Advanced Quantum Mechanics with Applications
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Lecture - 30
Linear Response Theory: Derivation of Kubo formula

Welcome back. So, we will discuss linear response theory and in particular Derivation of Kubo formula in the context of condensed matter physics.

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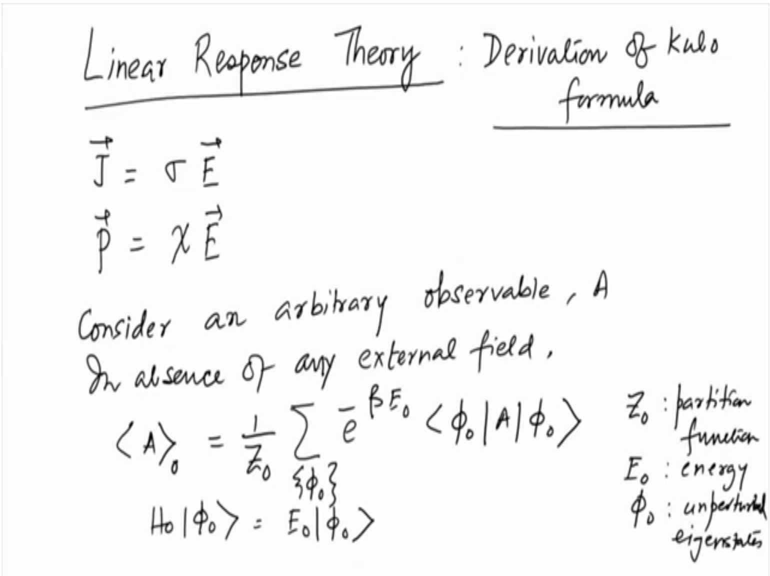

So, you can take the title as linear response theory and derivation of Kubo formula. However, in general the linear response theory goes beyond just the Kubo formula and it is applicable to various branches of physics.

So, what we mean by a linear response? So, in presence of an external field when the system responds to a given external field, and when the external field is small in magnitude, then there is a linear response that the system demonstrate or exhibits and this called as linear response theory. Such that say, the current density is given as this is called as a Omh's law; where J the current density is written as sigma E where sigma is the conductivity J is the current density and E is the applied electric field and this is valid for small electric fields small values of the electric fields. And if say another example is that the polarizability is or rather the polarization can be written as polarizability and the electric field in a dielectric material. And so, these are examples of linear response that we are familiar with.

Now, if the applied field is large then we actually may need to go to higher orders of the electric field which are like e square and E cube and so on; in which case we deviate from linear response theory. And there are examples of such non-linear materials which have their own domain of interest where people study non-linear responses of the system, and there are non-linear coefficients which are often of interest.

We will not go into that, but however we will derive formula for the linear response theory. And by doing so we will make grounds for arriving at the Kubo formula which establishes the connection between the current density and the electric field, which is what is written here is also alternately. Alternatively it is a the statement of Omh's law and this is what we are familiar with.

So, let us go into this linear response theory. So, any consider an arbitrary observable A. And in absence of any field, any external field the thermal average of this observable is written as A and this 0 in the subscript signify that there is no field. This is equal to 1 over Z 0 and this is phi 0 are the non-interacting Eigenstates or rather the Eigenstates in the absence of any external field. This is the Boltzmann weighting, and this is a value of the expectation value of A within the unperturbed states.

So, Z 0 is a partition function, E 0 energy and phi 0 are unperturbed Eigenstates. And assumably we know the problem of H 0 phi 0 equal to E 0 phi 0. So, that is a starting point, that we can solve the non-interacting or rather the unperturbed Hamiltonian that is without an external field, exactly and five 0's are the Eigenstates. Z 0 is the partition function which is the exponential minus beta H; H being the Hamiltonian of the; and summed over all the states and so on. And this is the thermal average of this quantity

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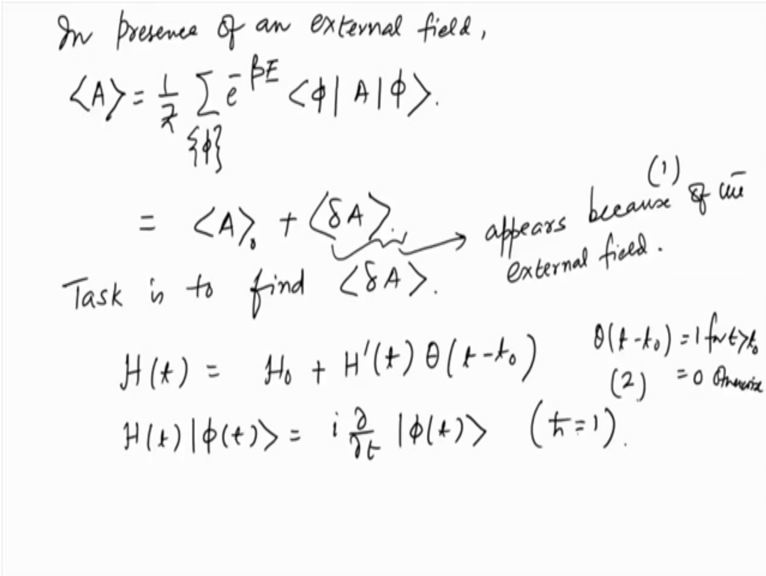

Now, if we apply an external field then the same expectation; so in presence of an external field. So, this the same observable at the thermal average of that is written as; so 1 over Z now is the partition function for the system; which is perturb perturbed by the external field. And, this is again having the same form accepting that all those 0's are now replaced by just the quantities such as Z 0 is now replaced by Z and phi 0 is replaced by phi. And these exponential minus beta E no longer beta E 0 where E 0 was the energy of the unperturbed state and this is a phi A phi.

So, this in the linear response regime when the external field is not too large, this we should be able to write it as A 0 plus a delta A ok. And it is important to find this delta A. So, our task at hand is to find this delta A ok. And which appears because of the field. So, this appears because of the external field.

So now, let us write down the Hamiltonian in presence of the field. That is the total Hamiltonian including the unperturbed term, plus the term that is arising out of the perturbation. So, that Hamiltonian is written as H of t, this is equal to H 0. Now H 0 can in principle include interaction terms and there is no embargo on that. So, H 0 is the Hamiltonian without an external field; which could have an electron interaction electron lattice interaction a single particle energies and so on, but is independent of time.

And the term that is, the term that depends on the external field is written as this where the perturbation or the external field is switched on at t 0 and before that it was nonexistent. So, a for t less than t 0 we have H of t equal to H 0. And at after t greater than or after t equal to t 0 or rather t greater than t 0 we have this Hamiltonian, which is H of t equal to H 0 plus H prime theta t minus t 0 where theta t minus t 0 is the theta function; which you all know that a theta t minus t 0 equal to 1 for t greater than t 0 equal to 0 otherwise ok.

So, this H satisfies this equation the Schrodinger equation which is i del t of y t and of course, we have taken H cross equal to 1 ok. So, the problems clear that we are talking about the thermal average of an observable which is given by A. And this observable can be written in the linear response regime as A 0 plus delta A. And we need to find delta A, and the Hamiltonian has a part which is independent of the external field which is H 0, and the part that depends upon the external perturbation or rather the external field is H prime t. And the whole Hamiltonian or rather the full Hamiltonian is H of t which satisfies the Schrodinger equation ht phi t equal to i del del t of phi t.

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In the interaction picture, the perturbed states are

$$|\phi(t)\rangle = e^{-iH_0 t}|\phi_0\rangle \qquad (3)$$

$$= e^{-iH_0 t}\, U(t,t_0)\, |\phi_0(t_0)\rangle$$

$$U(t,t_0) = 1 - i\int_{t_0}^{t} dt'\, H'(t') + \cdots \qquad (4)$$

Putting (3) & (4) in (1)

$$\langle A(t)\rangle = \langle A\rangle_0 - i\int_{t_0}^{t} dt' \sum_{\{\phi_0\}} \langle \phi_0 | [A(t), H'(t')] | \phi_0\rangle \frac{e^{-\beta E_0}}{Z_0}.$$

Retained upto linear term in $H'(t)$.

In a short hand notation,

$$\langle A(t)\rangle = \langle A\rangle_0 - i\underbrace{\int_{t_0}^{t} dt' \langle [A(t), H'(t')]\rangle}_{\text{Linear response theory.}}$$

Now, in the interaction picture the perturbed states are so, phi of t it is equal to exponential minus i H naught t and a phi 0 where again we have taken H equal to H cross equal to 1. So, this is equal to nothing but minus i H naught t U t of U t t 0 and a phi naught at t equal to t 0. So, where U of t t 0 is the same definition that we have seen earlier, it is a t 0 to t and a t t prime H t prime and plus other terms if we do not decide to stop at linear in the perturbation term which is equal to here H prime. So, H prime includes the perturbation term or the external field term.

So, if we substitute this phi t and this U t into this equation that we have we have written down here. So, let us write this down as equation 1, the Hamiltonian is say equation 2, and then we will talk about this as equation 3, and this as equation 4. If we put them down, and then we can write down A of t which is equal to a of 0 minus i t 0 to t dt prime and sum over phi 0. And there is a phi 0 A of t H prime t prime phi 0 and exponential minus beta E 0 over Z 0.

So, this is the term that is the first term is the term that is without any external field. And we have kept so, what we did is that putting 3 and 4 in 1. And we have retained linear terms in H prime. I have skipped a step which you should fill it in that there is a commutator bracket of A t and H prime t prime which are coming because of this 1 minus this which will be there on both sides, because there is a phi t and a phi. So, there is a phi there and a phi there. So, each one will involve a U t t 0, and then you will write it and then take the; so, keep terms up to linear in H prime. And then you will see that the commutator bracket comes out. So, just one step that has been skipped which you should fill up.

So, in a shorthand notation so, 80 equal to A 0 minus i t 0 t prime, sorry, t it is not p prime there is no. So, there is t prime is a dummy variable here as well I mean the t prime is a dummy variable in this step which is step just below the equation 4. And this is equal to we can skip those 5 0's understandable that it is the ground state or the unperturbed expectation values of this commutator A t and H prime t prime,.

So, this is the term that we wanted to find and this is the term that we get in linear response theory. So, this comes out as a commutator between the observable and the time dependent part of the Hamiltonian which is due to the external field. So, this is essentially the linear response theory.

Let us now write a particular form for H prime.

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Consider $H'(t) = \int \underbrace{\vec{f}(\vec{r},t)}_{\text{Coefficient}} \cdot \underbrace{\vec{B}(\vec{r})}_{\text{external field}} \, d\vec{r}$

$$\langle \delta A(\vec{r},t)\rangle = -i\int d\vec{r}\,' \int_0^t dt' \langle [A(\vec{r},t), B(\vec{r}\,',t')]\rangle f(\vec{r}\,',t') \underbrace{\frac{e^{-\beta E_0}}{Z_0}}.$$

$$= -i\int d\vec{r}\,' \int_{-\infty}^{\infty} dt' \, \underbrace{\theta(t-t')} \langle A(\vec{r},t), B(\vec{r}\,',t')\rangle f(\vec{r}\,',t')$$

$$= \int d\vec{r}\,' \, dt' \, \chi(\vec{r},t,\vec{r}\,',t') \, f(\vec{r}\,',t').$$

Where $\chi(\vec{r},\vec{r}\,',t,t') = -i\,\theta(t-t')\langle [A(\vec{r},t), B(\vec{r}\,',t')]\rangle$ (5)

$\longrightarrow$ Kubo formula.

So, consider H prime of t equal to some f r t and the B r and a d r. So, that is a volume integral, and this is a coefficient and this is the external field. At this moment it is nothing but just you know; I mean sort of this is actually a vector. So, this is a dot product of that. So, this b is not to be confused with magnetic field B is any field that you may want to consider.

So now our delta A r t this is equal to minus i dr prime and dt from 0 to t, and we have A r t B r r prime t prime I mean let us write it without this just to; so they look same and there is a f r prime t prime. And of course, we will have to write down the exponential minus beta Z, Z beta E 0 divided by Z 0, E 0 divided by Z 0. So, that is the thing that we want to write.

So now dropping this term for the moment, we will simply write it as d r prime and minus infinity to plus infinity, and dt prime is a prime here. And a theta t minus t prime and this is A r t B r prime t prime, and this and then you have a f r prime t prime. And so, this is this integral is taken from minus infinity to plus infinity by introducing the theta function that we see here.

Now, this can further be written as dr prime dt prime with appropriate limits of the integral, this is equal to chi r t r prime t prime, and f of r prime and t prime; where chi of r r prime t t prime. This is, t t prime this is equal to minus i theta t minus t minus t prime. And there is a A r t commuted with B r prime t prime and that is the form for this coefficient that we have written as chi

So, this equation let us call it give it a number let us call it as equation 5. Equation 5 is known as the Kubo formula.

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Kubo formula is applicable to

(i) density response function & dielectric constant.

(ii) Current response & Conductivity

(iii) Magnetic response & Susceptibility.

Kubo formula for the current response.

$$\vec{E}(\vec{r},t) = -\vec{\nabla}\phi - \frac{\partial \vec{A}}{\partial t} \quad ; \quad \vec{E}(\vec{r},t) = -\frac{\partial A(\vec{r},t)}{\partial t}.$$

$$\mathcal{H} = \int d\vec{r}\, \psi^{\dagger}(\vec{r}) \frac{(\vec{p} + e\vec{A})^2}{2m} \psi(\vec{r})$$

$$= H_0 + \frac{e}{2m}\int d\vec{r} \left(\psi^{\dagger} \vec{p}\cdot\vec{A}\psi + \psi^{\dagger}\vec{A}\cdot\vec{p}\psi\right) + \frac{e^2}{2m}\int d\vec{r}\, A^2 \psi^{\dagger}\psi$$

$$= H_0 + \delta H.$$

And this formula is applicable to a variety of situation say density response function and the chi is the dielectric constant. So, this A is the density response function and the chi is the dielectric constant which is the coefficient that appears in our discussion. Then we have current response and conductivity which is the coefficient. And then of course, we have other such as magnetic response and susceptibility and so on. So, for r case we shall consider this one, and we will compute the Kubo formula corresponding to the current response and conductivity.

So, let us take an external electric field to have the form E r t which is a derived from a scalar potential phi and a vector potential A. For the static case we have this minus grad phi only, and for the time dependent case we will have to include a del A del t. However, let us drop the first term by taking that you know by the potential since it is a quantity which can be set to 0, that you can set the potential to be 0 at a point that you want, and measure the potential from there. So, and so, basically this has a problem that this goes all the way up to infinity so, it is unbounded

So, let us drop this further for now, and let us write e equal to simply equal to minus del a del t. And the Hamiltonian is written as so, in presence of the field the Hamiltonian is written as d r; this is we are writing it in continuum notation which are like psi of r and there is a p plus e A divided square over 2 m and a psi of r. So, that is the Hamiltonian; this Hamiltonian can be expanded by opening up the square which will give us 2 thing 3 terms rather, a p square over 2 m, and e square a square over 2 m, and there is a p dot A and A dot p term. Not necessarily that p will come commute with A so, we will keep both these terms.

However, you see the p square by 2 m the first term is actually a part of H 0. So, this can be written as H 0 and plus e over 2 m and we have a dr and there is a psi dagger p dot A psi plus A psi dagger A dot p psi. And there is A plus e square over 2 m d r A square psi dagger psi. And so, this can be written as H 0 plus a delta H just the way we have segregated the unperturbed part of the Hamiltonian which is without the field, and the delta H coming from the term which includes a vector potential which comes because of the external field A or rather external field e.

So, what is the form of; so, H 0 is of course our nothing but a dr and a psi r and a p square over 2 m psi of r.

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$$\mathcal{H}_0 = \int d\vec{r}\, \psi^\dagger(\vec{r}) \frac{p^2}{2m} \psi(\vec{r}).$$

$$\delta H = \int d\vec{r}\, \psi^\dagger \left(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}\right)\psi + \int d\vec{r}\, \vec{A}^2 \psi^\dagger \psi$$

$$\vec{p} = -i\hbar\vec{\nabla}, \quad \text{use} \quad \vec{J} = \underbrace{\frac{1}{2mi}\left[\psi^\dagger \nabla\psi - (\nabla\psi^\dagger)\psi\right]}_{\text{paramagnetic } \vec{J}_p} + \underbrace{\frac{e}{m}\vec{A}\psi^\dagger\psi}_{\text{diamagnetic } \vec{J}_d}$$

The perturbation term can be written as,

$$\delta H = e\int d\vec{r}\, \vec{J}\cdot\vec{A}$$

A many body state $|n\rangle$ can be written as,

$$|n\rangle = |n^{(0)}\rangle + |n^{(1)}\rangle$$

[$|n^{(1)}\rangle$ includes correction upto first order]

And delta H is nothing but d r psi dagger and we have a p dot A plus A dot p psi. And plus a term which is dr a square psi dagger psi. Since p is equal to minus i h cross del, we can use the definition of J 1 by 2 mi and a psi dagger del psi minus del psi dagger psi and plus e by m a psi a psi dagger psi.

So, this is called as the paramagnetic current density. And this is known as the diamagnetic current density. So, this we will represent by a J p p for paramagnetic and this will represent by a J d. So, the perturbation term can be written as so, delta H which is the perturbation term which is equal to a dr a J dot A where J is the current density and a is the vector potential. And let us now write down the state; so, a many body state n n can be written as n equal to n 0 plus n 1 and. So, n 1 n 0 is of course, the unperturbed state which is same as phi 0 if you want, and n 1 includes the correction up to first order ok.

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$$\langle n|\vec{J}|n\rangle = \langle n^{(1)}|\vec{J}_p|n^{(0)}\rangle + \langle n^{(0)}|\vec{J}_d|n^{(0)}\rangle + \langle n^{(1)}|\vec{J}_p|n^{(1)}\rangle + O(A^2)$$

First term : $\langle n^{(0)}|\vec{J}_p|n^{(0)}\rangle = 0$ At equilibrium there is no current

2nd term

$$\langle n^{(0)}|\vec{J}_d|n^{(0)}\rangle = \frac{e}{m}\vec{A}(\vec{r},t)\langle\rho(\vec{r})\rangle$$

To establish contact with our earlier notation,

$$\vec{B}(\vec{r}) = \vec{J}_p(\vec{r})$$

$$\vec{f}(\vec{r},t) = e\vec{A}(\vec{r},t)$$

$$\vec{A} = \vec{J}_p^{\alpha}(\vec{r})$$

So, if that is the case my n J n so, this J now consists of a paramagnetic term which is coming from the current without a field, and the diamagnetic term is because of the field that is because of the vector potential A. And so, this is equal to n 0 J p n 0, plus n 0 J d n 0 plus n 1 J p n n 1 and plus n 1.

So now this term cannot be included because we have taken the corrections up to the first order. So, n 1 contains an order of A and J d will also contain an order of A. So, those terms will be of the second order and you have to neglect those term in a linear response theory. Thus n J n ideally should have 4 terms coming from J p and J d; however, because the n 1 is the correction up to first order in the external field, and J d is also includes a term which is linear in the external field; we will have to drop that term. So, any term that is of the order of a square has to be dropped.

Now, you look at the first term in this above. So, this can be said to be equal to 0 for the reason so, at equilibrium there is no current. So, this is equal to 0 so, the first term goes to 0, and then the thermal average of this the second term. So, this is the second term; which is because of the field is nothing but e by m A r t and a rho r. And this rho r is coming from psi dagger, psi and we have taken the thermal average.

So, now to establish a contact with our earlier notation that we have used; let us write, so, we have B of r which is equal to a paramagnetic J p of r, f of r t which is equal to e A r t. And a vector which is the left hand side of the linear response equation; which is equal to a J p alpha r.

So, the current the expectation value of the current or the thermal average of the current is written as rather thermal average is written as this.

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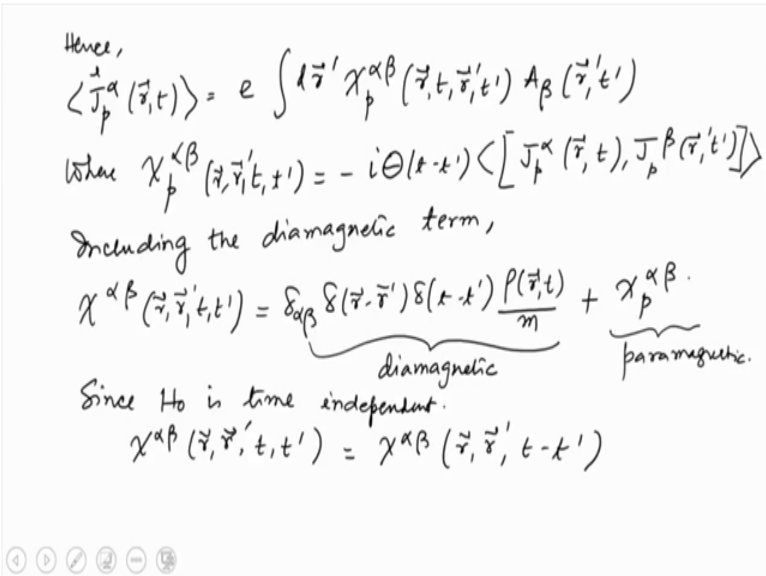

J p alpha r t, this is equal to e d r prime and a chi a p alpha beta r t r prime t prime A beta r prime t prime. We are almost there with the Kubo formula accepting that this a has to be now converted into e. So now, where our chi p alpha beta r, r prime t, t prime it is equal to minus i theta t minus t prime and J p alpha r t J p beta r prime t prime and this. So, this is your chi the paramagnetic part of the response. And including the diamagnetic term so, chi p alpha beta r, r prime t, t prime is written as delta alpha beta delta r minus r prime delta t minus t prime, and rho r t by m plus this chi. So, this is the not the paramagnetic, but this total chi. So, this is equal to p alpha beta. And this is coming from the diamagnetic term.

So, this is the diamagnetic contribution to the response and this is the paramagnetic. So, since H 0 is time independent this chi paramagnetic susceptibility, it does not depend upon 2 variables t and t prime the 2 the 2 time variables; rather, it depends on t minus t prime, so that we can write and in fact, the whole susceptibility, basically because of these factors. So, chi alpha beta r r prime t t prime t t prime it is equal to chi alpha beta r r prime t minus t prime. And this is.

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Fourier transform yields.

$$\langle \vec{J}^{\alpha}(\vec{r},\omega)\rangle = e\int d\vec{r}'\, \chi^{\alpha\beta}(\vec{r},\vec{r}',\omega)\, A_{\beta}(\vec{r}',\omega)$$

$$\vec{E}(\omega) = i\omega\vec{A}(\omega).$$

$$\vec{J}_e = -e\vec{J} \qquad [\vec{J}_e \text{ is the electronic current density}]$$

$$\langle \vec{J}_e^{\alpha}(\vec{r},\omega)\rangle = \int d\vec{r}'\, \underbrace{\sigma^{\alpha\beta}(\vec{r},\vec{r}',\omega)}_{\text{Conductivity tensor}}\, \vec{E}_{\beta}(\vec{r}',\omega)$$

$$\sigma^{\alpha\beta}(\vec{r},\vec{r}',\omega) = \frac{ie^2}{\omega}\chi_{\alpha\beta}(\vec{r},\vec{r}',\omega).$$

So now, Fourier transform of this J alpha r omega, it is equal to e d r prime chi alpha beta r r prime omega, and there is a A beta r prime omega. So, that is the contribution due to the external field.

Now the vector potential A is related to the electric field as follows. Your e omega it is equal to i omega A omega. So, the current density is actually written as so, the current density J the electronic current density is written as minus e J this is the J e is the electronic current density. And this J is the one that we have derived just in the last slides.

So, our J e alpha r omega it is equal to a d r prime a sigma p alpha beta r r prime omega e beta; so, this is not required, e is not required. So, it is equal to r prime omega. So, the conductivity tensor is written as this is called as the conductivity tensor. So, this conductivity tensor is defined as sigma alpha beta r r prime omega, it is equal to i e square by omega chi alpha beta r r prime omega.

So, in general this conductivity tensor is a non-local quantity; that is the contribution at a given point r depends on the neighbouring points r prime. And that is why you have to sum over all the neighbouring points in order to get the electronic current density.

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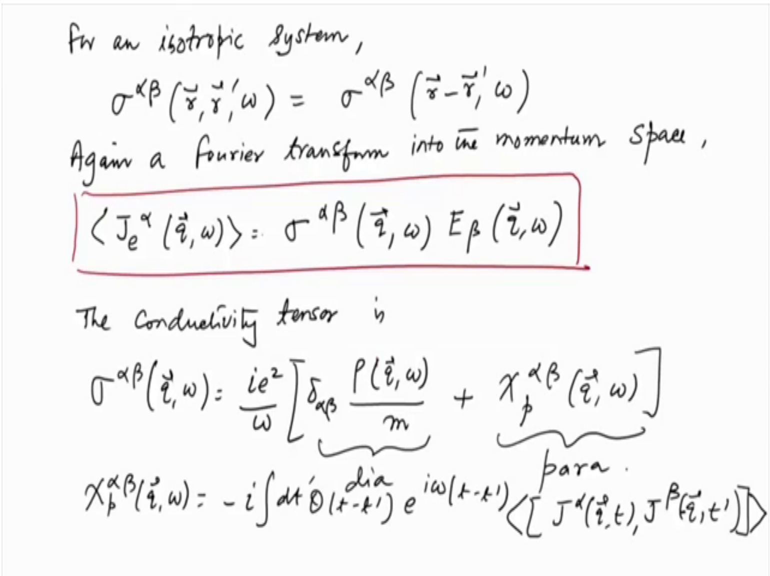

So, also for a homogenous system for an isotropic system or isotropic or homogeneous that is fine that is they mean the same. Sigma alpha beta r r prime omega that is equal to sigma alpha beta r minus r prime omega. So, the system is translationally invariant.

So, the quantity that is here the conductivity tensor does not depend upon 2 variables r and r prime; rather it depends on a single variable which is r minus r prime. And again a Fourier transform into the momentum space yields J e alpha q omega. It is equal to sigma alpha beta q omega and e beta q omega. So, this is our Kubo formula for the current response. So, the current response depends in the linear regime that is for small values of the electric field is linearly related to the current density or the thermal average of the current density, and the coefficient is known as the sigma which is that conductivity tensor. Remember it depends upon both momentum and frequency.

And let us see some of it is properties. So, the conductivity tensor actually i e square over omega delta alpha beta rho q omega by m and plus chi p alpha beta q omega. So, this is the diamagnetic contribution and this is the paramagnetic contribution; where we can write down this. So, chi p alpha beta q omega it is equal to a minus i dt prime theta t minus t prime exponential i omega my omega, omega t minus t prime and then the commutator. So, it is J alpha q t and J beta q prime my sorry minus q and t prime and this and so on. So, that is the paramagnetic part. And so, it is important to note that the diamagnetic part actually rather it is it vanishes for or rather it blows up.

So, what happens in the static limit? That is let us ask this question that as omega goes to 0, what happens to these 2 terms? So, it seems that as omega goes to 0 the diamagnetic part actually blows up, but that blowing up is compensated by a part of this paramagnetic susceptibility, and giving you a static DC conductivity or DC conductivity static conductivity.

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Static Case $\omega \to 0$.

The diamagnetic part diverges. for usual conductor, this divergence is canceled by a part of the paramagnetic term, yielding the D.C. conductivity finite.

In a superconductor (perfect diamagnet), the paramagnetic contribution becomes zero, the conductivity is purely imaginary.

$$\sigma^{\alpha\beta}_{SC}(\vec{q}, \omega) = \frac{ie^2}{\omega} \delta_{\alpha\beta} \frac{\rho(\vec{q}, \omega)}{m}$$

Imaginary conductivity implies an inductive behaviour

So, static case; omega going to 0 so, the diamagnetic part blows up diverges for usual conductor conductors, this divergence is cancelled by a part of the paramagnetic term; there by yielding the DC conductivity finite. Interestingly, in a superconductor which is a perfect diamagnet one gets the diamagnetic contribution dominates and the paramagnetic contribution vanishes and what one gets is the following.

The paramagnetic contribution becomes negligibly small or it becomes 0 and the DC and the conductivity; the conductivity not DC, but the conductivity is purely imaginary. So, sigma, alpha, beta for or we will writing it upstairs we will continue doing that. And for a superconductor is a q omega and it is i e square over omega and delta alpha beta rho q omega and divided by m.

And this is a purely imaginary thing; an imaginary conductivity implies conductivity implies an inductive behaviour which you know from electric study of electricity or rather these circuits LR circuits and LCR circuit etcetera. So, you have a the impedance which is a or rather the inverse of the impedance which is the conductance is a purely imaginary quantity. And so, this says it is a no dissipation of energy.

So, this implies that there is no dissipation of energy because of the flow of current and we know that these are called as the super current. And there persistent currents which would go for you know many years without any significant loss. And this arises because the paramagnetic part goes to 0 and only the diamagnetic contribution that remains. In diamagnets as we told earlier that the diamagnetic susceptibility or the diamagnetic response is far lower than that of a superconductor.

A superconductor has a diamagnetic susceptibility of minus 1 which means it exactly cancels out the external field the magnetization is just opposite to the field external field. And whereas, in normal metals or in the so called diamagnets it is of the order of 10 to the power minus 5; so there is it does not lead to dissipation less energy and like a superconductor.

So, to summarize we have looked at the Kubo formula within a linear response theory. The Kubo formula talks about the current and it is relationship to the applied field, and the proportionality or the coefficient that comes out is called as the conductivity tensor. And the conductivity is a momentum and frequency dependent quantity, and we have of course, the special interest is to talk about DC conductivity which is at the omega equal to 0 limits.

And this is what happens at a finite omega sigma will be a proportional to or rather will depend on q and omega. This is what we get from linear response theory where the response of the system to perturbation is linear to that of the external field.