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, V_I'(t)\right)|\Psi_n^{(I)}(t_0)\rangle. \quad \text{---}(9)$$

We are actually not going to evaluate how the state has evolved after the external perturbation is turned on. That's too hard and sometimes not needed for the purpose of measuring a few relevant properties which are affected by the external perturbation.

- Rather, we will study some physical operator $A(t)$

whose expectation value is what we measure. This is what we want to evaluate in the ground state, or in the thermal equilibrium. The operator $A(t)$ can be the density matrix of the state. For example, if we apply voltage, we measure current; or if we apply gate, we measure charge density, or for magnetic field perturbation, we measure magnetization. Then the linear relation between the ext voltage and the current is the conductivity, or between electrostatic potential and charge density is the dielectric constant ε, or between mag. field and magnetization is the spin susceptibility. (Notice a common feature among these external perturbation, material property, and the response function is that: external potential is like the intensive quantity and the material property is like the extensive quantity in the cannonical / grand cannonical ensemble theory, and the response function is the compressibility / susceptibility - which are commonly called the correlation function, and are evaluated by the 2nd derivative of the free energy.)

- Then the expectation value of some operator $A(t)$, which must be the same in any representation chosen, is given by

$$\langle A\rangle_n(t) = \langle \psi_n^{(I)}(t) \,|\, A_I(t) \,|\, \psi_n^{(I)}(t)\rangle$$

$$= \langle \psi_n^{(I)}(t_0)| \left(I + \frac{i}{\hbar}\int_{t_0}^{t} dt'\, \hat{V}_I(t')\right) \Big| A_I(t) \Big| \left(I - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, V_I(t')\, dt'\right) |\psi_n^{I}(t_0)\rangle$$

$$= \underbrace{\langle \psi_n^{(I)}(t_0) \,|\, A_I(t) \,|\, \psi_n^{(I)}(t_0)\rangle}_{\langle A_I\rangle_0} - \frac{i}{\hbar}\int_{t_0}^{t} dt' \langle \psi_n^{(I)}(t_0) | \big(A_I(t)\, V_I(t') - V_I(t')\, A_I(t)\big) | \psi_n^{(I)}(t_0)\rangle + O\left({H_I'}^2\, dt^2\right)$$

→ The first term is the expectation value of A with the ground state wave function (Ψ_n) of H_0 without the perturbation term. Since H_0 is time independent, the expectation value at t is simply governed by the time evolution w.r.to H_0.

→ We drop any $(V_I)^2$ or higher term since V_I is small. So, we only have one correction in the 2nd term due to the perturbation V_I, which is the expectation value of the commutator between A_I & V_I but in the interaction picture.

We write the final result in a concise form:

$$\langle A\rangle_n(t) = \langle A_I\rangle_0 - \frac{i}{\hbar}\int_{t_0}^{t} dt' \left\langle \left[A_I(t), V_I(t')\right]\right\rangle_0 \quad \text{--- (10a)}$$

where the expectation value is calculated with the unperturbed state $\Psi_n^{(I)}(t_0) \equiv \Psi_n^{(s)}(t_0)$.

[At finite temperature, the above expectation value is generated to include the thermal ensamble (Quantum Boltzmann probability)

$$\rho = \frac{1}{Z} e^{-\beta E_n} |n\rangle\langle n| , \quad \beta = k_B T ,$$

then one has $\langle A_I\rangle_0 = \frac{1}{Z}\, Tr\left(e^{-\beta H_0} A_I\right)$ and so on.].

→ Our ultimate goal is to evaluate the change in A due to perturbation with respect to its ground state expectation value (mean/average value in the statistical physics), which we denote as

$$\delta\langle A\rangle(t) = \langle A\rangle(t) - \langle A\rangle_0 = -\frac{i}{\hbar}\int_{t_0}^{t} dt\, \underbrace{\left\langle \left[A_I(t), V_I(t')\right]\right\rangle_0}_{\sim \chi_{AV}} . \quad \text{--- (10b)}$$

→ In the last term we define a response function of A due to V as.

Retarded

$$\chi^{(R)}_{A,V}(t,t') \equiv -\frac{i}{\hbar}\,\theta(t-t')\left\langle\left[A_I(t), V_I(t')\right]\right\rangle_0 \quad \text{---(11a)}.$$

Here basically we are saying, the perturbation is acted on at some time $t' < t$ in the past, and evaluating its response in the operator $A(t)$ at a future time $t > t'$. This is why the notation retarded "R" stands for, which says χ vanishes for $t < t'$. Needless to say there is also an advance response function, one generally define that for the response function and the difference between the retarded and advanced function gives the imaginary part of the response function in the frequency space, which is often called the spectral function.

→ The common perturbation term we encounter in experiment has often this particular form, i.e., V is split into a term corresponds to experimental probe and a term (operator) of the Hamiltonian that it couples to :

$$\hat{V}(t) = \hat{B}\, f(t) \quad \text{---(11b)}$$

, where $\hat{B}$ is time-independent operator, $f(t)$ is a c-number carrying the explicit time dependence.

- $f(t)$ is something that experimentalists can control, such as time-dependent electric field. Then B is the term corresponds to the Hamiltonian of system that f couples to. For f being the electric (magnetic) field, B would be the electric (magnetic) dipole moment of electrons and we will have $V(t) = -\vec{p}\cdot\vec{E}$ or $-\vec{m}\cdot\vec{B}$. For f being vector potential of light, B would be current of electrons : $V = -\vec{J}\cdot\vec{A}$. For f being electrostatic potential $\phi_{ext}(t)$, B is charge density of electron and so on.

Then substituting eq (11b) in (10b) and using eq(11a), we get

$$\delta\langle A\rangle(t) = -\frac{i}{\hbar}\int_{t_0}^{t} dt' \; \chi^{(R)}_{AB}(t,t') \; f(t') \qquad \text{--- (12a)}$$

where $$\chi^{(R)}_{AB}(t,t') = -i\,\theta(t-t')\,\langle[A_I(t), B_I(t')]\rangle_0 \qquad \text{--- (12b)}$$

- With a change of variable of $\tau = t-t' > 0$, and setting $B_I(t') = B_I(0)$, we can show that $\delta\langle A\rangle = -\frac{i}{\hbar}\int_0^{t-t_0} d\tau \; \chi^{(R)}_{AB}(\tau)\, f(t-\tau)\, d\tau$.

  Therefore, $\chi^{(R)}_{AB}(t-t')$, only depends on the relative time interval.
- We also extend $t_0 \to -\infty$, & $t \to \infty$, i.e., system goes back to unperturbed state as $t \to \infty$.
- This is like a convolution of the response function with the external probe function $f(t')$ to the property we measure at t. Owing to the time-translational invariance of the response function $\chi(t-t')$, this process becomes at the same frequency ω in the Fourier space:

$$\delta\langle A(\omega)\rangle = \chi^{(R)}_{AB}(\omega)\, f(\omega) \qquad \text{--- (13)}.$$

which is like a "resonance" condition or like a "elastic" scattering process that is the system is perturbed at a frequency ω, the corresponding response in the system as well as the measured property are obtained at the same frequency. This is due to the time-translational invariance, which means the energy remains conserved between the initial and final process. In other words, there is no "absorption" in this process. This will be constrasted with the "absorption" measured by the imaginary part of χ, but that absorption is ultimately compensated at the thermodynamic limit.

- The Kubo formula (eqs 12, 13) is like a generalization of the ohm's law to all momenta & frequency. So its a dissipative (absorption) process, but the conservation rule, called sum rule, prevail in a subtle way.

- Interestingly, the response function is determined by the commutator between the operators: $\vec{B}$ the probe field, and the operator $\vec{A}$ we measure in the detector. In most cases, A & B operators are the same operators, such as density-density, current-current, magnetization-magnetization, etc. But in the commutator, they sit at different time, meaning the same operator evolved by the probe field $f(t)$ to a value which does not commute with itself before the perturbation. But the expectation value is calculated with the unperturbed state. This means, the operator at different time does not commute. This happens when there is a correlation, in the theory between states at different time (and/or space) due to quantum effect in this case, such that an event at a later time (or different position) is affected by the state before (or another position). If the operators at two different times (or positions) commute, then they are like completely independent phenomena. Hence, it does not matter in which order one consider them. This is why the response function is sometimes called the correlation function. In classical analog, this response function or the correlation function measures the average deviation of the measure quantity or the expectation value from its mean value due to perturbation - like the standard deviation.
- Since, the "non-interacting" Hamiltonian is the full Hamiltonian without the external perturbation term (in this description, the interaction is the perturbation), so, the operators A_I, B_I in the interaction picture are actually same as those of the Heisenberg picture: $A_I(t) \equiv A_H(t)$ + same for B.

- One interesting fact about the linear response theory (Kubo formula) is that the response function does not depend on the probe field $f(t)$. This is true for the Ohm's law where the conductivity does not depend on external electric field. So, we can essentially set $f(t)=0$, and then we can interpret χ_{AB} as the intrinsic correlation function between the two operators A & B.

- If the fluctuation/correlations defined in eq(12b) are intrinsic, what's the origin of it if the system is in the ground state and/or in thermal equilibrium? There are essentially two sources of fluctuations here - quantum & classical. The quantum fluctuations are hidden in the commutator definition of χ. Even if $|\Psi_n\rangle$ are the eigenstates of H_0, but A and B don't necessarily commute with H_0, and hence $|\Psi_n\rangle$ is not an eigenstate of A and B. So, there will be fluctuation of A around its expectation value, which we are capturing here. Moreover, in most cases, we can not solve for the eigenstate of H_0, and then $|\Psi_n\rangle$ is some a variational ground state, which is neither an eigenstate of H_0, nor of A & B. So, all values fluctuate.

  The classical fluctuation is thermal fluctuations. At $T>0$, particles have thermal energy k_BT to visit nearby states and thus do not remain in a given state. Such a situation is captured by mixed state, density matrix, and one takes the thermal average. The thermal fluctuation is classical.

  Finally, note that unlike in atomic physics, where we have discrete energy levels, here in many-body theory, we have energy dispersions - a continuum of excited energy levels above the fermi sea. So, one has a continuum of low-energy excited states which the electron can access due to quantum and/or classical (thermal) fluctuations.

* We are now going to evaluate χ_{AB} for $A \equiv B \equiv n(t)$, the density operators for free electron gas and for the interacting electron gas. These are essentially the fluctuations across the Fermi-levels, where an electron moves across the Fermi level due to quantum and/or thermal fluctuations. They will have a continuum of fluctuations at different wavevectors - which are called particle-hole continuum. They are not localized or bound state in the non-interacting limit, but with Coulomb interaction, they can form bound states which are called excitons, plasmons in different cases.

The p-h spectrum, the plasmon dispersion also dictate if the material can be excited / shined with light at certain frequency and wavevector (momentum) or not, or the light can be absorbed or not, or the current can be induced by electric field or not, etc. In a given ground state, the correlation fluctuation can show singularity / divergence at some wavevector or finite frequency - signaling that the ground state is unstable to a phase transition to a different ground state.

Remarkable thing about many body fermionic system is that despite all these low-energy excitations, the system remains stable. That very much due to fermionic exclusion principle that the electrons occupy some exclusion volume on average.

Therefore, we will learn a rich information about the density fluctuations, instabilities, screening and other important properties about the materials

4.1B Density-Density correlation / Lindhard function of free-electron gas.

We will first consider a free electron gas without interaction:

$$H_0 = \sum_{k,\sigma} \varepsilon_k \underbrace{c_{k\sigma}^{\dagger} c_{k\sigma}}_{n_{k\sigma}}, \quad \varepsilon_k = \frac{\hbar^2 k^2}{2m}. \quad \text{--- (14)}$$

In this Hamiltonian, the momentum density $n_{k,\sigma} = c_{k\sigma}^{\dagger} c_{k\sigma}$ is conserved, i.e. $[H, n_{k,\sigma}] = 0$ at all k. But the local density $n(\vec{r}) = \psi_\sigma^{\dagger}(\vec{r})\psi_\sigma(\vec{r})$, i.e., its Fourier modes $n_\sigma(q)$ are not conserved. We are interested in the electron density fluctuation, i.e., the charge density fluctuation as $\rho(\vec{r}) = e\,n(\vec{r})$, and the density-density correlation function $\chi_{n,n}$.

Since the B-operator is the electron density operator ρ, it couples to external electrostatic potential ϕ_{ext}. So, $f(t) = \phi_{ext}(x,t)$. Therefore, the perturbation, that we assume to start at $t_0 = 0$ is

$$H'(t') = \int d^3r \; \underbrace{\phi_{ext}(\vec{r},t)}_{f(t)} \; \underbrace{\rho(\vec{r})}_{B = \rho = Q\sum_\sigma \psi_\sigma^{\dagger}(\vec{r})\psi_\sigma(\vec{r})} \quad \text{--- (15)}.$$

(set charge $Q = -e = 1$ for convenience)

Then $$\delta\langle \rho(\vec{r},t)\rangle_0 = \int d^3r' dt' \; \chi_0^{(R)}(\vec{r}-\vec{r}', t-t') \; \phi_{ext}(\vec{r}', t') \quad \text{--- (16)}$$

(Because the external perturbation is spatially varying, so, the response function is also a convolution in space, and we are capturing both spatial and temporal fluctuation here.)

Because of both spatial and temporal translational invariance, i.e. momentum and energy remain conserved, the above expression becomes "local" in the momentum & frequency space:

$$\delta \langle \rho(q,\omega) \rangle = \chi_0^{(R)}(q,\omega)\, \phi_{ext}(q,\omega) \quad --- \quad (17a)$$

where $\chi_0^{(R)}$ in time is

notice $-q$ here (H-W.)

$$\chi_0^{(R)}(q, t-t') = -\frac{i}{\hbar}\theta(t-t')\frac{1}{V}\langle [\rho_I(q,t), \rho_I(-q,t')] \rangle \quad --(17b)$$

(Note that the θ-function only exists in time, not in space, which is due to causality and time-ordering that is used in the derivation). Setting $t'=0$, the F.T. of χ in time is:

Then

$$\chi_0^{(R)}(q,\omega) = \int_{-\infty}^{\infty} dt\, \chi_0^{(R)}(q,t)\, e^{i\omega t}\, \underbrace{e^{-\eta t/\hbar}} \quad --- \quad (18)$$

Ad-hoc convergence term added.

The origin of this ad-hoc term, which essentially gives the decay term in time - causing dissipation / absorption that we talked about earlier. In an interacting system $\chi_0^{(R)}(q,t)$ sort of decay in time because the commutator $[\rho(t), \rho(t')]$ evaluated in the unperturbed ground state decays. Because, electrons move away from the specified ground state $|\psi_n(t)\rangle$ due to interaction. But for non-interacting (free-particle) system, electrons are infinitely long-lived on the ground state and hence the integrand oscillates in time at frequency ω and never decays. So, the integral becomes infinite. Therefore, to converge this integral, we have introduced an ad-hoc decay term $e^{-\eta t}$ with $\eta > 0$. This essentially shifts the pole in the complex integral from the real axis to inside the contour and we have a converged integral. $\tau = \eta^{-1}$ is like the life-time of the electron in the ground state, which is like the decay constant Drude introduced and is related to the mean-free path l as $l = v_F \tau$, v_F = Fermi-velocity. Generally, this happens in system due to the presence of impurity, defects etc which scatters an electron to other states. When we compute the density of states of electron, for non-interacting particles, one obtains δ-function, but then η is added to broaden the density of states in frequency/momentum, which is seen experimentally, as well.

We can eventually set $\eta \to 0$ after the calculation? Do we recover a fully energy conserved system from a dissipative/absorbing system by simply setting the dissipation term to zero? Where did the energy/particle go when η was finite and how do we recover them? This is kind of very subtle. For finite η, the lost energy/particle moved out of the finite volume V, absorbed by the confining potential $\to \infty$ at the wall. When we set $\eta \to 0$, the lost energy/particle are recoved from the potential reservoir at the wall. In what follows, in the limit $V \to \infty$, there is no loss. So, the ordering of limit $\eta \to 0$ & $V \to \infty$ do not commute as we will see further later.

- Now, we want to evaluate eq(18) for the density operator $\hat{\rho}$, which was written in terms of the field operator in eq(15), in the momentum space as

$$\rho(q,t) = \sum_{k,\sigma} c^{+}_{k\sigma}(t)\, c_{k+q,\sigma}(t) \,. \quad \text{---} (19a).$$

The time evolution of the creation and annihilator operators are evaluated as

$$c_k(t) = c_k e^{i\varepsilon_k t}, \quad c^{+}_k(t) = c^{+}_k e^{-i\varepsilon_k t}.$$

The creation/annihilator operators, evolve in time with only one unitary operator $e^{i\varepsilon_k t}$ as a state does, but not like other operator as $e^{iH_0 t} A e^{-iH_0 t}$. This is something subtle that needs to be derived carefully. c, c^{+} act on the Fock space, not the Hamiltonian's Hilbert space, and the Fock space does not evolve in time. Hence c, c^{+} evolve as state.

Then we get

$$\rho(q,t) = \sum_{k,\sigma} c^{+}_{k,\sigma}\, c_{k+q,\sigma}\, e^{i(\varepsilon_k - \varepsilon_{k+q})t} \quad \text{---} (19b)$$

(Notice that although ρ is defined in the interaction picture, but it evolves as in the Heisenberg picture. We discussed this before. This is due to the fact that the operators are evolved here with H_0 only, since H' is not an interaction term of the Hamiltonian, but a probe term which we eventually set to zero).

• Then substituting eq (19b) in eq (17b), we get

$$\chi_0^{(R)}(q, t-t') = -\frac{i}{\hbar}\,\theta(t-t')\,.\,\frac{1}{V}\,\times$$

$$\sum_{\substack{k,k'\\ \sigma,\sigma'}} \underbrace{\langle FS | [c^\dagger_{k\sigma} c_{k+q\sigma}, c^\dagger_{k'\sigma'} c_{k'-q\sigma'}] | FS\rangle}_{\star}\, e^{i(\varepsilon_k - \varepsilon_{k+q})t}\, e^{i(\varepsilon_{k'} - \varepsilon_{k'-q})t'}$$

Fermi sea in thermal equilibrium.

$\star = \langle FS | [c^\dagger_{k\sigma} c_{k+q\sigma}, c^\dagger_{k'\sigma'} c_{k'-q,\sigma} | FS\rangle$.

Now, we need to expand the commutator which will give us $c^\dagger c\, c^\dagger c$. Since the expectation value is evaluated in a single particle ground state, so, the Wick's theorem is applicable. So, $\langle c^\dagger c\, c^\dagger c\rangle = \langle c^\dagger c\rangle \langle c^\dagger c\rangle$. Using the momentum conservation we will end up with the density term n_k to survive here

H.W. show that $\star = \underbrace{\underbrace{\langle FS | c^\dagger_{k\sigma} c_{k\sigma} | FS\rangle}_{n_{k,\sigma}}}_{f(\varepsilon_k)} - \underbrace{\underbrace{\langle FS | c^\dagger_{k+q\sigma} c_{k+q\sigma} | FS\rangle}_{n_{k+q,\sigma}}}_{f(\varepsilon_{k+q})}$

= Fermi-Dirac distribution function at $T>0$

= $\theta(-\varepsilon_k)$ at $T=0$.

Then we get

$$\chi_0^{(R)}(q, t-t') = -\frac{i}{\hbar}\frac{\theta(t-t')}{V}\sum_{k,\sigma}\Big(f(\varepsilon_k) - f(\varepsilon_{k+q})\Big) \times e^{\frac{i}{\hbar}(\varepsilon_k - \varepsilon_{k+q})(t-t')} \quad \text{---(19c)}$$

So, we indeed get a term which does not explicitly depend on t & t', but its difference $t-t'$.

- Finally we perform the frequency Fourier transformation by substituting eq (19c) in eq (18). The time integral is of this form

$$-\frac{i}{\hbar}\int dt\ \theta(t)\, e^{i\left(\omega + \frac{\varepsilon_k - \varepsilon_{k+q}}{\hbar} + i\frac{\eta}{\hbar}\right)t}$$

The $\theta(t)$ dictates the integral only survives for $t>0$ from $t=0$ to ∞. Without η term, we can recognize the integral to be a delta function $2\pi\,\delta(\hbar\omega + \varepsilon_k - \varepsilon_{k+q})$. Clearly the imaginary $i\eta$ term broadens the δ-function to a Lorentzian with η being the broadening term. Ofcourse, $\eta>0$, otherwise the integrand diverges for $t>0$. Then this trivial integration gives $\dfrac{1}{\hbar\omega + \varepsilon_k - \varepsilon_{k+q} + i\eta}$.

Therefore, we get the final result as

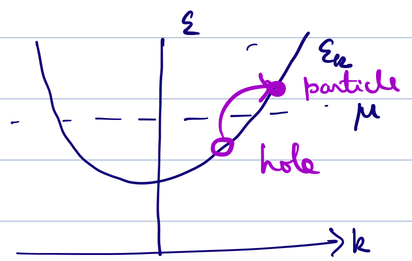
$$\boxed{\chi_0^{(R)}(q,\omega) = \frac{1}{V}\sum_{k,\sigma}\frac{f(\varepsilon_k) - f(\varepsilon_{k+q})}{\hbar\omega + \varepsilon_k - \varepsilon_{k+q} + i\eta}} \quad \text{--- (20).}$$

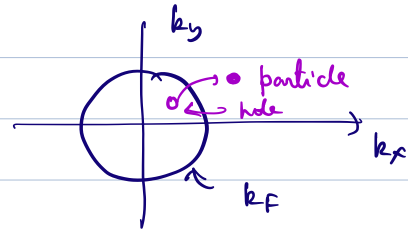
This is the famous Lindhard response function for density-density fluctuation of free-fermions. The expression seems simple to evaluate, but it encodes rich physical interpretations.

- ε_k is the electron dispersion with its wavevector k.
- ω and q are the frequency and wavevector (momentum) of the experimental perturbation $\phi_{ext}(\omega, q)$.

→ The denominator has poles at real frequency $\hbar\omega = \varepsilon_{k+q} - \varepsilon_k$, which is like a resonance condition or like an excitation from the energy level ε_k to ε_{k+q}. So, its like an oscillator between the two energy levels, except here the levels are not discrete, but have dispersion. So, we will have a spectrum of excitation depending on the incident light's frequency and momentum. q & ω are also interpreted as the inverse wavelength and frequency of density fluctuation - saying that its a collective fluctuation of electron's density in space and time. So, the resonance function has poles exactly at the resonance condition, except here one has a infinite set of resonance frequencies corresponding to different wave vectors. In fact, a relation of $\omega(q)$ can be obtained, which is however, not going to be sharp like an oscillator, as many k-values satisfy the same condition. As we will see below, we will get a broad continuum for $\omega(q)$.

→ But not all resonance conditions are satisfied due to the numerator. The fermi-function is 0, 1 if the state is empty or filled. Therefore, for a transition to occur both the states $|k\rangle$ & $|k+q\rangle$ cannot be simultaneously empty or occupied. In what follows, the transition takes place if the initial state is filled and the final state is empty. In fact, one does not create a single particle excitation here, rather an electron is moved from below the fermi level to above it, creating a particle in the empty state, and simultaneously leaving a hole in the Fermi sea. This is called the particle-hole excitation. Roughly, speaking one creates dipole between particle-hole across the Fermi surface.





- $\omega \geq 0$ as we cannot release energy by moving an electron to a lower level, because all states are filled inside the Fermi volume. Generally also excitation energy is measured with respect to the ground state energy and hence always positive.

- The presence of η term makes χ complex, with its imaginary part is proportional to η. Since η signifies dissipation / absorption, so, its obvious that $\text{Im}\,\chi$ gives the spectrum of the dissipation / absorption. In fact, the dissipation and fluctuation are related to each other through analyticity of χ – called Causality. This relation, called Kramer's-Kronig relation (KKR), is similar to the fluctuation-dissipation theorem.

  The $\text{Im}\,\chi$ is like a Lorentzian with η being its width and in the limit of $\eta \to 0$, a Lorentzian becomes a δ-function. This indeed happens here. Because, χ is of the following form:

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

$\mathcal{P}$ stands for Principal value.

  But $\delta(x)$ seems to signify infinite dissipation / absorption at $x=0$, i.e., $\omega = \varepsilon_{k+q} - \varepsilon_k$. But at the same time we have to take the volume $V \to \infty$, i.e., the wavevector $q \to 0$. Then with $q \to 0$ limit, we get a finite result.

- It is indeed surprising that a system with both spatial and temporal translational invariance, which dictates momentum and energy being conserved, automatically gives a dissipation / absorption term, i.e., loss of energy term. This we discussed briefly before that this dissipation arises because we are taking the long time limit before taking $V \to \infty$ or $q \to 0$ limit. Because if we wait long time, the energy will eventually come back and there is no dissipation. So, to recover the energy, we have to first take $q \to 0$ limit before taking the $\omega \to 0$ limit. This is like looking at the energy instantaneously and of course the energy may not be conserved at that position/state. Therefore, its extremely crucial to consider the ordering in taking the limits in order to obtain either a conserved system or a dissipative system.

- We will now evaluate the response function analytically, which is only possible in various limits of $q \to 0$, $\omega \to 0$, $\omega \to \infty$ etc. Each limit gives very interesting properties which are measurable or reveal important physical properties of the system.

I. Limit $q \to 0$, $\omega \neq 0$: we apply the perturbation at some finite frequency, but at zero momentum.

Since electrons are occupied at different momentum state, and excite a particle-hole, one needs to move an electron from one momentum state to another. But if the momentum transfer $q = 0$, then no excitation possible. In other words, there is no particle-hole excitation at $q \to 0$ and $\omega \neq 0$ as $\chi(q=0, \omega \neq 0) = 0$.

The physical interpretation of this limit is as follows. $\phi_{ext}(q=0)$ means a spatially uniform electrostatic potential $\phi_{ext}(x,t) = \phi_{ext}(t)$. Since an electrostatic potential shifts the chemical potential as $\mu(r) = \mu + \phi_{ext}(\vec{r}, t)$. Generally this is fine as the electrons will simply move from low-$\mu(\vec{r})$ to high-$\mu(\vec{r})$ region, but the total number of electron remains fixed. But for uniform $\phi_{ext}(t)$, we are saying the whole chemical potential is shifted, which is tied with changing the total number of electrons in the system. But since the total number of electron (called global charge) is conserved, so changing the global chemical potential without changing the global number of electron is not allowed. Therefore, the response function must vanish.

One can explicitly check it from eq (15) that

$$H'(x,t) = \int d^3x \, \phi_{ext}(x,t) \, \rho(x,t)$$

$$= \phi_{ext}(t) \underbrace{\int d^3x \, \rho(x,t)}_{N(t)} = \phi_{ext}(t) \, N(t)$$

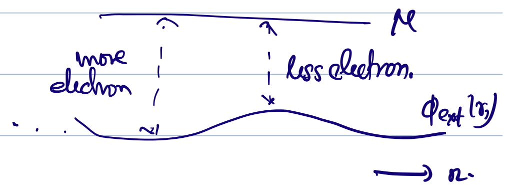
$N(t)$ = total number of electrons

which is not time dependent, as $[H_0, N] = 0$. So, $N(t) = N$.

II Limit ($q \to 0$ & $\omega \to 0$) or ($\omega \to 0$ & $q \to 0$) : Clearly if we first take the $q \to 0$ before $\omega \to 0$

limit, χ is zero and the whole function vanishes due to conservation of charge. If we reverse the order of the two limits, we get a finite result. As discussed before, as we take $\omega \to 0$ for $q \neq 0$, we are taking the long-time limit (so, the perturbation is static in time, but spatially modulated, and varying very very slowly in time such that the system has enough time to adjust its density.

- $$\chi(q, \omega=0) = \frac{1}{V} \sum_{k,\sigma} \frac{f(\varepsilon_k) - f(\varepsilon_{k+q})}{\varepsilon_k - \varepsilon_{k+q}}$$
(η is dropped)



Then as we take $q \to 0$ limit, so the numerator and denominator goes to zero. So, we have to use L'Hospital rule :

$$\chi(q \to 0, \omega = 0) = \frac{1}{V} \sum_{k,\sigma} \frac{\cancel{\varepsilon_k - \varepsilon_{k+q}}}{\cancel{\varepsilon_k - \varepsilon_{k+q}}} \left(\frac{\partial f}{\partial \varepsilon_k}\right) \quad \text{using Taylor expansion}$$

$$= \int \frac{d^3k}{(2\pi)^3} \frac{\partial f(\varepsilon_k)}{\partial \varepsilon_k} = -\int \frac{d^3k}{(2\pi)^3} \frac{\partial (\varepsilon_k)}{\partial \mu} = -\frac{\partial n}{\partial \mu}.$$

This static density fluctuation is also responsible for Thomas-Fermi screening.

- We can now convert the momentum summation to energy integral. In that case for each energy grid $d\varepsilon$, we need to take into account how many momentum states are there, i.e., the density of states.

$d(\varepsilon)$: $\frac{1}{V}\sum_k \to \frac{1}{(2\pi)^3}\int_0^{k_F} d^3k \to \int_0^{\mu} d(\varepsilon)\, d\varepsilon$, where $\frac{V}{(2\pi)^3}\int d^3k \; \delta(\varepsilon - \varepsilon_k) = d(\varepsilon)$.

(A factor of 2 is implicit in the density of states due to spin).

Then

$$\chi(q \to 0, \omega = 0) = \int_0^{\mu} d\varepsilon \; d(\varepsilon) \frac{\partial f}{\partial \varepsilon} = -\frac{\partial n}{\partial \mu} \xrightarrow{T=0} -d(\varepsilon_F).$$

as $\frac{\partial f}{\partial \varepsilon} = \delta(\varepsilon - \mu)$ at $T=0$.

as f is a step function so, $\frac{\partial f}{\partial T} \to -\delta(\varepsilon - \varepsilon_F)$.

--- (21) .

This result looks very much like (in fact same) the compressibility that we learned in stat mech course $\chi = -\partial n/\partial \mu \rightarrow$ DOS at $T=0$ for free electron gas. The negative sign makes sense because in grand cannonical Free energy we have $F \sim -\mu n$. Therefore, χ at $q\rightarrow 0$ & $\omega \rightarrow 0$ measures the stiffness or compressibility of the Fermi surface to change the total number of fermions per unit change in the chemical potential. Compressibility is same as the density of states for non-interacting Fermi gas.

It is a bit surprising that despite the fact the total number of electrons is conserved, by taking the limit $q\rightarrow 0$ first gives vanishing response function, while taking this limit after the long time ($t\rightarrow\infty$, ie, $\omega\rightarrow 0$) limit yields a finite compressibility. This has to do with the corresponding physical process. In the first case, we applied a uniform potential to begin with, which only can change the total number of electron in the system. In the second case, we applied a non-uniform (finite wavelength) potential and waited long enough for the electrons to move from high potential to low potential region and equilibrate. Then we made the wavelength goes to infinity. In this process the electrons have move locally according to the potential while the total number is still conserved. What the response function is capturing here a spatial average over $\langle \partial n(r)/\partial\phi(r)\rangle$, not $\partial\langle n\rangle/\partial\langle\phi\rangle$. This is finite even when $\partial\langle n\rangle/\partial\langle\phi\rangle = 0$. This is reflected by the fact that we summed over the k-variable over the entire Brillouin zone before taking the $q\rightarrow 0$ limit.

So, metal, ie, electron gas is a compressible system, unlike an insulator.

III Limit $\omega \to 0$ but finite q, at $T=0$:

$$\chi(q, \omega=0) = \frac{1}{V}\sum_{k,\sigma} \frac{f(\varepsilon_k) - f(\varepsilon_{k+q})}{\varepsilon_k - \varepsilon_{k+q}}$$

$$= \frac{2}{V}\sum_{k,\sigma} \frac{n(\varepsilon_k)}{\varepsilon_k - \varepsilon_{k+q}}$$

since the first and 2nd terms are the same after a change of dummy k variable.

For free electrons $\varepsilon_k - \varepsilon_{k+q} = \frac{k^2}{2m} - \frac{(k+q)^2}{2m} = -\frac{q^2 + 2\vec{k}\cdot\vec{q}}{2m}$.

& $\frac{1}{V}\sum_k \to \int \frac{d^3k}{(2\pi)^3}$, $\quad n(\varepsilon_k) = 1$ for $k < k_F$ at $T=0$.

So, $$\chi(q,0) = -4 \int_0^{k_F} \frac{d^3k}{(2\pi)^3} \frac{2m}{k^2 + 2k\cdot q},$$

factor of 2 for spin

$$= -8m \int_0^{k_F} 2\pi k^2 dk \int_{-1}^{1} \frac{1}{k^2 + 2kq\cos\theta} d(\cos\theta)$$

$$= -8m \int_0^{k_F} \frac{2\pi k^{\cancel{2}} dk}{2\cancel{k} q}\left[\log(k^2 + 2kq) - \log(k^2 - 2kq)\right]$$

$$= -16\pi m \underbrace{\int_0^{k_F} \frac{k\,dk}{2q}\left[\log(k+2q) - \log(k-2q)\right]}$$

We have done this integral in chapter 3.2 for the exchange energy and we obtained the $F(x)$ except here $x = q/2k_F$ and this gives an additional $1/2$ factor

$$F'(x) = \frac{1}{2}F(x).$$

We will continue to denote $F'(x)$ as $F(x)$ here as defined below.

$$= -4\pi m \, k_F \, F(x)$$

$$= -d(\varepsilon_F)\, F(x)$$

where $d(\varepsilon_F)$ is the density of states at the Fermi level. This is obtained as

for spin

$$d(\varepsilon) = \frac{2}{V}\sum_k \delta(\varepsilon - \varepsilon_k) = 2\int \frac{d^3k}{(2\pi)^3}\,\delta(\varepsilon - \varepsilon_k)$$

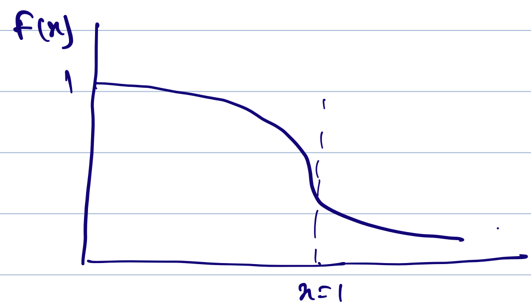
$$= \frac{2m}{2\pi^2\hbar^3}\,(2m\varepsilon)^{1/2}$$

$$\therefore\; d(\varepsilon_F) = \frac{m}{\pi^2\hbar^3}\left(2m\,\frac{\hbar^2 k_F^2}{2m}\right)^{1/2} = \frac{m}{\pi^2\hbar^2}\,k_F$$

$$= \frac{4\pi m k_F}{h^2}.$$

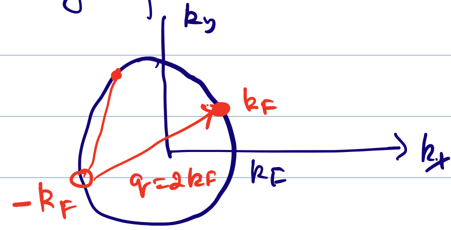
- And, $F(x) = \frac{1}{2} + \frac{1-x^2}{4x}\ln\left(\frac{1+x}{1-x}\right)$ for $x = q/2k_F$.

which is the same integral we saw before except here $x = q/2k_F$.



- At $x\to 0$, i.e., $q\to 0$, we get $F\to 1$ and $\chi(0,0)\to -d(\varepsilon_F)$ as obtained in the previous case.

• $F(x)$ has a log singularity in its first derivative at $x=1$, ie, $q = 2k_F$. This is very important and has to do with the Fermi statistics.



Because in a Fermi volume, at $\omega=0$, ie. with no energy transfer, one does not have inelastic scattering. Then the only allowed scattering is among the electrons on the Fermi surface. Here two electron can exchange momentum, and the maximum momentum transfer happen between two electrons sitting at k_F & $-k_F$, given a momentum transfer $q = k_F - (-k_F) = 2k_F$. $2k$ is the maximum value of q at $T=0$.

But the key point is that χ does not have a discontinuity at $q=2k_F$, but its first derivative has a log-divergence. This has important physical consequence that we will see later.

IV **Limit $q \neq 0$, $\omega \to \infty$** : when the external perturbation is oscillating too fast with time, which is to say the energy is too high $\omega \to \infty$. we get

$$\chi_0(q,\omega) = \frac{1}{V}\sum_{k,\sigma} \frac{f(\varepsilon_k) - f(\varepsilon_{k+q})}{\omega + \varepsilon_k - \varepsilon_{k+q}}$$, expand it upto 2nd order in ω.

$$\xrightarrow{\omega\to\infty} \frac{2}{V}\sum_k \underbrace{\frac{f(\varepsilon_k) - f(\varepsilon_{k+q})}{\omega}} - \frac{2}{V}\sum_k \frac{f(\varepsilon_k) - f(\varepsilon_{k+q})}{\omega^2}(\varepsilon_k - \varepsilon_{k+q}) + O\left(\frac{1}{\omega^3}\right).$$

$\frac{1}{\omega}\sum_k [f(\varepsilon_k) - f(\varepsilon_{k+q})] = 0$

due to sum over all filled and empty states.

$$= \frac{2}{V\omega^2}\sum_k f(\varepsilon_k)\left[\varepsilon_k - \varepsilon_{k+q} + \underbrace{\varepsilon_q - \varepsilon_{q-k}}\right]$$

By relabelling the 2nd term here

$\hbar^2 q^2/m$. for $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$

$$= \frac{n q^2}{m\omega^2}$$, where $n = \frac{2}{V}\sum_k f(\varepsilon_k)$.

This expression is also true for interacting electrons, because the external perturbation oscillates the electron so fast that the electron has no time to relax. So, it does not really matter if the electrons are interacting or non-interacting (i.e., it does not matter what's the Hamiltonian of the electron, as $e^{i(E+\omega)t} \approx e^{i\omega t}$ for $\omega \gg E$, where E is the energy eigenvalue of the electron. This is also connected to the f-sum rule, which is satisfied by all absorption at all frequencies - derived from the analyticity of χ

- The $\chi \sim q^2/\omega^2$ falls off as $1/\omega^2$ with the exponent '2' in frequency is an important exponent which people use as characterizing the free-electron like (quasiparticle) behavior of electron (Fermi liquid theory). In strongly correlated electronic system, it is sometimes seen the exponent changes to $\chi \sim 1/\omega$, which is called the non-Fermi liquid behavior. This requires more sophisticated theory to obtain and is a topic of research nowadays.

V Dynamical Response $\mathrm{Im}\,\chi_0^{(R)}(q,\omega)$.

Now we want to look at the finite frequency (and all momenta) response function. More specifically, we want to measure if the metal absorbs the incident light at some frequency ω and momentum q. In an atom, the absorptions are much more stable/long-lived, because an electron can simply be excited from some orbital to another orbitals. Since the orbital states are stationary eigenstates of the time-independent Schrödinger equation, the excited electron can stay in the excited state for long time before perhaps it emits the light to go back to its initial state. This happens only at discrete frequencies as atomic levels are discrete.

In metals, the electrons are below the fermi level, and for an incident photon, it can excite an electron to above the fermi level if the resonance condition $\hbar\omega = \varepsilon_{k+q} - \varepsilon_k$ as well as the state $\varepsilon_k < \mu$ is filled and $\varepsilon_{k+q} > \mu$ is empty. Moreover, this resonance condition is satisfied for a lot of states at k to $k+q$, and we have to sum over all such k-states. But the absorption will not be long-lived, unlike in a metal, because electrons are mobile and can move to another state and/or can scatter and screen each other. Moreover the excited states are not bound state, rather the excited electrons will quickly emit the energy and go back to the initial states. So, the absorption is not long-lived, and metals are shiny since the lights get emitted back (reflected) almost immediately. Only if we include coulomb interaction or other effects, the excited electrons and left behind hole can form a bound state - called excitons, or can move to different center of mass positions in space due to screening and hence creating permanent dipole moments. Such excitations are called plasmons. We will discuss these many body effects later, but returning to the metals, there can be weak and instantaneous absorption.

The absorption (loss of energy conservation) is introduced by the η-term in the derivation, and in the limit of $\eta \to 0$, it leaves behind an imaginary part of χ which we discussed earlier:

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

Using this formula we get

$$\mathrm{Im}\, \chi_0^{(R)}(q,\omega) = -\frac{\pi}{V} \sum_{k,\sigma} \left[f(\varepsilon_k) - f(\varepsilon_{k+q})\right] \delta\left(\omega + \varepsilon_k - \varepsilon_{k+q}\right). \quad \text{--(22a)}$$

This exactly satisfies the resonance condition for fermions in a Fermi sea that we just discussed above, we will get a continuum of absorption here - called particle-hole continuum, but short-lived. This is obtained by integrating over all possible k (σ summation gives a factor of 2). We will only discuss $T=0$ case where $f(\varepsilon_k) = \Theta(-\varepsilon_k)$.

- we will use a few tricks to evaluate it quickly. First thing we notice that $\mathrm{Im}\,\chi_0^{(R)}(q,\omega) = -\mathrm{Im}\,\chi_0^{(R)}(q,-\omega)$, is odd under ω, i.e., absorption & emission spectrum are exactly identical, due to space-time translational invariance.

Then for $\omega \geq 0$, the δ-function gives the resonance condition that

$$\varepsilon_{k+q} = \varepsilon_k + \omega > \varepsilon_k \quad \text{as } \omega \geq 0.$$

So, now since either ε_k state or ε_{k+q} state has to be filled and the other one to be empty and now $\varepsilon_k < \varepsilon_{k+q}$, so, ε_k state must be below the fermi level and $\varepsilon_{k+q} \geq \mu$ at $T=0$. Then $f(\varepsilon_k) = 1$ & $f(\varepsilon_{k+q}) = 0$ in our case.

So, we get

$$\boxed{\mathrm{Im}\,\chi_0^{(R)}(q,\omega) = 2\pi \int_{\substack{\varepsilon_k < \mu \\ \varepsilon_{k+q} > \mu}} \frac{d^3k}{(2\pi)^3}\, \delta^{(3)}(\omega + \varepsilon_k - \varepsilon_{k+q}) \qquad (22b)}$$

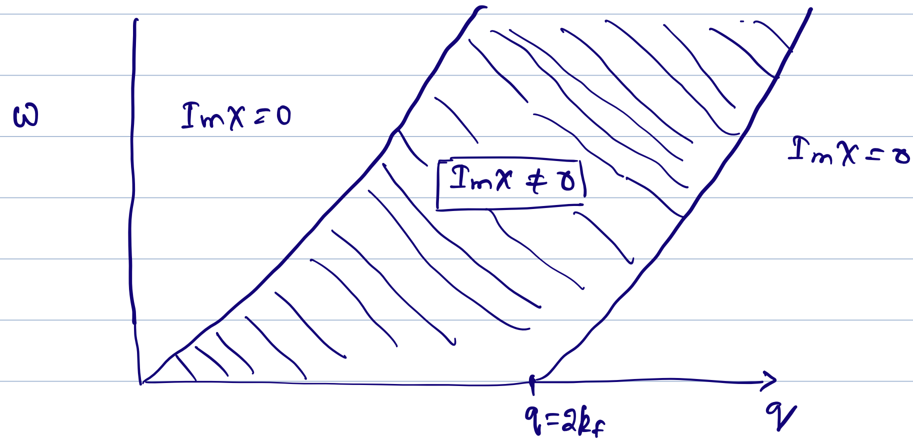
(2 for spin)

This integration can be done exactly, and the result is (P. Colemann book eq 8.180 page 229):

$$\mathrm{Im}\,\chi_0^{(R)}(q,\omega) = d(\varepsilon_F)\,\frac{\pi}{8x}\left[y_+\,\theta(y_+) - y_-\,\theta(y_-)\right].$$

$$\text{where } y_\pm = 1 - \left(x \pm \frac{\omega}{2\varepsilon_F x}\right)^2, \qquad x = q/2k_F.$$

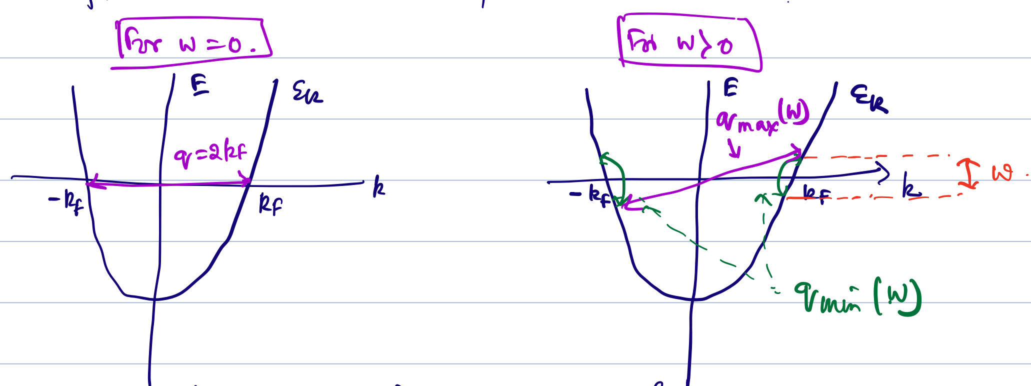
This final expression does not help much in understanding the absorption spectrum, but the plot of the function goes as



Im χ is finite when we have the resonance condition for q & ω,

$$\left.\begin{aligned} \epsilon_{k+q} &= \epsilon_k + \omega \\ \epsilon_{k+q} &> \mu \\ \epsilon_k &< \mu \end{aligned}\right\} \quad \text{--- (22c)}$$

Therefore, a particle hole excitation is possible at those k-values for which all the three conditions are satisfied. As we see earlier there is a upper bound for excitation at $q = 2k_F$ for $\omega \to 0$. At finite $\omega > 0$, in fact there are both lower and upper cut off momenta which are the solutions for $\frac{q^2}{2m} - v_F q < \omega < \frac{q^2}{2m} + v_F q$. This can be seen from the band structure plot as



There are continuum of particle hole excitations $q(\omega)$ which satisfy $q_{min}(\omega) \leq q(\omega) \leq q_{max}(\omega)$ as shown in the top figure.

We can obtain the $\mathrm{Im}\,\chi(q,\omega)$ for q_{min} and q_{max} lines, by expanding the expression near $q \to 0$ & $q \to 2k_F$. The result is one obtain gapless linear dispersion:

$$\mathrm{Im}\,\chi_0^{(R)}(q,\omega) \sim -\frac{\pi}{4} d(\varepsilon_F) \frac{\omega}{v_F q} \qquad \text{for } \omega < q v_F$$

$$= 0 \qquad \text{for } \omega > q v_F.$$

These excitations are clearly not sharp, unlike in atomic spectral line, and there is a continuum of excitations in the arbitrarily nearby energy and momentum. If we create such an excitation at some wavevector and frequency, it won't travel far, rather dissipate quickly. They are not bound state, unless coulomb interaction is included, which can confine these excitations to excitons or plasmons.